CHEM 856  
MOLECULAR SPECTROSCOPY  
Spring, 2016

Professor:  Carey K. Johnson, B039 Malott  
ckjohnson@ku.edu  
office hours: drop in or by appointment

Time and Place:  9:30 – 10:45 Tuesdays and Thursdays; 3059 Malott

Recommended Text:  Kelley, Condensed-Phase Molecular Spectroscopy and Photophysics (2013). This can be accessed online through the library catalog.

Catalog Description:  Quantitative molecular spectroscopy and its chemical applications. The basic principles of the molecular energy levels, selection rules and spectral transition intensities will be discussed and applied to rotational, vibrational, electronic, and nuclear magnetic spectroscopy. Linear and nonlinear spectroscopies will be addressed. Prerequisite: CHEM 750 or its equivalent.

Course Design:  The course will focus on the fundamentals of spectroscopy and applications of current interest. Then, depending on the time available, we will take up topics of current interest. The course will be highly interactive with presentations and papers by students. Participation in discussion will be expected, and students should prepare by reading text and other material so that they can contribute meaningfully to discussions and ask relevant questions.

Course Requirements:  (1) Problem sets (6 -- 8) will be assigned on a regular basis. (2) Two exams will be given in the course of the semester. (Portions may be take-home.) (3) Short reports (to be presented orally or in writing) will be assigned on journal articles or applications of spectroscopic topics. (4) Discussion: Journal articles or other materials will be assigned and discussed in class. (5) A paper (about 10 pages) exploring an aspect of modern molecular spectroscopy will be required. Presentations (about 15-20 min) on the topic of the papers will be scheduled during the final exam time (Wednesday, Dec. 16, 1 pm).

Grading:  

<table>
<thead>
<tr>
<th>Component</th>
<th>Points</th>
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<tbody>
<tr>
<td>Problem Sets</td>
<td>120 – 160</td>
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<tr>
<td>2 Exams (100 pts each)</td>
<td>200</td>
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<tr>
<td>Short reports, discussion, participation</td>
<td>50 – 100 pts (about)</td>
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<td>Paper and talk</td>
<td>100</td>
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<tr>
<td>Total</td>
<td>about 500 – 550</td>
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Solid, consistent effort will be awarded a B grade. Consistent excellent work will be awarded an A grade.
Some good references:
  Allen and Eberly: *Optical Resonance and Two-Level Atoms*
  Atkins and Friedman: *Molecular Quantum Mechanics*
  Cotton: *Chemical Applications of Group Theory* (3rd ed.)
  Harmony: *Introduction to Molecular Energies and Spectra* (text by a Professor, now Emeritus, at KU)
  Herzberg’s famous 3-volume set: *Spectra of Diatomic Molecules; Electronic Spectra of Polyatomic Molecules; Infrared and Raman Spectroscopy*
  Hochstrasser: *Molecular Aspects of Symmetry*
  McHale, *Molecular Spectroscopy*
  Milonni and Eberly: *Lasers* (good book on lasers)
  Mukamel: *Principles of Nonlinear Optical Spectroscopy* (an advanced treatment)
  Schonland: *Molecular Symmetry* (good group theory book)
  Struve, *Fundamentals of Molecular Spectroscopy*
  Tokmakoff, *Time-Dependent Quantum Mechanics and Spectroscopy* (available for download at https://tdqms.uchicago.edu/)
  Wilson, Decius, and Cross: *Molecular Vibrations*

**Academic Misconduct:** Academic misconduct – presenting someone else’s work as your own or giving or receiving unauthorized aid in exams, etc. – will not be tolerated and will result in a grade of zero for the assignment as well as prosecution as outlined in the KU Student Handbook (http://www.studenthandbook.ku.edu/codes.shtml#Academic_Misconduct).

**Disabilities:** Any student in this course who has a disability that may prevent him/her from fully demonstrating his/her abilities should contact me personally as soon as possible to discuss accommodations necessary to ensure full participation in the educational opportunity. Note that the Academic Achievement & Access Center Disability Resources (www.disability.ku.edu) can assist students with any needs they may have.
TOPICS

1. **Interaction of Molecules and Radiation**
electromagnetic radiation; electric and magnetic properties of matter;
interaction Hamiltonian; time-dependent perturbation theory
absorption and emission of light
theory of line shapes
density matrix representations

2. **Group Theory**
symmetry groups and representations
selection rules
(Note: If you are not familiar with molecular point-group classification and symmetry elements, you should study this background from a standard text–see reference list.)

3. **Vibrational Spectroscopy of Polyatomic Molecules**
Born-Oppenheimer approximation
normal modes, symmetry, and selection rules
vibrational infrared and Raman spectroscopy

5. **Electronic Spectroscopy of Polyatomic Molecules**
symmetry and selection rules
vibrational and rotational contributions, vibronic coupling
line broadening and line shapes
fluorescence spectroscopy
radiationless transitions

6. **Lasers, Ultrafast, and Nonlinear Spectroscopy**
lasers
nonlinear optics
two-photon processes, resonance Raman
ultrafast spectroscopy
coherence in spectroscopy

7. **Special Topics (if there is time)**
single-molecule spectroscopy
fluorescence microscopy
four-wave mixing spectroscopies