Supporting Information for:

Doubly Hybrid DFT: New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics

Yan Zhao, Benjamin J. Lynch, and Donald G. Truhlar

To be published in *J. Phys. Chem. A*

This supporting information was prepared on March 26, 2004 and consists of a total of 7 pages.

Contents: *page*

S1. AE109/3 Database: Zero-Point-Exclusive Atomization Energies 2

S2. BH42/03 Database 4

S3. SPG15/01 Database 5

S4. Geometric Parameters of the Saddle Points - I 6

S5. Geometric Parameters of the Saddle Points - II 7

Table S1. AE109/3 Database Zero-Point-Exclusive Atomization Energies (kcal/mol)

Molecule	D_e	Molecule	D_e	Molecule	D_e
CH (^{2})	84.00	S_2	101.67	H_2CCH	445.79
CH_2 ($^3B_1$)	190.97	Cl_2	57.97	$HCOOCH_3$	785.26
CH_2 ($^1A_1$)	181.50	SiO	192.08	HCOOH	500.98
CH_3 ($^2A''_2$)	307.46	SC	171.31	NF_3	204.53
CH_4	420.11	SO	125.00	PF_3	363.87
NH	83.67	ClO	64.49	SH	86.98
NH_2	181.90	ClF	61.36	$SiCl_4$	384.94
NH_3	297.90	Si_2H_6	530.81	SiF_4	574.35
OH	107.06	CH_3Cl	394.64	C_2H_5	603.75
OH_2	232.60	CH_3SH	473.84	C_4H_6 [d]	987.2
FH	141.05	HOCl	164.36	C_4H_6 [e]	1001.61
SiH_2 ($^1A_1$)	151.79	SO_2	257.86	HCOCOH	633.35
SiH_2 ($^3B_1$)	131.05	$AlCl_3$	306.26	CH_3CHO	677.03
SiH_3	227.37	AlF_3	426.50	C_2H_4O	650.70
SiH_4	322.40	BCl_3	322.90	C_2H_5O	698.64
PH_2	153.20	BF_3	470.04	H_3COCH_3	798.05
PH_3	242.55	C_2Cl_4	466.28	H_3CCH_2OH	810.36
SH_2	182.74	C_2F_4	583.96	C_3H_4 [f]	703.20
ClH	106.50	C_3H_4 [a]	704.79	C_3H_4 [g]	682.74
HCCH	405.39	C_4H_4O	993.74	H_3CCOOH	803.04
H_2CCH_2	563.47	C_4H_4S	962.73	H_3CCOCH_3	977.96
H_3CCH_3	712.80	C_4H_5N	1071.57	C_3H_6	853.41
CN	180.58	C_4H_6 [b]	1012.37	H_3CCHCH_2	860.61
HCN	313.20	C_4H_6 [c]	1004.13	C_3H_8	1006.87
CO	259.31	C_5H_5N	1237.69	$C_2H_5OCH_3$	1095.12
HCO	278.39	CCH	267.83	C_4H_{10} [h]	1303.04
H_2CO	373.73	CCl_4	312.74	C_4H_{10} [i]	1301.32

H_3COH	512.78	CF_3CN	639.85	C_4H_8 [j]	1149.01
N_2	228.46	CF_4	476.32	C_4H_8 [k]	1158.61
H_2NNH_2	438.60	CH_2OH	409.76	C_5H_8 [l]	1284.28
NO	155.22	CH_3CN	615.84	C_6H_6	1367.56
O_2	119.99	CH_3NH_2	582.56	CH_3CO	581.58
HOOH	268.57	CH_3NO_2	601.27	$(CH_3)_2CH$	900.75
F_2	38.20	$CHCl_3$	343.18	$(CH_3)_3C$	1199.34
CO_2	389.14	CHF_3	457.50	H_2CCO	532.73
Si_2	74.97	ClF_3	125.33		
P_2	117.09	H_2	109.48		

