Supplementary information for: "Improved interaction energy benchmarks for dimers of biological relevance"

Rafał Podeszwa

Institute of Chemistry, University of Silesia,

Szkolna 9, 40-006 Katowice, Poland and

Department of Physics and Astronomy,

University of Delaware, Newark, Delaware 19716

Konrad Patkowski and Krzysztof Szalewicz

Department of Physics and Astronomy,

University of Delaware, Newark, Delaware 19716

(Dated: March 23, 2010)

TABLE 1: Interaction energies (in kcal/mol) and estimated errors for the S22 database.

		SCF[a]			MP2[b]					
#	Complex (symmetry)	aTZ	aQZ	a5Z	aTZ	aQZ	a5Z	CBS(TQ)	CBS(Q5)	%err[c]
Hydrogen-bonded complexes										
1	$(NH_3)_2$ (C_{2h})	-1.397	-1.406	-1.407	-2.989	-3.088	-3.121	-3.156	-3.154	0.06%
2	$(H_2O)_2$ (C_s)	-3.547	-3.585	-3.585	-4.685	-4.855	-4.904	-4.961	-4.955	0.12%
3	Formic acid dimer (C_s)	-15.185	-15.283	-15.294	-17.544	-18.137	-18.330	-18.522	-18.525	-0.01%
4	Formamide dimer (C_{2h})	-12.097	-12.185	-12.189	-15.023	-15.493	-15.639	-15.794	-15.789	0.03%
5	Uracil dimer (C_{2h})	-16.198	-16.272		-19.594	-20.065		-20.372		
6	2-pyridone · 2-aminopyridine (C_1)	-10.425	-10.478		-16.633	-17.059		-17.344		
7	Adenine · Thymine WC (C_1)	-10.004	-10.058		-15.792	-16.229		-16.522		
Complexes with predominant dispersion contribution										
8	$(CH_4)_2$ (D_{3d})	0.371	0.368	0.367	-0.455	-0.477	-0.485	-0.492	-0.493	-0.11%
9	$(C_2H_4)_2$ (D_{2d})	0.835	0.829	0.828	-1.456	-1.532	-1.555	-1.584	-1.579	0.33%
10	Benzene · CH_4 (C_3)	1.177	1.170	1.169	-1.700	-1.769	-1.790	-1.815	-1.812	0.18%
11	Benzene dimer (C_{2h})	5.367	5.358	5.355	-4.693	-4.846	-4.901	-4.954	-4.955	-0.03%
12	Pyrazine dimer (C_s)	4.199	4.189	4.183	-6.565	-6.748	-6.831	-6.877	-6.913	-0.52%
13	Uracil dimer (C_2)	0.069	0.050		-10.605	-10.890		-11.088		
14	Indole · Benzene (C_1)	7.052	7.043	7.038	-7.728	-7.932	-8.006	-8.077	-8.081	-0.04%
15	Adenine · Thymine stack (C_1)	3.314	3.296		-14.235	-14.586		-14.834		
Mixed complexes										
16	Ethene · ethyne (C_{2v})	-0.432	-0.432	-0.431	-1.581	-1.627	-1.644	-1.661	-1.662	-0.08%
17	Benzene · H_2O (C_s)	-0.931	-0.937	-0.938	-3.349	-3.459	-3.497	-3.537	-3.537	0.00%
18	Benzene · NH_3 (C_s)	0.187	0.180	0.179	-2.512	-2.599	-2.627	-2.658	-2.656	0.11%
19	Benzene · HCN (C_s)	-1.996	-1.991	-1.990	-4.920	-5.057	-5.111	-5.159	-5.169	-0.19%
20	Benzene dimer (C_{2v})	1.518	1.517	1.516	-3.454	-3.554	-3.589	-3.626	-3.626	-0.02%
21	Indole · Benzene T-shape (C_s)	0.285	0.289		-6.707	-6.860		-6.975		
22	Phenol dimer (C_1)	-1.801	-1.838		-7.353	-7.587		-7.740		
									avg:[d]	0.12%

[a] RI-SCF results in aug-cc-pVXZ basis set, X = 3, 4, 5.

