CHM5300 Molecular Spectroscopy  
Fall 2003 Syllabus

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Office: 3420 Physical Science Bldg.  
Class meeting time: MWF at 9am Room 4125.

Web page: http://ux1.eiu.edu/~cfsap/chm5300.htm  
Solutions for homework assignments and other useful information will be posted to this site so check it often.

Office Hours: Will be announced in class; for up-to-date office hours, check my schedule on the web at http://ux1.eiu.edu/~cfsap/F2003.htm  
Please do not hesitate to come and see me at any time if you are having difficulties.


Prerequisites: CHM3920 or an equivalent Quantum Mechanics/Spectroscopy course

E-mail announcements: I may occasionally send e-mail announcements to the whole class so please be sure that you learn how to use your email and check it frequently.

Objective  
To study the quantum mechanical principles and theoretical foundations of important current spectroscopic techniques and to examine the applications of these methods. We will focus on microwave, vibrational and electronic spectroscopy with a briefer coverage of NMR (and other types of spin resonance) spectroscopy.

General Course Information  
Attendance is required in all classes on time. Absence from 5 or more lectures will generally result in a failing grade. The guide to the material that we will be covering in this class (given overleaf) is very approximate and we may deviate from it (maybe quite significantly). Given the complexity of the material that we will be covering in this course, there is considerable flexibility in the syllabus and no doubt we will spend more time on some areas than others. Please do not be afraid to ask questions or give me feedback (particularly on subtopics that you feel you would particularly like to cover) – feel free to send me questions via e-mail if you prefer since this gives me a better idea of where we should spend more time. Note that spectroscopy is a very wide-ranging field of study and no one text book can ever come anywhere close to covering everything. I encourage you to look in other texts in the library to further your understanding of various areas – I will try to point out useful additional texts in certain areas as we encounter them.

Exams  
The course will consist of three exams and a final comprehensive examination. The three midterm exams will contain material we have discussed in class as well as any material covered in the homework assignments. The grades will be determined as outlined in the section below. You are expected to take all exams as scheduled. If there is a compelling reason for missing an exam, you should prepare and submit to me a detailed description of the situation that necessitates your absence from the exam. All such submissions should be made several days in advance of the scheduled exam date. Final exam schedules may be found on the EIU web page at http://www.eiu.edu/~registra/fafinals.html. Cheating in any form will be dealt with severely; you run the risk of failing the course if caught cheating on any homework assignments or exam. Any suspected cases of cheating will be referred to the Office of Judicial Affairs.

Exam schedule: Three exams and the final exam will form the majority of the points in this class. The three exams given during the semester will be given around week 5, week 8 and week 12 and will cover the material in the weeks leading up to the exam – more details will be given closer to the exam. The final exam will be cumulative and will be given on Wednesday, 17-Dec-03 8:00-10:00 a.m. and will likely also have a take-home portion, the details of which we will decide in class nearer to the end of the semester.

Homework assignments: Some assignments (that are intended to be handed in and graded) will also be given throughout the semester. These homework assignments will contribute towards your final grade in this course and should be completed and turned in on time. The assignments may take a number of different formats, from problems to solve to short papers to write. Problem solutions and various other announcements (such as overall exam statistics) will be posted to the course web page so be sure to visit there at least once or twice a week. Please be sure to let me know (by e-mail or in person) if you should experience any difficulties in accessing materials on the web.

Grades  
The final grade will be determined approximately as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>Points</th>
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<tbody>
<tr>
<td>Three exams @ 100pts</td>
<td>300</td>
</tr>
<tr>
<td>Final Exam (including a take-home portion)</td>
<td>150</td>
</tr>
<tr>
<td>Homework assignments</td>
<td>100</td>
</tr>
</tbody>
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Tentative final grades for this class are as follows: A 90-100%, B 80-90%, C 65-80%, D 50-65%, F <50%.
Tentative schedule

**Week 1-2** – Chapter 1, Introduction: waves, interaction of radiation with matter, lineshape functions

**Week 2-4** – Chapters 2, 3, Symmetry and Group Theory: symmetry operations, point groups, character tables, matrix representation of Schrödinger equation, selection rules

**Week 4-7** – Chapter 4, Atomic spectroscopy: angular momentum, term symbols, H atom, spin-orbit coupling, selection rules, Zeeman effect; Chapter 9, Electronic spectroscopy of diatomics: vibrational structure, rotational structure, symmetry and parity; Chapter 10, Electronic spectroscopy of polyatomics: Walsh’s rules, Hückel MO theory, vibrational structure, vibronic coupling, Jablonski diagrams, photoelectron spectroscopy, rotational structure

**Week 8-10** – Chapter 6, Rotational spectroscopy: moment of inertia, diatomics/linear molecules, vibrational angular momentum, symmetric tops, asymmetric tops, Stark effect, nuclear quadrupole hyperfine structure, experimental techniques

**Week 10-11** – Chapter 7, Vibrational spectroscopy: diatomics, vibration-rotation spectra for diatomics, vibration of polyatomics, normal modes, vibration-rotation spectra of linear molecules, nuclear spin statistics, Coriolis and Fermi interactions, inversion doubling, fluxional behavior

**Week 12** – Chapter 8, Raman spectroscopy: classical and quantum mechanical description of the Raman effect, polarization, diatomics, vibration-rotation Raman

**Week 13-14** – Spin resonance techniques: NMR, ESR (not covered in Bernath).

**Fall 2003 holidays:**
Sept. 1, M – Labor Day – No Classes
Oct. 17, F – Fall Break – No Classes
Nov. 24-28, M-F – Thanksgiving Break – No Classes