[a] propyne

[b] *trans*-1,3-butadiene

[c] 2-butyne

[d] bicylobutane

[e] cyclobutene

[f] allene

[g] cyclopropene

[h] cyclobutane

[i] isobutane

[j] *trans*-2-butene

[k] isobutene

[l] spiropentane

Table S2. BH42/03 Database

Reaction	best estimate	
A + BC → AB + C	$V_f^{\neq}$	$V_r^{\neq}$
1. H + HCl → H_2 + Cl	5.7	8.7
2. OH + H_2 → H + H_2O	5.1	21.2
3. CH_3 + H_2 → H + CH_4	12.1	15.3
4. OH + CH_4 → CH_3 + H_2O	6.7	19.6
5. H + H_2 → H_2 + H	9.6	9.6
6. OH + NH_3 → H_2O + NH_2	3.2	12.7
7. HCl + CH_3 → Cl + CH_4	1.7	7.9
8. OH + C_2H_6 →H_2O + C_2H_5	3.4	19.9
9. F + H_2 → HF + H	1.8	33.4
10. O + CH_4 →OH + CH_3	13.7	8.1
11. H + PH_3→ PH_2 + H_2	3.1	23.2
12. H + ClH′ → HCl + H′	18.0	18.0
13. H + HO → H_2 +O	10.7	13.1
14. H + *trans*-N_2H_2→ H_2 + N_2H	5.9	40.9
15. H + H_2S → H_2 + HS	3.5	17.3
16. O + HCl → OH + Cl	9.8	10.4
17. NH_2 + CH_3→ CH_4 + NH	8.0	22.4
18. NH_2 + C_2H_5 → C_2H_6 + NH	7.5	18.3
19. C_2H_6 + NH_2 → NH_3 + C_2H_5	10.4	17.4
20. NH_2 + CH_4 → CH_3 + NH_3	14.5	17.8
21. *s-trans cis*-C_5H_8 → *s-trans cis*-C_5H_8	38.4	38.4

Table S3. SPG15/01 Database

Reaction	Best Estimate				
A + BC → AB + C	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	Ref.
H + HCl → H_2 + Cl	0.981	1.431	2.412	180	1
H + H_2 → H_2 + H	0.930	0.930	1.860	180	2
H + ClH' → HCl + H'	1.480	1.480	2.960	180	1
H + HO → H_2 +O	0.894	1.215	2.109	180	3
F + H_2 → HF + H	1.546	0.771	2.317	119	4

(1) Bian, W.; Werner, H.-J. *J. Chem. Phys.* **2000**, *112*, 220.
(2) Diedrich, D. L.; Anderson, J. B. *J. Chem. Phys.* **1994**, *100*, 8089.
(3) Peterson, K. A.; Dunning, T. H. *J. Phys. Chem. A* **1997**, *101*, 6280.
(4) Stark, R.; Werner, H.-J. *J. Chem. Phys.* **1996**, *104*, 6515.

Table S4. Geometric Parameters of the Saddle Points - I

Reaction	MC3BB				MC3MPW			
A + BC → AB + C	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$
H + HCl → H_2 + Cl	1.002	1.412	2.414	180	0.977	1.423	2.400	180
H + H_2 → H_2 + H	0.923	0.923	1.846	180	0.921	0.921	1.842	180
H + ClH' → HCl + H'	1.471	1.471	2.942	180	1.469	1.469	2.939	180
H + HO → H_2 +O	0.885	1.207	2.092	180	0.870	1.225	2.095	180
F + H_2 → HF + H	1.554	0.767	2.321	116	1.529	0.769	2.298	117

Table S5. Geometric Parameters of the Saddle Points - II

Reaction	MCG3/3				MC-QCISD/3				SAC-MP2/DIDZ			
A + BC → AB + C	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$	$R^{\neq}_{AB}$	$R^{\neq}_{BC}$	$R^{\neq}_{sum}$	$\theta^{\neq}_{ABC}$
H + HCl → H_2 + Cl	1.001	1.427	2.428	180	0.988	1.42	2.420	180	0.926	1.448	2.375	180
H + H_2 → H_2 + H	0.931	0.931	1.862	180	0.931	0.931	1.861	180	0.913	0.913	1.826	180
H + ClH' → HCl + H'	1.489	1.489	2.979	180	1.485	1.485	2.969	180	1.468	1.468	2.936	180
H + HO → H_2 + O	0.885	1.224	2.108	180	0.879	1.230	2.109	180	0.855	1.226	2.081	180
F + H_2 → HF + H	1.546	0.771	2.317	125	1.501	0.777	2.278	125	1.437	0.772	2.209	120