[b] RI-MP2 results in aug-cc-pVXZ basis set, X = 3, 4, 5 and CBS extrapolations.

[c] Percentage error of (TQ) CBS MP2 extrapolation with respect to the (Q5) one.

[d] Average magnitude of percentage deviation of the (TQ) CBS MP2 extrapolations with respect to (Q5) CBS.

TABLE 2: Interaction energies (in kcal/mol) and estimated errors for the S22 database, cont.

		MP2							
# Complex (symmetry)	X[a]	aXZ+mb[b]	CBS[c]	err[d]	$E_{\rm int}$ [e]	$\delta E_{\rm int}^{\rm CCSD(T)}$ [f]	err[g]	%err[h]	%unc[i]
Hydrogen bonded complexes									
1 $(NH_3)_2$ (C_{2h})	4	-3.105	-3.154	-1.55%	-3.145	0.009	0.000	0.00%	0.55%
2 $(H_2O)_2$ (C_s)	4	-4.877	-4.955	-1.58%	-5.004	-0.049	-0.001	0.02%	0.62%
3 Formic acid dimer (C_s)	3	-17.682	-18.525	-4.55%	-18.751	-0.226	-0.010	0.05%	0.53%
4 Formamide dimer (C_{2h})	3	-15.121	-15.789	-4.23%	-16.063	-0.274	-0.012	0.07%	0.59%
5 Uracil dimer (C_{2h})	3	-19.696	-20.372	-3.32%	-20.643	-0.271	-0.009	0.04%	0.77%
6 2-pyridone · 2-aminopyridine (C_1)	3	-16.715	-17.344	-3.63%	-16.938	0.406	0.015	-0.09%	0.77%
7 Adenine · Thymine WC (C_1)	2	-15.215	-16.522	-7.91%	-16.554	-0.033	-0.003	0.02%	0.77%
Complexes with predominant dispersion contribution									
8 $(CH_4)_2$ (D_{3d})	4	-0.485	-0.493	-1.44%	-0.529	-0.037	-0.001	0.10%	0.34%
9 $(C_2H_4)_2$ (D_{2d})	4	-1.545	-1.579	-2.12%	-1.482	0.096	0.002	-0.14%	0.62%
10 Benzene · CH_4 (C_3)	3	-1.753	-1.812	-3.26%	-1.448	0.364	0.012	-0.82%	1.02%
11 Benzene dimer (C_{2h})	3	-4.782	-4.955	-3.49%	-2.655	2.301	0.080	-3.02%	3.08%
12 Pyrazine dimer (C_s)	3	-6.753	-6.913	-2.31%	-4.256	2.658	0.062	-1.45%	1.64%
13 Uracil dimer (C_2)	3	-10.730	-11.088	-3.23%	-9.783	1.305	0.042	-0.43%	0.88%
14 Indole · Benzene (C_1)	3	-7.824	-8.081	-3.18%	-4.523	3.557	0.113	-2.50%	2.54%
15 Adenine · Thymine stack (C_1)	2	-13.636	-14.834	-8.08%	-11.857	2.978	0.241	-2.03%	2.17%
Mixed complexes									
16 Ethene · ethyne (C_{2v})	4	-1.637	-1.662	-1.54%	-1.503	0.159	0.002	-0.16%	0.52%
17 Benzene · H_2O (C_s)	3	-3.424	-3.537	-3.17%	-3.280	0.257	0.008	-0.25%	0.63%
18 Benzene · NH_3 (C_s)	3	-2.573	-2.656	-3.11%	-2.319	0.336	0.010	-0.45%	0.74%
19 Benzene · HCN (C_s)	3	-5.005	-5.169	-3.18%	-4.540	0.629	0.020	-0.44%	0.75%
20 Benzene dimer (C_{2v})	3	-3.519	-3.626	-2.96%	-2.717	0.909	0.027	-0.99%	1.15%
21 Indole · Benzene T-shape (C_s)	3	-6.790	-6.975	-2.65%	-5.627	1.348	0.036	-0.63%	1.00%
22 Phenol dimer (C_1)	3	-7.465	-7.740	-3.56%	-7.097	0.643	0.023	-0.32%	0.83%
							avg[j]:	0.64%	1.02%

[a] The aug-cc-pVXZ+mb level used in the MP2 and CCSD(T) calculations.

