Supplementary material to: Seeking for reliable double-hybrid density functionals without fitting parameters: The PBE0-2 functional

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TABLE I: Nonhydrogen transfer barrier heights (in kcal/mol) of the NHTBH38/04 set [1]. The notation used for characterizing statistical errors is as follows: mean signed errors (MSEs), mean absolute errors (MAEs), and root-mean-square (rms) errors.

Reactions		ΔE_{ref}	LDA	PBE	TPSS	PBE0	PBE0-DH	PBE0-2	B3LYP	B2PLYP	B2PLYP-D3	MP2
Heavy-atom transfer reactions												
$H + N_2O \rightarrow OH + N_2$	V^f	18.14	2.69	9.97	7.33	13.91	17.41	23.58	11.37	16.67	16.48	36.05
	V^r	83.22	32.09	52.46	60.16	68.79	76.63	81.25	72.81	76.62	76.34	88.32
$H + FH \rightarrow HF + H$	V^f	42.18	18.48	27.07	25.89	33.74	38.71	43.35	31.01	36.65	36.60	46.57
	V^r	42.18	18.48	27.07	25.89	33.74	38.71	43.35	31.01	36.65	36.60	46.57
$H + ClH \rightarrow HCl + H$	V^f	18.00	2.27	9.64	7.03	13.38	16.03	19.26	12.41	15.70	15.66	22.64
	V^r	18.00	2.27	9.64	7.03	13.38	16.03	19.26	12.41	15.70	15.66	22.64
$H + FCH_3 \rightarrow HF + CH_3$	V^f	30.38	13.36	18.51	16.40	25.71	30.23	33.87	21.79	26.55	26.26	36.14
	V^r	57.02	31.72	41.00	42.28	49.75	54.86	58.38	48.64	52.70	52.15	60.23
$H + F_2 \rightarrow HF + F$	V^f	2.27	-15.97	-9.86	-11.44	-4.60	-0.44	11.20	-7.54	0.86	0.78	28.32
	V^r	106.18	69.40	80.86	84.02	99.02	109.16	121.25	96.16	106.41	106.32	133.73
$CH_3 + FCl \rightarrow CH_3F + Cl$	V^f	7.43	-11.50	-6.48	-5.36	0.79	4.97	10.02	-1.58	2.51	1.81	18.72
	V^r	60.17	37.67	41.63	42.81	53.46	60.14	66.55	50.96	56.69	56.25	75.15
Nucleophilic substitution reactions												
$F^- + CH_3F \rightarrow FCH_3 + F^-$	V^f	-0.34	-12.18	-8.31	-8.80	-2.67	-0.71	0.00	-3.93	-3.20	-3.76	0.37
	V^r	-0.34	-12.18	-8.31	-8.80	-2.67	-0.71	0.00	-3.93	-3.20	-3.76	0.37
$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	V^f	13.38	6.55	7.06	6.24	11.69	13.57	14.40	10.23	11.30	11.43	14.75
	V^r	13.38	6.55	7.06	6.24	11.69	13.57	14.40	10.23	11.30	11.43	14.75
$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	V^f	3.10	-6.74	-3.80	-4.99	0.87	2.92	4.32	-0.57	1.02	0.12	5.50
	V^r	3.10	-6.74	-3.80	-4.99	0.87	2.92	4.32	-0.57	1.02	0.12	5.50
$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	V^f	13.61	6.74	7.15	5.68	11.29	13.41	15.14	9.22	11.36	11.32	16.54
	V^r	13.61	6.74	7.15	5.68	11.29	13.41	15.14	9.22	11.36	11.32	16.54
$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	V^f	-12.54	-23.45	-19.52	-20.87	-15.45	-13.75	-12.13	-16.55	-15.05	-15.78	-10.28
	V^r	20.11	10.10	12.31	13.42	19.44	21.77	21.83	18.26	18.63	17.85	20.70
$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	V^f	2.89	-1.04	-0.67	-2.18	1.66	2.96	4.29	0.31	1.74	1.75	5.66
	V^r	29.62	21.65	21.45	22.23	28.35	30.86	31.38	26.62	27.69	27.70	30.64
$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	V^f	-2.78	-14.36	-10.59	-10.74	-4.97	-2.97	-2.20	-5.83	-5.06	-5.77	-1.71
	V^r	17.33	5.70	9.14	8.02	15.94	18.22	18.50	14.13	14.60	13.98	17.96
$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	V^f	10.96	3.39	3.88	3.33	8.82	10.87	11.94	7.69	8.99	8.93	12.58
	V^r	47.20	47.53	43.21	40.74	49.06	51.09	51.22	45.46	46.16	45.89	50.20
Unimolecular and association reactions												
$H+N_2 \rightarrow HN_2$	V^f	14.69	-2.19	5.19	2.34	8.50	11.54	17.32	7.47	12.33	12.27	27.64
	V^r	10.72	9.44	9.09	8.87	11.64	12.55	11.91	10.88	10.71	10.66	8.64
$H + CO \rightarrow HCO$	V^f	3.17	-7.57	-1.69	-5.14	0.31	1.83	3.85	-0.59	1.82	1.59	5.93
	V^r	22.68	26.34	24.66	24.06	25.47	25.51	24.52	24.60	24.10	23.94	22.70
$H + C_2H_4 \rightarrow CH_3CH_2$	V^f	1.72	-5.34	-0.14	-4.34	0.67	1.50	4.24	-0.18	1.84	1.47	9.35
	V^r	41.75	39.21	40.20	40.29	44.12	45.72	46.18	41.73	42.53	42.31	46.58
$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	V^f	6.85	-5.81	1.50	2.92	4.02	5.24	7.93	6.00	7.16	6.07	12.87
	V^r	32.97	32.95	29.76	28.03	34.48	36.89	39.12	29.44	32.38	32.18	41.52
$HCN \rightarrow HCN$	V^f	48.16	44.83	45.60	46.96	46.37	47.30	49.35	47.38	48.68	48.73	52.21
	V^r	33.11	30.60	30.50	31.80	32.51	33.31	33.92	33.33	33.32	33.36	34.80

