Supporting Information for:

The 6-31B Basis Set and the BMC-QCISD and BMC-CCSD Multi-Coefficient Correlation Methods

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

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Table S1. Experimental Ionization Potentials and Electron Affinities (kcal/mol)

System	IP	EA	System	IP	EA
H		17.4[a]	NH_3	233.2	
Li	124.3	14.3	CN	313.7	89.0
Be	215.0		MgH		23.7
B	191.4	6.5	CF	209.4	
C	259.7	29.1	SiH	181.8	29.3
N	335.2		O_2	278.9	10.8
O	313.9	33.7	HNO		6.8
F	401.8	78.4	PH	234.1	23.2
BeH		15.5	FO	294.7	51.9
Na	118.5	12.6	SH	238.9	53.3
Mg	176.3		PH_2	226.3	29.4
Al	138.0	10.0	NaLi	116.8	
Si	187.9	31.9	NaF		11.9
P	241.9	17.2	LiCl		13.5
S	238.9	47.9	AlO	218.4	60.0
Cl	299.1	83.4	Na_2	112.7	9.8
CH		28.2	PO	193.5	25.2
CH_2		14.0	O_3	288.9	47.5
NH		8.4	Al_2	138.3	
CH_3	226.0		MgCl	176.8	36.4
OH	299.1	42.1	S_2	216.0	38.5
HF	369.7		Cl_2	265.3	55.6
AlF	224.2		Al_3		44.2

[a] This electron affinity is in Database/4MH but not in Database/4

Table S2. Best Estimate of Atomization Energies (kcal/mol)

Molecule	D_e	Molecule	D_e	Molecule	D_e
H_2	109.48	H_3CCH_3	712.80	Si_2	74.97
LiH	57.95	H_3COH	512.78	NaCl	97.79
BeH	49.94	H_2NNH_2	438.60	MgS	54.43
Li_2	24.36	HOOH	268.57	MgCl	74.46
$CH(^2P)$	84.00	F_2	38.20	P_2	117.09
BeLi	6.69	CH_3NH_2	582.56	C_4H_6[d]	1012.37
$CH_2(^3B_1)$	190.72	LiCl	113.90	C_4H_6[e]	1004.13
$CH_2(^1A_1)$	181.37	NaF	114.00	C_4H_6[f]	987.20
NH	83.67	NaOH	187.77	C_4H_6 [g]	1001.61
BH_3	281.08	MgO	59.19	$C_2H_2O_2$[h]	633.35
CH_3 ($^2A"_2$)	307.46	PC	124.63	PO_2	263.29
NH_2	181.90	AlO	122.31	S_2	101.67
OH	107.06	BeCl	90.20	SO_2	257.86
CH_4	420.11	MgF	110.86	BF_3	470.04
NH_3	297.90	MgOH	184.35	CH_3NO_2	601.27
H_2O	232.60	CO_2	389.14	$HCOOCH_3$	785.26
HF	141.05	SiO	192.08	H_3CCOOH	803.04
B_2	67.14	SC	171.31	H_3CCOCH_3	977.96
LiO	82.00	C_3H_4[a]	704.79	C_4H_8[i]	1149.01
BC	100.00	C_3H_4[b]	703.20	C_4H_8 [j]	1158.61
NaH	48.77	C_3H_4[c]	682.74	ClNO	192.04
LiF	138.92	CH_3CN	615.84	CH_3CONH_2	868.38
LiOH	211.68	H_2CCO	532.32	$(CH_3)_3C$	1199.34
BeO	104.77	N_2O	270.22	Cl_2	57.97
CN	180.58	HCP	250.50	Si_2H_6	530.81
CCH	267.83	Na_2	17.03	CHF_3	457.50
MgH	30.90	AlF	161.30	NF_3	204.53

