

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

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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<sup>a</sup>.

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<sup>a</sup>G. Gidofalvi and D. A. Mazziotti, *J. Chem. Phys.* 127, 244105 (2007)