Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Correction to DFT interaction energies by an empirical dispersion term valid for a range of intermolecular distances

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Supplementary Material

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TABLE SI: Mean absolute percent errors of dispersion corrected interaction energies in kcal/mol*

Method	Basis set	With BSSE correction			Without BSSE correction		
		Dispersion interacting	Mixed	Hydrogen bonded	Dispersion interacting	Mixed	Hydrogen bonded
B3LYP-DD	6-311G(d,p)	10.0	19.6	11.8	9.5	14.7	30.5
	6-311+G(d,p)	8.0	11.9	8.2	6.9	11.9	9.6

* The absolute error of the methane dimer was considered to be the average absolute error of the two methane dimers from the S22 and WI7 data sets.

TABLE SII: C6 [Jnm^6/mol] and r_0 [Å] parameters used in computation of present dispersion corrections originally reported by Grimme *et al.* [43] C6 parameters were converted to $kcal/mol * Å^6$ with a conversion factor of $10^6/4184$

Element	C6	r_0	Element	C6	r_0
H	0.14	1.001	F	0.75	1.287
He	0.08	1.012	Ne	0.63	1.243
Li	1.61	0.825	Na	5.71	1.144
Be	1.61	1.408	Mg	5.71	1.364
B	3.13	1.485	Al	10.79	1.639
C	1.75	1.452	Si	9.23	1.716
N	1.23	1.397	P	7.84	1.705
O	0.70	1.342			

TABLE SIII: Minima of the dispersion corrected interaction energy[†] and corresponding intermolecular distances [‡] for stacked adenine-thymine

Method	Interaction Energy [kcal/mol]	Intermolecular Distance [Å]
B3LYP-DD/6-311+G(d,p)	−12.97	3.26
B3LYP-DD/6-311+G(d,p) (Counterpoise)	−12.92	3.20
Best Estimate[*]	−12.23	3.19

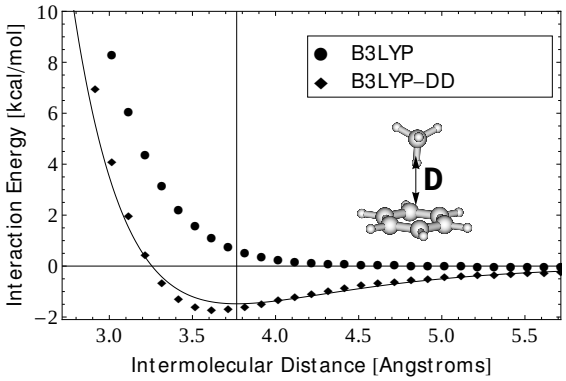
[†] The minima were found by linear least squares fitting a second order polynomial to seven data points, the minimum and three points on each side, of the adenine-thymine intermolecular interaction energy curve

[‡] The intermolecular distances were measured as the distance between thymine's C4 atom and adenine's C5 atom

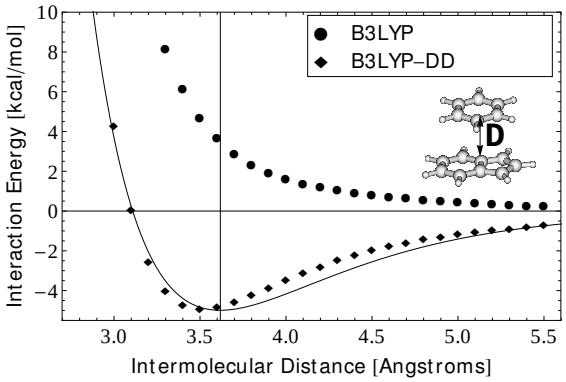
[*] Best estimate for the interaction energy was calculated at the CCSD(T)/CBS level with geometries obtained at the MP2/cc-pVTZ level with BSSE corrections

TABLE SIV: Interaction energies obtained for six bimolecular systems. The values reported are the lowest for the range of intermolecular distances repoted in Figures 4, 5, and 6. These are close to the minimum of the IES but do not strictly correspond to it. [†]Values obtained by fitting with a Morse potential the CCSD(T)/CBS reference data at the corresponding intermolecular distances are also shown

System	With BSSE correction		Without BSSE correction	
	B3LYP-DD/6-311+G(d,p) with dispersion	CCSD(T)/CBS[†]	B3LYP-DD/6-311+G(d,p) with dispersion	CCSD(T)/CBS[†]
benzene-methane	−1.68	−1.40	−1.60	−1.47
indole-benzene stack	−4.89	−4.83	−5.15	−4.99
benzene-dimer-C2v	−3.04	−2.78	−3.04	−2.81
indole-benzene t-shape	−6.05	−5.97	−5.93	−5.97
2 pyridoxine-2 aminopyridine	−17.97	−16.69	−18.06	−16.69
ammonia-dimer	−3.88	−3.27	−3.74	−3.25

