

Supporting Information for:

W1X-1 and W1X-2: W1-Quality Accuracy With an Order Of Magnitude Reduction in Computational Cost

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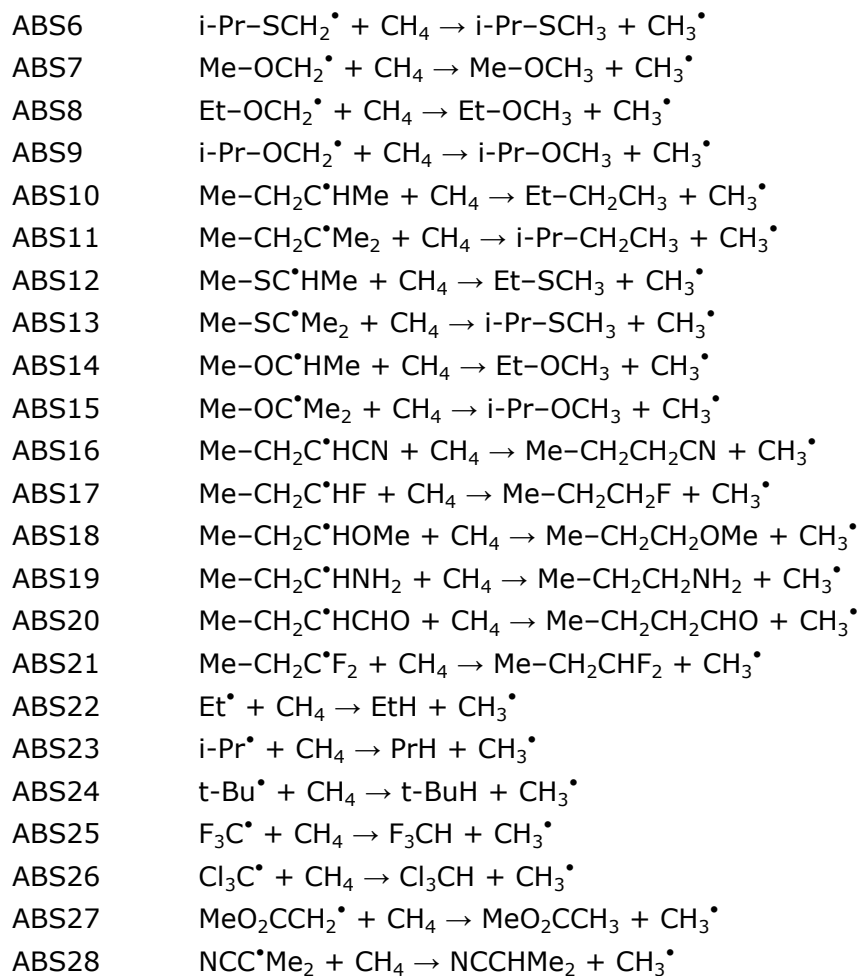
Table S3. Deviations from Benchmark Values (kJ mol^{-1})

Table S1. Reactions in the DBH24, RR49 and PR8 Sets**DBH24**

DBH24-1	$\text{H} + \text{N}_2\text{O} \rightarrow \text{OH} + \text{N}_2$
DBH24-2	$\text{H} + \text{ClH} \rightarrow \text{HCl} + \text{H}$
DBH24-3	$\text{CH}_3 + \text{FCl} \rightarrow \text{CH}_3\text{F} + \text{Cl}$
DBH24-4	$\text{Cl}\cdot\text{CH}_3\text{Cl}^- \rightarrow \text{ClCH}_3\cdot\text{Cl}^-$
DBH24-5	$\text{F}\cdot\text{CH}_3\text{Cl}^- \rightarrow \text{FCH}_3\cdot\text{Cl}^-$
DBH24-6	$\text{OH}^- + \text{CH}_3\text{F} \rightarrow \text{HOCH}_3 + \text{F}^-$
DBH24-7	$\text{H} + \text{N}_2 \rightarrow \text{HN}_2$
DBH24-8	$\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_5$
DBH24-9	$\text{HCN} \rightarrow \text{HNC}$
DBH24-10	$\text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O}$
DBH24-11	$\text{H} + \text{OH} \rightarrow \text{O} + \text{H}_2$
DBH24-12	$\text{H} + \text{H}_2\text{S} \rightarrow \text{H}_2 + \text{HS}$

