Supporting Information for: "Understanding the many-body expansion for large systems. III. Critical role of four-body terms, counterpoise corrections, and cutoffs"

Kuan-Yu Liu and John M. Herbert[*]

Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio 43210 USA
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TABLE S1: Comparison of δE^{CP} and MBCP(2) for $(\mathrm{H_2O})_N$ clusters, $N = 6$–37.

N	CP correction (Hartree)		difference
	δE^{CP}	MBCP(2)	(kcal/mol/monomer)
6	0.005	0.005	0.060
7	0.006	0.006	0.027
8	0.007	0.007	0.024
9	0.008	0.008	0.020
10	0.009	0.009	0.020
11	0.011	0.011	0.041
12	0.012	0.013	0.047
13	0.013	0.014	0.033
14	0.014	0.015	0.041
15	0.016	0.017	0.035
16	0.017	0.019	0.062
17	0.018	0.020	0.044
18	0.019	0.021	0.051
19	0.021	0.022	0.041
20	0.022	0.023	0.048
21	0.024	0.026	0.050
22	0.025	0.026	0.042
23	0.026	0.028	0.053
24	0.027	0.029	0.051
25	0.028	0.029	0.034
26	0.030	0.032	0.042
27	0.032	0.034	0.049
28	0.033	0.036	0.056
29	0.034	0.035	0.041
30	0.037	0.040	0.051
31	0.038	0.041	0.060
32	0.040	0.042	0.050
33	0.042	0.044	0.048
34	0.043	0.046	0.048
35	0.044	0.047	0.046
36	0.046	0.049	0.059
37	0.046	0.049	0.043

[*] herbert@chemistry.ohio-state.edu

TABLE S2: Interaction energies (in kcal/mol) arising from sub-clusters separated by 8–9Å, for the four structural motifs in $(H_2O)_{20}$ clusters.

Isomer	fused cubes	dodecahedra	face-sharing pentagonal prisms	edge-sharing pentagonal prisms
1	−0.544	0.000	−0.917	−0.455
2	−1.251	0.000	−2.064	−0.455
3	−0.737	0.000	−1.992	−0.454
4	0.521	0.241	−0.963	0.033
5	−0.565	0.000	−1.335	0.513
6	−0.579	0.000	−0.942	−0.455
7	−2.001	0.000	−0.916	−0.454
8	−0.738	0.000	−1.986	−0.028
9	−1.300	0.000	−1.986	−0.454
10	0.024	0.000	−0.917	−4.422
11	−0.615	0.000	−0.917	−0.028
12	−1.813	0.000	−1.064	0.031
13	−1.328	0.000	−1.799	0.032
14	−2.920	0.000	−2.064	−0.248
15	−0.076	0.216	−2.057	−0.029
16	0.508	0.000	−2.063	0.032
17	−0.753	0.000	−0.942	−0.028
18	−2.004	0.000	−2.057	−4.111
19	−0.951	0.000	−1.852	−0.028
20	−0.747	0.000	−1.828	−0.378