

## Supplementary material to: Self-consistent determination of the fictitious temperature in thermally-assisted-occupation density functional theory

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References (S2).

FIG. S1. Potential energy curves for the ground state of H<sub>2</sub> (S3).

FIG. S2. Occupation numbers of the 1σ<sub>g</sub> orbital for the ground state of H<sub>2</sub> as a function of the internuclear distance *R* (S4).

FIG. S3. Potential energy curves for the ground state of N<sub>2</sub> (S4 to S5).

FIG. S4. Occupation numbers of the 3σ<sub>g</sub> orbital for the ground state of N<sub>2</sub> as a function of the internuclear distance *R* (S5 to S6).

FIG. S5. Occupation numbers of the 1π<sub>ux</sub> orbital for the ground state of N<sub>2</sub> as a function of the internuclear distance *R* (S6).

FIG. S6. Torsion potential energy curves for the ground state of twisted ethylene as a function of the HCCH torsion angle (S7).

FIG. S7. Occupation numbers of the π (1b<sub>2</sub>) orbital for the ground state of twisted ethylene as a function of the HCCH torsion angle (S8).

TABLE S1. Reaction energies of the 30 chemical reactions in the NHTBH38/04 and HTBH38/04 sets (S8 to S9).

TABLE S2. Non-hydrogen transfer barrier heights of the NHTBH38/04 set (S9 to S10).

TABLE S3. Hydrogen transfer barrier heights of the HTBH38/04 set (S10 to S11).

TABLE S4. Interaction energies of the S22 set (S11 to S12).

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## FIGURES

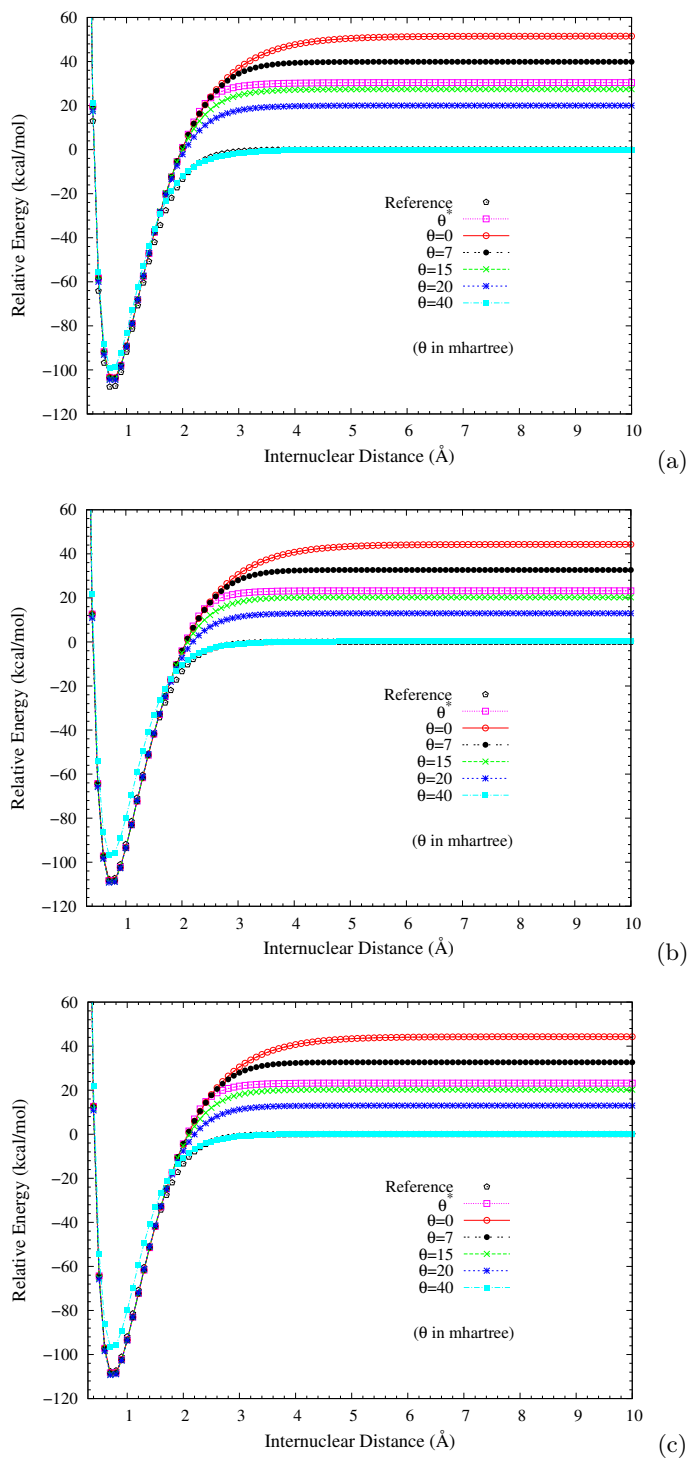


FIG. S1. Potential energy curves (in relative energy) for the ground state of  $\text{H}_2$ , calculated using spin-restricted (a) TAO-PBE, (b) TAO-BLYP, and (c) TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE, (b) KS-BLYP, and (c) KS-BLYP-D, respectively. The reference curve is calculated using the CCSD theory (exact for any two-electron system). The zeros of energy are set at the respective spin-unrestricted dissociation limits.

