The aug-cc-pVnZ-F12 Basis Set Family: Correlation Consistent Basis Sets for Explicitly Correlated Benchmark Calculations on Anions and Noncovalent Complexes

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We have developed a new basis set family, denoted aug-cc-pVnZ-F12 (or aVnZ-F12 for short), for explicitly correlated calculations. The sets included in this family were constructed by supplementing the corresponding cc-pVnZ-F12 sets with additional diffuse functions on the higher angular momenta (i.e., additional d-h functions on non-hydrogen atoms, and p-g on hydrogen), optimized for the MP2-F12 energy of the relevant atomic anions. The new basis sets have been benchmarked against electron affinities of the first- and second-row atoms, the W4-17 dataset of total atomization energies, the S66 dataset of noncovalent interactions, the BEGDB water clusters subset, and the WATER23 subset of the GMTKN24 and GMTKN30 benchmark suites. The aVnZ-F12 basis sets displayed excellent performance, not just for electron affinities but also for noncovalent interaction energies of neutral and anionic species. Appropriate CABS (complementary auxiliary basis sets) were explored for the S66 noncovalent interactions benchmark: between similar-sized basis sets, CABS were found to be more transferable than generally assumed.