Molecular Structure & Energetics II

Instructor: Andrei Kutateladze, SGM 230, x2995. Office hours: Friday 12-2pm
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.
QM Software package: Gaussian 03 (Gaussian, Inc.)

Introduction

- Overview of computational methods (molecular mechanics, Hückel, semi-empirical and ab initio). Introduction to the Hückel theory.
- 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 G03 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)

Grading:

Final Exam: 35% (the date for which is to be determined)
Weekly Quizzes: 30% (two lowest scores are dropped, no make-up quizzes)
Homeworks:10%
Class Project: 25%