ACHIEVING THE COMPLETE-BASIS LIMIT IN LARGE MOLECULAR CLUSTERS: COMPUTATIONALLY EFFICIENT PROCEDURES TO ELIMINATE BASIS-SET SUPERPOSITION ERROR

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Previous electronic structure studies that have relied on fragmentation have been primarily interested in those methods' abilities to replicate the supersystem energy (or a related energy difference) without recourse to the ability of those supersystem results to replicate experiment or high accuracy benchmarks. Here we focus on replicating accurate *ab initio* benchmarks, that are suitable for comparison to experimental data. In doing this it becomes imperative that we correct our methods for basis-set superposition errors (BSSE) in a computationally feasible way. This criterion leads us to develop a new method for BSSE correction, which we term the many-body counterpoise correction, or MBn for short. MBn is truncated at order n, in much the same manner as a normal many-body expansion leading to a decrease in computational time. Furthermore, its formulation in terms of fragments makes it especially suitable for use with pre-existing fragment codes. A secondary focus of this study is directed at assessing fragment methods' abilities to extrapolate to the complete basis set (CBS) limit as well as compute approximate triples corrections. Ultimately, by analysis of $(H_2O)_6$ and $(H_2O)_{10}F^-$ systems, it is concluded that with large enough basis-sets (triple or quad zeta) fragment based methods can replicate high level benchmarks in a fraction of the time.