

Supplementary material to: Long-Range Corrected Hybrid Density Functionals with Damped Atom-Atom Dispersion Corrections

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TABLE I: Interaction energies (in kcal/mol) for the S22 set [1]. The counterpoise corrections are used to reduce the basis set superposition errors. Monomer deformation energies are not included. The results for the ω B97X and ω B97 are taken from Ref. [2].

Complex [Symmetry]	ΔE_{ref}	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
Hydrogen bonded complexes							
(NH ₃) ₂ [C _{2h}]	-3.17	-3.07	-3.15	-3.65	-3.44	-3.58	-3.64
(H ₂ O) ₂ [C _s]	-5.02	-4.97	-4.32	-5.30	-4.92	-5.59	-5.64
Formic acid dimer [C _{2h}]	-18.61	-19.30	-17.48	-19.93	-18.50	-19.96	-20.13
Formamide dimer [C _{2h}]	-15.96	-16.16	-14.62	-16.76	-15.63	-16.65	-16.78
Uracil dimer [C _{2h}]	-20.65	-20.44	-18.99	-21.38	-20.22	-20.30	-20.31
2-pyridoxine·2-aminopyridine [C ₁]	-16.71	-17.06	-16.46	-17.89	-17.28	-16.37	-16.40
Adenine·thymine WC [C ₁]	-16.37	-16.45	-15.60	-17.27	-16.50	-15.91	-16.05
MSE		-0.14	0.84	-0.81	0.00	-0.27	-0.35
MAE		0.24	0.84	0.81	0.28	0.60	0.63
Dispersion complexes							
(CH ₄) ₂ [D _{3d}]	-0.53	-0.57	-0.54	-0.47	-0.32	-0.57	-0.44
(C ₂ H ₄) ₂ [D _{2d}]	-1.51	-1.78	-1.48	-1.73	-1.44	-1.77	-1.92
Benzene·CH ₄ [C ₃]	-1.50	-1.68	-1.41	-1.47	-1.23	-1.41	-1.55
Benzene dimer [C _{2h}]	-2.73	-3.19	-2.40	-2.15	-1.91	-1.57	-2.33
Pyrazine dimer [C _s]	-4.42	-4.25	-3.88	-3.99	-3.71	-2.86	-3.68
Uracil dimer [C ₂]	-10.12	-9.79	-9.37	-10.33	-9.68	-7.84	-8.90
Indole·benzene [C ₁]	-5.22	-5.05	-4.35	-4.18	-3.97	-2.39	-3.58
Adenine·thymine stack [C ₁]	-12.23	-11.81	-11.42	-12.47	-11.88	-8.40	-10.26
MSE		0.02	0.43	0.18	0.52	1.43	0.70
MAE		0.25	0.43	0.35	0.52	1.51	0.82
Mixed complexes							
Ethene·ethine [C _{2v}]	-1.53	-1.64	-1.63	-1.69	-1.49	-1.67	-1.63
Benzene·H ₂ O [C _s]	-3.28	-3.50	-3.42	-3.67	-3.30	-3.39	-3.56
Benzene·NH ₃ [C _s]	-2.35	-2.54	-2.36	-2.48	-2.19	-2.31	-2.46
Benzene·HCN [C _s]	-4.46	-4.79	-4.70	-5.18	-4.65	-4.61	-4.89
Benzene dimer [C _{2v}]	-2.74	-2.89	-2.75	-2.80	-2.51	-2.11	-2.38
Indole·benzene T-shape [C ₁]	-5.73	-5.63	-5.86	-6.07	-5.68	-4.44	-4.82
Phenol dimer [C ₁]	-7.05	-6.98	-6.03	-7.23	-6.65	-6.49	-6.93
MSE		-0.12	0.06	-0.28	0.10	0.30	0.07
MAE		0.17	0.24	0.28	0.16	0.42	0.33
MSE		-0.08	0.44	-0.28	0.22	0.53	0.16
MAE		0.22	0.50	0.48	0.33	0.87	0.60
rms		0.27	0.69	0.60	0.44	1.30	0.80
Max(-)		-0.69	-0.24	-1.32	-0.57	-1.35	-1.52
Max(+)		0.42	1.66	1.04	1.25	3.83	1.97

TABLE II: Binding energies (in kcal/mol) of several sets of noncovalent interactions. The first three sets are taken from Ref. [3] with monomer deformation energies taken into considerations. The last three sets are taken from Ref. [1] without considering monomer deformation energies. The counter-point corrections are applied for all the cases. The results for the ω B97X and ω B97 are taken from Ref. [2].

