SUPPORTING INFORMATION

Gauge Effects in Local Hybrid Functionals Evaluated for Weak Interactions and the GMTKN30 Test Set

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Table S1. List of semi-empirical parameters used in the local hybrids validated in this work^a

<i>Lh</i> -LSDA, <i>t</i> -LMF	$b = 0.48$
<i>Lh</i> -LSDA, <i>s</i> -LMF	$b_s = 0.22$
<i>Lh</i> -LSDA, <i>ct</i> -LMF	$b = 0.534$
<i>Lh</i> -LSDA, ζ - <i>t</i> -LMF	$b = 0.446, d = 0.0531$
<i>Lh</i> -LSDA, ζ - <i>s</i> -LMF	$b = 0.197, d = 0.0423$
<i>Lh</i> -LSDA-SIF-SRc	$b = 0.709$ $\mu = 0.8, \lambda = 1.0$
<i>Lh</i> -LSDA-SIR-SRc	$b = 0.646$ $\mu = 0.8, \lambda = 0.646$
<i>Lh</i> -BLYP-CG	$b = 0.488, \text{nlx} = 0.206, \text{nlc} = 0.497$ CG: $\eta = 0.5, c = -0.000894$
<i>Lh</i> -PBE-CG	$b = 0.50, \text{nlx} = 0.507, \text{nlc} = 0.451$ CG: $\eta = 0.12, c = -0.00238$

^a nlx and nlc are the coefficients of GGA corrections to exchange and correlation [eq. (14) in main text], respectively. b_s is the prefactor of the *s*-LMF [eq. (8)], b that of the *t*-LMF [eqs. (5,6,9)], c is the prefactor of the calibration function [eq. (14)], d controls the spin polarization contribution to the ζ -*t*-LMF [eq. (9)], μ is the range-separation parameter for correlation eq. (11)] and λ is the prefactor of the short-range correlation SIE correction [eq. (11)].

Table S2. MAE/MSE values for a selection of functionals (in kcal/mol) for eight subsets of the GMTKN30 database concerning “basic properties” (atomization energies, reaction barriers, ionization potentials, electron and proton affinities, etc.), with and without DFT-D3 corrections.

	MB08-165	W4-08	G21IP	G21EA	PA	SIE11	BHPERI	BH76
global and double hybrids								
B3LYP	8.14 /-6.79	3.94 /-2.35	3.55 /-0.09	1.92 / 0.48	2.23 / 1.90	7.63 / 6.17	5.80 / 5.36	4.67 /-4.57
+D3	6.38 /-3.97	3.86 /-2.14	3.55 /-0.10	1.93 / 0.48	2.38 / 2.06	8.70 / 7.32	2.78 / 2.18	5.21 /-5.14
PBE0	8.65 /-0.42	3.70 /-1.88	3.68 / 0.03	2.61 /-0.46	2.66 / 2.66	7.13 / 6.38	2.37 / 1.07	4.11 /-3.86
+D3	8.66 / 1.30	3.67 /-1.76	3.69 / 0.02	2.61 / -0.46	2.76 / 2.76	7.79 / 7.06	2.58 / -2.12	4.43 /-4.20
PW6B95	4.78 /-0.77	2.38 /-0.87	2.78 / 0.99	1.24 / 0.06	2.45 / 2.30	7.02 / 6.21	3.53 / 2.98	3.21 /-3.14
+D3	4.69 / 0.53	2.37 /-0.77	2.78 / 0.99	1.25 / 0.06	2.52 / 2.37	7.54 / 6.76	2.34 / 1.55	3.47 /-3.40
DSD-BLYP	4.15 /-3.90	2.49 /-1.70	2.06 /-0.92	1.98 /-1.52	1.19 / 1.01	3.01 / 0.71	1.91 / 1.16	1.18 / 0.00
+D3	3.38 /-2.89	2.45 /-1.61	2.06 /-0.92	1.98 /-1.51	1.24 / 1.06	3.10 / 1.15	1.19 / 0.04	1.21 /-0.21
Local hybrids								
<i>Lh</i> -LSDA, <i>t</i> -LMF	8.79 /-4.31	3.46 /-1.50	4.57 / 3.64	4.11 / 4.11	1.48 / 0.12	6.39 / 4.75	5.90 / 5.48	2.55 /-2.00
+D3	7.31 /-0.68	3.49 /-1.17	4.58 / 3.63	4.12 / 4.11	1.55 / 0.38	7.69 / 6.27	1.92 / 0.99	3.19 /-2.85
<i>Lh</i> -LSDA, <i>s</i> -LMF	9.34 /-7.89	4.13 /-1.19	4.00 / 2.25	3.39 / 3.38	1.72 / 0.90	6.75 / 4.95	6.20 / 5.34	3.39 /-3.01
+D3	6.64 /-2.12	4.29 /-0.48	3.99 / 2.24	3.41 / 3.40	1.89 / 1.44	8.82 / 7.30	2.14 /-1.88	4.76 /-4.51

