Chem279
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November 8th, 2024

Chem 279 Assignment 3

In this assignment, we were to implement our own version of the CNDO/2 method to evaluate the total energy of a dimer. We had to generate the fock matrix (f), density matrices (p_a and p_b), the hamiltonian core (h), and use our overlap matrix (s) from the previous assignment. The SCF program is different from Hartree-Fock in its speed and simplicity, owing to the fact that empirical values are integrated into the evaluation (namely, the values for electron-electron interactions and ionization energies).

After setting the initial probability matrices to zero and defining the overlap matrix, we were then able to calculate the fock matrix for the alpha and beta electrons from both atoms.We could then find the eigenvectors from equation 2.1 and 2.2, which were needed to solve for the coefficients to update the probability matrices. The updated probability matrices were then used to re-calculate the fock matrix upon subsequent iterations. At convergence, one can calculate the total energy of the interaction.

In my implementation, I had time to focus solely on the H_2 dimer, and was able to approximate the total energy of the interaction. In addition, I decided to forgo nuclear-repulsion energy, being that it seemed negligible to the general evaluation of the problem. Of course, for more accurate predictions in the future, I would include it in my program. Another piece I did not get to add was the tolerance level (10^{-6}) to indicate convergence within the probability matrices.

Github: https://github.com/lkollmorgen/chem279_hw4