MSE	-12.41	-8.52	-9.09	-3.13	-0.32	2.34	-4.57	-2.00	-2.29	5.37
MAE	12.62	8.62	9.16	3.63	1.57	2.44	4.69	2.19	2.44	5.48
rms	16.13	10.61	10.55	4.63	2.19	3.71	5.71	2.69	2.95	8.45

TABLE II: Hydrogen transfer barrier heights (in kcal/mol) of the HTBH38/04 set [1, 2]. The notation used for characterizing statistical errors is as follows: mean signed errors (MSEs), mean absolute errors (MAEs), and root-mean-square (rms) errors.

Reactions		ΔE_{ref}	LDA	PBE	TPSS	PBE0	PBE0-DH	PBE0-2	B3LYP	B2PLYP	B2PLYP-D3	MP2
$H + HCl \rightarrow H_2 + Cl$	V^f	5.70	-3.14	0.56	-3.91	2.94	4.88	7.64	-0.77	2.84	2.74	10.68
	V^r	-8.70	8.70	-1.95	-1.10	1.66	3.90	5.90	3.73	5.45	5.34	7.45
$OH + H_2 \rightarrow H + H_2O$	V^f	5.10	-18.39	-6.36	-3.88	-0.02	3.16	5.51	0.51	2.92	2.74	7.27
	V^r	21.20	11.33	13.69	8.04	17.31	20.24	25.39	13.36	18.55	18.37	31.87
$CH_3 + H_2 \rightarrow H + CH_4$	V^f	12.10	-5.35	3.82	5.12	6.89	8.83	10.84	8.73	10.23	9.95	12.76
	V^r	15.30	4.94	9.32	5.58	11.90	13.92	16.73	9.53	12.78	12.52	19.76
$OH + CH_4 \rightarrow CH_3 + H_2O$	V^f	6.70	-17.22	-5.65	-1.77	1.62	4.91	6.50	1.92	3.89	3.44	7.19
	V^r	19.60	2.21	8.91	9.69	13.94	16.90	20.50	13.98	16.96	16.51	24.79
$H + H_2 \rightarrow H_2 + H$	V^f	9.60	-2.70	3.64	-0.86	5.63	7.47	10.24	4.22	7.12	7.09	13.24
	V^r	9.60	-2.70	3.64	-0.86	5.63	7.47	10.24	4.22	7.12	7.09	13.24
$OH + NH_3 \rightarrow H_2O + NH_2$	V^f	3.20	-23.88	-11.94	-7.99	-2.28	2.16	4.60	-2.62	0.12	-0.36	6.40
	V^r	12.70	-10.71	-0.71	2.29	7.41	11.49	14.91	7.32	10.41	9.93	18.62
$HCl + CH_3 \rightarrow Cl + CH_4$	V^f	1.70	-13.74	-5.94	-4.04	-2.49	-0.67	0.74	-1.59	-0.19	-0.76	1.87
	V^r	-7.90	7.90	-2.95	-0.77	1.24	3.45	4.88	3.70	4.96	4.41	5.64
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	V^f	3.40	-20.98	-9.03	-5.00	-1.23	2.22	4.00	-1.05	1.12	0.55	4.94
	V^r	19.90	4.79	10.76	11.26	15.66	18.30	21.52	15.63	18.20	17.44	25.50
$F + H_2 \rightarrow HF + H$	V^f	1.80	-24.20	-12.97	-10.36	-4.90	-0.73	2.44	-6.03	-1.67	-1.85	4.37
