CH4412
Spring (!) Semester 2003/2004

Instructor: Dr. Dallas K. Bates
dates@mtu.edu

Office Hours: 10:00-10:30 am MWF and by arrangement

Office: 19-708A (behind the 7th floor elevators). The lab doors
leading to my office will normally be locked. If you want
to come to my office, ring the doorbell in the corridor (the
button is near the lab door closest to the elevator). If there
is no answer-leave me a note indicating when and where I
can reach you. In spite of this inconvenience, please feel
free to see me about any questions or difficulties you have
with the material.

Text(s): Organic Structure Analysis, Crews, Rodriguez, Jaspars,

Useful REFERENCE texts: Silverstein and Webster,
Spectroscopic Identification of Organic Compounds, 6th
edition; Breitmaier, Structure Elucidation by NMR in
Organic Chemistry: A Practical Guide; Nelson, Nuclear

Software: Introduction to Spectroscopy-Mass Spec, IR, 1H and 13C
NMR (10 licenses)
MestRe-C (freeware)
nmrsm (NMR spectrum simulator) (freeware)
ChemSketch (ACD Labs) (freeware) + others as available
vanPelt Library: Aldrich/ACD NMR database

CH4412 is designed to make you proficient at interpretation of organic spectral data and, as such, is very
problem solving oriented. Little emphasis is placed on instrument theory, operation or design. This course
is not a course to provide training for hands-on operation of chemistry instrumentation. If you wish
to learn to use any departmental equipment, please see me. I can arrange training independent of this class.
Those of you who are using, or will be using, the Varian 400 MHz NMR can process NMR data “at your
desk.” I will show anyone wishing to develop this feature how it is done.

There will be no class for the first week to allow you time to begin working through the 4 “Introduction to
Spectroscopy” modules (IR, MS, 1H NMR, and 13C NMR). This software is available in the Chemistry
Computer Lab (ChemSci 719) and the Studio Lab (ChemSci 708); plan to work on this software at your
own pace, but finish the IR and 1H NMR modules by Sunday, January 18, 2004. Class will begin on
January 19, 2004 to begin work on IR problems in class.
TOPICS
Beginning January 19, lecture material, homework problems and in-class group problem assignments will cover the following topics:

- Infrared Spectroscopy  ~ 0.5 week
- Mass Spectroscopy 2.5 weeks
- $^1$H NMR 3 weeks
- $^{13}$C NMR 3 weeks
- 2D NMR techniques 2 weeks
- Combination problems 3 weeks

As time allows, computational chemistry and dynamic NMR (including line-shape analysis software) will be introduced to the class for use in problem solving.

GRADING

<table>
<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Quizzes</td>
<td>70%</td>
</tr>
<tr>
<td>Poster presentation</td>
<td>*</td>
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<tr>
<td>Final</td>
<td>30%</td>
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* For use in the case of borderline grades to determine whether a “bump” is appropriate, participation is required.

Quizzes may be written (taken by the entire class) or oral (taken individually in my office). The final exam is typically a larger version of problems worked in class and on quizzes. A hand-written “Blue Book of Useful Spectroscopic Information” may be used on quizzes and the final exam. You may include any information in the blue book (some potentially useful data is posted on the CH4412 bulletin board in the 7th floor corridor). The ONLY source that may be used on tests and quizzes is your blue book and all information in the blue book must be hand-written by the individual using it. You can add new material to your bluebook at anytime- plan ahead for expansion of each section during the semester. Make sure you understand what is allowed: USE OF 'UNAUTHORIZED' MATERIALS ON A QUIZ OR THE FINAL WILL RESULT IN A GRADE OF ZERO (0) FOR THAT EXERCISE.

The poster presentations will be in class during the last lab session of the term. The poster project involves solving an assigned problem, preparing a poster showing how the spectroscopic data from the problem supports the structure you propose as the answer, and orally discussing the poster with other students and with me during the presentations. I will discuss in class the poster format and answer any questions you have later in the term. Some examples of previous year’s spectroscopy posters are posted on the walls on the north end of the 7th floor corridor.

CH4412 information will be posted on the CH4412 bulletin board (by the drinking fountain in the 7th floor corridor) AND to the course webpage (Go to the MTU Chemistry homepage, click on “course” in the menu on the left side of the page, then click on CH4412.

FN: CH4412SYL_04.doc

MTU complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act. If you have a disability and need a reasonable accommodation for equal access to education or services at MTU, please call Gloria Melton at 72212. For other concerns you may contact your academic advisor, department chair, or the Affirmative Action Office.