Analytic Derivatives of Quartic-Scaling Doubly Hybrid XYGJ-OS Functional: Benchmark for Nonbonded Complexes

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Analytic gradients of XYGJ-OS[1], an opposite-spin (OS) ansatz[2] applied doubly hybrid functional with quartic scaling, is derived and implemented into Q-Chem quantum chemistry package[3]. The calculation of the first gradients scales quartically as the functional itself, with aid of Laplace transformation and resolution-of-identity technique. The assessment of XYGJ-OS optimized geometries for nonbonded complexes was performed by direct comparison with CCSD(T) geometries firstly, and CCSD(T)-F12 energy comparison with M06-2X and RI-MP2 geometries. The result showed that XYGJ-OS produced high quality geometries comparable to CCSD(T) ones, for both weakly bound complexes and molecules in S66 benchmark set[4], and were the most stable among the geometries obtained by three aforementioned methods.

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