	V^r	33.40	25.72	25.12	19.19	28.41	31.46	37.89	23.76	30.40	30.22	46.07
$O + CH_4 \rightarrow OH + CH_3$	V^f	13.70	-10.69	-0.79	4.14	7.16	11.53	14.42	6.79	10.47	10.15	15.88
	V^r	8.10	-9.27	-0.57	0.51	3.94	6.48	8.93	4.44	6.76	6.42	11.49
$H + PH_3 \rightarrow PH_2 + H_2$	V^f	3.10	-7.35	-1.79	-5.21	0.35	1.86	3.70	-1.10	1.28	1.10	5.50
	V^r	23.20	9.24	17.91	17.68	20.12	21.43	22.79	22.72	23.48	23.25	24.04
$H + HO \rightarrow H_2 + O$	V^f	10.70	-1.69	3.75	-1.31	7.13	9.66	13.34	4.14	8.17	8.05	17.76
	V^r	13.10	-13.40	-1.98	1.86	5.33	9.62	12.94	5.69	9.34	9.21	15.15
$H + H_2S \rightarrow H_2 + HS$	V^f	3.50	-6.73	-1.22	-4.71	1.05	2.69	4.69	-0.58	1.93	1.71	6.66
	V^r	-17.30	17.30	9.10	10.13	12.06	13.75	15.13	15.54	16.22	15.98	16.11
$O + HCl \rightarrow OH + Cl$	V^f	9.80	-23.13	-10.55	-3.92	2.22	14.62	12.39	0.96	13.30	13.21	15.25
	V^r	-10.40	10.40	-7.33	-4.28	2.74	13.69	11.04	3.90	14.75	14.66	14.63
$NH_2 + CH_3 \rightarrow CH_4 + NH$	V^f	8.00	-8.37	0.71	2.46	5.05	7.26	9.00	6.13	7.74	7.28	10.61
	V^r	22.40	2.16	10.56	15.34	16.42	19.62	22.03	17.09	19.58	19.13	23.70
$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	V^f	7.50	-5.76	2.89	4.57	6.89	8.71	9.86	8.20	9.14	8.39	10.93
	V^r	18.30	-1.57	7.51	12.64	13.70	16.98	19.38	14.54	16.98	16.41	21.06
$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	V^f	10.40	-9.69	1.44	5.61	7.26	9.81	10.87	8.73	9.85	9.17	11.19
	V^r	17.40	2.91	9.99	11.59	14.45	16.57	18.08	15.47	16.64	15.77	19.54
$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	V^f	14.50	-6.16	4.39	8.33	9.87	12.37	13.49	11.27	12.47	11.92	13.84
	V^r	17.80	0.10	7.71	9.51	12.50	15.03	17.18	13.39	15.26	14.71	19.23
s-trans cis-$C_5H_8 \rightarrow$ *s-trans cis*-C_5H_8	V^f	38.40	25.00	31.19	34.13	35.57	37.35	36.46	38.77	38.06	37.99	33.30
	V^r	38.40	25.00	31.19	34.13	35.57	37.35	36.46	38.77	38.06	37.99	33.30
MSE			-15.60	-9.67	-8.68	-4.60	-1.52	0.50	-4.48	-1.66	-1.99	2.56
MAE			15.60	9.67	8.68	4.60	2.01	1.39	4.56	2.17	2.45	3.38
rms			17.47	10.37	9.14	4.88	2.31	1.74	5.10	2.40	2.65	4.27