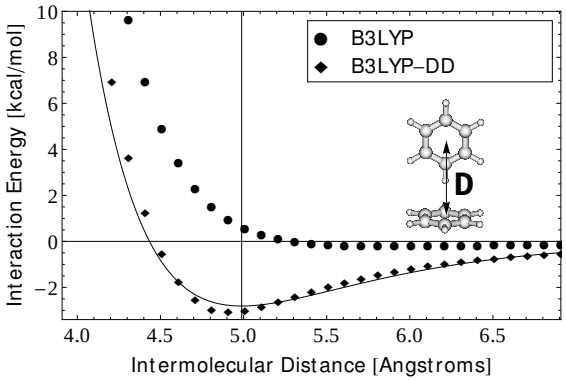


(a)benzene-methane

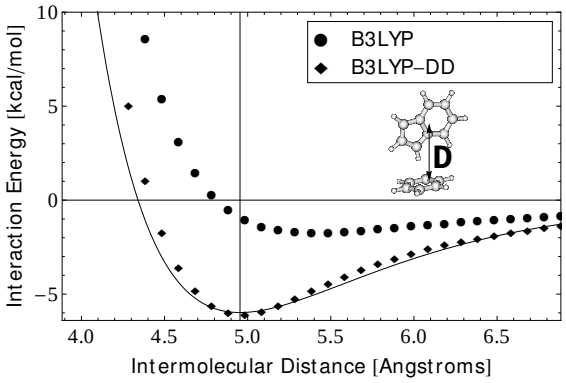


(b)indole-benzene stack

FIG. S1: Interaction energy surfaces for two dispersion-interacting systems (benzene-methane and indole-benzene stack). Calculations were done at the B3LYP/6311+G(d,p) and B3LYP-DD/6311+G(d,p) levels with BSSE correction. Solid lines are Morse potentials fitted to CCSD(T)/CBS data. [46] Distance dependent B3LYP, B3LYP-DD, and Morse potential energies given in Supplementary Tables SVI and SVIII.

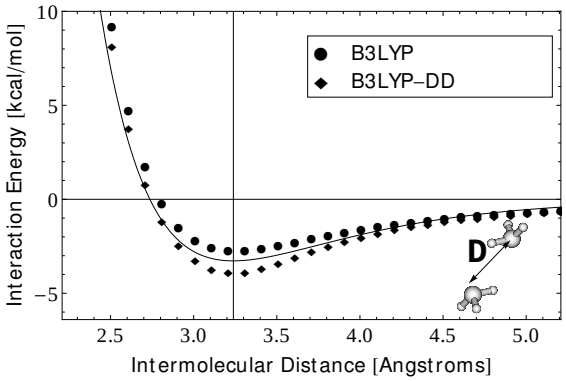


(a)benzene dimer C2v

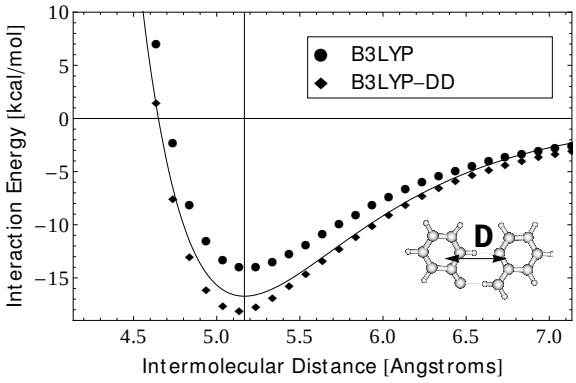


(b)indole-benzene T shape

FIG. S2: Interaction energy surfaces for two mixed systems (benzene dimer C2v and indole-benzene T shape). Calculations were done at the B3LYP/6311+G(d,p) and B3LYP-DD/6311+G(d,p) levels with BSSE correction. Solid lines are Morse potentials fitted to CCSD(T)/CBS data. [46] Distance dependent B3LYP, B3LYP-DD, and Morse potential energies given in Supplementary Tables SX and SXII.



(a)ammonia dimer



(b)2 pyridoxine-2 aminopyridine

FIG. S3: Interaction energy surfaces for the two hydrogen systems (namely ammonia dimer and 2 pyridoxine-2 aminopyridine). Calculations were done at the B3LYP/6311+G(d,p) and B3LYP-DD/6311+G(d,p) levels with BSSE correction. Solid lines are Morse potentials fitted to CCSD(T)/CBS data. [46] respectively. [47] Distance dependent B3LYP, B3LYP-DD, and Morse potential energies given in Supplementary Tables SXIV and SXVI.

