

**Supplementary information for: “Predictions for water clusters
from a first-principles two- and three-body force field”**

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TABLE 1. Comparisons of three-body nonadditive interaction energies (in kcal/mol) for a set of trimers from cage and prism hexamers. The geometries of trimers corresponding the labels given in the first column for each hexamer are listed in the Supplementary Information. The next column contains CBS extrapolated interaction energies, obtained in a hybrid way as described in the text. All the remaining columns list errors with respect to CBS benchmarks and are computed using the MP2, CCSD(T), and the hybrid method defined in the text. The last line lists the total three-body contributions to hexamer energies.

trimer	cage							prism						
	MP2		CCSD(T)				hybrid	MP2		CCSD(T)				hybrid
	CBS	aTZ	aDZ	haTZ	aTZ	aQZ	aT-DZ	CBS	aTZ	aDZ	haTZ	aTZ	aQZ	aT-DZ
123	0.667	-0.006	-0.004	-0.002	-0.002	-0.000	-0.004	0.512	-0.067	-0.044	-0.008	-0.004	-0.001	-0.008
124	-0.973	-0.017	0.013	-0.006	0.003	0.001	0.004	-1.120	-0.012	0.021	0.001	0.008	0.003	0.010
125	-1.165	-0.052	0.003	0.000	0.002	0.000	-0.000	-0.184	-0.007	0.003	0.001	0.002	0.001	0.002
126	0.039	0.003	0.003	0.002	0.001	0.000	0.000	-1.213	-0.026	0.016	0.003	0.005	0.002	0.006
134	0.015	-0.003	-0.005	-0.003	-0.001	-0.000	-0.000	-0.011	-0.002	-0.001	0.001	0.001	0.000	0.001
135	-0.633	-0.017	0.002	-0.009	-0.002	-0.001	-0.003	-0.947	-0.012	0.014	0.004	0.003	0.001	0.003
136	-0.035	0.004	0.004	0.002	0.002	0.001	0.003	-1.326	-0.010	0.025	0.005	0.008	0.003	0.010
145	-0.953	-0.018	0.011	-0.004	0.007	0.003	0.009	0.059	-0.002	0.000	-0.001	0.000	0.000	0.000
146	-0.109	-0.001	-0.001	-0.000	0.001	0.001	0.002	-1.089	-0.015	0.021	0.001	0.008	0.003	0.010
156	0.005	-0.006	-0.001	-0.003	-0.003	-0.001	-0.003	-1.086	-0.028	0.007	-0.011	0.004	0.001	0.006
234	-1.205	-0.022	0.015	-0.001	0.005	0.002	0.006	-0.488	-0.019	-0.004	-0.011	-0.001	-0.001	-0.001
235	0.574	-0.048	-0.033	-0.009	-0.001	-0.000	-0.003	0.543	-0.027	-0.021	-0.008	-0.001	-0.000	-0.003
236	-1.071	-0.005	0.011	0.002	0.005	0.002	0.006	0.048	-0.010	0.001	-0.001	0.000	0.000	-0.001
245	-1.125	-0.057	0.004	-0.001	0.000	-0.000	-0.002	-0.650	-0.022	0.012	0.005	0.002	0.001	0.001
246	-1.319	-0.004	0.015	-0.000	0.006	0.002	0.009	-1.006	-0.027	0.016	0.004	0.004	0.001	0.004
256	0.084	-0.006	0.006	0.000	0.001	0.000	0.001	0.007	-0.017	-0.002	-0.005	-0.001	-0.001	-0.004
345	0.617	-0.018	-0.010	-0.005	-0.001	0.000	-0.003	0.687	0.002	0.001	0.000	0.000	0.001	-0.001
346	-1.322	-0.017	0.018	-0.000	0.006	0.002	0.008	-0.159	-0.008	0.003	-0.000	0.001	0.000	0.001
356	-0.738	-0.019	0.011	0.004	0.004	0.001	0.003	-0.924	-0.020	0.013	-0.002	0.004	0.001	0.004
456	0.525	-0.030	-0.022	-0.003	0.001	0.000	-0.000	0.348	-0.073	-0.048	-0.019	-0.007	-0.002	-0.013
$E_{\text{int}}[3, 6]$	-8.121	-0.341	0.039	-0.036	0.036	0.013	0.031	-7.999	-0.405	0.032	-0.040	0.037	0.014	0.028

TABLE 2. Comparison of performance of various methods of computing three-body pairwise nonadditive interaction energies on the trimers extracted from the cage and prism hexamers. The order of trimers is the same as in Table 1. CC stands for CCSD(T). See text for definitions of other methods.