Complex	ΔE_{ref}	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
Charge-transfer complexes							
C ₂ H ₄ ···F ₂	1.06	0.78	3.02	2.20	3.53	1.03	1.09
NH ₃ ···F ₂	1.81	1.50	4.33	3.20	5.32	1.93	1.98
C ₂ H ₂ ···ClF	3.81	3.66	4.57	4.49	5.18	4.43	4.50
HCN···ClF	4.86	4.21	3.87	4.76	5.00	5.32	5.42
NH ₃ ···Cl ₂	4.88	4.81	6.36	6.06	7.15	5.18	4.89
H ₂ O···ClF	5.36	5.18	5.31	5.98	6.43	6.16	6.21
NH ₃ ···ClF	10.62	11.12	14.16	13.54	15.48	11.10	10.49
MSE		-0.16	1.32	1.12	2.24	0.39	0.31
MAE		0.31	1.61	1.15	2.24	0.40	0.35
Dipole-dipole interaction complexes							
H ₂ S···H ₂ S	1.66	1.54	1.59	1.58	1.50	1.99	1.99
HCl···HCl	2.01	1.69	1.63	1.88	1.77	2.30	2.33
H ₂ S···HCl	3.35	3.38	3.46	3.57	3.58	3.90	3.93
CH ₃ Cl···HCl	3.55	3.17	3.11	3.52	3.41	3.82	3.97
HCN···CH ₃ SH	3.59	3.72	3.65	3.95	3.74	3.99	4.05
CH ₃ SH···HCl	4.16	4.87	5.17	5.29	5.36	5.28	5.38
MSE		0.01	0.05	0.25	0.17	0.50	0.56
MAE		0.28	0.35	0.33	0.35	0.50	0.56
Weak interaction complexes							
He···Ne	0.04	0.00	0.09	0.04	0.01	0.01	-0.05
He···Ar	0.06	0.00	0.07	0.01	-0.05	0.05	-0.03
Ne···Ne	0.08	-0.02	0.17	0.14	0.11	-0.02	-0.07
Ne···Ar	0.13	-0.01	0.19	0.16	0.10	0.05	-0.04
CH ₄ ···Ne	0.22	0.13	0.30	0.24	0.17	0.10	0.00
C ₆ H ₆ ···Ne	0.47	0.24	0.50	0.60	0.47	0.30	0.32
CH ₄ ···CH ₄	0.51	0.60	0.51	0.51	0.33	0.64	0.55
MSE		-0.08	0.04	0.03	-0.05	-0.05	-0.12
MAE		0.11	0.05	0.04	0.06	0.09	0.13
Hydrogen-bonded DNA base pairs							
G···A HB	-11.30	-13.48	-13.02	-14.19	-13.72	-12.29	-12.44
C···G WC	-30.70	-32.45	-30.00	-33.36	-31.55	-31.92	-32.12
G···C WC	-31.40	-32.28	-29.70	-33.14	-31.28	-31.85	-32.07
MSE		-1.60	0.23	-2.43	-1.05	-0.89	-1.08
MAE		1.60	1.37	2.43	1.13	0.89	1.08
Interstrand base pairs							
G···G IS	-5.20	-5.43	-5.35	-5.30	-5.08	-4.83	-4.70
G···G IS	0.80	1.15	1.04	1.30	1.31	2.21	2.13
C···C IS	3.10	3.29	2.87	3.26	3.06	3.62	3.69
MSE		0.10	-0.05	0.18	0.20	0.77	0.80
MAE		0.25	0.20	0.25	0.23	0.77	0.80
Stacked base pairs							
A···G S	-6.50	-6.66	-6.22	-6.55	-6.25	-3.46	-4.62
C···G S	-12.40	-10.83	-10.11	-10.56	-10.10	-8.57	-9.61
G···C S	-11.60	-11.06	-10.31	-10.71	-10.21	-8.77	-9.69
MSE		0.65	1.29	0.89	1.31	3.23	2.19
MAE		0.76	1.29	0.93	1.31	3.23	2.19
MSE		-0.14	0.49	0.19	0.61	0.51	0.36
MAE		0.43	0.77	0.73	0.90	0.73	0.65
rms		0.68	1.19	1.15	1.51	1.18	0.93

TABLE III: Comparison of errors of different functionals for the reaction energies (in kcal/mol) of the 30 chemical reactions in the NHTBH38/04 and HTBH38/04 database [4, 5]. The results for the ω B97X and ω B97 are taken from Ref. [2].

