SYLLABUS

Time:	Mon./Wed./Fri. 9:40-10:30 am
Location:	PS H433
Instructor:	Prof. Dmitry Matyushov Office: PS D202E Phone: (480)9650057 E-mail: dmitrym@asu.edu Office hours: Mondays and Wednesdays, 10:30 - 11:30 am
Text:	"Symmetry and Spectroscopy", D. C. Harris & M. D. Bertolucci, Dover, NY 1978
Web page:	`http://www.public.asu.edu/~dmatyus/teaching/chm545/chm545.html`
Additional Text:	"Quantum Mechanics in Chemistry" by G. C. Schatz and M. A. Ratner (Dover, NY, 2002)

GRADING:

Homework: One in-class presentation and three homework assignments will be given during the semester. Each of homework assignments must be turned in by 6:00 PM on the due date. The homework assignments and the presentation will make 50 % of the grade. In addition, each week a homework assignment from the text will be given which will not be graded, but must be returned on time for a passing grade.

Mid-term exam: A one-hour mid-term exam (open-book and open-notes, 25 % of the grade).

Final exam: A cumulative assignment for an in-class presentation based on the material of the course, 25 % of the grade (May 8, 7:40-9:30am).

ABSTRACT:

This class is designed with the aim to teach basics of spectroscopy of polyatomic molecules. Minimum necessary background from quantum mechanics is provided with the main focus on the understanding of origin and quantitative description of molecular spectra. The use of symmetry in interpreting of electronic, IR, and Raman spectra is explained. Also included are the basics of the molecular orbital theory, Hückel formalism, and the buildup of Franck-Condon envelopes in electronic spectroscopy.

TENTATIVE LIST OF TOPICS

1. Principles of Quantum Mechanics
    - Properties of light
    - Schrödinger equation
    - Postulates of quantum mechanics
    - Dirac notation
2. Atomic Orbitals
    - Hydrogen atom and spherical functions
    - Atomic orbitals
    - Atomic configurations
    - Photoelectron spectroscopy
3. Theory of point groups
    - Symmetry operations
    - Groups
    - Point groups
    - Classification of molecules into point groups
    - Matrix representation
    - Decomposition into irreducible representations
4. Molecular orbital theory
    - The LCAO molecular orbitals
    - Diatomic molecules
    - Polyatomic molecules
    - The Hückel method
    - Transition metal complexes
5. Transitions between stationary states (Fermi Golden Rule)
6. Vibrational spectra
    - IR and Raman spectra
    - Harmonic oscillator and vibrational states
    - The normal modes of polyatomic molecules
    - Selection Rules
    - Symmetry coordinates and normal modes
    - The resonance Raman effect
7. Electronic spectra
    - Selection rules
    - Intensities of transitions
    - Franck-Condon envelope and vibronic analysis