[b] The MP2 aug-cc-pVXZ+mb energy.

[c] The CBS extrapolated values, same as in the column with the identical header in Table 1 of the main text.

[d] Percentage error of the MP2/aug-cc-pVXZ+mb result with respect to MP2/CBS.

[e] The total interaction energies calculated using Eq. (1) of the main paper, same as in the column with the identical header in Table 1 of the main text.

[f] Calculated in the aug-cc-pVXZ+mb basis set.

[g] Error of $\delta E_{\rm int}^{\rm CCSD(T)}$ estimated by multiplying the MP2/aug-cc-pVXZ+mb error (column 6) by $\delta E_{\rm int}^{\rm CCSD(T)}$.

[h] Ratio of the previous column to $E_{\rm int}$, in percent.

[i] Total percentage uncertainties computed as $\sqrt{\sigma_{\rm MP2}^2 + \sigma_{\delta_{\rm CCSD(T)}}^2 + \sigma_{\rm FC}^2 + \sigma_{\rm exc}^2}$, where $\sigma_{\rm MP2}$ is the estimated MP2 CBS error (last column of Table 1) or 0.5%, $\sigma_{\delta_{\rm CCSD(T)}}$ is the preceding column, $\sigma_{\rm FC}$ are the values in the last column of Table 3 or 0.5%, and $\sigma_{\rm exc} = 0.3\%$ are the uncertainties resulting from excitations beyond the CCSD(T) level.

[j] Average magnitude of the percentage deviations in this column.

TABLE 3: CCSD(T) frozen-core and all-electron results (in kcal/mol). Aug-cc-pCVTZ+mb basis set was used for all studied systems, except for indole-benzene, where aug-cc-pCVDZ+mb was used.

#	Complex (symmetry)	AE[a]	FC[b]	%diff[c]
Hydrogen bonded complexes				
1	$(NH_3)_2$ (C_{2h})	-3.068	-3.053	0.46%
2	$(H_2O)_2$ (C_s)	-4.880	-4.854	0.53%
3	Formic acid dimer (C_s)	-18.004	-17.927	0.43%
4	Formamide dimer (C_{2h})			
5	Uracil dimer (C_{2h})			
6	2-pyridone · 2-aminopyridine (C_1)			
7	Adenine · Thymine WC (C_1)			
	MUE/MURE			
Complexes with predominant dispersion contribution				
8	$(CH_4)_2$ (D_{3d})	-0.520	-0.520	-0.03%
9	$(C_2H_4)_2$ (D_{2d})	-1.432	-1.426	0.40%
10	Benzene · CH_4 (C_3)			
11	Benzene dimer (C_{2h})			
12	Pyrazine dimer (C_s)			
13	Uracil dimer (C_2)			
14	Indole · Benzene (C_1)	-4.028	-4.013	0.36%
15	Adenine · Thymine stack (C_1)			
	MUE/MURE			
Mixed complexes				
16	Ethene · ethyne (C_{2v})	-1.465	-1.460	0.38%
17	Benzene · H_2O (C_s)			
18	Benzene · NH_3 (C_s)			
19	Benzene · HCN (C_s)			
20	Benzene dimer (C_{2v})			
21	Indole · Benzene T-shape (C_s)			
22	Phenol dimer (C_1)			
			avg[d]:	0.37%

[a] All electron.

[b] Frozen core.

[c] Percentage contribution of the AE-FC effect to the all-electron interaction energy.

[d] Average magnitude of the percentage deviations in this column.