Table S2 continued.....

	MB08-165	W4-08	G21IP	G21EA	PA	SIE11	BHPERI	BH76
local hybrids								
<i>Lh</i> -LSDA, <i>ct</i> -LMF +D3	10.77 /-6.32 8.70 /-1.99	2.98 / 0.54 3.12 / 0.90	5.11 / 4.76 5.11 / 4.75	4.89 / 4.89 4.89 / 4.89	1.59 / 0.67 1.66 / 0.92	5.78 / 3.79 7.72 / 5.64	7.48 / 7.31 2.75 / 2.50	1.69 /-0.68 2.15 /-1.58
<i>Lh</i> -LSDA, ζ - <i>t</i> -LMF +D3	7.68 /-2.95 6.74 / 0.08	2.74 /-1.03 2.73 /-0.78	4.47 / 3.49 4.47 / 3.48	4.14 / 4.14 4.14 / 4.14	1.53 /-0.24 1.51 /-0.04	6.94 / 5.45 8.02 / 6.70	4.98 / 4.33 1.84 / 0.64	2.95 /-2.62 3.53 /-3.28
<i>Lh</i> -LSDA, ζ - <i>s</i> -LMF +D3	8.43 /-6.30 6.61 /-1.48	3.18 /-0.51 3.36 /-0.01	3.94 / 2.09 3.94 / 2.08	3.47 / 3.41 3.48 / 3.42	1.62 / 0.51 1.69 / 0.90	7.35 / 5.62 9.10 / 7.63	5.27 / 4.12 2.08 /-1.88	3.85 /-3.63 4.92 /-4.81
<i>Lh</i> -LSDA-SIF-SRc +D3	9.48/-5.85 6.63/ 1.30	3.69/-1.51 4.04/-0.13	3.41/ 1.65 3.37/ 1.67	2.56/ 2.39 2.60/ 2.45	1.71/-0.90 1.69/ 0.17	4.58/ 1.66 6.90/ 4.73	7.53/ 7.25 2.77/-2.07	1.79/ 1.43 1.98/-0.84
<i>Lh</i> -LSDA-SIR-SRc +D3	9.73/-5.91 6.53/ 0.82	3.13/-0.65 3.68/ 0.65	3.81/ 2.74 3.79/ 2.75	3.40/ 3.39 3.45/ 3.44	1.59/-0.36 1.67/ 0.65	4.98/ 2.42 7.30/ 5.28	6.92/ 6.69 2.59/-2.11	1.55/ 0.67 2.25/-1.47
<i>Lh</i> -BLYP-CG +D3	6.89 /-2.49 6.17 / 0.18	2.69 /-1.98 2.60 /-1.78	3.35 /-0.26 3.36 /-0.26	1.95 / 1.00 1.96 / 1.00	2.02 /-1.16 2.01 /-0.99	6.87 / 5.39 7.80 / 6.45	3.03 / 2.33 1.15 /-0.85	3.22 /-2.94 3.72 /-3.49
<i>Lh</i> -PBE-CG +D3	5.98 /-0.50 5.83 / 1.23	3.42 /-2.85 3.35 /-2.73	4.46 / 3.46 4.47 / 3.46	3.84 / 3.75 3.84 / 3.75	1.40 / 0.71 1.44 / 0.80	6.98 / 5.98 7.60 / 6.65	1.33 / 0.44 1.60 /-1.57	3.16 /-2.83 3.46 /-3.17

Table S3. MAE/MSE values for a selection of functionals (in kcal/mol) for twelve subsets of the GMTKN30 database concerning “reaction energies”, with and without DFT-D3 corrections.

