CASSCF CALCULATIONS VIA VARIATIONAL TWO-ELECTRON REDUCED-DENSITY-MATRIX THEORY

GERGELY GIDOFALVI, *Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439*; DAVID A. MAZZIOTTI, *Department of Chemistry and The James Franck Institute, The University of Chicago, Chicago, IL 60637*.

Variational reduced-density-matrix theory allows the computation of ground-state energies without the explicit construction of the N-electron wavefunction, and, with the incorporation of orbital rotations, may be employed in CASSCF calculations. The implementation and application of the method will be presented[a].

[a] G. Gidofalvi and D. A. Mazziotti, J. Chem. Phys. 127, 244105 (2007)