Programming Project 4: RMP2
Second-order Møller-Plesset perturbation theory (closed-shell)

Let $\{\phi_p\}$ be RHF spatial orbitals with orbital energies $\{\epsilon_p\}$ and basis expansion coefficients $C_{\mu p}$.

$$\langle \phi_p \phi_q | \phi_r \phi_s \rangle = \sum_{\mu\nu\rho\sigma} C^*_{\mu p} C^*_{\nu q} C_{\rho r} C_{\sigma s} \langle \chi_\mu \chi_\nu | \chi_\rho \chi_\sigma \rangle \tag{1}$$

$$E^{(2)} = \sum_{ijab} \frac{\langle \phi_i \phi_j | \phi_a \phi_b \rangle \left(\langle \phi_i \phi_j | \phi_a \phi_b \rangle - \langle \phi_i \phi_j | \phi_b \phi_a \rangle \right)}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b} \tag{2}$$

Procedure

1. Run RHF code to obtain MO coefficients $\{C_{\mu p}\}$ and orbital energies $\{\epsilon_p\}$.
2. Transform two-electron integrals from the AO basis $\{\chi_\mu\}$ to the MO basis $\{\phi_p\}$ (equation 1)
3. Evaluate MP2 energy expression (equation 2)