SYLLABUS – CHM6490, Spring 2023
Introduction to Molecular Spectroscopy

Instructor: Prof. Russ Bowers, Department of Chemistry
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Office Hours: TBA
Class meetings: MWF Period 5 (11:45 – 12:35), Dauer Rm. 342
Class dates: 01/09/23-4/26/23

OBJECTIVES
To introduce the following topics: molecular energy levels and orbitals; group theory and spectroscopic selection rules; time-dependent perturbation theory and transition rates; theory of rotational, vibrational, electronic, spectra of diatomic and polyatomic molecules; electron spin resonance; and nuclear magnetic resonance spectroscopy.

PREREQUISITES
An undergraduate level understanding of quantum mechanics is recommended. Key principles of quantum mechanics will be reviewed. Spin systems provide an excellent platform for learning quantum mechanics.

PLACE IN CURRICULUM
This course satisfies the spectroscopy course requirement to qualify for the PhD in the Division of Physical Chemistry.

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

SUPPLEMENTAL TEXTS (used to prepare lectures and assignments)
Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Edgar Bright Wilson.
Spin Dynamics: Basics of Nuclear Magnetic Resonance, Malcolm H. Levitt.

SOFTWARE (used in lecture demonstrations, homework assignments, and exams)

- Wolfram's Mathematica (purchase or access via UFApps)
- Python
- Matlab (UF Chemistry site-license available)
- Spinach (free, www.spindynamics.org)
- MestReNova (UF Chemistry site-license)

OPTIONAL SOFTWARE
PDF Scan Software - for scanning your homework pages into PDF for uploading onto Canvas. Genius Scan, by Grizzly Labs, for IOS or Android phones, is recommended. PDF scans can be uploaded to Cloud Storage such as UF Google Drive, Dropbox, or UF OneDrive.
Word Processing – Neatly hand-written homework is acceptable. Typesetting is optional.
In chemistry, the standard is MS Word with the built-in equation editor. In physics and chemical physics, LaTeX is also widely used.
UFApps - UFApps offers a large number of different software packages to UF students free of charge.
UF OneDrive - required for transferring files between your local computer and UFApps. Assignments, lecture notes and other course materials may be distributed via OneDrive.

GRADING SCHEME

Midterm Exam	30%
Final Exam	30%
Pop quizzes	30%
Term Project	10%

QUIZZES
There will be 5 (unannounced) in-class quizzes. The best 4/5 will be used in grade calculation.

TERM PAPER
A term paper will be prepared 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

Homework will be assigned but not graded. Homework solutions will be provided.

MAKE-UP EXAMS

Must be arranged in advance of the scheduled date. No make-up exams are allowed otherwise except for emergency situations.

LATE SUBMISSION POLICY

Late assignments will receive a late penalty of 10% per day past the scheduled due date. If something arises that prevents you from completing the assignment on time, contact the instructor as soon as possible to request an extension.

GRADING POLICIES: https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

ATTENDANCE

If you're going to miss any lecture for any reason, please let the instructor know in advance. Don't be late. I keep tabs on that.

TENATIVE TOPIC 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