Syllabus

Instructor: Alexander I. Boldyrev

Office: ML 369

Email: a.i.boldyrev@usu.edu

Class times:  TR  5:30pm – 7:00pm

Office hours:  ML369  MWF  any time

I will be happy to make appointments with anyone who has unavoidable conflicts at these times. The best way to contact me outside office hours is by email.

The last day to add this class is the September 16. Attending this class beyond that date without being officially registered will not be approved by the Dean’s Office.

The last day to withdraw from this class (W on transcript) is the October 25, 2013.

In accordance with the Americans with Disabilities Act, reasonable accommodation will be provided for all persons with disabilities in order to ensure equal participation in this course.

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Text: Molecular Spectroscopy (1-st edition) by Jeanne L. McHale

I will make reading assignments from the textbook. You are responsible for all material in these assignments even if it isn't covered in lecture.

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Course content: Approximately the first 2 weeks of Chemistry 6020 will be devoted to review of molecular symmetry. The following topics will be covered:

- Symmetry Point Groups
- Character Tables, Irreducible Representations
- Projector Operators, Symmetry Adapted Linear Combinations of Atomic Orbitals
- Symmetry of Molecular Orbitals
- Symmetry of Normal Vibrational Modes
- Finding the Symmetries of Normal Modes

The next 2 weeks will be devoted to introduction of Rotations and Vibrations in Molecules. The following topics will be covered:

- The Born-Oppenheimer Approximation and Its Consequences
- Multiple Global and Local Minima on Potential Energy Surfaces
- Permutational-Inversion Groups
- The Harmonic Oscillator Model
- Selection Rules for Vibrational Transitions
- Infrared Spectroscopy
- Raman Spectroscopy
- Beyond the Rigid Rotor - Harmonic Oscillator Approximation
- Perturbation Theory of Vibration-Rotation Energy
- The Morse Oscillator and Other Anharmonic Potentials

The next 2 weeks will be devoted to rotational spectroscopy. The following topics will be covered:

- Energy Levels of Free Rigid Rotors
- Diatomic Rotations
- Polyatomic Rotations
- Angular Momentum Coupling in Non-$^1\Sigma$ Electronic States
- Nuclear Statistics and J States of Homonuclear Diatomics
- Rotational Absorption and Emission Spectroscopy
- Rotational Raman Spectroscopy
- Corrections to the Rigid-Rotator Approximation
- Internal Rotation
The next 3 weeks will be devoted to vibrational spectroscopy. The following topics will be covered:

- Normal Modes of Vibration
- Classical Equations of Motion for Normal Modes
- Normal Modes of a Linear Triatomic Molecule
- The Wilson F and G Matrices
- Group Theoretical Treatment of Vibrations
- Finding the Symmetries of Normal Modes
- Symmetries of Vibrational Wavefunctions
- Rotational Structure
- Anharmonicity
- Floppy Molecules
- Selection Rules at Work: Benzene

The next 2 weeks will be devoted to atomic spectroscopy. The following topics will be covered:

- The hydrogen atom: Energy Levels and Selection Rules
- Many-Electron Atoms
- Spin-Orbit Coupling
- Selection Rules for Atomic Absorption and Emission
- Hyperfine Structure
- The Effect of External Fields

The next 3 weeks will be devoted to electron spectroscopy. The following topics will be covered:

- Diatomic Molecules: Electronic States and Selection Rules
- Molecular Orbitals and Electronic Configurations
- Term Symbols for Diatomics
- Selection Rules
- Examples of Selection Rules at Work: O₂ and I₂
- Vibrational Structure in Electronic Spectra of Diatomics
- Polyatomic Molecules: Electronic States and Selection Rules
- Molecular Orbitals and Electronic States of H₂O
- Franck-Condon Progressions in Electronic Spectra of Polyatomics
- Benzene: Electronic Spectra and Vibronic Activity of Nontotally Symmetric Modes
- Photoelectron Spectroscopy

After every section there will be a test (50 pts.).
Final grades will be computed with an A, A- >90%, a B+, B, B- > 80% and a C+, C, C- >70%. These cutoffs may be revised slightly downwards.

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