THE DEVELOPMENT AND INITIAL APPLICATIONS OF A DOUBLE GROUP TWO-COMPONENT CI

<u>JEPPE OLSEN</u>, *Dept. of Chemistry, University of Aarhus*; TIMO FLEIG, *Dept. of Theoretical Chemistry, Bonn*; CHRISTEL M. MARIAN, *GMD St. Augustin (Germany)*.

We have recently developed and implemented an algorithm for performing extended CI calculations using a two-component formulation. In contrast to most previous approaches our program allows the use of general spinors as one-electron basis functions, and is accordingly based on the use of double group symmetry. The major advantage of using general spinors as basis functions is that orbital-contractions and -expansions due to spin-orbit coupling can be introduced in the orbital optimization. The CI-expansion of the wave function has then to account only for dynamic correlation, instead of dynamic correlation and orbital relaxation. We will discuss our calculations on Uranium- and Thallium - compounds, and show how the use of a general spinbasis does shorten the size of the required CI expansions.