Supporting Information for:

Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics

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Table S1. Barrier Heights and Energies of Reaction (kcal/mol) for the Kinetics9 database[a]

	Best Estimates			BB1K/DIDZ			MPW1K/DIDZ		
Reaction	$V_f^{\neq}$	$Vr^{\neq}$	ΔE	$V_f^{\neq}$	$Vr^{\neq}$	ΔE	$V_f^{\neq}$	$Vr^{\neq}$	ΔE
$OH + CH_4 \rightarrow CH_3 + H_2O$	6.7	19.6	-12.9	7.1	15.7	-8.6	7.6	16.6	-9.0
$H + OH \rightarrow O + H_2$	10.7	13.1	-2.4	7.7	13.1	-5.5	8.1	12.5	-4.4
$H + H_2S \rightarrow H_2 + HS$	3.5	17.3	-13.7	3.0	17.7	-14.7	2.3	17.1	-14.8

[a]These barrier heights and energies of reaction are calculated from the geometries consistently optimized by the sepecified method.

Table S2. Geometric Parameters of the Saddle Points (BB1K and B97-2)

Reaction	BB1K/DIDZ				BB1K/MG3S				B97-2/DIDZ				B97-2/MG3S			
A + BC → AB + C	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$
H + HCl → H_2 + Cl	1.076	1.384	2.459	180	1.030	1.399	2.429	180	1.201	1.352	2.553	180	1.155	1.358	2.514	180
H + H_2 → H_2 + H	0.928	0.928	1.856	180	0.927	0.927	1.853	180	0.930	0.930	1.859	180	0.928	0.928	1.857	180
H + ClH′ → HCl + H′	1.480	1.480	2.961	180	1.472	1.472	2.944	180	1.483	1.483	2.966	180	1.474	1.474	2.948	180
H + HO → H_2 +O	0.930	1.164	2.095	180	0.914	1.178	2.091	180	0.986	1.125	2.110	180	0.945	1.151	2.096	180
F + H_2 → HF + H	1.559	0.766	2.325	120	1.554	0.769	2.322	120	-	-	-	-	-	-	-	-

Table S3. Geometric Parameters of the Saddle Points (BB95 and B1B95)

Reaction	BB95/DIDZ				BB95/MG3S				B1B95/DIDZ				B1B95/MG3S			
A + BC → AB + C	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$
H + HCl → H_2 + Cl	1.344	1.345	2.689	180	1.287	1.346	2.632	180	1.134	1.372	2.507	180	1.084	1.383	2.467	180
H + H_2 → H_2 + H	0.939	0.939	1.878	180	0.937	0.937	1.873	180	0.931	0.931	1.861	180	0.930	0.930	1.859	180
H + ClH′ → HCl + H′	1.504	1.504	3.008	180	1.495	1.495	2.991	180	1.488	1.488	2.975	180	1.479	1.479	2.958	180
H + HO → H_2 +O	0.938	1.190	2.129	180	0.885	1.252	2.138	180	0.932	1.173	2.105	180	0.912	1.189	2.1001	180
F + H_2 → HF + H	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S4. 42 Barrier Heights from Best Estimate, BB1K/DIDZ// QCISD/MG3 and BB1K/MG3S// QCISD/MG3 for the BH42/03 Database

Reaction	best estimate		BB1K/DIDZ		BB1K/MG3S	
A + BC → AB + C	$V_f^{\neq}$	$Vr^{\neq}$	$V_f^{\neq}$	$Vr^{\neq}$	$V_f^{\neq}$	$Vr^{\neq}$
1. H + HCl → H_2 + Cl	5.7	8.7	2.8	7.3	4.4	5.6
2. OH + H_2 → H + H_2O	5.1	21.2	5.4	18.6	4.8	19.5
3. CH_3 + H_2 → H + CH_4	12.1	15.3	9.8	14.4	9.9	14.7
4. OH + CH_4 → CH_3 + H_2O	6.7	19.6	7.2	15.8	6.8	16.8
5. H + H_2 → H_2 + H	9.6	9.6	8.5	8.5	8.6	8.6
6. OH + NH_3 → H_2O + NH_2	3.2	12.7	4.1	11.3	4.4	12.6
7. HCl + CH_3 → Cl + CH_4	1.7	7.9	-0.9	8.2	0.4	6.5
8. OH + C_2H_6 →H_2O + C_2H_5	3.4	19.9	4.3	17.3	4.0	18.5
9. F + H_2 → HF + H	1.8	33.4	-0.1	27.3	-0.2	29.1
10. O + CH_4 →OH + CH_3	13.7	8.1	14.6	4.6	14.3	5.8
11. H + PH_3→ PH_2 + H_2	3.1	23.2	2.1	23.8	2.7	23.1
12. H + ClH′ → HCl + H′	18.0	18.0	18.9	18.9	18.2	18.2
13. H + HO → H_2 +O	10.7	13.1	7.6	13.1	8.7	12.3
14. H + *trans*-N_2H_2→ H_2 + N_2H	5.9	40.9	1.6	39.9	1.7	40.2
15. H + H_2S → H_2 + HS	3.5	17.3	2.9	17.6	3.6	15.9
16. O + HCl → OH + Cl	9.8	10.4	9.1	10.0	7.7	10.1
17. NH_2 + CH_3→ CH_4 + NH	8.0	22.4	6.1	22.9	7.2	22.4
18. NH_2 + C_2H_5 → C_2H_6 + NH	7.5	18.3	7.9	20.2	9.1	19.8
19. C_2H_6 + NH_2 → NH_3 + C_2H_5	10.4	17.4	11.4	17.2	11.7	17.9
20. NH_2 + CH_4 → CH_3 + NH_3	14.5	17.8	13.9	15.3	14.2	15.9
21. *s-trans cis*-C_5H_8 → *s-trans cis*-C_5H_8	38.4	38.4	39.6	39.6	39.8	39.8