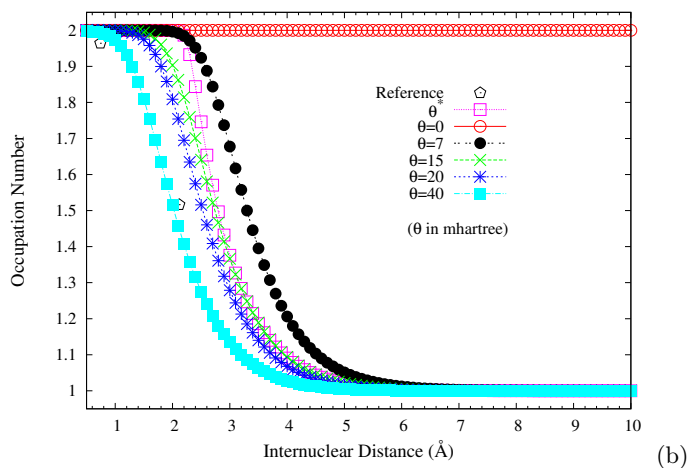
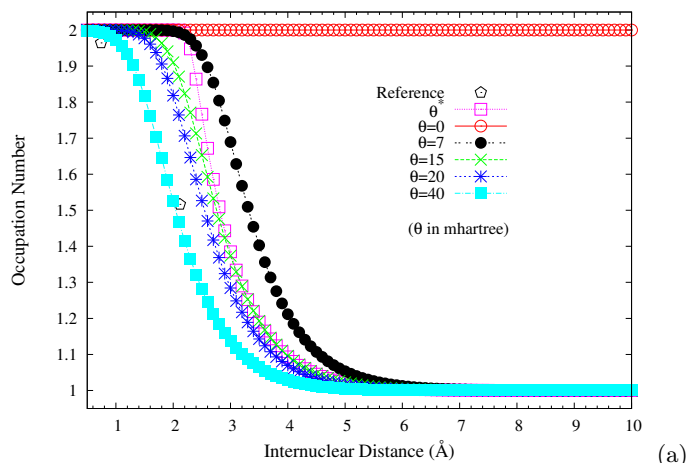
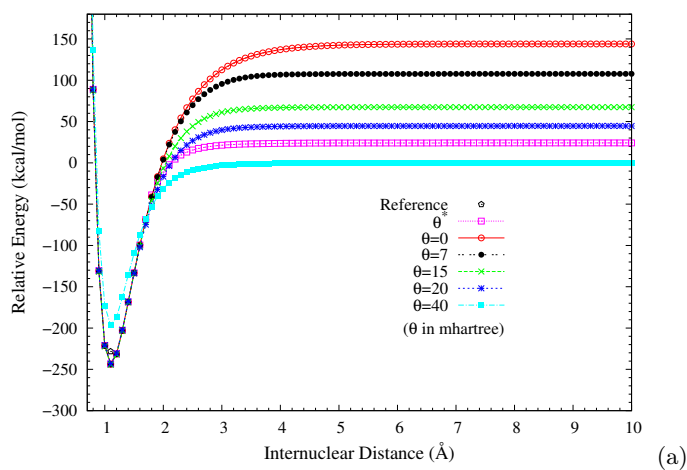


FIG. S2. Occupation numbers of the  $1\sigma_g$  orbital for the ground state of  $H_2$  as a function of the internuclear distance  $R$ , calculated using spin-restricted (a) TAO-PBE and (b) TAO-BLYP/TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE and (b) KS-BLYP/KS-BLYP-D, respectively. The reference data are the FCI NOONs [1].



