Chemical species that display multiconfigurational character are some of the most difficult to treat theoretically, and different methods have over the years been devised to address this issue. One of the most successful approaches includes all possible configurations within a complete active space (CAS). However, the computational effort increases dramatically with the size of active space, which is a large hindrance for the use of CAS methods, which in practice is limited by 16 active orbitals.

The Density Matrix Renormalization Group (DMRG) method is a very efficient approximation to a CAS, making it possible to reach larger active spaces. DMRG is still under development, and is defined in different formalisms in a number of different programs. In all formalisms, both the efficiency and accuracy of the approximation relies on a few technical parameters (e.g. the number of renormalized states). We have here benchmarked the convergence of DMRG-SCF ground-state energies with respect to these technical parameters for three different implementations of DMRG (QCMaquis[1], cheMPS2[2] and Block[3]), integrated into the MOLCAS [4] code.

* Set of molecules:
  * Small-medium-large active space
  * Different flavours of DMRG
  * Dependence on \( m \)
  * Energy accuracy
  * Convergence
  * Faulty minima
  * Speed
  * Other limitations

**References:**