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Atomization energies using analytic density functional theory[1]
RAJENDRA ZOPE, George Washington University, Washington DC , BRETT DUNLAP, US Naval Research Laboratory, Washington DC — Our recent formulation of analytic and variational Slater-Roothaan (SR) method uses Gaussian basis sets to express the molecular orbitals, electron density and the one-body effective potential of density functional theory. It allows arbitrary scaling of the exchange potential around each atom in heteroatomic systems. We examine the performance of the SR method for atomization energies using values of Slaters scaling parameters determined from the Hartree-Fock and the exact total atomic energies. We also present another set of scaling parameters for atomization energies. The performance of the computationally efficient SR method for the atomization energies of a set of 148 molecules using this third set of parameters is comparable to that of the Perdew-Burke-Ernzerhof generalized gradient approximation.

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