UTAH STATE UNIVERSITY

CHEMISTRY 6020: MOLECULAR SPECTROSCOPY

SPRING SEMESTER 2019

Syllabus

Instructor: Alexander I. Boldyrev

Office: ML 369

Email: a.i.boldyrev@usu.edu

Class times: Monday 3:30 pm - 5:00 pm ML151 and Friday 3:30 pm - 5:00 pm

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 January 11. 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 March 20, 2019.

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.

No classes on Martin Luther King, Jr. Day January 21, Presidents' Day February 18, and Spring Break March 11 – March 15.
Last day of classes April 23.

Text: Molecular Spectroscopy (any 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.

Course content: Approximately the first 3-4 weeks of Chemistry 6020 will be devoted to review of Rotational-Vibrational Spectroscopy.

The Born-Oppenheimer Approximation and Its Consequences
Multiple Global and Local Minima on Potential Energy Surfaces
Permutational-Inversion Groups
The Harmonic Oscillator Model for Diatomic Molecules
Selection Rules for Vibrational Transitions for Diatomic Molecules
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 2-3 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 for polyatomic molecules. 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 3-4 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: O_2 and I_2
Vibrational Structure in Electronic Spectra of Diatomics
Polyatomic Molecules: Electronic States and Selection Rules
Molecular Orbitals and Electronic States of H_2O
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.).

Learning Objectives for Molecular Spectroscopy

Divisional level learning objectives in molecular spectroscopy are as follows. After completing the course students will be able to:

1. Determine a point group of any molecule.
2. Understand and use Character Tables and irreducible representations.
3. Know how to use projector operators for making symmetry adapted linear combinations of atomic orbitals.
4. Determine symmetry of molecular orbitals and normal vibrational modes.
5. Find symmetry of normal vibrational modes of any molecule.
6. Understand the Born-Oppenheimer approximation and its consequences.
7. Know the harmonic oscillator model and selection rules for vibrational transitions.
8. Understand perturbation theory of vibration-rotation energy.
9. Capable of finding energy levels of free rigid rotors and know the selection rules for rotational transitions.
10. Understand rotational absorption and emission spectroscopy, and rotational Raman spectroscopy.

11. Understand normal modes of vibrations in polyatomic molecules and the selection rules for vibrational transitions.
12. Know energy levels and selection rules for hydrogen atom.
13. Understand spin-orbit coupling and be capable of finding term symbol from an atomic electron configuration.
14. Understand molecular orbitals in diatomic and polyatomic molecules.
15. Know how to determine a term symbol and selection rules in diatomic and polyatomic molecules.

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.
