UTAH STATE UNIVERSITY

CHEMISTRY 6020: MOLECULAR SPECTROSCOPY

FALL SEMESTER 2009

Syllabus

Instructor: Alexander I. Boldyrev

Office: ML 369

Email: boldyrev@cc.usu.edu

Class times: W333 TR 4:30pm – 6:00pm

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 August 28. Attending this class beyond that date without being officially registered will not be approved by the Dean's Office.

The last day to submit a Petition for Late Drop Form is November 9, 2009.

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.

Text: Molecular Spectroscopy (1-st edition) by Jeanne L. McHale and Quantum Chemistry (5-th edition) by Ira N. Levine.

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

Course content: Approximately the first 6 weeks of Chemistry 6020 will be devoted to molecular symmetry and quantum chemistry (Quantum Chemistry (5-th edition) by Ira N. Levine. Chapters 12-15). The following topics will be covered:

Symmetry Point Groups
Character Tables, Irreduciable Representations
Symmetry of Molecular Vibrations
Symmetry of Molecular Orbitals
Schrodinger Equation
The Born-Oppenheimer Approximation
The Hartree-Fock Method
Molecular Orbital and Electron Density
Density Functional Methods
Configuration Interaction
Moller-Plesset Perturbation Theory
The Coupled-Cluster Method

The next 3 weeks will be devoted to rotational spectroscopy (Molecular Spectroscopy (1-st edition) by Jeanne L. McHale). 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 of diatomics (Molecular Spectroscopy (1-st edition) by Jeanne L. McHale). The following topics will be covered:

The Born-Oppenheimer Approximation and Its Consequences
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 3 weeks will be devoted to vibrational and electron spectroscopy of polyatomic molecules (Molecular Spectroscopy (1-st edition) by Jeanne L. McHale). 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
Selection Rules at Work: Benzene
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

After every section there will be a test (50 pts.) including the final exam (100 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.