	BH76RC	RSE43	O3ADD6	G2RC	AL2X	NBPRC	ISO34	ISOL22	DC9	DARC	ALK6	BSR36
global and double hybrids												
B3LYP +D3	2.32/-0.24 2.25/-0.28	2.37/-2.37 1.97/-1.97	1.99/-0.88 2.75/-2.75	2.64/ 0.46 2.76/ 0.21	8.46/-8.46 4.28/-4.28	4.78/ 3.99 3.02/ 1.67	2.28/-0.23 1.86/-0.09	9.08/-5.53 6.96/-4.39	15.10/ 6.92 11.92/ 4.68	15.28/ 15.28 10.11/ 10.11	9.23/-9.14 4.82/-4.63	11.32/-11.32 6.00/-6.00
PBE0 +D3	2.52/-0.01 2.55/-0.03	2.00/-2.00 1.76/-1.76	4.81/-4.59 5.71/-5.71	6.47/-3.52 6.77/-3.67	2.68/-1.80 1.89/ 0.75	2.61/ 0.19 3.27/-1.21	1.81/-0.22 1.61/-0.14	4.15/-1.87 2.94/-1.18	10.41/ 1.89 9.36/ 0.45	3.52/ 0.00 3.32/-3.19	2.42/ 0.81 3.50/ 3.33	8.24/-8.24 4.73/-4.73
PW6B95 +D3	1.53/ 0.12 1.56/ 0.10	2.63/-2.63 2.44/-2.44	3.52/-3.47 4.31/-4.31	3.21/-1.15 3.36/-1.26	2.33/-1.59 1.25/ 0.36	2.07/ 0.74 1.80/-0.36	1.36/-0.50 1.20/-0.44	5.52/-3.50 4.57/-2.96	8.42/ 3.23 6.96/ 2.22	5.84/ 5.76 3.61/ 3.41	2.79/ 2.51 4.73/ 4.73	6.63/-6.63 4.06/-4.06
DSD-BLYP +D3	0.99/-0.12 1.01/-0.14	0.95/-0.23 0.85/-0.08	2.03/ 0.24 2.38/-0.42	1.85/-0.98 1.89/-1.07	2.30/-2.12 0.95/-0.63	1.32/ 1.12 0.83/ 0.27	1.06/ 0.39 0.96/ 0.43	3.85/-2.08 3.08/-1.66	4.04/ 1.58 3.04/ 0.83	3.96/ 3.96 2.23/ 2.16	2.36/-1.73 1.22/ 0.06	2.93/-2.93 1.10/-1.10
local hybrids												
<i>Lh</i> -LSDA, <i>t</i> -LMF +D3	2.96/-0.93 2.78/-0.99	1.92/-1.92 1.34/-1.32	1.64/ 0.08 2.45/-2.43	2.60/ 0.42 2.79/ 0.00	8.13/-8.13 3.14/-3.14	5.56/ 4.54 2.28/ 1.40	1.73/-0.60 1.33/-0.40	6.97/-4.51 4.27/-2.87	8.68/ 6.48 5.20/ 3.59	11.18/ 11.18 4.14/ 4.14	7.43/-7.43 3.42/-3.16	6.41/-6.38 0.48/-0.15
<i>Lh</i> -LSDA, <i>s</i> -LMF +D3	3.01/-0.86 2.84/-0.93	2.22/-2.22 1.32/-1.32	1.82/ 1.09 3.19/-3.05	2.81/-0.09 3.64/-0.91	9.89/-9.89 2.97/-2.97	5.35/ 4.91 0.98/ 0.01	1.92/-0.56 1.40/-0.32	6.78/-4.52 2.91/-1.56	9.32/ 7.09 5.59/ 2.44	10.09/ 10.09 1.79/-0.92	9.14/-9.14 3.71/-1.64	10.33/-10.33 2.06/-2.06
<i>Lh</i> -LSDA, <i>ct</i> -LMF +D3	2.31/-0.63 2.11/-0.69	2.26/-2.26 1.65/-1.62	1.49/ 1.39 1.52/-1.43	3.07/ 1.23 2.84/ 0.84	9.72/-9.72 3.40/-3.40	7.23/ 5.79 3.53/ 2.21	1.85/-0.67 1.41/-0.48	7.50/-5.11 4.56/-3.34	9.19/ 7.23 4.52/ 4.08	13.65/ 13.65 6.04/ 6.04	8.98/-8.98 4.64/-1.28	7.05/-7.01 0.99/ 0.50

