

Accurate and Efficient Treatment of Relativistic Effects Using an Exact Two-component Approach with Atomic-mean-field Integrals

CHAOQUN ZHANG, LAN CHENG

Department of Chemistry, Johns Hopkins University, Baltimore, MD, USA.

Relativistic effects play important roles in molecules containing heavy atoms. An exact two-component approach with atomic-mean-field integrals (the X2CAMF scheme) is presented with an efficient implementation to treat relativistic effects, including scalar relativistic effects, spin-orbit coupling, and Breit interaction. The accuracy of X2CAMF approach is demonstrated with benchmarks calculations of equilibrium bond lengths, harmonic frequencies, and dipole moments of selected small molecules. The X2CAMF scheme is generally compatible with quantum chemistry methods. It is combined with spin-orbit coupled-cluster (SO-CC) method together with analytical gradient techniques for highly accurate calculations of molecular equilibrium structures of heavy-atom-containing molecules.