SUPPORTING INFORMATION

for

Physical Molecular Mechanics Method for Damped Dispersion

Pragya Verma, Bo Wang,[‡] Laura E. Fernandez,[†] and Donald G. Truhlar*

Department of Chemistry, Nanoporous Materials Genome Center, Chemical Theory Center, and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455-0431

*E-mail: truhlar@umn.edu

Present Addresses:
[‡]BW: Global Energy Interconnection Research Institute, State Grid Corporation of China, San Jose, CA
[†]LEF: American Chemical Society, Washington, D.C. 20036

Date and time of finalization of Supporting Information: Mar. 6, 2017, 11:57 pm.

Table S1 shows how damped dispersion contributions to the binding of two monomers are affected by the geometry of the monomer. The first column (**1**) with each DFT-D3 method refers to the case in which the geometries of the monomers are separately optimized and the second column (**2**) with each DFT-D3 method (and also SAPT(DFT)) refers to the case in which the geometries of the monomers are the same as in the complex.

Table S1. Damped dispersion contributions ($\Delta E_{\text{dampdisp}}$ in kcal/mol)[a] for the NCCE31/05 database.

Complex	SAPT(DFT) Disp + Exch-Disp[b]	DD3S		OLYP -D3(BJ)		OPBE -D3(BJ)	
	2	**1**	**2**	**1**	**2**	**1**	**2**
$(NH_3)_2$	–2.11	–2.05	–2.05	–1.73	–1.73	–1.77	–1.77
$(HF)_2$	–1.66	–1.77	–1.77	–1.17	–1.17	–1.12	–1.12
$(H_2O)_2$	–2.30	–2.30	–2.30	–1.69	–1.69	–1.66	–1.66
$NH_3…H_2O$	–3.03	–2.84	–2.85	–2.13	–2.13	–2.11	–2.11
$(HCONH_2)_2$	–7.41	–7.29	–7.26	–5.71	–5.71	–5.78	–5.78
$(HCOOH)_2$	–8.78	–7.90	–8.02	–5.94	–6.00	–5.93	–5.97
$C_2H_4…F_2$	–1.63	–1.19	–1.19	–1.16	–1.16	–1.24	–1.24
$NH_3…F_2$	–1.80	–0.98	–0.98	–0.88	–0.88	–0.90	–0.90
$C_2H_2…ClF$	–5.01	–5.27	–5.29	–4.28	–4.28	–4.23	–4.23
HCN…ClF	–4.18	–3.52	–3.53	–2.67	–2.68	–2.61	–2.61
$NH_3…Cl_2$	–4.70	–3.51	–3.55	–2.93	–2.94	–2.95	–2.96
$H_2O…ClF$	–4.05	–3.27	–3.28	–2.54	–2.54	–2.49	–2.49
$NH_3…ClF$	–9.16	–5.82	–5.88	–4.20	–4.21	–4.02	–4.03
$(H_2S)_2$	–2.05	–2.28	–2.28	–2.16	–2.16	–2.30	–2.30
$(HCl)_2$	–2.05	–2.59	–2.59	–2.22	–2.22	–2.28	–2.28
$HCl…H_2S$	–2.96	–3.40	–3.40	–2.86	–2.86	–2.92	–2.92
$CH_3Cl…HCl$	–3.63	–4.58	–4.60	–3.93	–3.93	–4.02	–4.03
$HCN…CH_3SH$	–2.69	–3.70	–3.72	–3.36	–3.37	–3.51	–3.52
$CH_3SH…HCl$	–4.61	–5.49	–5.49	–4.66	–4.65	–4.76	–4.76
HeNe	–0.08	–0.08	–0.08	–0.08	–0.08	–0.09	–0.09
HeAr	–0.13	–0.13	–0.13	–0.13	–0.13	–0.15	–0.15
Ne_2	–0.16	–0.17	–0.17	–0.17	–0.17	–0.18	–0.18
NeAr	–0.27	–0.28	–0.28	–0.29	–0.29	–0.32	–0.32
$CH_4…Ne$	–0.33	–0.36	–0.36	–0.38	–0.38	–0.41	–0.41
$C_6H_6…Ne$	–1.00	–1.03	–1.03	–1.09	–1.09	–1.20	–1.21
$(CH_4)_2$	–1.26	–1.57	–1.58	–1.63	–1.63	–1.78	–1.78
$(C_2H_2)_2$	–1.42	–1.82	–1.83	–1.84	–1.85	–2.00	–2.00
$(C_2H_4)_2$	–2.60	–3.92	–3.93	–3.84	–3.84	–4.11	–4.11
sandwich $(C_6H_6)_2$	–4.72	–5.89	–5.29	–6.04	–5.78	–6.69	–6.48
T-shaped $(C_6H_6)_2$	–4.07	–6.02	–5.42	–5.73	–5.47	–6.14	–5.94
parallel-displaced $(C_6H_6)_2$	–5.82	–7.31	–6.71	–7.50	–7.25	–8.30	–8.09
Average[c]	–3.09	–3.17	–3.12	–2.74	–2.72	–2.84	–2.82
Method MUE[d]	0.00	0.63	0.57	0.87	0.84	0.98	0.96

[a] $\Delta E_{\text{dampdisp}}$ is defined as $E_{\text{dampdisp}}^{\text{complex}} - E_{\text{dampdisp}}^{\text{monomer\_1}} - E_{\text{dampdisp}}^{\text{monomer\_2}}$.

[b] Ref. 20 of the paper.

[c]The average for each method is taken over all 31 complexes.
[d]MUE = mean unsigned error.