Programming Project 8: CCD
Coupled-cluster doubles

Equations

$$E_c = \tfrac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_{kl}^{cd} \tag{1}$$

$$t_{ij}^{ab} = \mathcal{E}_{ij}^{ab}\Bigg(\langle ab||ij\rangle + \tfrac{1}{2}\sum_{cd}\langle ab||cd\rangle t_{ij}^{cd} + \tfrac{1}{2}\sum_{kl}\langle kl||ij\rangle t_{kl}^{ab} + \hat{P}(ij|ab)\sum_{kc}\langle ak||ic\rangle t_{jk}^{bc} - \tfrac{1}{2}\hat{P}(ab)\sum_{klcd}\langle kl||cd\rangle t_{ij}^{ac}t_{kl}^{bd} - \tfrac{1}{2}\hat{P}(ij)\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ab}t_{jl}^{cd} + \tfrac{1}{4}\sum_{klcd}\langle kl||cd\rangle t_{ij}^{cd}t_{kl}^{ab} + \hat{P}(ij)\sum_{klcd}\langle kl||cd\rangle t_{ik}^{ac}t_{jl}^{bd}\Bigg) \tag{2}$$

$$\mathcal{E}_{ij}^{ab} \equiv \frac{1}{\varepsilon_i + \varepsilon_i - \varepsilon_a - \varepsilon_b}$$

Procedure

1. Set $t_{ij}^{ab} = 0$ as a starting guess.
2. Update amplitudes (equation 2)
3. Evaluate correlation energy (equation 1)
4. If energy is not converged, return to step 2