

QUANTUM CHEMISTRY AND SPECTROSCOPY
(CHEMISTRY 571)
Fall 2017

Instructor: Dr. Kostas Vogiatzis
Office: Bu 319; Office Hours (open door or by appointment)
Phone: N/A

Textbooks: A. "Spectra of Atoms and Molecules; Second Edition"
Peter F. Bernath (Oxford University Press, New York, NY 2005).
B. "Modern Quantum Chemistry"
Szabo and Ostlund (Dover Publications, New York, 1996).
C. "Molecular Electronic Structure Theory"
Helgaker, Jorgensen, Olsen (Wiley, New Jersey, 2004).

Grading: Midterm Exam: 25%
Final Exam: 25%
Problem Sets: 25%
Computational Exercises: 25%

Class Schedule: Every Tuesday and Thursday, 11:10-12:25, Buehler 472

Topics: 1. Modern electronic structure theory
2. The electromagnetic spectrum, characteristics of radiation
3. Symmetry and group theory
4. Introduction to rovibrational spectroscopy
5. Electronic spectroscopy for atoms and molecules
6. Computational chemistry and spectroscopy

LECTURES

TOPICS

- I. Modern Electronic Structure Theory (Chapters from books B and C)
 - 1 Introduction - Foundations of Molecular Orbital Theory
 - 1 Second Quantization
 - 1 Exact and Approximate Wave Functions
 - 1 Atomic Basis Functions and Basis Sets
 - 1 Hartree-Fock Theory
 - 1 Multiconfigurational Quantum Chemistry
 - 1 Coupled-Cluster Theory – Perturbation Theory

- II. Electromagnetic Interactions (Book A, Chapter 1)
 - 1 Charge Distributions and their interaction with radiation fields
 - 1 Weak Field Electromagnetic Radiation and Optical Transitions

III. Symmetry and Group Theory (Book A, Chapters 2-4)

- 1 Symmetry Operators and Point Groups
- 2 Matrix Representation of Operators and Groups
- 2 Quantum Mechanics and Group Theory

IV. Rotational Spectroscopy (Book A, Chapter 6)

- 1 Structure and Rotation of Rigid Bodies
- 1 Pure Rotational Spectra of Diatomics and linear Polyatomics

V. Vibrational Spectroscopy (Book A, Chapters 7-8)

- 1 Vibrational Wavefunctions and Energy Expressions
- 1 Vibrational-Rotational Spectra in Diatomics
- 2 Polyatomic Normal Modes and Vibrational Transitions
- 1 Raman Spectroscopy
Calculation of rovibrational spectra of diatomic molecules

VI. Electronic Spectroscopy of Diatomic Molecules (Book A, Chapter 9)

- 1 Molecular Orbitals, Configurations and States - Vibrational Fine Structure in an Electronic Transition
- 1 Rotational Fine Structure in a Vibrational Transition

VII. Electronic Spectra of Polyatomic Molecules (Book A, Chapter 10)

- 1 Molecular Orbitals, Configurations and States
- 1 Electronic Structure and Spectra of Triatomic Molecules; Walsh's Rules
- 1 Categorizing Transitions: Allowed, Symmetry Forbidden, Vibronically Allowed, and Spin Forbidden
- 1 Electronic Structure and Spectra of larger polyatomics
Calculation of adsorption spectra of polyatomic molecules

VIII. Computational Spectroscopy (Notes)

Total:

27 lectures

2 lectures dedicated to exercises and computational spectroscopy