TABLE SV: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for benzene-methane. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E_{CCSD(T)}^{Morse\ Fit}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E_{CCSD(T)}^{c}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
3.316	2.96	-0.07	-0.43	82.74	0.36	-0.40	0.33
3.416	2.07	-0.85	-0.93	8.40	0.08		
3.516	1.44	-1.32	-1.24	-6.58	-0.08	-1.24	-0.08
3.616	0.98	-1.54	-1.40	-9.86	-0.14	-1.41	-0.13
3.716 (d_{min})[b]	0.67	-1.60	-1.47	-8.50	-0.13	-1.48	-0.12
3.816	0.44	-1.55	-1.47	-5.33	-0.08	-1.48	-0.07
3.916	0.29	-1.45	-1.43	-1.63	-0.02	-1.43	-0.02
4.016	0.19	-1.33	-1.36	2.02	0.03		
4.116	0.12	-1.20	-1.27	5.45	0.07	-1.26	0.06
4.216	0.08	-1.07	-1.17	8.59	0.10		
4.316	0.06	-0.95	-1.07	11.03	0.12		
4.416	0.04	-0.85	-0.97	12.72	0.12	-0.95	0.10
4.516	0.03	-0.75	-0.87	14.25	0.12		
4.616	0.02	-0.66	-0.79	15.67	0.13		
4.716	0.01	-0.59	-0.70	16.05	0.11	-0.70	0.11
4.816	0.00	-0.53	-0.62	15.08	0.09		
4.916	-0.01	-0.48	-0.55	13.60	0.07		
5.016	-0.01	-0.43	-0.49	12.28	0.06		
5.116	-0.01	-0.39	-0.43	10.79	0.04		
5.216	-0.02	-0.35	-0.38	8.16	0.03	-0.40	0.05
5.316	-0.02	-0.32	-0.34	5.07	0.02		
5.416	-0.02	-0.29	-0.30	2.19	0.01		
5.516	-0.02	-0.26	-0.26	-0.23	0.00		
5.616	-0.02	-0.24	-0.23	-2.96	-0.01		
5.716	-0.02	-0.22	-0.20	-6.82	-0.02	-0.24	0.02
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				0.84	0.06		
$d_{min.}-0.30 \leftrightarrow d_{min.}+2.00$				7.61	0.05		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SVI: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for benzene-methane. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
3.316	3.17	-0.61	-0.43	-42.34	-0.18	-0.40	-0.21
3.416	2.26	-1.25	-0.93	-34.53	-0.32		
3.516	1.60	-1.57	-1.24	-26.98	-0.33	-1.24	-0.33
3.616	1.13	-1.68	-1.40	-19.38	-0.28	-1.41	-0.27
3.716 (d_{min})[b]	0.80	-1.65	-1.47	-12.29	-0.18	-1.48	-0.17
3.816	0.56	-1.56	-1.47	-6.00	-0.09	-1.48	-0.08
3.916	0.40	-1.44	-1.43	-0.62	-0.01	-1.43	-0.01
4.016	0.29	-1.30	-1.36	3.95	0.06		
4.116	0.22	-1.17	-1.27	7.93	0.10	-1.26	0.09
4.216	0.17	-1.04	-1.17	11.31	0.13		
4.316	0.13	-0.92	-1.07	13.98	0.15		
4.416	0.11	-0.81	-0.97	16.10	0.16	-0.95	0.14
4.516	0.09	-0.72	-0.87	17.89	0.15		
4.616	0.08	-0.63	-0.79	19.26	0.16		
4.716	0.07	-0.56	-0.70	19.81	0.14	-0.70	0.14
4.816	0.06	-0.50	-0.62	19.73	0.12		
4.916	0.05	-0.45	-0.55	19.54	0.10		
5.016	0.04	-0.40	-0.49	19.17	0.09		
5.116	0.04	-0.36	-0.43	18.07	0.07		
5.216	0.03	-0.32	-0.38	15.67	0.06	-0.40	0.08
5.316	0.02	-0.29	-0.34	13.12	0.05		
5.416	0.02	-0.26	-0.30	10.86	0.04		
5.516	0.01	-0.24	-0.26	8.51	0.02		
5.616	0.01	-0.22	-0.23	5.08	0.01		
5.716	0.00	-0.20	-0.20	0.25	0.00	-0.24	0.04
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				6.27	0.09		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				17.39	0.16		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SVII: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for indole-benzene. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
3.098	13.35	1.44	0.29	-404.46	1.15	0.28	1.16
3.198	9.69	-1.67	-2.03	17.51	0.36		
3.298	7.04	-3.60	-3.51	-2.56	-0.09	-3.52	-0.08