Reactions	ΔE_{ref}^a	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
H + N ₂ O → OH + N ₂	-65.08	4.80	13.72	3.69	12.02	3.72	3.82
H + FCH ₃ → HF + CH ₃	-26.64	2.18	-1.14	-0.08	0.63	3.37	4.27
H + F ₂ → HF + F	-103.91	-0.70	5.35	0.20	10.08	0.50	2.21
CH ₃ + FCl → CH ₃ F + Cl	-52.74	-1.02	1.79	-0.03	3.75	-1.85	-2.60
F ⁻ + CH ₃ Cl → FCH ₃ + Cl ⁻	-32.65	-2.18	-1.16	-2.09	0.36	-1.29	0.78
F ⁻ ···CH ₃ Cl → FCH ₃ ···Cl ⁻	-26.73	-0.80	1.80	0.41	4.03	-0.23	1.17
OH ⁻ + CH ₃ F → HOCH ₃ + F ⁻	-20.11	-1.25	0.82	-0.31	0.73	-1.22	-1.80
OH ⁻ ···CH ₃ F → HOCH ₃ ···F ⁻	-36.24	-2.44	-0.93	-1.54	-0.28	-1.62	-1.36
H + N ₂ → HN ₂	3.97	-5.06	-7.59	-7.41	-7.27	-4.30	-3.57
H + CO → HCO	-19.51	-3.28	-5.93	-5.76	-5.87	-2.66	-1.91
H + C ₂ H ₄ → CH ₃ CH ₂	-40.03	-2.47	-1.52	-2.42	0.60	-2.97	-3.52
CH ₃ + C ₂ H ₄ → CH ₃ CH ₂ CH ₂	-26.12	-2.90	2.29	0.50	3.48	-4.05	-5.65
HCN → HNC	15.05	-1.85	-0.44	-0.94	0.09	-1.87	-1.97
H + HCl → H ₂ + Cl	-3.0	2.71	-2.38	-1.49	-1.28	3.09	3.18
OH + H ₂ → H + H ₂ O	-16.1	-0.41	2.87	3.23	2.20	-0.84	-1.02
CH ₃ + H ₂ → H + CH ₄	-3.2	-1.33	3.83	2.29	2.55	-2.30	-2.86
OH + CH ₄ → CH ₃ + H ₂ O	-12.9	0.92	-0.96	0.95	-0.36	1.46	1.84
OH + NH ₃ → H ₂ O + NH ₂	-9.5	-0.17	-1.89	-0.37	-1.43	0.15	0.23
HCl + CH ₃ → Cl + CH ₄	-6.2	1.38	1.45	0.80	1.27	0.79	0.33
OH + C ₂ H ₆ → H ₂ O + C ₂ H ₅	-16.5	0.22	-2.33	0.41	-1.31	0.54	1.04
F + H ₂ → HF + H	-31.6	-1.09	-0.27	1.81	-0.71	-1.46	-1.96
O + CH ₄ → OH + CH ₃	5.6	-0.92	-2.32	-3.14	-5.70	-0.50	0.03
H + PH ₃ → PH ₂ + H ₂	-20.1	-0.09	-5.25	-3.06	-3.35	0.61	0.74
H + HO → H ₂ + O	-2.4	2.26	-1.51	0.85	3.14	2.80	2.82
H + H ₂ S → H ₂ + HS	-13.8	1.60	-3.73	-2.12	-2.17	2.17	2.32
O + HCl → OH + Cl	-0.6	0.46	-0.87	-2.34	-4.43	0.29	0.36
NH ₂ + CH ₃ → CH ₄ + NH	-14.4	1.53	2.09	3.35	4.55	1.49	1.28
NH ₂ + C ₂ H ₅ → C ₂ H ₆ + NH	-10.8	2.23	3.46	3.89	5.50	2.41	2.08
C ₂ H ₆ + NH ₂ → NH ₃ + C ₂ H ₅	-7.0	0.39	-0.44	0.78	0.13	0.39	0.81
NH ₂ + CH ₄ → CH ₃ + NH ₃	-3.3	0.99	0.83	1.22	0.98	1.21	1.50
MSE		-0.21	-0.01	-0.29	0.73	-0.07	0.09
MAE		1.66	2.70	1.92	3.01	1.74	1.97
rms		2.06	3.81	2.56	4.19	2.10	2.36
Max(-)		-5.06	-7.59	-7.41	-7.27	-4.30	-5.65
Max(+)		4.80	13.72	3.89	12.02	3.72	4.27

TABLE IV: Non-hydrogen transfer barrier heights (in kcal/mol) of the NHTBH38/04 set [5]. The results for the ω B97X and ω B97 are taken from Ref. [2].

