Chem 3320
Wntr 2001

Molecular Structure & Energetics II

Instructor: Andrei Kutateladze, SGM 230, x2995
Text: (a) Ira Levine, "Quantum Chemistry", Fifth Edition, Prentice Hall, 2000 (b) J. B. Foresman, A. Frish, "Exploring Chemistry with Electronic Structure Methods", Second Edition, Gaussian, Inc.
Programs: Gaussian 98 (Gaussian, Inc.), Gamess (Mark Gordon's group at Iowa State), Spartan (Wavefunction, Inc)

Introduction

- Overview of computational methods (molecular mechanics, Hückel, semi-empirical and ab initio)
- Molecular geometry specification: Cartesian coordinates, internal coordinates, Z-matrix input; redundant coordinates, constraining molecular symmetry, "ghost" atoms;

Electronic Structure of Small Molecules

- Single point energy computations: choosing the level of theory (Hartree-Fock, electron correlation/post HF methods, Møller-Plesset perturbational treatment, configuration interaction methods, CI, MCSCF, the Density Functional Theory), basis set (Slater orbitals, minimal bases, split valence, polarized, diffuse functions); locating results in G98 output
- Geometry optimizations (locating minima on potential energy hypersurfaces, convergence criteria)
- Studying chemical reactions (potential energy surface scans, reaction path following)
- Frequency calculations, predicting IR and Raman spectra (input/output, normal modes, thermochemistry, zero-point energy)
- Excited States (input/output, CIS, CASSCF, excited state optimizations, triplet-singlet energy gaps and spin-orbit coupling)

Modeling Large Molecules

- Theory/limitations of force field methods (MM2, Sybyl etc.)
- Limitations of Hückel theory
- Theoretical basis and limitations of semi-empirical methods (CNDO, INDO, MINDO, MNDO, AM1, PM3 etc)
- Modeling conformational behavior of bio-molecules.

Grading:

Final Exam: 35%
Weekly Quizzes: 25%
Homeworks: 15%
Class Project: 25%