Chemistry 441: Instrumental Analysis  
Spring 2013

Instructor: Dr. Stephen D. Starnes  
Office: STC 339  
Research lab: STC 329  
Phone: 903-886-5389, e-mail: stephen.starnes@tamuc.edu  
Office Hours: MWR 12:00-1:00 p.m., F 10:00-10:50 am and by appointment

Lectures: MW 2:00-3:15, Room: Science 123  
Lab: T 2-5:50 pm, Room: Varies


The purpose of this course is to introduce the student to the subject of Spectroscopy as it relates to the identification and characterization of organic and biological compounds. This semester we will cover $^1$H-, $^{13}$C-, and variable temperature NMR spectroscopy. We will also cover several advanced NMR techniques like NOE, COSY, HETCOR, and HMQC. We will cover the basic principles of IR, Uv/Vis, mass spectroscopy, CD spectroscopy, fluorescence spectroscopy, and polarimetry. We will examine in general terms how the instrument functions and in more detail how to interpret the spectroscopic data generated by the instrument.

**Grading**

There will be several take-home problem sets assigned throughout the semester that will constitute 20% of the grade. You are encouraged to form study groups and to work together on these problems. There will be two exams (20% each) and a final exam (20%) which will be in part take-home (spectroscopy problems) and part in-class. The lab will constitute 20% of the course grade. The final letter grade will be based on a standard scale 90-100% A, 80-89% B, 70-79% C, 60-69% D, and below 60% F. The grades may be curved, if warranted.

Friday, March 29, 2013 is the last day to drop the course and receive a drop.

There will be absolutely no make-ups for exams. If you miss an examination, you will be assigned a zero for that assignment. Problem sets not submitted on time may receive a grade of zero.

**Tentative Schedule**

<table>
<thead>
<tr>
<th>Date</th>
<th>Topic</th>
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<tbody>
<tr>
<td>January 14</td>
<td>Theory of 1H-NMR spectroscopy – nuclear spin flip</td>
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<tr>
<td>January 16</td>
<td>Theory of 1H-NMR spectroscopy – chemical shift, correlation tables</td>
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<tr>
<td>January 21</td>
<td>Theory of 1H-NMR spectroscopy – integration</td>
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<tr>
<td>January 23</td>
<td>Theory of 1H-NMR spectroscopy – spin-spin splitting</td>
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<tr>
<td>January 28</td>
<td>Theory of 1H-NMR spectroscopy – spin-spin splitting, coupling constants</td>
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<td>January 30</td>
<td>Theory of 1H-NMR spectroscopy – alcohols and related</td>
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<td>February 4</td>
<td>Theory of 1H-NMR spectroscopy –</td>
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<tr>
<td>February 6</td>
<td>Theory of $^{13}$C-NMR Spectroscopy</td>
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<tr>
<td>February 11</td>
<td>Theory of $^{13}$C-NMR Spectroscopy</td>
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<tr>
<td>February 13</td>
<td>Learn to use the 90 MHz and 400 MHz NMR - training</td>
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<tr>
<td>February 18</td>
<td>Learn to use the 90 MHz and 400 MHz NMR - training</td>
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<tr>
<td>February 20</td>
<td>COSY</td>
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<tr>
<td>February 25</td>
<td>HETCOR, HMQC</td>
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February 27 – Exam 1, NMR spectroscopy
March 4 – IR spectroscopy
March 6 – IR spectroscopy
March 11 – No class – Spring Break
March 13 – No class – Spring Break
March 18 – IR spectroscopy
March 20 – UV/Vis spectroscopy
March 25 – UV/Vis spectroscopy
March 27 – Learn to use the IR and Uv/Vis instruments
April 1 – Mass spectroscopy
April 3 – Mass spectroscopy
April 8 – Mass spectroscopy
April 10 – Mass spectroscopy, elemental analysis
April 15 –Solving spectroscopy problems
April 17 – Polarimetry
April 22 – Exam 2, IR, UV/vis and Mass Spectroscopy
April 24 – Fluorescence spectroscopy
April 29 – CD spectroscopy
May 1 – Learn to use the Fluorimeter, Polarimeter, CD instrument
May – 6 – Final Exam

Course Objectives

By the end of the semester I intend for my students to have realized a number of objectives.

1. Know how to determine the structure of an organic molecule using spectroscopic techniques such as NMR, IR, UV/vis and MS.
2. Know how to interpret NMR, IR, Uv/Vis and MS data.
3. Understand the theory behind several spectroscopic techniques such as NMR, IR, UV/vis and MS.

CLASS ATTENDANCE POLICY: All students are expected to attend classes on a regular basis and attendance will be recorded. Being late by more than 10 minutes is equivalent to missing a lecture. Excessive absence is defined as missing more than 10% of the lectures without excusable reasons. Excessive absence will be reported to the Dean of Graduate Studies and Research. In addition, according to the TAMU-Commerce Procedure A13.02., good class attendance will be necessary in order to pass the course.

CLASSROOM BEHAVIOR: Disorderly conduct which interferes with the normal classroom atmosphere will not be tolerated. The classroom instructor is the judge of such behavior and may instruct a disorderly student to leave the room with an unexcused absence or in more serious situations a student may be removed from the class with a failing grade.

CHEATING AND OTHER BREACHES OF ACADEMIC CONDUCT: Academic cheating, plagiarism, and other forms of academic misconduct may result in removal of the student from class with a failing grade or may in extreme cases result in suspension or expulsion from the University as described in the “Code of Student Conduct” section of the “Student's Guidebook”.

ADA ELIGIBLE STUDENTS: ADA eligible students should make arrangements with the instructor in the first week of the semester about special arrangements needed for classroom or testing facilities and procedures to accommodate the disability.