Reactions		ΔE_{ref}	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
Heavy-atom transfer reactions								
H + N ₂ O → OH + N ₂	V^f	18.14	17.45	12.93	11.05	8.18	19.22	20.67
	V^r	83.22	77.73	64.29	72.44	61.24	80.57	81.93
H + FH → HF + H	V^f	42.18	40.54	33.86	30.77	25.76	43.10	44.78
	V^r	42.18	40.54	33.86	30.77	25.76	43.10	44.78
H + ClH → HCl + H	V^f	18.00	18.24	13.81	12.36	9.74	20.73	23.17
	V^r	18.00	18.24	13.81	12.36	9.74	20.73	23.17
H + FCH ₃ → HF + CH ₃	V^f	30.38	30.10	20.48	21.09	15.32	32.14	33.46
	V^r	57.02	54.56	48.26	47.81	41.33	55.41	55.83
H + F ₂ → HF + F	V^f	2.27	-0.64	-6.26	-7.65	-11.79	0.86	1.96
	V^r	106.18	103.97	92.30	96.06	82.04	104.27	103.66
CH ₃ + FCl → CH ₃ F + Cl	V^f	7.43	2.84	-6.56	-2.85	-8.42	3.93	4.62
	V^r	60.17	56.60	44.39	49.91	40.57	58.52	59.96
Nucleophilic substitution reactions								
F ⁻ + CH ₃ F → FCH ₃ + F ⁻	V^f	-0.34	-1.36	-5.99	-4.85	-8.95	-2.27	-2.60
	V^r	-0.34	-1.36	-5.99	-4.85	-8.95	-2.27	-2.60
F ⁻ ···CH ₃ F → FCH ₃ ···F ⁻	V^f	13.38	12.91	8.56	10.51	6.82	13.28	13.32
	V^r	13.38	12.91	8.56	10.51	6.82	13.28	13.32
Cl ⁻ + CH ₃ Cl → ClCH ₃ + Cl ⁻	V^f	3.10	3.71	-4.14	-2.09	-5.70	4.71	6.21
	V^r	3.10	3.71	-4.14	-2.09	-5.70	4.71	6.21
Cl ⁻ ···CH ₃ Cl → ClCH ₃ ···Cl ⁻	V^f	13.61	14.37	6.99	9.15	5.64	16.09	17.74
	V^r	13.61	14.37	6.99	9.15	5.64	16.09	17.74
F ⁻ + CH ₃ Cl → FCH ₃ + Cl ⁻	V^f	-12.54	-13.47	-19.02	-17.72	-20.69	-13.11	-11.72
	V^r	20.11	21.36	14.79	17.01	11.60	20.83	20.15
F ⁻ ···CH ₃ Cl → FCH ₃ ···Cl ⁻	V^f	2.89	3.16	-0.93	0.40	-1.56	4.23	5.39
	V^r	29.62	30.70	24.00	26.72	21.14	31.19	30.95
OH ⁻ + CH ₃ F → HOCH ₃ + F ⁻	V^f	-2.78	-3.32	-8.75	-7.40	-11.57	-3.70	-4.05
	V^r	17.33	18.05	10.54	13.02	7.80	17.64	17.86
OH ⁻ ···CH ₃ F → HOCH ₃ ···F ⁻	V^f	10.96	10.50	4.83	7.21	3.18	11.47	11.52
	V^r	47.20	49.18	42.01	44.98	39.69	49.33	49.13
Unimolecular and association reactions								
H + N ₂ → HN ₂	V^f	14.69	12.32	7.59	7.32	5.08	13.99	15.47
	V^r	10.72	13.42	11.21	10.76	8.38	14.32	15.06
H + CO → HCO	V^f	3.17	3.37	0.87	-0.86	-2.26	4.55	5.65
	V^r	22.68	26.16	26.31	24.41	23.12	26.72	27.07
H + C ₂ H ₄ → CH ₃ CH ₂	V^f	1.72	2.99	0.58	-1.17	-1.83	4.07	4.94
	V^r	41.75	45.49	42.13	41.28	37.60	47.07	48.49
CH ₃ + C ₂ H ₄ → CH ₃ CH ₂ CH ₂	V^f	6.85	4.57	1.00	3.14	1.45	5.04	4.81
	V^r	32.97	33.59	24.84	28.75	24.10	35.21	36.59
HCN → HNC	V^f	48.16	46.43	46.68	47.54	46.95	46.29	45.89
	V^r	33.11	33.22	32.08	33.43	31.81	33.12	32.80
MSE			-0.42	-6.22	-5.13	-9.32	0.56	1.32
MAE			1.51	6.46	5.24	9.34	1.75	2.31
rms			2.00	7.58	6.17	10.82	2.08	2.82
Max(-)			-5.49	-18.93	-11.41	-24.14	-3.50	-2.81
Max(+)			3.74	3.63	1.73	0.44	5.32	6.74

