

Optional homework #10

Derive the coupled-perturbed Hartree–Fock (CPHF) equation for the first derivatives of density matrix elements with static nuclear displacement ($\omega = 0$). What are the corresponding quantities with normal-mode displacement at its frequency ω ?

J. A. Pople, R. Krishnan, H. B. Schlegel, and J. S. Binkley, *Int. J. Quantum Chem. Symp.* **13**, 225 (1979).