3.398	5.12	-4.66	-4.38	-6.37	-0.28	-4.45	-0.21
3.498 (d_{min})[b]	3.74	-5.11	-4.83	-5.79	-0.28	-4.87	-0.24
3.598	2.77	-5.15	-4.99	-3.36	-0.16	-5.00	-0.15
3.698	2.09	-4.95	-4.94	-0.24	-0.01	-4.89	-0.06
3.798	1.61	-4.62	-4.75	2.81	0.13		
3.898	1.25	-4.25	-4.49	5.41	0.24	-4.42	0.17
3.998	1.00	-3.86	-4.18	7.67	0.32		
4.098	0.82	-3.47	-3.84	9.66	0.37		
4.198	0.69	-3.11	-3.50	11.12	0.39	-3.46	0.35
4.298	0.58	-2.80	-3.17	11.86	0.37		
4.398	0.49	-2.51	-2.86	12.07	0.35		
4.498	0.42	-2.25	-2.56	12.05	0.31	-2.50	0.25
4.598	0.37	-2.01	-2.28	11.82	0.27		
4.698	0.33	-1.80	-2.03	11.31	0.23		
4.798	0.29	-1.62	-1.80	10.33	0.18		
4.898	0.26	-1.46	-1.60	8.80	0.14		
4.998	0.23	-1.32	-1.41	6.73	0.09	-1.47	0.15
5.098	0.20	-1.19	-1.24	4.26	0.05		
5.198	0.17	-1.08	-1.10	1.51	0.02		
5.298	0.15	-0.98	-0.96	-1.43	-0.02		
5.398	0.14	-0.89	-0.85	-4.48	-0.04		
5.498	0.13	-0.80	-0.74	-8.10	-0.06	-0.92	0.12
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				1.16	0.11		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				12.81	0.21		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SVIII: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for indole-benzene. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
3.098	14.66	0.12	0.29	57.57	-0.17	0.28	-0.16
3.198	10.92	-2.51	-2.03	-23.63	-0.48		
3.298	8.18	-3.99	-3.51	-13.78	-0.48	-3.52	-0.47
3.398	6.20	-4.69	-4.38	-6.98	-0.31	-4.45	-0.24
3.498 (d_{min})[b]	4.76	-4.89	-4.83	-1.19	-0.06	-4.87	-0.02
3.598	3.71	-4.79	-4.99	3.88	0.20	-5.00	0.21
3.698	2.95	-4.53	-4.94	8.31	0.41	-4.89	0.36
3.798	2.39	-4.18	-4.75	12.15	0.57		
3.898	1.98	-3.79	-4.49	15.48	0.70	-4.42	0.63
3.998	1.67	-3.42	-4.18	18.21	0.76		
4.098	1.43	-3.06	-3.84	20.30	0.78		
4.198	1.24	-2.73	-3.50	21.98	0.77	-3.46	0.73
4.298	1.10	-2.43	-3.17	23.44	0.74		
4.398	0.98	-2.15	-2.86	24.58	0.71		
4.498	0.87	-1.92	-2.56	25.05	0.64	-2.50	0.58
4.598	0.77	-1.72	-2.28	24.81	0.56		
4.698	0.69	-1.54	-2.03	24.32	0.49		
4.798	0.62	-1.37	-1.80	23.82	0.43		
4.898	0.56	-1.23	-1.60	23.14	0.37		
4.998	0.51	-1.10	-1.41	21.94	0.31	-1.47	0.37
5.098	0.46	-1.00	-1.24	19.97	0.24		
5.198	0.40	-0.91	-1.10	17.36	0.19		
5.298	0.36	-0.82	-0.96	14.62	0.14		
5.398	0.33	-0.74	-0.85	12.28	0.11		
5.498	0.30	-0.67	-0.74	10.04	0.07	-0.92	0.25
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				5.62	0.06		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				16.84	0.28		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SIX: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for benzene dimer C2v. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.509	4.41	-0.07	-0.91	92.42	0.84	0.44	-0.51
4.609	2.94	-1.32	-1.77	25.61	0.45		
4.709	1.88	-2.18	-2.32	6.06	0.14	-1.89	-0.29
4.809	1.12	-2.72	-2.63	-3.23	-0.09	-2.43	-0.29
4.909 (d_{min})[b]	0.59	-2.98	-2.78	-7.38	-0.20	-2.72	-0.26
5.009	0.22	-3.04	-2.81	-8.15	-0.23	-2.83	-0.21
5.109	-0.03	-2.94	-2.76	-6.82	-0.18	-2.83	-0.11
5.209	-0.19	-2.77	-2.65	-4.53	-0.12		
5.309	-0.29	-2.56	-2.50	-2.02	-0.06	-2.57	0.01
5.409	-0.34	-2.33	-2.34	0.31	0.01		
5.509	-0.36	-2.12	-2.17	2.38	0.05		
5.609	-0.37	-1.91	-1.99	4.16	0.08	-2.04	0.13
5.709	-0.36	-1.72	-1.82	5.36	0.10		
5.809	-0.35	-1.56	-1.65	5.94	0.09		
