CHEM 461/867AB: Computational Chemistry (Fall 2025)
Professor: Dr. Allan East, Room RI312

Computational Chemistry is the use of computers to predict the properties of molecules. The course consists of Wednesday 08h30-09h45 lectures (CL206) and Friday 08h00-09h15 tutorials (computer room CL136), to allow lots of practical experience; we will use the computational chemistry software package Gaussian and its graphical user interface GaussView. The text is Essentials of Computational Chemistry, 2nd edition, by C. J. Cramer, and I will follow it closely.

1. Grading Scheme

Computational Assignments 40%, Midterm (Oct. 17) 20%, Exam (Dec. 10 14h00) 40%
The midterm and exam are hand-written. You must achieve 40% on EACH of the 3 components (and an overall 50%) to pass the course; otherwise, a grade of no more than 45% will be issued.

2. Computational Assignments

The assignments involve computations on the PCs in CL136, as well as some writeup of results. You can freely use CL136 whenever there is NOT a lecture going on; consult the schedule on the CL136 door to find out when other classes are scheduled there.

You will need a USB memory stick for your input and output files, because user files cannot be kept on those PCs (which are periodically cleaned by system administrators); please bring one every Tuesday to CL136. You may be asked to e-mail output files to the instructor as part of an assignment. There is a printer in CL136 as well, if you need.

Each student MUST prepare their own input files, do their own runs, and do their own assignment writeups.

3. Course Outline

Week 1: Ch. 1: Introduction
Week 2: Ch. 2: Molecular Mechanics (eg. AMBER, CHARMM, MM3)
Week 3: Ch. 4: Molecular Orbital (MO) Theory
Week 4: Ch. 5: Semi-Empirical MO methods (eg. INDO, AM1, PM3)
Week 5: Ch. 6: Ab Initio MO methods, including basis sets
Week 6: Ch. 7: Advanced MO methods (MCSCF, CI)
Week 7: Ch. 7: Advanced MO methods (MP2, CCSD)
Week 8: Ch. 8: Density Functional Theory
Week 9: Ch. 9: Spectroscopic Prediction (IR, NMR, ...) *[Chem867: X-ray?]*
Week 10: Ch. 10: Thermochemical Prediction (U, H, S, G) *[Chem867: Eigen ion and pKa?]*
Autumn Break: Nov. 10-14
Week 11: Ch. 14: Excited Electronic States
Week 12: Ch. 11: Implicit Solvent Models
Week 13: course review

4. Further Information

Office Hours: 14h30-15h20 weekdays. Office: RI312; go up the elevator, turn left, and then left through the nearest door, and down the hall.
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