RR49

ADD1	$\text{Me}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{Me}-\text{CH}_2\text{CH}_2\cdot$
ADD2	$\text{Et}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{Et}-\text{CH}_2\text{CH}_2\cdot$
ADD3	$i\text{-Pr}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow i\text{-Pr}-\text{CH}_2\text{CH}_2\cdot$
ADD4	$\text{Me}\cdot + \text{S}=\text{CH}_2 \rightarrow \text{Me}-\text{SCH}_2\cdot$
ADD5	$\text{Et}\cdot + \text{S}=\text{CH}_2 \rightarrow \text{Et}-\text{SCH}_2\cdot$
ADD6	$i\text{-Pr}\cdot + \text{S}=\text{CH}_2 \rightarrow i\text{-Pr}-\text{SCH}_2\cdot$
ADD7	$\text{Me}\cdot + \text{O}=\text{CH}_2 \rightarrow \text{Me}-\text{OCH}_2\cdot$
ADD8	$\text{Et}\cdot + \text{O}=\text{CH}_2 \rightarrow \text{Et}-\text{OCH}_2\cdot$
ADD9	$i\text{-Pr}\cdot + \text{O}=\text{CH}_2 \rightarrow i\text{-Pr}-\text{OCH}_2\cdot$
ADD10	$\text{Me}\cdot + \text{CH}_2=\text{CHMe} \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HMe}$
ADD11	$\text{Me}\cdot + \text{CH}_2=\text{CMe}_2 \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{Me}_2$
ADD12	$\text{Me}\cdot + \text{S}=\text{CHMe} \rightarrow \text{Me}-\text{SC}\cdot\text{HMe}$
ADD13	$\text{Me}\cdot + \text{S}=\text{CMe}_2 \rightarrow \text{Me}-\text{SC}\cdot\text{Me}_2$
ADD14	$\text{Me}\cdot + \text{O}=\text{CHMe} \rightarrow \text{Me}-\text{OC}\cdot\text{HMe}$
ADD15	$\text{Me}\cdot + \text{O}=\text{CMe}_2 \rightarrow \text{Me}-\text{OC}\cdot\text{Me}_2$
ADD16	$\text{Me}\cdot + \text{CH}_2=\text{CHCN} \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HCN}$
ADD17	$\text{Me}\cdot + \text{CH}_2=\text{CHF} \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HF}$
ADD18	$\text{Me}\cdot + \text{CH}_2=\text{CHOMe} \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HOMe}$
ADD19	$\text{Me}\cdot + \text{CH}_2=\text{CHNH}_2 \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HNNH}_2$
ADD20	$\text{Me}\cdot + \text{CH}_2=\text{CHCHO} \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{HCHO}$
ADD21	$\text{Me}\cdot + \text{CH}_2=\text{CF}_2 \rightarrow \text{Me}-\text{CH}_2\text{C}\cdot\text{F}_2$
ABS1	$\text{Me}-\text{CH}_2\text{CH}_2\cdot + \text{CH}_4 \rightarrow \text{Me}-\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot$
ABS2	$\text{Et}-\text{CH}_2\text{CH}_2\cdot + \text{CH}_4 \rightarrow \text{Et}-\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot$
ABS3	$i\text{-Pr}-\text{CH}_2\text{CH}_2\cdot + \text{CH}_4 \rightarrow i\text{-Pr}-\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot$
ABS4	$\text{Me}-\text{SCH}_2\cdot + \text{CH}_4 \rightarrow \text{Me}-\text{SCH}_3 + \text{CH}_3\cdot$
ABS5	$\text{Et}-\text{SCH}_2\cdot + \text{CH}_4 \rightarrow \text{Et}-\text{SCH}_3 + \text{CH}_3\cdot$