5.909	-0.34	-1.40	-1.50	6.33	0.10	-1.52	0.12
6.009	-0.31	-1.26	-1.35	6.65	0.09		
6.109	-0.29	-1.14	-1.21	6.30	0.07		
6.209	-0.28	-1.04	-1.09	4.88	0.05		
6.309	-0.27	-0.95	-0.98	2.95	0.03		
6.409	-0.26	-0.86	-0.87	1.03	0.01	-0.90	0.04
6.509	-0.24	-0.79	-0.78	-1.03	-0.01		
6.609	-0.23	-0.72	-0.69	-4.01	-0.03		
6.709	-0.22	-0.66	-0.62	-7.67	-0.04		
6.809	-0.21	-0.61	-0.55	-11.44	-0.06		
6.909	-0.20	-0.56	-0.49	-15.08	-0.07	-0.53	-0.03
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				3.85	0.06		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				20.35	0.26		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SX: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for benzene dimer C2v. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.509	4.94	-0.49	-0.91	46.42	0.42	0.44	-0.93
4.609	3.44	-1.72	-1.77	2.94	0.05		
4.709	2.34	-2.51	-2.32	-8.28	-0.19	-1.89	-0.62
4.809	1.55	-2.92	-2.63	-10.89	-0.29	-2.43	-0.49
4.909 (d_{min})[b]	0.98	-3.04	-2.78	-9.34	-0.26	-2.72	-0.32
5.009	0.59	-2.98	-2.81	-5.98	-0.17	-2.83	-0.15
5.109	0.31	-2.81	-2.76	-2.07	-0.05	-2.83	0.02
5.209	0.13	-2.60	-2.65	1.73	0.05		
5.309	0.01	-2.38	-2.50	5.10	0.12	-2.57	0.19
5.409	-0.06	-2.15	-2.34	7.96	0.19		
5.509	-0.11	-1.94	-2.17	10.40	0.23		
5.609	-0.13	-1.75	-1.99	12.38	0.24	-2.04	0.29
5.709	-0.15	-1.57	-1.82	13.78	0.25		
5.809	-0.15	-1.41	-1.65	14.68	0.24		
5.909	-0.16	-1.27	-1.50	15.26	0.23	-1.52	0.25
6.009	-0.15	-1.14	-1.35	15.52	0.21		
6.109	-0.15	-1.03	-1.21	15.21	0.18		
6.209	-0.15	-0.93	-1.09	14.30	0.16		
6.309	-0.14	-0.85	-0.98	13.14	0.13		
6.409	-0.14	-0.77	-0.87	11.81	0.10	-0.90	0.13
6.509	-0.13	-0.70	-0.78	10.06	0.08		
6.609	-0.13	-0.64	-0.69	7.45	0.05		
6.709	-0.13	-0.59	-0.62	4.44	0.03		
6.809	-0.12	-0.54	-0.55	1.42	0.01		
6.909	-0.12	-0.50	-0.49	-1.74	-0.01	-0.53	0.03
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.} + 2.00$				3.80	0.13		
$d_{min.} - 0.30\text{Å} \leftrightarrow d_{min.} + 2.00$				2.34	0.03		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXI: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies (kcal/mol) for indole-benzene T shape. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.484	4.66	-1.22	-3.04	59.83	1.82	-3.02	1.80
4.584	2.42	-3.17	-4.37	27.52	1.20		
4.684	0.81	-4.46	-5.22	14.63	0.76	-5.33	0.87
4.784	-0.31	-5.27	-5.71	7.74	0.44	-5.85	0.58
4.884 (d_{min})[b]	-1.07	-5.74	-5.94	3.41	0.20	-6.00	0.26
4.984	-1.56	-5.93	-5.97	0.71	0.04	-5.99	0.06
5.084	-1.85	-5.90	-5.87	-0.53	-0.03	-5.83	-0.07
5.184	-2.01	-5.69	-5.67	-0.47	-0.02		
5.284	-2.07	-5.38	-5.40	0.46	0.02	-5.26	-0.12
5.384	-2.08	-5.02	-5.09	1.52	0.07		
5.484	-2.04	-4.63	-4.77	2.91	0.14		
5.584	-1.96	-4.24	-4.43	4.16	0.19	-4.23	-0.01
5.684	-1.87	-3.88	-4.09	5.11	0.21		
5.784	-1.77	-3.55	-3.77	5.78	0.22		
5.884	-1.67	-3.24	-3.45	6.10	0.21	-3.34	0.10
5.984	-1.57	-2.96	-3.15	5.94	0.19		
6.084	-1.48	-2.72	-2.87	5.33	0.15		
6.184	-1.38	-2.49	-2.61	4.45	0.12		
6.284	-1.30	-2.29	-2.36	3.26	0.07		
6.384	-1.22	-2.11	-2.14	1.59	0.03	-2.24	0.13
6.484	-1.15	-1.95	-1.93	-0.60	-0.02		
6.584	-1.08	-1.80	-1.75	-3.11	-0.05		
6.684	-1.02	-1.66	-1.57	-5.73	-0.09		