TABLE V: Hydrogen transfer barrier heights (in kcal/mol) of the HTBH38/04 set [4, 5]. The results for the ω B97X and ω B97 are taken from Ref. [2].

Reactions	ΔE_{ref}	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
H + HCl \rightarrow H ₂ + Cl	V^f 5.7	4.22	-1.58	-0.89	-2.60	5.33	6.68
	V^r 8.7	4.51	3.80	3.60	1.69	5.24	6.49
OH + H ₂ \rightarrow H + H ₂ O	V^f 5.1	2.24	-1.45	0.11	-3.95	2.56	3.27
	V^r 21.2	18.76	11.78	12.98	9.96	19.50	20.39
CH ₃ + H ₂ \rightarrow H + CH ₄	V^f 12.1	9.14	7.82	7.69	5.96	9.63	10.29
	V^r 15.3	13.67	7.20	8.61	6.60	15.13	16.35
OH + CH ₄ \rightarrow CH ₃ + H ₂ O	V^f 6.7	3.19	-3.11	0.81	-4.02	3.97	4.53
	V^r 19.6	15.17	10.75	12.76	9.24	15.41	15.59
H + H ₂ \rightarrow H ₂ + H	V^f 9.6	9.22	6.47	4.05	2.67	10.74	12.38
	V^r 9.6	9.22	6.47	4.05	2.67	10.74	12.38
OH + NH ₃ \rightarrow H ₂ O + NH ₂	V^f 3.2	0.01	-9.03	-3.73	-10.47	1.62	2.83
	V^r 12.7	9.68	2.37	6.14	0.47	10.97	12.10
HCl + CH ₃ \rightarrow Cl + CH ₄	V^f 1.7	-1.67	-4.75	-2.95	-5.06	-1.07	-0.47
	V^r 7.9	3.15	0.01	2.45	-0.13	4.34	5.41
OH + C ₂ H ₆ \rightarrow H ₂ O + C ₂ H ₅	V^f 3.4	0.33	-6.54	-2.32	-7.57	1.26	1.85
	V^r 19.9	16.61	12.29	13.77	10.24	17.22	17.31
F + H ₂ \rightarrow HF + H	V^f 1.8	-3.70	-8.98	-6.25	-11.87	-3.89	-3.76
	V^r 33.4	28.98	22.89	23.54	20.45	29.17	29.80
O + CH ₄ \rightarrow OH + CH ₃	V^f 13.7	9.36	3.07	5.97	0.51	9.94	10.45
	V^r 8.1	4.69	-0.21	3.51	0.61	4.85	4.82
H + PH ₃ \rightarrow PH ₂ + H ₂	V^f 3.1	3.22	-0.82	-1.49	-3.07	4.62	5.88
	V^r 23.2	23.41	24.52	21.67	20.38	24.11	25.25
H + HO \rightarrow H ₂ + O	V^f 10.7	8.78	1.76	4.04	1.48	9.79	10.68
	V^r 13.1	8.92	5.67	5.58	0.74	9.38	10.26
H + H ₂ S \rightarrow H ₂ + HS	V^f 3.5	4.07	0.12	-0.88	-2.54	5.54	6.94
	V^r 17.3	16.27	17.65	15.03	13.42	17.16	18.42
O + HCl \rightarrow OH + Cl	V^f 9.8	5.63	-5.26	0.92	-8.82	7.07	14.21
	V^r 10.4	5.77	-3.79	3.86	-3.79	7.38	14.45
NH ₂ + CH ₃ \rightarrow CH ₄ + NH	V^f 8.0	5.67	0.83	4.59	1.81	6.50	6.95
	V^r 22.4	18.54	13.14	15.64	11.66	19.42	20.07
NH ₂ + C ₂ H ₅ \rightarrow C ₂ H ₆ + NH	V^f 7.5	7.38	2.91	6.10	3.54	8.48	8.82
	V^r 18.3	15.95	10.26	13.01	8.84	16.87	17.54
C ₂ H ₆ + NH ₂ \rightarrow NH ₃ + C ₂ H ₅	V^f 10.4	8.81	3.43	6.80	3.04	10.16	11.01
	V^r 17.4	15.42	10.88	13.02	9.91	16.77	17.21
NH ₂ + CH ₄ \rightarrow CH ₃ + NH ₃	V^f 14.5	11.39	6.45	9.56	6.03	12.64	13.49
	V^r 17.8	13.70	8.93	11.64	8.35	14.72	15.29
<i>s-trans cis</i> -C ₅ H ₈ \rightarrow <i>s-trans cis</i> -C ₅ H ₈	V^f 38.4	39.06	34.63	37.81	34.72	41.44	42.84
	V^r 38.4	39.06	34.63	37.81	34.72	41.44	42.84
MSE		-2.52	-7.33	-5.39	-8.89	-1.51	-0.34
MAE		2.64	7.41	5.39	8.89	2.24	2.24
rms		3.04	8.09	5.80	9.52	2.58	2.62
Max(-)		-5.50	-15.06	-9.86	-18.62	-5.69	-5.56
Max(+)		0.66	1.32	-0.59	-2.82	3.04	4.44

