Performance of ANO-VT-XZ basis sets in the description of the density and potential energy curves

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We assessed the quality of the density obtained at the CCSD(T)/ANO-VT-XZ level of theory, with different sizes of the ANO-VT-XZ basis sets (X=D, T, Q). The results are evaluated in terms of the ability of the basis set to retrieve the features of the set of primitive functions, which is achieved by the computation of the corresponding contraction errors. The density is sampled in different regions of space through calculation of the contraction errors in $\langle r^n \rangle$, $-3 \leq n \leq 3$. Likewise, the contraction errors in ω_e and $\omega_e x_e$ obtained via two different approaches (DVR and Dunham) for a group of diatomic molecules are also computed. In both cases the results are compared to contraction errors similarly obtained using Dunning's correlation consistent basis sets (cc-pVXZ) of the same size. Overall, the ANO-VT-XZ series has superior performance in terms of the density in both short- and long-range regions of space and also in the abovementioned spectroscopic constants.