Supplementary Information for "Analysis of two overlapping fragmentation approaches in density matrix construction: GMBE-DM vs ADMA"

Francisco Ballesteros and Ka Un Lao*
Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284 USA

TABLE S1: MAEs in millihartree (mH) for $(H_2O)_{N=6-55}$ at the level of HF/6-31G(d) and HF/def2-TZVPPD using the DM-based GMBE(1)-DM, ADMA, ADMA-S, ADMA-F, and ADMA-F-S approaches with respect to the supersystem results.

Method	MAE
GMBE(1)-DM[a]	16.3
ADMA[a]	101.5
ADMA-S[a]	434.5
ADMA-F[a]	86.0
ADMA-F-S[a]	319.6
GMBE(1)-DM[b]	19.5
ADMA[b]	613.0
ADMA-S[b]	2524.0
ADMA-F[b]	650.1
ADMA-F-S[b]	2214.0

TABLE S2: MAEs in milliHartree (mH) for $(H_2O)_{30}$ with a single ion including eight anions (F^-, Cl^-, Br^-, NO_3^-, $H_2PO_4^-$, SCN^-, CO_3^{2-}, and SO_4^{2-}) and and four cations (Li^+, Na^+, K^+, and NH_4^+) being inside or outside of the water cluster using the DM-based GMBE(1)-DM, ADMA, ADMA-S, ADMA-F, and ADMA-F-S approaches with respect to the supersystem calculations at the level of HF/6-31G(d) and HF/def2-TZVPPD.

Method	Cation	Anion	Inside	Outside	Overall
GMBE(1)-DM[a]	31.2	16.1	28.4	13.8	21.1
ADMA[a]	64.2	58.9	59.2	62.0	60.6
ADMA-S[a]	213.1	517.8	466.9	365.6	416.2
ADMA-F[a]	73.9	42.3	51.2	54.5	52.8
ADMA-F-S[a]	540.0	398.9	585.8	306.1	445.9
GMBE(1)-DM[b]	7.3	27.0	29.1	11.9	20.5
ADMA[b]	354.0	403.3	311.7	462.1	386.9
ADMA-S[b]	1859.0	2075.4	1577.4	2429.1	2003.3
ADMA-F[b]	466.0	700.0	633.2	610.8	622.0
ADMA-F-S[b]	2087.4	2503.8	2677.9	2052.1	2365.0

[a]HF/6-31G(d). [b]HF/def2-TZVPPD.

* email: laoku@vcu.edu