PR10

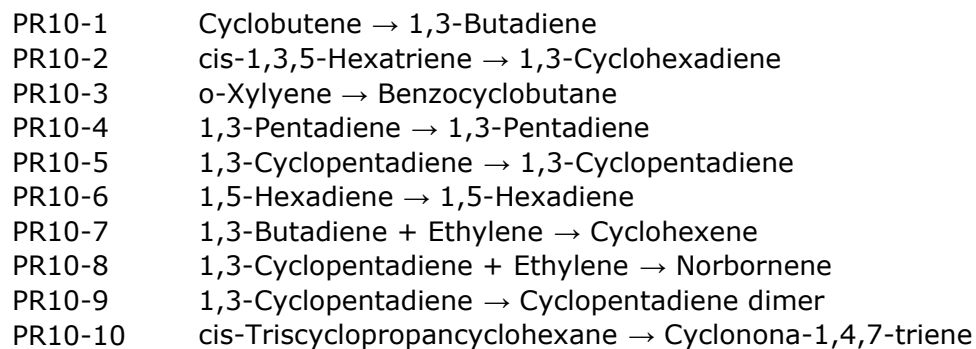


Table S2. Zero-Point Vibrational Energies (ZPVEs), Enthalpy Corrections at 298

Molecule	ZPVE	ΔH_{298}	W1w	W1-F12
atoms				
H (² S)	0.0	6.2	-0.49999	-0.49997
He (¹ S)	0.0	6.2	-2.90380	-2.90362
Li (² S)	0.0	6.2	-7.47205	-7.47224
Be (¹ S)	0.0	6.2	-14.66341	-14.66232
B (² P)	0.0	6.2	-24.65381	-24.65221
C (³ P)	0.0	6.2	-37.85304	-37.85072
N (⁴ S)	0.0	6.2	-54.61121	-54.60834
O (³ P)	0.0	6.2	-75.11168	-75.10843
F (² P)	0.0	6.2	-99.81216	-99.80887
Ne (¹ S)	0.0	6.2	-129.00494	-129.06088
Na (² S)	0.0	6.2	-162.05739	-162.34135
Mg (¹ S)	0.0	6.2	-199.93945	-200.22147
Al (² P)	0.0	6.2	-242.64419	-242.65024
Si (³ P)	0.0	6.2	-289.83393	-289.82996
P (⁴ S)	0.0	6.2	-341.94945	-341.93782
S (³ P)	0.0	6.2	-399.06685	-399.05204
Cl (² P)	0.0	6.2	-461.43609	-461.41715
Ar (¹ S)	0.0	6.2	-528.64782	-529.20487
atomic cations				
He ⁺ (² S)	0.0	6.2	-2.00021	-2.00002
Li ⁺ (¹ S)	0.0	6.2	-7.27410	-7.27440
Be ⁺ (² S)	0.0	6.2	-14.32084	-14.32017
B ⁺ (¹ S)	0.0	6.2	-24.34955	-24.34778
C ⁺ (² P)	0.0	6.2	-37.43966	-37.43728
N ⁺ (³ P)	0.0	6.2	-54.07731	-54.07438
O ⁺ (⁴ S)	0.0	6.2	-74.61190	-74.60829
F ⁺ (³ P)	0.0	6.2	-99.17224	-99.16873
Ne ⁺ (² P)	0.0	6.2	-128.21255	-128.26865
Na ⁺ (¹ S)	0.0	6.2	-162.18025	-162.15719
Mg ⁺ (² S)	0.0	6.2	-199.96847	-199.94431
Al ⁺ (¹ S)	0.0	6.2	-242.42510	-242.43078
Si ⁺ (² P)	0.0	6.2	-289.53523	-289.53072
P ⁺ (³ P)	0.0	6.2	-341.56465	-341.55236
S ⁺ (⁴ S)	0.0	6.2	-398.68652	-398.67170
Cl ⁺ (³ P)	0.0	6.2	-460.95975	-460.94159
Ar ⁺ (² P)	0.0	6.2	-528.06887	-528.62729
atomic anions				
Li ⁻ (¹ S)	0.0	6.2	-7.49478	-7.49489
B ⁻ (³ P)	0.0	6.2	-24.66331	-24.66075