6.784	-0.95	-1.54	-1.42	-8.50	-0.12		
6.884	-0.90	-1.42	-1.27	-11.61	-0.15	-1.48	0.06
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				7.51	0.18		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				19.57	0.68		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXII: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for indole-benzene T shape. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.484	5.43	-1.67	-3.04	45.28	1.37	-3.02	1.35
4.584	3.13	-3.54	-4.37	18.90	0.83		
4.684	1.48	-4.79	-5.22	8.25	0.43	-5.33	0.54
4.784	0.32	-5.57	-5.71	2.53	0.14	-5.85	0.28
4.884 (d_{min})[b]	-0.48	-5.97	-5.94	-0.46	-0.03	-6.00	0.03
4.984	-1.01	-6.05	-5.97	-1.22	-0.08	-5.99	-0.06
5.084	-1.35	-5.88	-5.87	-0.27	-0.01	-5.83	-0.05
5.184	-1.55	-5.57	-5.67	1.63	0.10		
5.284	-1.65	-5.19	-5.40	3.84	0.21	-5.26	0.07
5.384	-1.68	-4.79	-5.09	5.94	0.30		
5.484	-1.67	-4.40	-4.77	7.78	0.37		
5.584	-1.62	-4.02	-4.43	9.25	0.41	-4.23	0.21
5.684	-1.56	-3.67	-4.09	10.31	0.42		
5.784	-1.49	-3.35	-3.77	10.97	0.42		
5.884	-1.42	-3.06	-3.45	11.27	0.39	-3.34	0.28
5.984	-1.34	-2.80	-3.15	11.18	0.35		
6.084	-1.27	-2.56	-2.87	10.68	0.31		
6.184	-1.19	-2.35	-2.61	9.85	0.26		
6.284	-1.12	-2.16	-2.36	8.73	0.20		
6.384	-1.06	-1.98	-2.14	7.30	0.16	-2.24	0.26
6.484	-1.00	-1.83	-1.93	5.46	0.10		
6.584	-0.94	-1.69	-1.75	3.20	0.06		
6.684	-0.89	-1.56	-1.57	0.68	0.01		
6.784	-0.84	-1.45	-1.42	-2.06	-0.03		
6.884	-0.79	-1.34	-1.27	-5.10	-0.07	-1.48	0.14
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				2.32	0.02		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				12.00	0.45		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXIII: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for ammonia-dimer. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
2.809	-0.61	-1.32	-1.13	-17.39	-0.19	-0.78	-0.54
2.909	-1.79	-2.48	-2.19	-13.61	-0.29		
3.009	-2.46	-3.18	-2.82	-12.77	-0.36	-2.65	-0.53
3.109	-2.79	-3.56	-3.15	-13.10	-0.41	-2.99	-0.57
3.209 (d_{min})[b]	-2.90	-3.73	-3.27	-14.09	-0.46	-3.10	-0.63
3.309	-2.86	-3.74	-3.25	-15.07	-0.49	-3.07	-0.67
3.409	-2.73	-3.61	-3.13	-15.24	-0.48	-2.94	-0.67
3.509	-2.56	-3.38	-2.96	-14.30	-0.42		
3.609	-2.36	-3.10	-2.75	-12.57	-0.35	-2.56	-0.54
3.709	-2.16	-2.80	-2.53	-10.64	-0.27		
3.809	-1.97	-2.51	-2.30	-8.97	-0.21		
3.909	-1.79	-2.25	-2.08	-7.82	-0.17	-1.94	-0.31
4.009	-1.62	-2.01	-1.87	-7.25	-0.14		
4.109	-1.46	-1.80	-1.68	-7.32	-0.12		
4.209	-1.33	-1.61	-1.49	-8.09	-0.12	-1.43	-0.18
4.309	-1.21	-1.45	-1.33	-9.45	-0.12		
4.409	-1.10	-1.31	-1.17	-11.40	-0.14		
4.509	-1.00	-1.18	-1.04	-14.10	-0.14		
4.609	-0.92	-1.07	-0.91	-17.49	-0.16		
4.709	-0.84	-0.98	-0.81	-21.33	-0.17	-0.87	-0.11
4.809	-0.77	-0.89	-0.71	-25.81	-0.18		
4.909	-0.71	-0.81	-0.62	-31.16	-0.19		
5.009	-0.66	-0.75	-0.54	-37.18	-0.21		
5.109	-0.61	-0.69	-0.48	-43.73	-0.21		
5.209	-0.56	-0.63	-0.42	-51.06	-0.21	-0.56	-0.07
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				18.49	0.33		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				18.73	0.04		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXIV: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for ammonia-dimer. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E^{\text{Morse Fit}}_{CCSD(T)}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E^{c}_{CCSD(T)}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
