ACCURATE PREDICTION OF EQUILIBRIUM STRUCTURE FOR HEAVY ELEMENT CONTAINING MOLECULES

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Accurate prediction of molecular geometries is a central subject in electronic structure theory. For accurate calculations of vibronic branching ratios in laser coolable molecules, it requires accurate calculations of molecular geometries for both electronic ground states and excited states. Using exact two-component theory with atomic-mean-field (X2CAMF) framework and analytical gradient techniques for spin-orbit coupled-cluster (SO-CC) method, we can obtain molecular equilibrium structures with accurate treatment of electron correlation and relativistic effects. By comparing with the experimental measurements of period-four-element containing diatomic molecules, the calculated bond lengths are accurate to 0.001 Å and the calculated harmonic frequencies are accurate to a few cm^{-1}.