Computational Spectroscopy
Chemistry 3150:713

Purpose: A workshop style course to give hands-on experience with methods for computing molecular spectra.

Instructor: David Perry
KNCL 302
X 6825
dperry@uakron.edu

Time and Location: Tu, Th 10:45 AM - noon, CBA 134

Text: Foresman and Frisch, *Exploring Chemistry with electronic structure methods: A guide to using Gaussian*. See the Gaussian web site at *www.gaussian.com/allbooks.htm*
Supplementary text: Zare, *Angular Momentum, Understanding spatial aspects of chemistry and physics*

Course Credit: Student will undertake two projects, one small and one larger, and complete a few homework assignments designed to build the skills needed for the projects.

Large project		50%
Small Project	25%	
Assignments	25%	

Syllabus
Computational Spectroscopy
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I. *Introduction*
   a. What is Spectroscopy?
   b. Model Chemistries

II. *Ab initio methods for the computation of molecular spectra*
   a. Use of the Gaussian and Spartan programs.
      - Assignment 1: Spartan and Gaussian Tutorials
   b. Optimized structures and Rotational constants
      - Assignment 2: Optimized structures
   c. Infrared and Raman Spectra
      - Assignment 3: Calculated vibrational spectra
   d. Electronic Spectra
      - guest lecture by Ed Lim
      - Assignment 4: Calculated electronic spectra
   e. NMR spectra
   f. Convergence of results and computation cost.
      -Assignment 5: Basis set and correlation level convergence of ozone
   g. Advanced methods for thermochemistry
   h. Other available *ab initio* software and choice of software
      -Introduction to multi-reference methods and MolPro- guest lecture by Trocia Clasp

III. *Spectroscopic Hamiltonians*
   a. Introduction to MatLab
   b. Matrix operations
   c. Programming
      - Assignment 6: MatLab Tutorial
   d. Basis sets and Hamiltonian matrices
   e. Elementary operators for the harmonic oscillator
   f. Elementary operators for the asymmetric rotor
   g. Implementation of complex spectroscopic Hamiltonians
      - Assignment 7: The asymmetric rotor
   h. Matrix diagonalization methods: Jacobi, Householder, and Lanczos
   i. Symmetry and wave function diagnostics
   j. Selection rules

IV. *Atmospheric Spectra*
   a. Atmospheric constituents and absorption spectra
   b. The HITRAN database and the Javahawks software

Reserve Reading List

3150:713 Spring 2008
ST: Computational Spectroscopy
Instructor: David S. Perry

Angular Momentum: Understanding Spatial Aspects In Chemistry And Physics / Richard N. Zare
Zare, Richard N
New York: Wiley, c1988
QC793.3.A5 Z37 1988

Exploring Chemistry With Electronic Structure Methods / James B. Foresman, Æleen Frisch
Foresman, James B
Pittsburgh, PA: Gaussian, Inc., 1996
QD461 .F674 1996

Ab Initio Molecular Orbital Theory / Warren J. Hehre ... [Et Al.]
POPLE, JOHN A
New York: Wiley, c1986
QD461 .A185 1986

A Guide To Molecular Mechanics and Quantum Chemical Calculations / Warren J. Hehre
Hehre, Warren J
Irvine, CA: Wavefunction, c2003
QD462.6.D38 H447 2003 (book)
QD462.6.D38 H447 2003 (CD-ROM, DISC)

Additional Reading List

(not on reserve*)

Essentials of Computational Chemistry - Theories and Models, C. J. Cramer, Wiley 2004. Available through OhioLink – 15 libraries, or paperback from Amazon for $60.

Introduction to Computational Chemistry, Frank Jensen, Wiley, 2007.
UA call #: QD455.3.E4 J46 2007; also in 7 OhioLink libraries or paperback on Amazon for $64.

* I will have all of these books in my office. You can read any of them there.