Introduction to Computational Quantum Chemistry

Lesson 11: ADF

Amsterdam Density Functional

- "user-friendly DFT software for chemists"
- `https://www.scm.com/`
- Free trial licence for 30 days
- The licence for our clusters expires 20. December (negotiations under way, full licence coming no time soon)
- GUI available only at wolf23

Introduction

- Very fast code
- Uses Slater-type basis functions
- Functionalities:
  - Optimizations
  - Response properties (NMR, EPR, UV-VIS, IR, Mössbauer..)
  - NOCV
  - EDA
  - COSMO model of solvation
  - ZORA scalar and spin-orbit relativistic approach

GUI

- Nice and clear interface
- adfinput
- adfview
- adfoutput
- Only single licence

Running ADF jobs

- Input: keywords in blocks
- adf {-n nproc} < input.adf > output.out
- nmr {-n nproc} < input_nmr.adf > output_ nmr.out
- INFINITY takes care of the number of CPUs
- Tape files: binaries containing the orbitals
- `http://www.scm.com/Doc/Doc2014/ADF/ADFUsersGuide/page262.html#keyscheme%20SAVE`

NMR

- TAPE10 is required
- Separate input file with NMR keywords
- `http://www.scm.com/Doc/Doc2014/ADF/ADFUsersGuide/page188.html`

SCF calculations

- Use the prepared input files distributed in IS
- Write the molecular geometry in same format as .xyz (Å)
- Bond lengths:
  - HCl(scalar): 1.276930
  - HI(scalar) : 1.606800
  - HCl(SO): 1.276467
  - HI(SO): 1.609681

NMR calculations

- Calculate the NMR properties of hydrogen in HI and HCl
- For relativity use ZORA Scalar and ZORA Spin-Orbit approximations
- Compare the Experimental, Nonrelativistic, ECP, and Two component approach
- Chemical shielding for benzene ^{1}H nuclei: