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 $C_{\mu P}$.

$$\langle \phi_P \phi_Q | \phi_R \phi_S \rangle = \sum_{\mu\nu\rho\sigma} \langle \chi_\mu \chi_\nu | \chi_\rho \chi_\sigma \rangle C^*_{\mu P} C^*_{\nu Q} C_{\rho R} C_{\sigma S} \tag{1}$$

$$E^{(2)} = \sum_{IJAB} \frac{\langle \phi_I \phi_J | \phi_A \phi_B \rangle \left(\langle \phi_I \phi_J | \phi_A \phi_B \rangle - \langle \phi_I \phi_J | \phi_B \phi_A \rangle \right)}{\epsilon_I + \epsilon_J - \epsilon_A - \epsilon_B} \tag{2}$$

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)