TABLE III: Interaction energies (in kcal/mol) of the S22 set [3, 4]. The counterpoise corrections are used to reduce the basis set superposition errors. Monomer deformation energies are not included. The notation used for characterizing statistical errors is as follows: mean signed errors (MSEs), mean absolute errors (MAEs), and root-mean-square (rms) errors.

Complex	ΔE_{ref}	LDA	PBE	TPSS	PBE0	PBE0-DH	PBE0-2	B3LYP	B2PLYP	B2PLYP-D3	MP2
Hydrogen bonded complexes											
$(NH_3)_2$ [C_{2h}]	-3.17	-5.10	-2.83	-2.29	-2.77	-2.83	-2.93	-2.19	-2.56	-3.04	-2.92
$(H_2O)_2$ [C_s]	-5.02	-7.78	-4.91	-4.44	-4.92	-4.96	-4.89	-4.49	-4.66	-5.05	-4.61
Formic acid dimer [C_{2h}]	-18.80	-26.82	-18.08	-17.61	-18.86	-19.21	-18.75	-17.29	-17.52	-18.75	-17.16
Formamide dimer [C_{2h}]	-16.12	-21.82	-14.69	-14.02	-15.27	-15.64	-15.55	-13.97	-14.49	-15.85	-14.68
Uracil dimer [C_{2h}]	-20.69	-26.15	-18.45	-17.76	-19.16	-19.72	-19.91	-17.87	-18.67	-20.44	-19.22
2-pyridoxine2-aminopyridine [C_1]	-17.00	-22.77	-15.27	-14.38	-15.35	-15.84	-16.42	-13.72	-14.93	-16.97	-16.29
Adeninethymine WC [C_1]	-16.74	-21.99	-14.29	-13.28	-14.50	-15.09	-15.69	-12.82	-14.15	-16.37	-15.47
MSE		-4.98	1.29	1.97	0.96	0.61	0.49	2.17	1.51	0.15	1.03
MAE		4.98	1.29	1.97	0.97	0.72	0.49	2.17	1.51	0.16	1.03
Dispersion complexes											
$(CH_4)_2$ [D_{3d}]	-0.53	-0.83	-0.08	0.18	-0.04	-0.09	-0.25	0.40	0.06	-0.36	-0.42
$(C_2H_4)_2$ [D_{2d}]	-1.50	-2.49	-0.31	0.33	-0.35	-0.58	-1.00	0.51	-0.28	-1.40	-1.35
BenzeneCH_4 [C_3]	-1.45	-2.01	-0.01	0.52	-0.08	-0.41	-1.04	0.82	-0.13	-1.32	-1.64
Benzene dimer [C_{2h}]	-2.62	-2.62	1.90	3.00	1.80	0.60	-1.94	3.84	0.82	-2.21	-4.58
Pyrazine dimer [C_s]	-4.20	-4.46	0.73	1.91	0.52	-0.82	-3.57	2.56	-0.69	-3.86	-6.38
Uracil dimer [C_2]	-9.74	-10.15	-2.69	-0.96	-3.29	-4.99	-7.91	-0.86	-4.72	-9.34	-10.32
Indolebenzene [C_1]	-4.59	-4.38	2.24	3.69	2.02	0.17	-3.67	4.81	0.34	-4.01	-7.56
Adeninethymine stack [C_1]	-11.66	-11.96	-1.33	0.75	-2.14	-4.86	-9.69	1.46	-4.55	-10.93	-13.87
MSE		-0.33	4.59	5.71	4.34	3.17	0.90	6.23	3.39	0.36	-1.23
MAE		0.38	4.59	5.71	4.34	3.17	0.90	6.23	3.39	0.36	1.29
Mixed complexes											
Etheneethine [C_{2v}]	-1.51	-2.27	-1.16	-0.84	-1.18	-1.26	-1.41	-0.64	-0.99	-1.53	-1.52
BenzeneH2O [C_s]	-3.29	-4.44	-2.04	-1.44	-2.21	-2.54	-2.98	-1.21	-2.04	-3.21	-3.25
BenzeneNH3 [C_s]	-2.32	-3.03	-0.92	-0.35	-1.03	-1.36	-1.94	-0.08	-1.01	-2.22	-2.43
BenzeneHCN [C_s]	-4.55	-5.85	-2.81	-2.26	-3.28	-3.83	-4.46	-1.93	-3.07	-4.56	-4.78
Benzene dimer [C_{2v}]	-2.71	-3.05	-0.10	0.59	-0.28	-0.95	-2.19	1.02	-0.63	-2.58	-3.36
Indolebenzene T-shape [C_1]	-5.62	-6.26	-2.03	-1.08	-2.36	-3.32	-5.03	-0.50	-2.79	-5.35	-6.53
Phenol dimer [C_1]	-7.09	-9.01	-3.87	-2.93	-4.18	-4.96	-6.23	-2.94	-4.71	-6.95	-7.23
MSE		-0.98	2.03	2.68	1.80	1.27	0.41	2.97	1.69	0.10	-0.29
MAE		0.98	2.03	2.68	1.80	1.27	0.41	2.97	1.69	0.11	0.30
MSE		-2.01	2.72	3.56	2.46	1.75	0.61	3.90	2.25	0.21	-0.21
MAE		2.03	2.72	3.56	2.46	1.78	0.61	3.90	2.25	0.22	0.89
rms		3.08	3.72	4.64	3.45	2.49	0.78	5.02	2.79	0.29	1.23