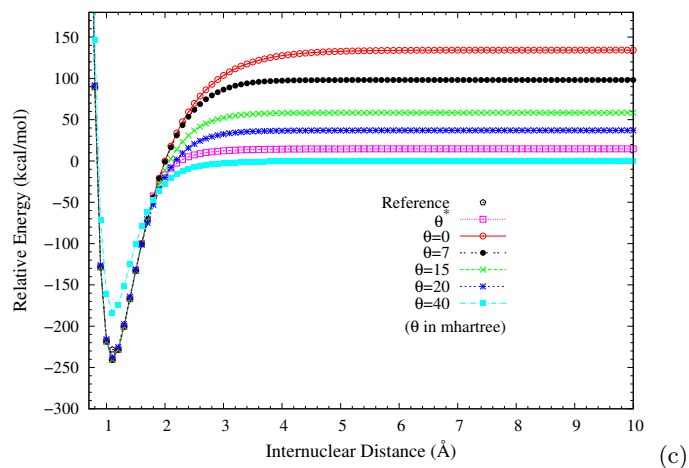
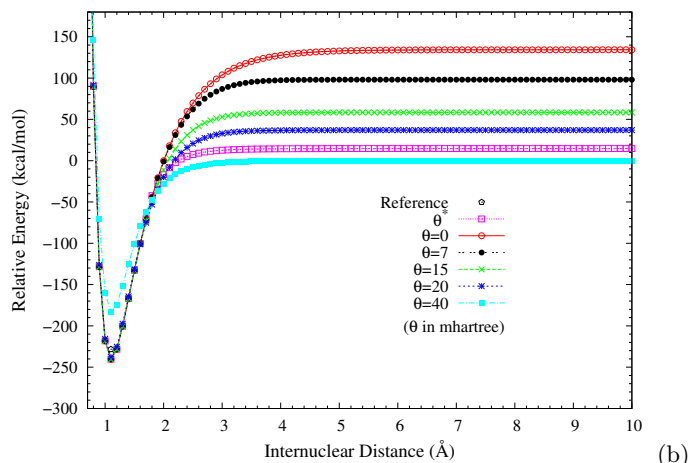
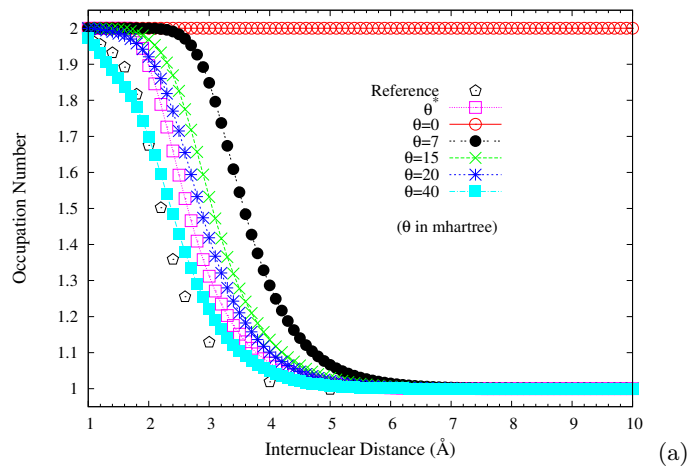


FIG. S3. Potential energy curves (in relative energy) for the ground state of  $N_2$ , calculated using spin-restricted (a) TAO-PBE, (b) TAO-BLYP, and (c) TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE, (b) KS-BLYP, and (c) KS-BLYP-D, respectively. The reference data ( $-228.3$  kcal/mol) at  $R = 1.098$   $\text{\AA}$  (i.e., the equilibrium bond length) are the experimental results [2, 3]. The zeros of energy are set at the respective spin-unrestricted dissociation limits.



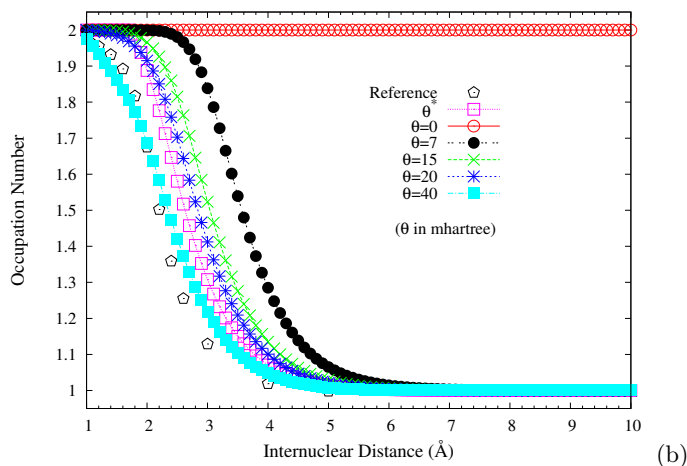


FIG. S4. Occupation numbers of the  $3\sigma_g$  orbital for the ground state of  $N_2$  as a function of the internuclear distance  $R$ , calculated using spin-restricted (a) TAO-PBE and (b) TAO-BLYP/TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE and (b) KS-BLYP/KS-BLYP-D, respectively. The reference data are the NOONs of the MRCI method [4].

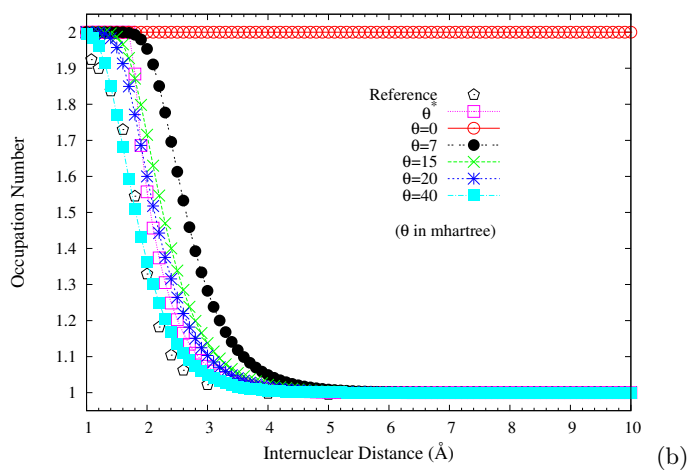
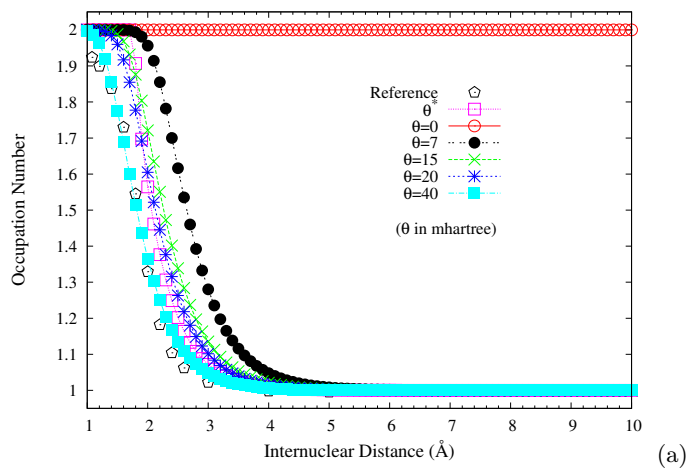


