On the interaction-induced electric properties of linear $(HCN)_n$ clusters

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ABSTRACT

We report the results of calculations of the interaction energy and the incremental static electronic electric properties of linear hydrogen cyanide dimer and trimer. The nonadditivity of the interaction-induced electric properties in the studied HB trimer is analyzed in terms of the incremental properties obtained in the finite field differencing procedure of the interaction energy components obtained in the hybrid variational-perturbational interaction energy decomposition scheme at the Coupled-Cluster with noniterative triples CCSD(T) calculations.

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