TABLE IV: Interaction energies (in kcal/mol) of the S66 set [5]. The counterpoise corrections are used to reduce the basis set superposition errors. Monomer deformation energies are not included. The notation used for characterizing statistical errors is as follows: mean signed errors (MSEs), mean absolute errors (MAEs), and root-mean-square (rms) errors.

	ΔE_{ref}	LDA	PBE	TPSS	PBE0	PBE0-DH	PBE0-2	B3LYP	B2PLYP	B2PLYP-D3	MP2
Hydrogen bonded complexes											
Water → Water	-4.92	-7.64	-4.87	-4.41	-4.90	-4.94	-4.88	-4.48	-4.66	-5.04	-4.62
Water → MeOH	-5.59	-8.47	-5.16	-4.63	-5.20	-5.33	-5.43	-4.71	-5.08	-5.71	-5.31
Water → MeNH2	-6.91	-10.61	-7.15	-6.66	-7.01	-7.01	-6.94	-6.34	-6.55	-7.16	-6.64
Water → Peptide	-8.10	-11.73	-7.28	-6.57	-7.49	-7.72	-7.82	-6.73	-7.22	-8.19	-7.52
MeOH → MeOH	-5.76	-8.46	-5.08	-4.51	-5.10	-5.26	-5.46	-4.54	-5.02	-5.80	-5.45
MeOH → MeNH2	-7.55	-11.28	-7.19	-6.50	-7.05	-7.16	-7.32	-6.08	-6.63	-7.65	-7.23
MeOH → Peptide	-8.23	-11.86	-7.18	-6.39	-7.30	-7.56	-7.78	-6.40	-7.04	-8.27	-7.62
MeOH → Water	-5.01	-7.62	-4.78	-4.28	-4.79	-4.85	-4.87	-4.33	-4.58	-5.07	-4.69
MeNH2 → MeOH	-3.06	-4.65	-2.22	-1.62	-2.17	-2.31	-2.61	-1.54	-2.14	-3.02	-2.81
MeNH2 → MeNH2	-4.16	-6.56	-3.08	-2.27	-3.01	-3.24	-3.67	-2.08	-2.91	-4.04	-3.94
MeNH2 → Peptide	-5.42	-7.74	-3.39	-2.40	-3.53	-3.98	-4.67	-2.39	-3.59	-5.32	-5.09
MeNH2 → Water	-7.27	-11.10	-7.14	-6.52	-7.06	-7.15	-7.22	-6.27	-6.67	-7.45	-7.03
Peptide → MeOH	-6.19	-8.33	-4.53	-3.76	-4.72	-5.09	-5.63	-3.88	-4.82	-6.07	-5.93
Peptide ... MeNH2	-7.45	-10.30	-6.12	-5.32	-6.12	-6.44	-6.96	-4.95	-5.94	-7.35	-7.22
Peptide ... Peptide	-8.63	-11.10	-6.36	-5.46	-6.64	-7.16	-7.84	-5.43	-6.65	-8.48	-8.14
Peptide ... Water	-5.12	-7.05	-4.32	-3.75	-4.46	-4.64	-4.83	-3.87	-4.37	-5.04	-4.84
Uracil ... Uracil (BP)	-17.18	-22.91	-15.49	-14.74	-15.98	-16.47	-16.69	-14.73	-15.55	-17.29	-16.10
Water ... Pyridine	-6.86	-10.21	-6.82	-6.33	-6.64	-6.69	-6.76	-6.10	-6.42	-7.14	-6.63