FIG. S5. Occupation numbers of the  $1\pi_{ux}$  orbital for the ground state of  $N_2$  as a function of the internuclear distance  $R$ , calculated using spin-restricted (a) TAO-PBE and (b) TAO-BLYP/TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE and (b) KS-BLYP/KS-BLYP-D, respectively. The reference data are the NOONs of the MRCI method [4].

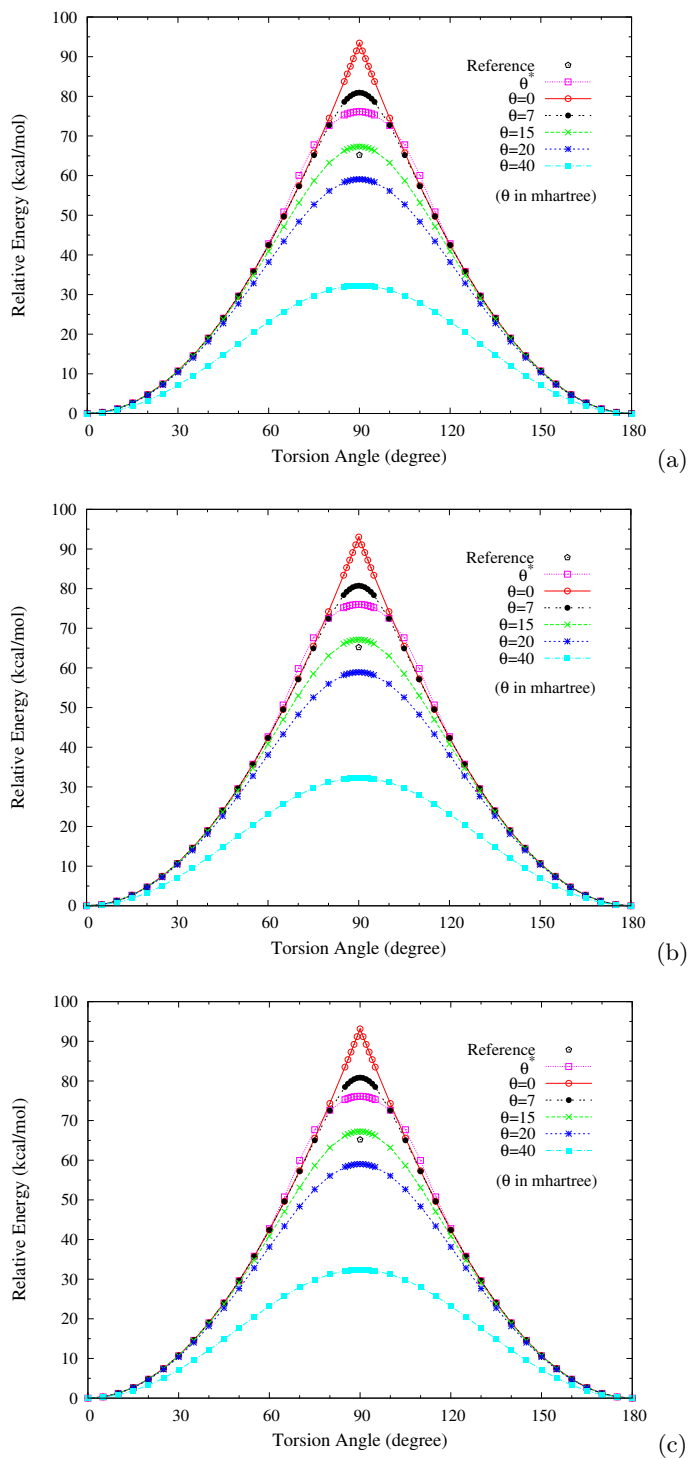


FIG. S6. Torsion potential energy curves (in relative energy) for the ground state of twisted ethylene as a function of the HCCH torsion angle, calculated using spin-restricted (a) TAO-PBE, (b) TAO-BLYP, and (c) TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE, (b) KS-BLYP, and (c) KS-BLYP-D, respectively. The reference data are the CASPT2 results [5]. The zeros of energy are set at the respective minimum energies.

