CHM 6490: Molecular Spectroscopy, Spring 2014

CHM6490 is a 3-credit hour "core" graduate course covering the theory of the various forms of molecular spectroscopy.

Instructor: Prof. Clifford R Bowers
2360 NPB
bowers@chem.ufl.edu

Office Hours: MW 7-8th periods

Meeting Place and Time:
T, 7th period: MCCB, 1108
R: 7-8th period: MAT 0116

Primary Course Text: *Symmetry and Spectroscopy, An Introduction to Vibrational and Electronic Spectroscopy*, Daniel C. Harris and Michael D. Bertolucci.

Additional Texts to be used to prepare lectures:

Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Edgar Bright Wilson.
Spin Dynamics: Basics of Nuclear Magnetic Resonance, Malcolm H. Levitt.

Grading scheme:

Midterm Exam	30%
Final Exam	30%
In-class quizzes	30%
Term Project	10%

Quizzes: There will be 5 (unannounced) in-class quizzes. The best 3/5 will be used in grade calculation.

Term Paper: Each student will prepare a written term paper on a specific application of molecular spectroscopy. Students will present a summary of their paper in front of the class in the final week of the semester.

Homework: Will be regularly assigned but not collected or graded.

Tentative schedule

Weeks 1-2: Propagation of electromagnetic waves and optics

Maxwell's Equations
Plane waves in isotropic media
Polarization Vector
Birefringence and index ellipsoid
Polarization states of photons
Ray propagation

Week 3: Transitions rates and selection rules

Time-dependent perturbation theory
Transition dipole moment
Selection rules
Examples

Weeks 4-5: Group Theory

Symmetry elements/operations
Point groups
Character tables
Reducible representations

Weeks 6-7: Vibrational spectroscopy

Infrared and Raman spectroscopy
Diatomic molecules
Anharmonic corrections
Population distributions
Diatomics
Normal modes
Selection rules and polarization
Overtone transitions and combination bands
Vibrational analysis
Computation of vibrational spectra

Weeks 8-9: Electronic spectroscopy

Molecular orbitals and term symbols
Selection rules
Franck-Condon principle
Spin selection rules
Orbital selection rules

Weeks 10-13: Magnetic Resonance Spectroscopy

Magnetic moments
Spin dynamics - Bloch equations
Rotating frame transformation
Spin functions
Spin Hamiltonians
Transition intensities
Density matrix formalism
Liouville-von Neumann equations
Relaxation

Week 14: Term paper presentations