Table S3 continued.....

	BH76RC	RSE43	O3ADD6	G2RC	AL2X	NBPRC	ISO34	ISOL22	DC9	DARC	ALK6	BSR36
local hybrids												
<i>Lh</i> -LSDA, ζ - <i>t</i> -LMF +D3	2.39/-0.62 2.25/-0.67	2.08/-2.08 1.58/-1.58	1.96/-0.75 2.83/-2.83	2.74/-0.09 3.07/-0.41	7.14/-7.14 2.72/-2.72	4.51/ 3.75 2.04/ 1.15	1.67/-0.56 1.31/-0.38	6.66/-4.14 4.30/-2.81	8.17/ 5.82 5.83/ 3.29	9.62/ 9.62 3.64/ 3.64	6.45/-6.45 2.91/-2.88	6.00/-5.98 0.68/-0.52
<i>Lh</i> -LSDA, ζ - <i>s</i> -LMF +D3	2.35/-0.45 2.27/-0.51	2.46/-2.46 1.68/-1.68	2.18/ 0.29 3.19/-3.07	3.37/-0.51 4.05/-1.10	8.81/-8.81 2.56/-2.56	4.48/ 4.09 0.98/-0.06	1.92/-0.53 1.42/-0.30	6.50/-3.87 3.14/-1.66	9.20/ 6.46 6.44/ 2.69	8.77/ 8.61 1.82/-0.55	8.14/-8.14 3.53/-2.05	9.56/-9.56 1.85/-1.85
<i>Lh</i> -LSDA-SIF-SRc +D3	2.21/-1.03 1.82/-1.16	2.28/-2.28 1.38/-1.28	2.94/ 2.58 4.07/-3.46	2.85/-0.68 3.83/-2.31	11.13/-11.13 3.47/-2.96	8.23/ 7.01 2.27/ 0.81	2.28/-0.33 1.88/ 0.15	6.31/-4.09 2.39/-0.28	8.80/ 8.61 7.35/ 1.02	11.42/ 11.42 4.11/-4.11	10.45/-10.45 4.02/ 0.10	5.81/-5.63 3.14/ 3.14
<i>Lh</i> -LSDA-SIR-SRc +D3	2.23/-0.88 1.81/-1.00	2.29/-2.29 1.40/-1.33	2.42/ 2.16 3.97/-3.51	2.54/ 0.00 3.09/-1.54	10.61/-10.61 3.38/-3.09	7.85/ 6.56 1.97/ 0.74	2.01/-0.44 1.58/-0.01	6.70/-4.45 2.39/-0.86	7.89/ 7.29 6.82/ 1.28	12.22/ 12.22 2.39/-2.39	9.91/-9.91 3.58/-0.23	6.23/-6.10 1.95/ 1.95
<i>Lh</i> -BLYP-CG +D3	2.30/-0.61 2.19/-0.66	1.91/-1.91 1.49/-1.48	2.86/-1.91 3.72/-3.72	2.52/-0.25 2.73/-0.51	6.79/-6.79 2.80/-2.80	4.11/ 3.43 1.95/ 1.17	1.58/-0.50 1.21/-0.33	6.67/-3.98 5.27/-1.89	7.91/ 5.37 4.94/ 3.07	9.57/ 9.57 4.30/ 4.30	7.43/-7.43 4.21/-4.21	5.81/-5.80 0.92/-0.84
<i>Lh</i> -PBE-CG +D3	2.10/-0.45 2.08/-0.48	1.48/-1.46 1.24/-1.21	4.08/-3.71 4.88/-4.88	3.34/-0.83 3.58/-0.97	4.10/-4.07 1.66/-1.44	2.46/ 1.99 1.57/ 0.55	1.44/-0.60 1.22/-0.49	5.43/-3.31 4.03/-2.61	6.54/ 3.19 5.86/ 1.64	5.55/ 5.52 2.60/ 2.14	2.81/-2.81 1.24/-0.52	5.94/-5.94 2.33/-2.33

