

**The Pariser-Parr-Pople model for trans-polyenes-III: derivation of equations of motion for excited state dynamics using two-determinantal and MCSCF type electronic wave functions.** Foerner, Wolfgang.

**Abstract**

An SCF treatment for excited two-determinantal states and for multiconfiguration SCF (MCSCF), including single excitations within the framework of the semiempirical PPP Hamiltonian is derived. Anal. gradients of the electronic energy with respect to the geometrical variables can be calcd. and the formation for the two-determinantal state is applied to the dynamics of singlet and triplet excited Bu states of polyenes. Due to tech. difficulties concerning orbital ordering, the inclusion of all single excitations in the excited state wave functions via an MCSCF treatment is necessary.