Coupled-Cluster-based basis sets for valence correlation calculations

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New Gaussian atomic basis sets were developed whose primary focus is the description of the so-called valence correlation energy for first- and second-row atoms. The primitive functions in the Dunning's correlation consistent family (cc-pVXZ, X=D, T, Q, and so on) were used to generate new contraction coefficients according to the Atomic Natural Orbitals (ANO) scheme using Coupled-Cluster density matrices. The satisfaction of the Virial Theorem at the atomic level was subsequently carried out by scaling the exponents of the primitive functions. This approach was evaluated through the calculation of the contraction error for both the cc-pVXZ original functions and the herein proposed basis sets. The contraction errors obtained with the use of basis sets developed in this work are consistently smaller than those from the popular cc-pVXZ series, not only for atoms H-Ar, but also for a set of 13 diatomic molecules comprised of some of these atoms.