Table S4. MAE/MSE values for a selection of functionals (in kcal/mol) for ten subsets of the GMTKN30 database concerning energies of non-covalent interactions, with and without DFT-D3 corrections.

	IDISP	WATER27	S22	ADIM6	RG6	HEAVY2 8	PCONF	ACONF	SCONF	CYCONF
Global hybrids										
B3LYP +D3	17.46/ 3.75 6.62/ 3.58	6.50/-6.20 4.26/ 4.12	3.79/-3.79 0.36/ 0.17	5.02/-5.02 0.43/ 0.43	0.80/-0.80 0.07/ 0.01	1.37/-1.37 0.16/-0.05	3.98/-3.98 0.34/-0.26	0.96/ 0.96 0.14/ 0.14	0.98/-0.70 0.52/-0.52	0.46/-0.38 0.24/-0.14
PBE0 +D3	10.59/ 0.78 3.48/ 0.70	2.80/-0.76 6.46/ 6.10	2.38/-2.34 0.57/ 0.29	3.41/-3.41 0.36/ 0.36	0.43/-0.43 0.03/ 0.03	0.66/-0.66 0.17/ 0.11	3.33/-3.33 0.89/-0.89	0.64/ 0.64 0.10/ 0.10	0.47/-0.39 0.32/-0.30	0.58/ 0.36 0.55/ 0.49
PW6B95 +D3	8.19/ 1.78 3.54/ 1.77	5.91/-5.74 1.66/-0.96	1.95/-1.95 0.34/-0.13	2.01/-2.01 0.58/ 0.58	0.39/-0.37 0.03/ 0.02	0.68/-0.68 0.13/-0.03	1.24/-1.24 0.51/ 0.37	0.21/ 0.21 0.15/-0.15	0.51/-0.37 0.31/-0.27	0.31/ 0.22 0.31/ 0.30
DSD-BLYP +D3	5.05/ 0.40 1.37/ 0.36	2.54/-2.19 1.50/ 1.22	1.04/-1.04 0.28/ 0.27	1.89/-1.89 0.13/-0.13	0.32/-0.32 0.07/-0.01	0.42/-0.42 0.11/ 0.09	1.17/-1.17 0.16/ 0.03	0.32/ 0.32 0.06/ 0.06	0.53/-0.32 0.25/-0.23	0.15/-0.15 0.09/-0.08
Local hybrids										
<i>Lh</i> -LSDA, <i>t</i> -LMF +D3	15.92/ 2.35 2.93/ 2.22	17.00/-16.98 3.86/-3.68	4.92/-4.92 0.33/-0.06	6.64/-6.64 0.17/-0.01	1.10/-1.10 0.25/-0.25	1.88/-1.88 0.44/-0.44	4.57/-4.57 0.34/-0.10	1.27/ 1.27 0.19/ 0.19	1.02/-0.54 0.32/-0.22	0.52/-0.14 0.31/ 0.20
<i>Lh</i> -LSDA, <i>s</i> -LMF	19.74/	22.79/-22.76	6.27/-6.27	8.76/-8.76	1.30/-1.30	2.24/-2.24	6.31/-6.31	1.61/ 1.61	1.34/-0.71	0.70/-0.06

+D3	2.17 1.48/ 1.42	3.48/-3.00	0.31/ 0.01	0.64/-0.64	0.24/-0.14	0.28/-0.13	0.82/-0.80	0.04/-0.03	0.82/ 0.13	0.55/ 0.53
<i>Lh</i> -LSDA, <i>ct</i> -LMF	17.81/ 2.68	22.92/-22.92	5.69/-5.69	7.44/-7.44	1.24/-1.24	2.19/-2.19	4.83/-4.83	1.44/ 1.44	1.44/-0.75	0.56/-0.40
+D3	3.47/ 2.35	8.89/-8.88	0.54/-0.31	0.46/-0.46	0.42/ 0.12	0.38/-0.05	0.43/ 0.28	0.29/ 0.29	0.36/-0.35	0.31/-0.06

Table S4 continued....