CBS	CC/(T-D)	HF(45)	MP2(45)	CC(34)	CCpol3	SAPT-3B	WHBB5	WHBB6	HBB2-pol
cage									
0.667	-0.004	0.042	-0.007	0.000	-0.019	0.089	-0.002	0.009	0.046
-0.973	0.004	-0.003	-0.018	-0.000	0.015	-0.013	0.004	0.029	-0.081
-1.165	-0.000	-0.053	-0.051	-0.001	-0.001	0.013	-0.072	-0.038	-0.034
0.039	0.000	0.022	0.002	-0.000	0.007	0.038	-0.037	-0.037	0.019
0.015	-0.000	-0.011	-0.002	0.000	-0.004	-0.014	-0.015	-0.010	0.016
-0.633	-0.003	-0.020	-0.015	-0.000	-0.000	-0.006	-0.052	0.003	-0.016
-0.035	0.003	-0.000	0.002	0.000	-0.004	0.010	0.034	0.029	-0.005
-0.953	0.009	-0.028	-0.022	0.000	0.024	-0.087	0.005	-0.022	-0.096
-0.109	0.002	-0.011	-0.002	-0.000	0.006	-0.064	0.101	0.099	-0.038
0.005	-0.003	0.004	-0.004	-0.000	-0.014	-0.075	-0.003	-0.005	-0.006
-1.205	0.006	-0.051	-0.024	-0.000	0.013	-0.021	-0.010	0.016	-0.012
0.574	-0.003	-0.104	-0.046	0.000	-0.014	-0.147	-0.096	-0.072	-0.036
-1.071	0.006	-0.004	-0.009	-0.000	0.029	0.138	0.029	0.034	0.037
-1.125	-0.002	-0.036	-0.055	-0.001	0.003	0.010	-0.036	0.010	0.050
-1.319	0.009	-0.015	-0.008	-0.000	0.028	0.157	-0.023	-0.001	0.059
0.084	0.001	-0.003	-0.006	-0.000	0.001	-0.039	-0.035	-0.023	0.029
0.617	-0.003	-0.016	-0.017	0.001	-0.038	-0.139	-0.074	-0.008	-0.039
-1.322	0.008	-0.052	-0.020	-0.000	0.009	0.021	-0.009	0.021	-0.014
-0.738	0.003	-0.006	-0.022	-0.000	0.040	0.057	-0.016	0.026	-0.035
0.525	-0.000	-0.081	-0.030	0.000	-0.018	-0.098	-0.036	-0.054	-0.032
-8.122	0.033	-0.426	-0.354	-0.001	0.063	-0.170	-0.343	0.006	-0.188
prism									
0.512	-0.008	-0.132	-0.061	0.001	-0.033	-0.400	-0.188	-0.073	0.018
-1.120	0.010	-0.015	-0.017	-0.000	0.002	-0.088	0.033	0.002	-0.059
-0.184	0.002	-0.006	-0.008	-0.000	0.009	0.015	0.032	0.016	-0.014
-1.213	0.006	-0.012	-0.030	-0.001	0.029	0.150	0.000	-0.001	0.110
-0.011	0.001	-0.007	-0.003	0.000	0.010	-0.056	0.012	-0.052	0.004
-0.947	0.003	0.010	-0.015	-0.000	0.015	0.128	0.018	0.030	0.047
-1.326	0.010	-0.006	-0.016	-0.000	0.032	0.195	0.019	0.019	0.096
0.059	0.000	0.000	-0.002	-0.000	0.005	-0.022	-0.031	-0.011	-0.011
-1.089	0.010	-0.022	-0.020	-0.000	-0.014	-0.186	0.030	-0.004	-0.084
-1.086	0.006	-0.035	-0.030	-0.000	0.019	-0.001	-0.058	-0.025	-0.134
-0.488	-0.001	-0.038	-0.018	-0.000	-0.006	-0.158	-0.011	0.010	-0.081
0.543	-0.003	-0.077	-0.025	0.000	-0.019	-0.111	-0.040	-0.042	-0.106
0.048	-0.001	-0.013	-0.010	0.000	-0.024	-0.078	-0.061	-0.035	-0.033
-0.650	0.001	-0.002	-0.023	-0.000	0.007	0.051	-0.023	0.016	-0.012
-1.006	0.004	-0.008	-0.030	-0.001	0.017	0.117	0.005	-0.013	0.083
0.007	-0.004	-0.011	-0.016	-0.000	-0.015	-0.065	-0.006	-0.010	0.009
0.687	-0.001	0.026	0.000	0.000	-0.009	0.025	-0.065	-0.026	-0.010
-0.159	0.001	-0.003	-0.009	-0.000	-0.006	-0.042	0.010	0.005	0.007
-0.924	0.004	-0.002	-0.022	-0.000	0.028	0.036	0.061	0.020	-0.065
0.348	-0.013	-0.113	-0.065	0.001	-0.031	-0.321	-0.163	-0.063	-0.054
-7.999	0.027	-0.466	-0.420	0.000	0.016	-0.811	-0.426	-0.237	-0.289