Supporting Information for:

Multi-Coefficient Extrapolated Density Functional Theory for Thermochemistry and Thermochemical Kinetics

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Table S1: MGAE109/04 Database of Zero-Point-Exclusive Atomization Energies (kcal/mol)

Molecule	D_e	Molecule	D_e	Molecule	D_e
CH ($^2\Pi$)	83.94	S_2	101.67	H_2CCH	445.79
CH_2 ($^3B_1$)	190.97	Cl_2	57.98	$HCOOCH_3$	785.26
CH_2 ($^1A_1$)	181.51	SiO	192.08	HCOOH	500.98
CH_3 ($^2A"_2$)	307.44	SC	171.11	NF_3	204.53
CH_4	420.11	SO	125.22	PF_3	363.87
NH	83.67	ClO	64.49	SH	86.98
NH_2	181.90	ClF	61.48	$SiCl_4$	384.94
NH_3	297.90	Si_2H_6	534.66	SiF_4	574.35
OH	107.09	CH_3Cl	395.51	C_2H_5	603.75
OH_2	232.60	CH_3SH	473.84	C_4H_6 *d*	987.20
FH	141.18	HOCl	164.81	C_4H_6 *e*	1001.61
SiH_2 ($^1A_1$)	151.79	SO_2	258.62	HCOCOH	633.35
SiH_2 ($^3B_1$)	131.05	$AlCl_3$	306.26	CH_3CHO	677.03
SiH_3	227.58	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	241.56	C_2Cl_4	466.28	H_3CCH_2OH	810.36
SH_2	182.60	C_2F_4	589.36	C_3H_4 *f*	703.20
ClH	106.48	C_3H_4 *a*	704.79	C_3H_4 *g*	682.74
HCCH	405.36	C_4H_4O	993.74	H_3CCOOH	803.04
H_2CCH_2	563.51	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	313.05	C_4H_6 *c*	1004.13	C_3H_8	1006.87
CO	259.27	C_5H_5N	1237.69	$C_2H_5OCH_3$	1095.12
HCO	278.39	CCH	265.19	C_4H_{10} *h*	1303.04
H_2CO	373.82	CCl_4	312.74	C_4H_{10} *i*	1301.32
H_3COH	513.22	CF_3CN	639.85	C_4H_8 *j*	1149.01

N_2	228.42	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	152.54	CH_3CN	615.84	C_6H_6	1367.56
O_2	120.22	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	532.32
Si_2	75.72	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: HTBH38/04 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 + HO → H_2 +O	10.7	13.1
13. H + H_2S → H_2 + HS	3.5	17.3
14. O + HCl → OH + Cl	9.8	10.4
15. NH_2 + CH_3→ CH_4 + NH	8.0	22.4
16. NH_2 + C_2H_5 → C_2H_6 + NH	7.5	18.3
17. C_2H_6 + NH_2 → NH_3 + C_2H_5	10.4	17.4
18. NH_2 + CH_4 → CH_3 + NH_3	14.5	17.8
19. *s-trans cis*-C_5H_8 → *s-trans cis*-C_5H_8	38.4	38.4

Table S3: Zero-point-exclusive Ionization Potentials (IP13/3) and Electron Affinities (EA13/3) Databases (kcal/mol)

	IP	EA
C	259.7	29.1
S	238.9	47.9
SH	238.9	53.3
Cl	299.1	83.4
Cl_2	265.3	55.6
OH	299.1	42.1
O	313.9	33.7
O_2	278.9	10.8
P	241.9	17.2
PH	234.1	23.2
PH_2	226.3	29.4
S_2	216.0	38.5
Si	187.9	31.9