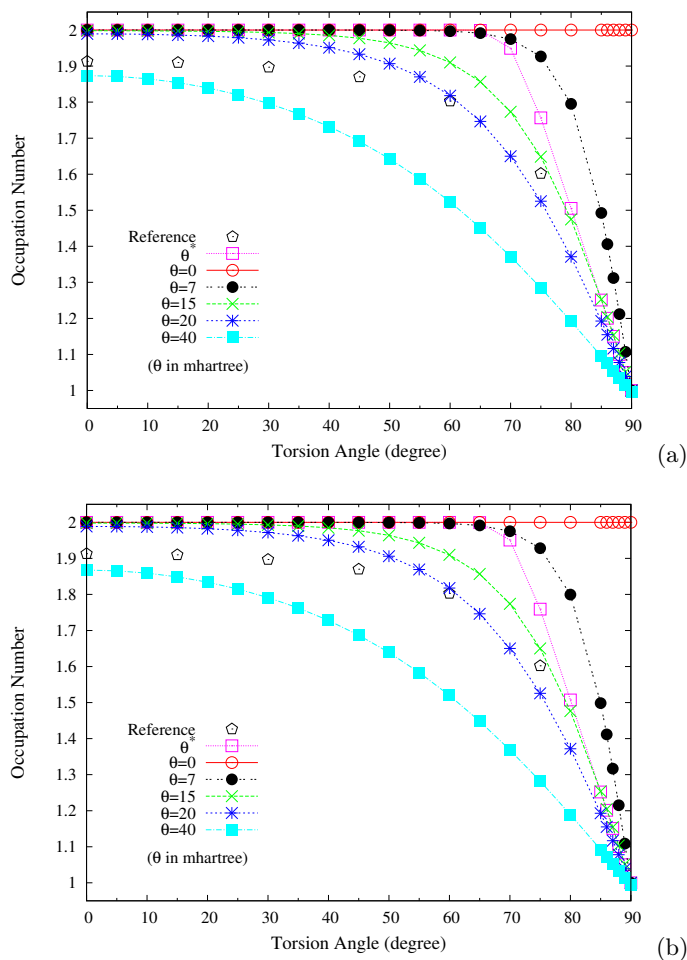


FIG. S7. Occupation numbers of the  $\pi$  ( $1b_2$ ) orbital for the ground state of twisted ethylene as a function of the HCCH torsion angle, calculated using spin-restricted (a) TAO-PBE and (b) TAO-BLYP/TAO-BLYP-D with the  $\theta^*$  and system-independent  $\theta$  values. The  $\theta = 0$  cases correspond to spin-restricted (a) KS-PBE and (b) KS-BLYP/KS-BLYP-D, respectively. The reference data are the half-projected NOONs of the CASSCF method (HPNO-CAS) [6].

## TABLES

TABLE S1. Comparison of errors of the reaction energies (in kcal/mol) of the 30 chemical reactions in the NHTBH38/04 and HTBH38/04 sets [7, 8].

Reactions	$\Delta E_{ref}$	with $\theta^*$			
		TAO-LDA	TAO-PBE	TAO-BLYP	TAO-BLYP-D
$\text{H} + \text{N}_2\text{O} \rightarrow \text{OH} + \text{N}_2$	-65.08	35.68	22.59	11.96	12.03
$\text{H} + \text{FCH}_3 \rightarrow \text{HF} + \text{CH}_3$	-26.64	8.28	4.16	0.49	0.63
$\text{H} + \text{F}_2 \rightarrow \text{HF} + \text{F}$	-103.91	18.54	13.19	10.10	10.10
$\text{CH}_3 + \text{FCl} \rightarrow \text{CH}_3\text{F} + \text{Cl}$	-52.74	3.56	4.63	4.00	3.85
$\text{F}^- + \text{CH}_3\text{Cl} \rightarrow \text{FCH}_3 + \text{Cl}^-$	-32.65	-0.90	0.82	0.27	0.37
$\text{F}^- \cdots \text{CH}_3\text{Cl} \rightarrow \text{FCH}_3 \cdots \text{Cl}^-$	-26.73	3.98	4.41	3.83	3.90
$\text{OH}^- + \text{CH}_3\text{F} \rightarrow \text{HOCH}_3 + \text{F}^-$	-20.11	-0.74	-1.09	-0.41	-0.92
$\text{OH}^- \cdots \text{CH}_3\text{F} \rightarrow \text{HOCH}_3 \cdots \text{F}^-$	-36.24	-11.06	-8.12	-5.50	-5.52