MeOH ... Pyridine	-7.41	-10.64	-6.92	-6.32	-6.73	-6.86	-7.14	-6.03	-6.58	-7.61	-7.21
AcOH ... AcOH	-19.09	-27.31	-18.59	-17.99	-19.24	-19.58	-19.20	-17.72	-18.01	-19.34	-17.73
AcNH2 ... AcNH2	-16.27	-22.15	-15.02	-14.27	-15.48	-15.85	-15.85	-14.21	-14.80	-16.25	-15.08
AcOH ... Uracil	-19.49	-26.45	-18.31	-17.64	-18.96	-19.39	-19.28	-17.59	-18.11	-19.64	-18.21
AcNH2 ... Uracil	-19.19	-25.20	-17.67	-16.94	-18.31	-18.79	-18.83	-16.97	-17.64	-19.26	-18.00
MSE		-3.67	0.88	1.55	0.74	0.50	0.31	1.63	1.04	-0.06	0.51
MAE		3.67	0.90	1.55	0.76	0.55	0.32	1.63	1.04	0.12	0.51
Dispersion complexes											
Benzene ... Benzene (pi-pi)	-2.82	-2.42	1.22	2.23	1.18	0.18	-2.04	2.91	0.30	-2.34	-4.41
Pyridine ... Pyridine (pi-pi)	-3.90	-3.66	0.48	1.54	0.34	-0.79	-3.17	2.20	-0.63	-3.47	-5.65
Uracil ... Uracil (pi-pi)	-9.83	-10.27	-2.51	-0.75	-3.14	-4.90	-7.90	-0.64	-4.59	-9.33	-10.34
Benzene ... Pyridine (pi-pi)	-3.44	-3.15	0.81	1.86	0.72	-0.36	-2.68	2.53	-0.22	-2.99	-5.11
Benzene ... Uracil (pi-pi)	-5.71	-5.51	0.35	1.75	0.01	-1.49	-4.34	2.31	-1.25	-5.01	-7.00
Pyridine ... Uracil (pi-pi)	-6.82	-6.73	-0.74	0.65	-1.12	-2.63	-5.44	1.06	-2.46	-6.17	-8.04
Benzene ... Ethene	-1.43	-1.80	0.76	1.50	0.82	0.32	-0.84	2.03	0.54	-1.02	-2.08
Uracil ... Ethene	-3.38	-3.94	-0.34	0.58	-0.52	-1.22	-2.51	0.88	-0.91	-2.99	-3.65
Uracil ... Ethyne	-3.74	-4.44	-1.03	-0.18	-1.24	-1.88	-3.00	0.06	-1.55	-3.32	-3.96
Pyridine ... Ethene	-1.87	-2.37	0.44	1.23	0.48	-0.06	-1.28	1.72	0.15	-1.48	-2.56
Pentane ... Pentane	-3.78	-5.27	0.42	2.02	0.38	-0.45	-2.12	2.33	-0.12	-3.52	-3.64
Neopentane ... Pentane	-2.61	-3.70	0.14	1.26	0.18	-0.35	-1.45	1.58	-0.07	-2.47	-2.46
Neopentane ... Neopentane	-1.78	-2.52	0.05	0.86	0.16	-0.15	-0.89	1.20	0.06	-1.65	-1.60
Cyclopentane ... Neopentane	-2.40	-3.47	0.18	1.25	0.23	-0.26	-1.31	1.55	-0.02	-2.25	-2.27
Cyclopentane ... Cyclopentane	-3.00	-4.16	0.11	1.36	0.18	-0.42	-1.69	1.59	-0.25	-2.85	-2.88