Table S5. 42 Barrier Heights Calculated by BB95and B1B95 (QCISD/MG3 geometries) for the BH42/03 Database

Reaction	BB95/DIDZ		BB95/MG3S		B1B95/DIDZ		B1B95/MG3S	
A + BC → AB + C	$V_f^{\neq}$	$Vr^{\neq}$	$V_f^{\neq}$	$Vr^{\neq}$	$V_f^{\neq}$	$Vr^{\neq}$	$V_f^{\neq}$	$Vr^{\neq}$
1. H + HCl → H_2 + Cl	-1.3	1.2	0.4	-1.4	1.5	5.8	3.2	4.1
2. OH + H_2 → H + H_2O	-3.9	12.2	-4.5	13.6	2.6	16.7	2.0	17.9
3. CH_3 + H_2 → H + CH_4	5.7	9.8	5.8	10.3	8.6	13.0	8.6	13.3
4. OH + CH_4 → CH_3 + H_2O	-3.9	8.1	-4.1	9.5	3.8	13.5	3.5	14.7
5. H + H_2 → H_2 + H	5.1	5.1	5.4	5.4	7.4	7.4	7.6	7.6
6. OH + NH_3 → H_2O + NH_2	-11.2	-1.4	-10.5	0.4	-0.7	7.4	-0.2	8.9
7. HCl + CH_3 → Cl + CH_4	-6.0	0.6	-4.6	-1.8	-2.4	6.2	-1.1	4.6
8. OH + C_2H_6 →H_2O + C_2H_5	-7.5	10.0	-7.6	11.6	0.8	15.2	0.5	16.5
9. F + H_2 → HF + H	-12.1	21.7	-12.1	24.0	-3.5	26.0	-3.5	28.0
10. O + CH_4 →OH + CH_3	2.3	-2.1	2.2	-0.6	10.8	2.6	10.6	3.9
11. H + PH_3→ PH_2 + H_2	-1.6	21.1	-0.8	20.5	1.1	23.1	1.7	22.4
12. H + ClH′ → HCl + H′	12.2	12.2	12.3	12.3	16.8	16.8	16.3	16.3
13. H + HO → H_2 +O	1.8	2.1	3.3	1.5	5.9	9.7	7.1	9.0
14. H + *trans*-N_2H_2→ H_2 + N_2H	-5.3	35.0	-4.9	35.3	-0.4	38.5	-0.2	38.8
15. H + H_2S → H_2 + HS	-1.1	13.6	-0.1	12.1	1.7	16.4	2.5	14.8
16. O + HCl → OH + Cl	-10.6	-8.3	-9.4	-9.4	4.6	5.1	5.1	4.1
17. NH_2 + CH_3→ CH_4 + NH	-0.5	13.9	0.9	13.7	4.1	20.1	5.3	19.7
18. NH_2 + C_2H_5 → C_2H_6 + NH	2.0	10.8	3.6	10.7	6.1	17.4	7.5	17.0
19. C_2H_6 + NH_2 → NH_3 + C_2H_5	2.7	10.5	3.2	11.5	8.7	15.2	9.1	16.0
20. NH_2 + CH_4 → CH_3 + NH_3	5.7	7.9	6.1	8.8	11.4	13.0	11.7	13.8
21. *s-trans cis*-C_5H_8 → *s-trans cis*-C_5H_8	32.3	32.3	32.6	32.6	37.1	37.1	37.3	37.3

Table S6. Experimental Data for G45/04 database

Molecules	Geometirc Parameter	Experimental Data
H2	R_{H-H}	0.741
CH4	R_{C-H}	1.094
NH3	R_{N-H}	1.012
	θ_{HNH}	106.67
H2O	R_{O-H}	0.956
	θ_{HOH}	105.2
HF	R_{H-F}	0.917
CO	R_{C-O}	1.128
N2	R_{N-N}	1.098
F2	R_{F-F}	1.412
C2H2	R_{C-C}	1.203
	R_{C-H}	1.063
HCN	R_{C-H}	1.064
	R_{C-N}	1.156
H2CO	R_{C-H}	1.111
	R_{C-O}	1.205
	θ_{HCH}	116.1
	θ_{HCO}	121.9
CO2	R_{C-O}	1.162
N2O	R_{N-N}	1.128
	R_{N-O}	1.184
SiH4	R_{Si-H}	1.480
SiO	R_{Si-O}	1.510
H2S	R_{S-H}	1.328
	θ_{HSH}	92.2
S2	R_{S-S}	1.889
C3H4	R_{C-H}	1.105
	R_{C-H}	1.056
	R_{C-C}	1.459
	R_{C-C}	1.206
	θ_{HCH}	110.2
	θ_{HCC}	108.73
C2H2O2	R_{C-C}	1.526
	R_{C-O}	1.212
	R_{C-H}	1.132
	θ_{CCO}	121.2

	θ_{HCC}	112.2
C4H8	R_{C-C}	1.555
	R_{C-H}	1.093
	R_{C-H}	1.091
	θ_{HCH}	106.4
OH	R_{O-H}	0.970
SH	R_{S-H}	1.341
CH3	R_{C-H}	1.079
	θ_{HCH}	120.0