H + N <sub>2</sub> → HN <sub>2</sub>	3.97	-15.60	-7.86	-7.24	-7.28
H + CO → HCO	-19.51	-14.40	-6.84	-5.78	-5.87
H + C <sub>2</sub> H <sub>4</sub> → CH <sub>3</sub> CH <sub>2</sub>	-40.03	-4.52	-0.31	1.22	0.62
CH <sub>3</sub> + C <sub>2</sub> H <sub>4</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub>	-26.12	-12.64	-2.14	5.96	3.47
HCN → HNC	15.05	-0.83	0.06	0.02	0.09
H + HCl → H <sub>2</sub> + Cl	-3.0	11.13	5.51	-1.29	-1.29
OH + H <sub>2</sub> → H + H <sub>2</sub> O	-16.1	-13.62	-3.95	2.22	2.19
CH <sub>3</sub> + H <sub>2</sub> → H + CH <sub>4</sub>	-3.2	-7.09	-2.30	2.70	2.55
OH + CH <sub>4</sub> → CH <sub>3</sub> + H <sub>2</sub> O	-12.9	-6.53	-1.65	-0.48	-0.36
OH + NH <sub>3</sub> → H <sub>2</sub> O + NH <sub>2</sub>	-9.5	-3.67	-1.73	-1.51	-1.43
HCl + CH <sub>3</sub> → Cl + CH <sub>4</sub>	-6.2	4.04	3.21	1.41	1.26
OH + C <sub>2</sub> H <sub>6</sub> → H <sub>2</sub> O + C <sub>2</sub> H <sub>5</sub>	-16.5	-9.27	-3.29	-1.97	-1.30
F + H <sub>2</sub> → HF + H	-31.6	-18.31	-6.49	-0.72	-0.72
O + CH <sub>4</sub> → OH + CH <sub>3</sub>	5.6	-7.02	-5.83	-5.84	-5.69
H + PH <sub>3</sub> → PH <sub>2</sub> + H <sub>2</sub>	-20.1	3.51	0.40	-4.10	-3.42
H + HO → H <sub>2</sub> + O	-2.4	14.11	8.12	3.14	3.14
H + H <sub>2</sub> S → H <sub>2</sub> + HS	-13.8	7.93	3.48	-2.41	-2.15
O + HCl → OH + Cl	-0.6	-2.98	-2.61	-4.43	-4.43
NH <sub>2</sub> + CH <sub>3</sub> → CH <sub>4</sub> + NH	-14.4	3.87	4.55	4.66	4.56
NH <sub>2</sub> + C <sub>2</sub> H <sub>5</sub> → C <sub>2</sub> H <sub>6</sub> + NH	-10.8	6.62	6.19	6.15	5.49
C <sub>2</sub> H <sub>6</sub> + NH <sub>2</sub> → NH <sub>3</sub> + C <sub>2</sub> H <sub>5</sub>	-7.0	-5.61	-1.55	-0.46	0.14
NH <sub>2</sub> + CH <sub>4</sub> → CH <sub>3</sub> + NH <sub>3</sub>	-3.3	-2.96	-0.02	0.94	0.97
MSE		-0.55	0.85	0.56	0.50
MAE		8.63	4.57	3.37	3.19
rms		11.19	6.39	4.47	4.31
Max(-)		-18.31	-8.12	-7.24	-7.28
Max(+)		35.68	22.59	11.96	12.03

TABLE S2. Non-hydrogen transfer barrier heights (in kcal/mol) of the NHTBH38/04 set [7, 8].

Reactions	$\Delta E_{ref}$	with $\theta^*$				
		TAO-LDA	TAO-PBE	TAO-BLYP	TAO-BLYP-D	
<b>Heavy-atom transfer reactions</b>						
H + N <sub>2</sub> O → OH + N <sub>2</sub>	$V^f$	18.14	2.69	9.97	8.54	8.19
	$V^r$	83.22	32.09	52.46	61.67	61.24
H + FH → HF + H	$V^f$	42.18	18.48	27.07	26.03	25.76
	$V^r$	42.18	18.48	27.07	26.03	25.76
H + ClH → HCl + H	$V^f$	18.00	2.27	9.64	9.80	9.74
	$V^r$	18.00	2.27	9.64	9.80	9.74
H + FCH <sub>3</sub> → HF + CH <sub>3</sub>	$V^f$	30.38	13.36	18.51	16.12	15.33
	$V^r$	57.02	31.72	41.00	42.27	41.33
H + F <sub>2</sub> → HF + F	$V^f$	2.27	-15.97	-9.86	-11.66	-11.78
	$V^r$	106.18	69.40	80.86	82.15	82.03
CH <sub>3</sub> + FCl → CH <sub>3</sub> F + Cl	$V^f$	7.43	-10.90	-6.01	-6.39	-7.87
	$V^r$	60.17	38.28	42.10	42.35	41.02
<b>Nucleophilic substitution reactions</b>						
F <sup>-</sup> + CH <sub>3</sub> F → FCH <sub>3</sub> + F <sup>-</sup>	$V^f$	-0.34	-12.18	-8.31	-7.90	-8.95
	$V^r$	-0.34	-12.18	-8.31	-7.90	-8.95
F <sup>-</sup> ...CH <sub>3</sub> F → FCH <sub>3</sub> ...F <sup>-</sup>	$V^f$	13.38	6.34	6.41	5.72	6.07
	$V^r$	13.38	6.34	6.41	5.72	6.07
Cl <sup>-</sup> + CH <sub>3</sub> Cl → ClCH <sub>3</sub> + Cl <sup>-</sup>	$V^f$	3.10	-6.73	-3.80	-3.95	-5.69