	IDISP	WATER27	S22	ADIM6	RG6	HEAVY2 8	PCONF	ACONF	SCONF	CYCONF
Local hybrids										
<i>Lh</i> -LSDA, ζ - <i>t</i> -LMF	14.73/ 2.14	13.31/-13.24	4.44/-4.44	6.13/-6.13	1.00/-1.00	1.68/-1.68	4.42/-4.42	1.16/ 1.16	0.75/-0.40	0.51/ 0.02
+D3	3.19/ 2.18	2.25/-1.77	0.27/ 0.00	0.17/ 0.08	0.24/-0.24	0.43/ 0.43	0.41/-0.29	0.25/ 0.25	0.35/-0.22	0.46/ 0.33
<i>Lh</i> -LSDA, ζ - <i>s</i> -LMF	18.30/ 1.96	19.35/-19.26	5.83/-5.83	8.37/-8.37	1.26/-1.26	2.10/-2.10	6.12/-6.12	1.48/ 1.48	0.98/-0.52	0.75/ 0.14
+D3	1.86/ 1.54	3.08/-2.38	0.29/-0.01	0.67/-0.67	0.24/-0.20	0.31/-0.22	0.86/-0.83	0.08/ 0.08	0.70/ 0.03	0.64/ 0.59
<i>Lh</i> -LSDA-SIF-SRc	19.39/ 1.38	32.11/-32.11	7.00/-7.00	9.23/-9.23	1.59/-1.59	2.89/-2.89	5.72/-5.72	1.77/1.77	1.85/-0.72	0.61/-0.42
+D3	3.20/-0.13	5.75/-5.53	0.47/-0.09	0.76/-0.76	0.39/-0.37	0.53/-0.51	0.57/-0.47	0.13/- 0.13	1.31/ 0.53	0.65/ 0.65
<i>Lh</i> -LSDA-SIR-SRc	19.50/ 1.91	28.85/-28.85	6.54/-6.54	8.59/-8.59	1.46/-1.46	2.67/-2.67	5.41/-5.41	1.65/1.65	1.73/-0.84	0.59/-0.41
		4.08/-3.84	0.44/-0.11	0.68/-0.68	0.37/-0.37	0.50/-0.49	0.60/-0.56	0.14/-	1.35/ 0.59	0.60/ 0.60

+D3	2.41/ 1.76							0.14		
<i>Lh</i> -BLYP-CG +D3	13.76/ 2.09 8.54/ 8.26	9.49/-9.32 1.62/ 0.97	3.99/-3.99 0.28/ 0.10	5.70/-5.70 0.20/ 0.13	0.95/-0.95 0.25/-0.25	1.61/-1.61 0.49/-0.49	4.15/-4.15 0.43/-0.34	1.04/ 1.04 0.22/ 0.22	0.50/-0.27 0.37/-0.17	0.43/ 0.03 0.45/ 0.32
<i>Lh</i> -PBE-CG +D3	10.36/ 1.79 2.93/ 1.81	5.07/-4.69 2.79/ 2.58	2.71/-2.71 0.25/ 0.12	3.81/-3.81 0.36/ 0.36	0.56/-0.56 0.12/-0.11	0.87/-0.87 0.22/-0.12	3.17/-3.17 0.56/-0.56	0.71/ 0.71 0.16/ 0.16	0.40/-0.31 0.31/-0.27	0.39/ 0.10 0.38/ 0.26

Table S5. Deviations from S22 reference values (in kcal/mol) for two uncalibrated and two calibrated local hybrids, with and without D3 corrections.