Benzene ... Cyclopentane	-3.58	-4.01	0.30	1.41	0.18	-0.72	-2.52	1.93	-0.43	-3.29	-4.26
Benzene ... Neopentane	-2.90	-3.27	0.10	1.01	0.00	-0.67	-2.04	1.49	-0.35	-2.65	-3.36
Uracil ... Pentane	-4.85	-5.62	0.52	2.09	0.27	-0.91	-3.09	2.41	-0.62	-4.52	-4.99
Uracil ... Cyclopentane	-4.14	-4.59	0.58	1.96	0.44	-0.58	-2.54	2.22	-0.43	-3.81	-4.31
Uracil ... Neopentane	-3.71	-4.15	0.08	1.21	-0.07	-0.87	-2.39	1.47	-0.66	-3.46	-3.73
Ethene ... Pentane	-2.01	-3.12	0.01	0.93	0.03	-0.36	-1.17	1.20	-0.09	-1.87	-1.92
Ethyne ... Pentane	-1.75	-2.52	-0.10	0.65	-0.06	-0.39	-1.12	1.00	-0.12	-1.48	-1.85
Peptide ... Pentane	-4.26	-5.66	0.07	1.61	-0.07	-0.97	-2.65	1.83	-0.65	-4.00	-4.09
MSE		-0.55	3.72	4.86	3.61	2.77	1.11	5.24	3.01	0.34	-0.46
MAE		0.66	3.72	4.86	3.61	2.77	1.11	5.24	3.01	0.34	0.54
Mixed complexes											
Benzene ... Benzene (TS)	-2.88	-3.17	-0.19	0.56	-0.36	-1.03	-2.29	0.96	-0.73	-2.72	-3.50
Pyridine ... Pyridine (TS)	-3.54	-4.14	-0.75	0.08	-0.97	-1.68	-2.95	0.34	-1.38	-3.43	-4.09
Benzene ... Pyridine (TS)	-3.33	-3.75	-0.61	0.14	-0.84	-1.53	-2.78	0.53	-1.17	-3.20	-3.90
Benzene ... Ethyne (CH-pi)	-2.87	-3.66	-1.23	-0.68	-1.48	-1.94	-2.64	-0.36	-1.47	-2.84	-3.19
Ethyne ... Ethyne (TS)	-1.52	-2.35	-1.20	-0.88	-1.21	-1.28	-1.39	-0.70	-1.01	-1.52	-1.47
Benzene ... AcOH (OH-pi)	-4.71	-5.94	-2.32	-1.57	-2.65	-3.28	-4.18	-1.16	-2.61	-4.41	-4.78
Benzene ... AcNH2 (NH-pi)	-4.36	-5.73	-2.34	-1.55	-2.59	-3.10	-3.86	-1.36	-2.60	-4.23	-4.38
Benzene ... Water (OH-pi)	-3.28	-4.58	-1.98	-1.36	-2.17	-2.52	-2.98	-1.11	-1.99	-3.20	-3.25
Benzene ... MeOH (OH-pi)	-4.19	-5.46	-1.86	-0.99	-2.03	-2.61	-3.58	-0.58	-2.07	-3.95	-4.37