2.809	-0.21	-1.13	-1.13	-0.54	0.00	-0.78	-0.35
2.909	-1.45	-2.42	-2.19	-10.56	-0.23		
3.009	-2.17	-3.23	-2.82	-14.43	-0.41	-2.65	-0.58
3.109	-2.55	-3.69	-3.15	-17.17	-0.54	-2.99	-0.70
3.209 (d_{min})[b]	-2.69	-3.88	-3.27	-18.75	-0.61	-3.10	-0.78
3.309	-2.68	-3.85	-3.25	-18.61	-0.60	-3.07	-0.78
3.409	-2.58	-3.66	-3.13	-16.78	-0.53	-2.94	-0.72
3.509	-2.43	-3.38	-2.96	-14.06	-0.42		
3.609	-2.26	-3.06	-2.75	-11.26	-0.31	-2.56	-0.50
3.709	-2.07	-2.75	-2.53	-8.86	-0.22		
3.809	-1.89	-2.47	-2.30	-7.07	-0.17		
3.909	-1.72	-2.21	-2.08	-5.97	-0.13	-1.94	-0.27
4.009	-1.57	-1.98	-1.87	-5.53	-0.11		
4.109	-1.42	-1.77	-1.68	-5.74	-0.09		
4.209	-1.29	-1.59	-1.49	-6.64	-0.10	-1.43	-0.16
4.309	-1.18	-1.43	-1.33	-8.11	-0.10		
4.409	-1.07	-1.29	-1.17	-10.14	-0.12		
4.509	-0.98	-1.17	-1.04	-12.89	-0.13		
4.609	-0.90	-1.06	-0.91	-16.31	-0.15		
4.709	-0.82	-0.97	-0.81	-20.15	-0.16	-0.87	-0.10
4.809	-0.76	-0.88	-0.71	-24.62	-0.17		
4.909	-0.70	-0.81	-0.62	-29.97	-0.19		
5.009	-0.65	-0.74	-0.54	-36.02	-0.20		
5.109	-0.60	-0.68	-0.48	-42.62	-0.20		
5.209	-0.55	-0.63	-0.42	-50.02	-0.21	-0.56	-0.07
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				15.64	0.20		
$d_{min.}-0.30\text{Å} \leftrightarrow d_{min.}+2.00$				19.73	0.01		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXV: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for 2 pyridoxine-2 aminopyridine. Energies computed with 6311+G(d,p) basis without BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E_{CCSD(T)}^{Morse\ Fit}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E_{CCSD(T)}^{c}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.736	-3.22	-7.57	-6.57	-15.33	-1.00	-5.96	-1.61
4.836	-8.93	-13.04 1	-11.55	-12.93	-1.49		
4.936	-12.26	-16.15	-14.54	-11.04	-1.61	-14.76	-1.39
5.036	-13.97	-17.65 2	-16.11	-9.53	-1.54	-16.37	-1.28
5.136 (d_{min})[b]	-14.59	-18.06	-16.69	-8.22	-1.37	-16.76	-1.30
5.236	-14.50	-17.75	-16.59	-7.00	-1.16	-16.60	-1.15
5.336	-13.95	-16.96	-16.03	-5.82	-0.93	-15.81	-1.15
5.436	-13.14	-15.89	-15.18	-4.66	-0.71		
5.536	-12.20	-14.69	-14.16	-3.68	-0.53	-13.84	-0.85
5.636	-11.20	-13.46	-13.07	-2.99	-0.39		
5.736	-10.22	-12.27	-11.95	-2.72	-0.32		
5.836	-9.27	-11.16	-10.85	-2.86	-0.31	-10.52	-0.64
5.936	-8.39	-10.12	-9.79	-3.29	-0.33		
6.036	-7.57	-9.13	-8.80	-3.83	-0.33		
6.136	-6.83	-8.22	-7.87	-4.45	-0.35	-7.80	-0.42
6.236	-6.16	-7.39	-7.02	-5.23	-0.37		
6.336	-5.55	-6.64	-6.25	-6.28	-0.39		
6.436	-5.01	-5.97	-5.54	-7.68	-0.43		
6.536	-4.53	-5.37	-4.91	-9.50	-0.46		
6.636	-4.10	-4.85	-4.34	-11.77	-0.51	-4.79	-0.06
6.736	-3.73	-4.39	-3.83	-14.51	-0.56		
6.836	-3.39	-3.98	-3.38	-17.72	-0.60		
6.936	-3.09	-3.61	-2.97	-21.42	-0.64		
7.036	-2.82	-3.29	-2.62	-25.63	-0.67		
7.136	-2.58	-3.00	-2.30	-30.41	-0.70	-3.00	0.00
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				11.00	0.33		
$d_{min.}-0.30 \leftrightarrow d_{min.}+2.00$				8.74	0.40		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].

