

1. Show that the canonical Hartree-Fock equations can be expressed in terms of spatial orbitals as follows.

$$\begin{aligned} \hat{f}_\alpha \phi_{p_\alpha} &= \epsilon_{p_\alpha} \phi_{p_\alpha} & \hat{f}_\alpha &= \hat{h} + \sum_{i_\alpha}^{n_\alpha} (\hat{J}_{i_\alpha} - \hat{K}_{i_\alpha}) + \sum_{i_\beta}^{n_\beta} \hat{J}_{i_\beta} \\ \hat{f}_\beta \phi_{p_\beta} &= \epsilon_{p_\beta} \phi_{p_\beta} & \hat{f}_\beta &= \hat{h} + \sum_{i_\alpha}^{n_\alpha} \hat{J}_{i_\alpha} + \sum_{i_\beta}^{n_\beta} (\hat{J}_{i_\beta} - \hat{K}_{i_\beta}) \end{aligned}$$

2. Expand the spatial orbitals in problem 1. as $\phi_{p_\omega} = \sum_\nu \chi_\nu C_{\mu p_\omega}$ and project each equation by χ_ν in order to arrive at the Pople-Nesbet equations.
3. Write out a complete algorithm for solving the Pople-Nesbet equations.