Benzene ... MeNH2 (NH-pi)	-3.23	-4.08	-0.77	0.08	-0.90	-1.48	-2.55	0.47	-1.08	-3.00	-3.52
Benzene ... Peptide (NH-pi)	-5.28	-6.04	-1.68	-0.66	-2.01	-2.90	-4.45	-0.14	-2.32	-5.00	-5.79
Pyridine ... Pyridine (CH-N)	-4.15	-5.61	-2.49	-1.81	-2.60	-3.02	-3.66	-1.75	-2.79	-4.01	-4.04
Ethyne ... Water (CH-O)	-2.85	-4.31	-2.63	-2.29	-2.74	-2.81	-2.81	-2.34	-2.57	-2.93	-2.68
Ethyne ... AcOH (OH-pi)	-4.87	-7.50	-4.10	-3.50	-4.30	-4.50	-4.62	-3.26	-3.80	-4.83	-4.44
Pentane ... AcOH	-2.91	-3.97	0.07	1.24	0.02	-0.57	-1.71	1.42	-0.32	-2.71	-2.71
Pentane ... AcNH2	-3.53	-4.95	-0.26	1.04	-0.32	-0.98	-2.23	1.25	-0.66	-3.31	-3.30
Benzene ... AcOH	-3.80	-4.39	-0.52	0.41	-0.81	-1.60	-2.99	0.80	-1.15	-3.49	-4.19
Peptide ... Ethene	-3.00	-4.17	-0.95	-0.06	-1.06	-1.49	-2.25	0.06	-1.18	-2.88	-2.86
Pyridine ... Ethyne	-3.99	-5.74	-3.64	-3.31	-3.65	-3.78	-3.94	-3.10	-3.51	-4.14	-3.93
MeNH2 ... Pyridine	-3.97	-5.48	-1.73	-0.79	-1.73	-2.25	-3.28	-0.58	-2.03	-3.78	-4.20
MSE		-1.14	2.05	2.82	1.89	1.40	0.56	3.08	1.79	0.13	-0.12
MAE		1.14	2.05	2.82	1.89	1.40	0.56	3.08	1.79	0.16	0.26
MSE		-1.82	2.22	3.09	2.09	1.56	0.66	3.33	1.96	0.14	-0.02
MAE		1.85	2.23	3.09	2.10	1.58	0.67	3.33	1.96	0.21	0.45
rms		2.52	2.75	3.63	2.61	1.98	0.81	3.89	2.25	0.25	0.62

[1] Y. Zhao, N. González-García, D.G. Truhlar, J. Phys. Chem. A 109 (2005) 2012; 110 (2006) 4942(E).

[2] Y. Zhao, B.J. Lynch, D.G. Truhlar, J. Phys. Chem. A 108 (2004) 2715.

[3] P. Jurečka, J. Šponer, J. Černý, P. Hobza, Phys. Chem. Chem. Phys. 8 (2006) 1985.

[4] T. Takatani, E.G. Hohenstein, M. Malagoli, M.S. Marshall, C.D. Sherrill, J. Chem. Phys. 132 (2010) 144104.

[5] J. Rezac, K.E. Riley, P. Hobza, J. Chem. Theory Comput. 7 (2011) 2427.