	ref. values ^a	<i>Lh</i> -LSDA-SIF-SRc <i>Lh</i> -LSDA-SIR-SRc			
		deviations			
H-bonded complexes		+D3		+D3	
(NH ₃) ₂	-3.17	3.29	1.00	2.99	0.83
(H ₂ O) ₂	-5.02	2.79	0.58	2.48	0.40
formic acid dimer	-18.80	5.33	-0.77	4.82	-0.87
formamide dimer	-16.12	6.30	-0.16	5.79	-0.25
uracil dimer	-20.69	7.22	-0.05	6.72	-0.07
2-pyridoxine-2-aminopyridine	-17.00	7.78	-0.11	7.24	-0.13
adenine*thymine WC	-16.74	8.99	0.72	8.39	0.67
dispersion-dominated complexes					
(CH ₄) ₂	-0.53	2.12	0.82	1.94	0.73
(C ₂ H ₄) ₂	-1.50	4.38	0.47	4.05	0.42
benzene*CH ₄	-1.45	4.14	0.60	3.86	0.57
PD benzene dimer	-2.62	9.46	0.47	8.90	0.55
pyrazine dimer	-4.20	10.08	0.21	9.48	0.33
stacked uracil dimer	-9.74	13.51	-0.76	12.72	-0.52
stacked indole*benzene	-4.59	13.34	0.25	12.61	0.45
stacked adenine*thymine	-11.66	19.00	-0.88	17.95	-0.50
mixed complexes					
ethene*ethine	-1.51	2.28	0.51	2.10	0.45
benzene*H ₂ O	-3.29	3.65	-0.35	3.37	-0.36
benzene*NH ₃	-2.32	3.87	0.08	3.60	0.07
benzene*HCN	-4.55	4.77	-0.58	4.47	-0.51
T-shaped benzene dimer	-2.71	6.05	0.16	5.69	0.20
T-shaped indole benzene	-5.62	7.86	-0.54	7.43	-0.44
phenol dimer	-7.09	7.85	0.31	7.33	0.29

cont....

Table S5 continued...

	ref. values ^a	<i>Lh</i> -BLYP-CG		<i>Lh</i> -PBE-CG	
		deviations			
H-bonded complexes		+D3		+D3	
(NH ₃) ₂	-3.17	1.43	0.52	0.80	0.19
(H ₂ O) ₂	-5.02	0.72	-0.01	0.27	-0.20
formic acid dimer	-18.80	1.05	-1.35	0.14	-1.37
formamide dimer	-16.12	2.32	-0.31	1.24	-0.46
uracil dimer	-20.69	3.04	-0.29	2.02	-0.30
2-pyridoxine-2-aminopyridine	-17.00	3.55	-0.40	2.35	-0.43
adenine*thymine WC	-16.74	4.45	0.12	3.07	0.03
dispersion-dominated complexes					
(CH ₄) ₂	-0.53	1.26	-0.26	0.79	0.03
(C ₂ H ₄) ₂	-1.50	2.53	-0.11	1.56	0.12
benzene*CH ₄	-1.45	2.53	-0.18	1.65	0.03
PD benzene dimer	-2.62	6.30	-0.06	4.43	-0.05
pyrazine dimer	-4.20	6.60	-0.02	4.70	0.17
stacked uracil dimer	-9.74	8.73	0.76	6.37	-0.25
stacked indole*benzene	-4.59	9.02	-0.16	6.57	0.34
stacked adenine*thymine	-11.66	12.49	0.49	9.28	0.36
mixed complexes					
ethene*ethine	-1.51	1.22	-0.12	0.67	-0.09
benzene*H ₂ O	-3.29	1.96	0.42	1.12	-0.55
benzene*NH ₃	-2.32	2.29	0.13	1.43	-0.27
benzene*HCN	-4.55	2.79	-0.04	1.73	-0.04
T-shaped benzene dimer	-2.71	3.91	-0.21	2.73	0.07
T-shaped indole benzene	-5.62	5.13	-0.18	3.62	0.03
phenol dimer	-7.09	4.44	-0.03	3.16	0.11

^a Relative energies were calculated as E(dimer) - ΣE(monomers).