# A New Database and Benchmark of the Bond Energies of Noble-Gas Containing Molecules

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**Abstract**

We have developed a new database of structures and bond energies of 45 noble-gas containing molecules. The structures were calculated by CCSD(T)/aug-cc-pVTZ methods and the bond energies were obtained using CCSD(T)/CBS (complete basis set) method. Many wavefunction-based and density functional theory methods have been benchmarked against the 45 accurate bond energies. Our result showed that the MPW1B95, B2GP-PLYP, and DSD-BLYP functionals with the aug-cc-pVTZ basis set excel on predicting the bond energies of the noble-gas molecules with MUEs (mean unsigned errors) of 1.5-1.9 kcal/mol. When combinations of Dunning's basis sets are used, the MPW1B95, MPW1PW91, and B2GP-PLYP functional give significantly lower MUEs of 1.1-1.3 kcal/mol. Doubly hybrid methods using B2GP-PLYP and DSD-BLYP functionals and MP2 calculation also provide satisfactory accuracy with MUEs of 1.3-1.4 kcal/mol. If the noble-gas bond energies and the total atomization energies of a group of 109 main-group molecules are considered at the same time, the MPW1B95/aug-cc-pVTZ single-level method (MUE = 2.7 kcal/mol) and the B2GP-PLYP functional with combinations of basis sets (MUEs = 1.8 kcal/mol) give the overall best result.

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