	$V^r$	3.10	-6.73	-3.80	-3.95	-5.69
$\text{Cl}^- \cdots \text{CH}_3\text{Cl} \rightarrow \text{ClCH}_3 \cdots \text{Cl}^-$	$V^f$	13.61	6.70	7.07	5.58	5.41
	$V^r$	13.61	6.70	7.07	5.58	5.41
$\text{F}^- + \text{CH}_3\text{Cl} \rightarrow \text{FCH}_3 + \text{Cl}^-$	$V^f$	-12.54	-23.45	-19.52	-19.35	-20.67
	$V^r$	20.11	10.10	12.31	13.03	11.62
$\text{F}^- \cdots \text{CH}_3\text{Cl} \rightarrow \text{FCH}_3 \cdots \text{Cl}^-$	$V^f$	2.89	-1.13	-0.94	-2.01	-1.89
	$V^r$	29.62	21.62	21.38	20.89	20.94
$\text{OH}^- + \text{CH}_3\text{F} \rightarrow \text{HOCH}_3 + \text{F}^-$	$V^f$	-2.78	-15.12	-11.99	-11.35	-13.14
	$V^r$	17.33	5.73	9.21	9.17	7.89
$\text{OH}^- \cdots \text{CH}_3\text{F} \rightarrow \text{HOCH}_3 \cdots \text{F}^-$	$V^f$	10.96	0.23	-1.14	-1.49	-2.05
	$V^r$	47.20	47.53	43.23	40.25	39.71
<b>Unimolecular and association reactions</b>						
$\text{H} + \text{N}_2 \rightarrow \text{HN}_2$	$V^f$	14.69	-2.19	5.19	5.24	5.08
	$V^r$	10.72	9.44	9.08	8.51	8.38
$\text{H} + \text{CO} \rightarrow \text{HCO}$	$V^f$	3.17	-7.57	-1.69	-1.95	-2.25
	$V^r$	22.68	26.34	24.66	23.34	23.13
$\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{CH}_3\text{CH}_2$	$V^f$	1.72	-5.34	-0.14	-0.69	-1.78
	$V^r$	41.75	39.21	40.20	38.11	37.63
$\text{CH}_3 + \text{C}_2\text{H}_4 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2$	$V^f$	6.85	-5.81	1.50	4.73	1.48
	$V^r$	32.97	32.95	29.76	24.88	24.13
$\text{HCN} \rightarrow \text{HNC}$	$V^f$	48.16	44.83	45.60	46.76	46.94
	$V^r$	33.11	30.60	30.50	31.68	31.80
MSE			-12.50	-8.71	-8.89	-9.53
MAE			12.71	8.81	8.93	9.55
rms			16.16	10.75	10.42	10.98
Max(-)			-51.13	-30.76	-24.03	-24.15
Max(+)			3.66	1.98	0.66	0.45

TABLE S3. Hydrogen transfer barrier heights (in kcal/mol) of the HTBH38/04 set [7, 8].

Reactions	$\Delta E_{ref}$	with $\theta^*$				
		TAO-LDA	TAO-PBE	TAO-BLYP	TAO-BLYP-D	
$\text{H} + \text{HCl} \rightarrow \text{H}_2 + \text{Cl}$	$V^f$	5.7	-3.14	0.56	-2.45	-2.58
	$V^r$	8.7	-11.27	-1.95	1.84	1.71
$\text{OH} + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$	$V^f$	5.1	-18.39	-6.36	-3.49	-3.95
	$V^r$	21.2	11.33	13.69	10.39	9.96
$\text{CH}_3 + \text{H}_2 \rightarrow \text{H} + \text{CH}_4$	$V^f$	12.1	-5.35	3.82	7.14	5.96
	$V^r$	15.3	4.94	9.32	7.65	6.61
$\text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	$V^f$	6.7	-17.22	-5.65	-2.75	-4.01
	$V^r$	19.6	2.21	8.91	10.63	9.24
$\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$	$V^f$	9.6	-2.70	3.64	2.86	2.67
	$V^r$	9.6	-2.70	3.64	2.86	2.67
$\text{OH} + \text{NH}_3 \rightarrow \text{H}_2\text{O} + \text{NH}_2$	$V^f$	3.2	-23.88	-11.94	-9.20	-10.46
	$V^r$	12.7	-10.71	-0.71	1.81	0.47
$\text{HCl} + \text{CH}_3 \rightarrow \text{Cl} + \text{CH}_4$	$V^f$	1.7	-13.74	-5.94	-3.51	-5.09
	$V^r$	7.9	-11.58	-2.95	1.29	-0.15
$\text{OH} + \text{C}_2\text{H}_6 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_5$	$V^f$	3.4	-20.98	-9.03	-6.12	-7.54
	$V^r$	19.9	4.79	10.76	12.36	10.26
$\text{F} + \text{H}_2 \rightarrow \text{HF} + \text{H}$	$V^f$	1.8	-24.20	-12.97	-11.61	-11.86
	$V^r$	33.4	25.71	25.12	20.70	20.45
$\text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$	$V^f$	13.7	-10.69	-0.79	1.44	0.52