BeF	137.84	NaLiO	145.00	$C_2H_5OCH_3$	1095.12
BeOH	216.86	BeF_2	305.22	C_4H_{10}[k]	1303.04
BO	193.12	Be(OH)2	464.08	C_4H_{10}[l]	1301.32
HCCH	405.39	CH_3CO	581.58	C_4H_4O	993.74
HCN	313.20	NO2	228.25	C_4H_5N	1071.57
CO	259.31	PO	141.55	C_5H_8[m]	1284.28
N2	228.46	SO(3)	125.00	AlF_3	426.50
AlH	70.22	HCOOH	500.98	$ClNO_2$	262.60
BF	182.10	CH_3CHO	677.03	C_5H_5N	1237.69
HCO	278.39	C_2H_4O	650.70	CF_4	476.32
NO	155.22	C_3H_6	853.41	PF_3	363.87
H_2CCH	445.79	H_3CCHCH_2	860.61	C_6H_6	1367.56
SiH_2 ($^1A_1$)	151.79	$(C_2H_4)NH$	718.81	C_4H_4S	962.73
SiH_2 ($^3B_1$)	131.05	O_3	146.10	ClF_3	125.33
H_2CCH_2	563.47	NaCN	280.00	CF_3CN	639.85
H_2CO	373.73	ClO	64.49	C_2F_4	589.36
O_2	119.99	C_2H_5O	698.64	$BFCl_2$	371.21
SiH_3	227.37	$(CH_3)_2CH$	900.75	SiF_4	574.35
PH_2	153.20	ClF	61.36	BCl_3	322.90
CH_2OH	409.76	CH_3Cl	394.64	$CHCl_3$	343.18
SH	86.98	CH_3SH	473.84	$AlCl_3$	306.26
C_2H_5	603.75	HOCl	164.36	SF_6	477.96
FO	53.40	H_3COCH3	798.05	CCl_4	312.74
SiH_4	322.40	H_3CCH_2OH	810.36	C_2Cl_4	466.28
PH_3	242.55	C_3H_8	1006.87	$SiCl_4$	384.94
H_2S	182.74	NCCN	500.89		
HCl	106.51	Al_2	31.10		

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[a] propyne
[b] Allene
[c] cyclopropene
[d] *trans*-butadiene
[e] 2- butyne
[f] bicyclobutane
[g] cyclobutene
[h] glyoxal
[i] cyclobutane
[j] isobutene
[k] isobutane
[l] *n*-butane
[m] spiropentane

Table S3. Barrier Heights (kcal/mol)

Reaction	$V_f^{\ddagger}$	$V_r^{\ddagger}$
1. $Cl + H_2 \rightarrow HCl + H$	8.7	5.6
2. $OH + H_2 \rightarrow H + H_2O$	5.7	22.0
3. $CH_3 + H_2 \rightarrow H + CH_4$	11.4	14.6
4. $OH + CH_4 \rightarrow CH_3 + H_2O$	6.7	20.2
6. $H + H_2 \rightarrow H_2 + H$	9.6	9.6
7. $OH + NH_3 \rightarrow H_2O + NH_2$	3.2	13.2
8. $HCl + CH_3 \rightarrow Cl + CH_4$	1.8	7.8
9. $OH + C_2H_6 \rightarrow H_2O + C_2H_5$	3.4	20.7
10. $F + H_2 \rightarrow H + HF$	1.8	33.2
11. $OH + CH_3 \rightarrow O + CH_4$	7.8	13.7
12. $H + PH_3 \rightarrow PH_2 + H_2$	3.2	25.5
13. H + ClH´ → HC1 + H´	18.0	18.0
14. $OH + H \rightarrow H_2 + O$	10.1	13.1
15. H + *trans*-$N_2H_2 \rightarrow H_2 + N_2H$	5.9	41.0
16. $H + H_2S \rightarrow H_2 + HS$	3.6	17.4
17. $O + HCl \rightarrow OH + Cl$	9.8	9.9
18. $CH_4 + NH \rightarrow NH_2 + CH_3$	8.4	22.7
19. $C_2H_6 + NH \rightarrow NH_2 + C_2H_5$	8.0	18.4
20. $C_2H_6 + NH_2 \rightarrow C_2H_5 + NH_3$	10.4	17.8
21. $NH_2 + CH_4 \rightarrow CH_3 + NH_3$	14.5	17.9
22. *s-trans cis*-$C_5H_8 \rightarrow$ *s-trans cis*-C_5H_8	38.4	38.4