TABLE SXVI: Intermolecular distances (Å), B3LYP interaction energies, and B3LYP-DD interaction energies for 2 pyridoxine-2 aminopyridine. Energies computed with 6311+G(d,p) basis with BSSE correction.

Intermolecular distance (Å)	E_{B3LYP} [kcal/mol]	$E_{B3LYP-DD}$ [kcal/mol]	$E_{CCSD(T)}^{Morse\ Fit}$ [kcal/mol]	% Error[a]	Abs. Error[a] [kcal/mol]	$E_{CCSD(T)}^{c}$ [kcal/mol]	Abs. Error[d] [kcal/mol]
4.736	-2.22	-7.43	-6.57	-13.10	-0.86	-5.96	-1.47
4.836	-8.02	-12.93	-11.55	-11.93	-1.38		
4.936	-11.43	-16.07	-14.54	-10.49	-1.53	-14.76	-1.31
5.036	-13.21	-17.58	-16.11	-9.08	-1.47	-16.37	-1.21
5.136 (d_{min})[b]	-13.90	-17.97	-16.69	-7.67	-1.28	-16.76	-1.21
5.236	-13.88	-17.62	-16.59	-6.20	-1.03	-16.60	-1.02
5.336	-13.40	-16.79	-16.03	-4.75	-0.76	-15.81	-0.98
5.436	-12.65	-15.70	-15.18	-3.45	-0.52		
5.536	-11.76	-14.52	-14.16	-2.49	-0.36	-13.84	-0.68
5.636	-10.81	-13.33	-13.07	-1.96	-0.26		
5.736	-9.85	-12.17	-11.95	-1.83	-0.22		
5.836	-8.93	-11.05	-10.85	-1.86	-0.20	-10.52	-0.53
5.936	-8.07	-9.98	-9.79	-1.85	-0.19		
6.036	-7.27	-8.96	-8.80	-1.86	-0.16		
6.136	-6.55	-8.03	-7.87	-2.02	-0.16	-7.80	-0.23
6.236	-5.90	-7.20	-7.03	-2.48	-0.18		
6.336	-5.31	-6.45	-6.25	-3.31	-0.20		
6.436	-4.80	-5.80	-5.54	-4.57	-0.26		
6.536	-4.34	-5.22	-4.91	-6.28	-0.31		
6.636	-3.93	-4.71	-4.34	-8.46	-0.37	-4.79	0.08
6.736	-3.57	-4.26	-3.83	-11.11	-0.43		
6.836	-3.24	-3.86	-3.38	-14.23	-0.48		
6.936	-2.96	-3.51	-2.97	-17.85	-0.54		
7.036	-2.70	-3.19	-2.62	-22.00	-0.57		
7.136	-2.48	-2.92	-2.30	-26.70	-0.62	-3.00	0.08
				MAD	MAD		
$d_{min.} \leftrightarrow d_{min.}+2.00$				9.52	0.33		
$d_{min.}-0.30 \leftrightarrow d_{min.}+2.00$				7.39	0.38		

[a] B3LYP-DD error relative to fit with a Morse potential to CCSD(T)/CBS distance-dependent data.
[b] Intermolecular distance at minimum interaction energy as reported for S22 data set. [47]
[c] CCSD(T),CBS interaction energies from extrapolation with BSSE corrections reported in [46].
[d] B3LYP-DD error relative to CCSD(T),CBS energies reported in [46].