	$V^r$	8.1	-9.27	-0.57	1.68	0.61
H + PH <sub>3</sub> → PH <sub>2</sub> + H <sub>2</sub>	$V^f$	3.1	-7.35	-1.79	-2.63	-3.14
	$V^r$	23.2	9.24	17.91	21.58	20.38
H + HO → H <sub>2</sub> + O	$V^f$	10.7	-1.69	3.75	1.60	1.48
	$V^r$	13.1	-13.40	-1.98	0.86	0.74
H + H <sub>2</sub> S → H <sub>2</sub> + HS	$V^f$	3.5	-6.73	-1.22	-2.20	-2.59
	$V^r$	17.3	-0.86	9.10	14.00	13.36
O + HCl → OH + Cl	$V^f$	9.8	-23.13	-10.54	-8.78	-8.86
	$V^r$	10.4	-19.55	-7.33	-3.75	-3.83
NH <sub>2</sub> + CH <sub>3</sub> → CH <sub>4</sub> + NH	$V^f$	8.0	-8.37	0.71	3.57	1.82
	$V^r$	22.4	2.16	10.56	13.31	11.66
NH <sub>2</sub> + C <sub>2</sub> H <sub>5</sub> → C <sub>2</sub> H <sub>6</sub> + NH	$V^f$	7.5	-5.76	2.89	5.94	3.56
	$V^r$	18.3	-1.57	7.51	10.59	8.87
C <sub>2</sub> H <sub>6</sub> + NH <sub>2</sub> → NH <sub>3</sub> + C <sub>2</sub> H <sub>5</sub>	$V^f$	10.4	-9.69	1.44	5.25	3.08
	$V^r$	17.4	2.91	9.99	12.72	9.94
NH <sub>2</sub> + CH <sub>4</sub> → CH <sub>3</sub> + NH <sub>3</sub>	$V^f$	14.5	-6.16	4.39	7.99	6.04
	$V^r$	17.8	0.10	7.71	10.36	8.37
<i>s-trans cis</i> -C <sub>5</sub> H <sub>8</sub> → <i>s-trans cis</i> -C <sub>5</sub> H <sub>8</sub>	$V^f$	38.4	25.00	31.19	35.82	34.69
	$V^r$	38.4	25.00	31.19	35.82	34.69
MSE			-17.90	-9.67	-7.84	-8.89
MAE			17.90	9.67	7.84	8.89
rms			18.92	10.37	8.66	9.52
Max(-)			-32.93	-20.34	-18.58	-18.66
Max(+)			-7.69	-4.61	-1.56	-2.82

TABLE S4. Interaction energies (in kcal/mol) of the S22 set [9]. The counterpoise corrections are used to reduce the basis set superposition errors. Monomer deformation energies are not included.

Complex [Symmetry]	$\Delta E_{ref}$	with $\theta^*$			
		TAO-LDA	TAO-PBE	TAO-BLYP	TAO-BLYP-D
<b>Hydrogen bonded complexes</b>					
(NH <sub>3</sub> ) <sub>2</sub> [C <sub>2h</sub> ]	-3.17	-5.10	-2.83	-1.78	-3.44
(H <sub>2</sub> O) <sub>2</sub> [C <sub>s</sub> ]	-5.02	-7.78	-4.91	-3.99	-4.92
Formic acid dimer [C <sub>2h</sub> ]	-18.61	-26.82	-18.08	-15.48	-18.50
Formamide dimer [C <sub>2h</sub> ]	-15.96	-21.82	-14.69	-12.44	-15.63
Uracil dimer [C <sub>2h</sub> ]	-20.65	-26.15	-18.46	-16.21	-20.21
2-pyridoxine-2-aminopyridine [C <sub>1</sub> ]	-16.71	-22.74	-15.24	-12.48	-17.25
Adenine-thymine WC [C <sub>1</sub> ]	-16.37	-21.91	-14.21	-11.33	-16.42
<b>Dispersion complexes</b>					
(CH <sub>4</sub> ) <sub>2</sub> [D <sub>3d</sub> ]	-0.53	-0.83	-0.08	0.68	-0.31
(C <sub>2</sub> H <sub>4</sub> ) <sub>2</sub> [D <sub>2d</sub> ]	-1.51	-2.49	-0.31	1.12	-1.44
Benzene·CH <sub>4</sub> [C <sub>3</sub> ]	-1.50	-2.01	-0.01	1.39	-1.23
Benzene dimer [C <sub>2h</sub> ]	-2.73	-2.63	1.90	4.93	-1.93
Pyrazine dimer [C <sub>s</sub> ]	-4.42	-4.40	0.76	3.82	-3.63
Uracil dimer [C <sub>2</sub> ]	-10.12	-10.14	-2.69	1.13	-9.68
Indole·benzene [C <sub>1</sub> ]	-5.22	-4.37	2.26	6.33	-3.91
Adenine·thymine stack [C <sub>1</sub> ]	-12.23	-11.92	-1.30	4.10	-11.77
<b>Mixed complexes</b>					
Ethene·ethine [C <sub>2v</sub> ]	-1.53	-2.27	-1.16	-0.29	-1.49
Benzene·H <sub>2</sub> O [C <sub>s</sub> ]	-3.28	-4.44	-2.04	-0.49	-3.30
Benzene·NH <sub>3</sub> [C <sub>s</sub> ]	-2.35	-3.03	-0.92	0.55	-2.18

Benzene·HCN [ $C_s$ ]	-4.46	-5.85	-2.81	-0.94	-4.65
Benzene dimer [ $C_{2v}$ ]	-2.74	-3.06	-0.10	1.86	-2.52
Indole·benzene T-shape [ $C_1$ ]	-5.73	-6.07	-1.86	0.84	-5.52
Phenol dimer [ $C_1$ ]	-7.05	-8.99	-3.85	-1.73	-6.64
MSE		-1.95	2.78	5.07	0.24
MAE		2.07	2.78	5.07	0.34
rms		3.17	3.90	6.33	0.45
Max(-)		-8.21	0.11	1.03	-0.54
Max(+)		0.85	10.93	16.33	1.31