TABLE VI: Comparison of errors of different functionals for the intermolecular bond lengths (in Å) of the 12 weakly bound complexes on the S22 set [1]. For the hydrogen bonded complexes, the hydrogen bond lengths are computed, while for other complexes, the distances of the centers of mass of the monomers are computed.

Complex [Symmetry]	Reference	MP2	ω B97X-D	B97-D	B3LYP-D	BLYP-D	ω B97X	ω B97
Hydrogen bonded complexes								
(NH ₃) ₂ [C _{2h}]	2.504	0.010	0.032	0.043	-0.006	0.002	-0.019	-0.033
(H ₂ O) ₂ [C _s]	1.952	-0.017	-0.017	0.014	-0.039	-0.028	-0.030	-0.029
Formic acid dimer [C _{2h}]	1.670	-0.015	-0.003	-0.019	-0.019	-0.020	0.008	0.019
Formamide dimer [C _{2h}]	1.841	-0.011	0.005	0.003	-0.015	-0.014	0.015	0.020
MSE		-0.008	0.005	0.010	-0.020	-0.015	-0.006	-0.006
MAE		0.013	0.014	0.020	0.020	0.016	0.018	0.025
Dispersion complexes								
(CH ₄) ₂ [D _{3d}]	3.718	-0.113	-0.198	0.042	-0.267	-0.200	-0.231	-0.362
(C ₂ H ₄) ₂ [D _{2d}]	3.718	-0.066	-0.064	-0.114	-0.218	-0.194	-0.080	-0.140
Benzene·CH ₄ [C ₃]	3.716	-0.175	-0.088	-0.041	-0.133	-0.103	0.043	-0.090
Benzene dimer [C _{2h}]	3.765	-0.231	0.056	0.125	0.043	0.079	0.177	0.077
MSE		-0.146	-0.074	0.003	-0.144	-0.104	-0.022	-0.129
MAE		0.146	0.101	0.080	0.166	0.144	0.133	0.167
Mixed complexes								
Ethene·ethine [C _{2v}]	4.422	-0.102	-0.050	-0.092	-0.140	-0.124	-0.073	-0.102
Benzene·H ₂ O [C _s]	3.380	-0.144	-0.144	-0.084	-0.162	-0.117	-0.129	-0.192
Benzene·NH ₃ [C _s]	3.560	-0.204	-0.082	-0.093	-0.171	-0.140	-0.059	-0.131
Benzene·HCN [C _s]	3.950	0.024	0.024	-0.032	-0.074	-0.056	0.003	-0.143
MSE		-0.107	-0.063	-0.075	-0.137	-0.109	-0.065	-0.142
MAE		0.119	0.075	0.075	0.137	0.109	0.066	0.142
MSE		-0.087	-0.044	-0.021	-0.100	-0.076	-0.031	-0.092
MAE		0.093	0.064	0.058	0.107	0.090	0.072	0.111
rms		0.121	0.085	0.071	0.136	0.111	0.100	0.145
Max(-)		-0.231	-0.198	-0.114	-0.267	-0.200	-0.231	-0.362
Max(+)		0.024	0.056	0.125	0.043	0.079	0.177	0.077