C ⁻ (⁴ S)	0.0	6.2	-37.89904	-37.89594
O ⁻ (² P)	0.0	6.2	-75.16481	-75.16093
F ⁻ (¹ S)	0.0	6.2	-99.93746	-99.93359
Na ⁻ (¹ S)	0.0	6.2	-162.38873	-162.36642
Al ⁻ (³ P)	0.0	6.2	-242.65937	-242.66520
Si ⁻ (⁴ S)	0.0	6.2	-289.88459	-289.88057
P ⁻ (³ P)	0.0	6.2	-341.97648	-341.96387
S ⁻ (² P)	0.0	6.2	-399.14331	-399.12709
Cl ⁻ (¹ S)	0.0	6.2	-461.56943	-461.54859

W4/08

B ₂ H ₆	164.7	11.9	-53.27513	-53.26989
BHF ₂	47.2	10.7	-225.43265	-225.42227
BF ₃	32.8	11.7	-324.83995	-324.82563
C ₂ H ₆	192.9	11.6	-79.84247	-79.83591
H ₂ CN	65.6	10.2	-94.01122	-94.00521
NCCN	43.5	12.3	-185.72688	-185.71556
CH ₂ NH ₂	130.0	11.6	-95.23276	-95.22587
CH ₃ NH	126.9	11.5	-95.22039	-95.21381
CH ₃ NH ₂	165.9	11.6	-95.89238	-95.88525
CF ₂	18.8	10.3	-237.88846	-237.87850
N ₂ H	35.4	10.0	-110.07997	-110.07358
N ₂ H ₂	74.5	10.0	-110.69462	-110.68786
N ₂ H ₄	139.8	11.1	-111.92119	-111.91342
FO ₂	16.1	10.9	-250.24449	-250.23421
F ₂ O ₂	24.7	12.7	-350.08621	-350.07253
AlF ₃	20.2	14.3	-542.76224	-542.75569
Si ₂ H ₆	133.8	15.7	-583.51885	-583.50879
P ₄	15.2	14.7	-1368.25806	-1368.21114
SO ₂	18.7	10.5	-549.70030	-549.67872
SO ₃	33.2	11.7	-624.94739	-624.92217
OCS	24.4	9.9	-512.56433	-512.54298
CS ₂	18.3	10.6	-836.42967	-836.39719
S ₂ O	13.6	11.2	-873.57193	-873.53854
S ₃	9.2	12.0	-1197.46170	-1197.41658
S ₄	14.8	15.4	-1596.63020	-1596.57027
BeCl ₂	12.2	12.2	-937.89177	-937.85092
CCl ₂	11.1	11.5	-961.00343	-960.96274
AlCl ₃	12.6	16.6	-1627.44554	-1627.39121
CICN	23.0	10.7	-554.35260	-554.32794
OCIO	14.8	10.8	-611.85787	-611.83303
CIOO	13.1	11.6	-611.85347	-611.82777
Cl ₂ O	10.5	11.6	-998.14134	-998.09980
H ₂	26.3	8.7	-1.17459	-1.17418
OH	22.3	8.7	-75.78229	-75.77841
HF	24.5	8.7	-100.53779	-100.53350

H ₂ O	56.2	9.9	-76.48307	-76.47840
CH	16.6	8.7	-38.48697	-38.48447
CH ₂	44.6	10.0	-39.15687	-39.15396
CH ₃	76.8	10.5	-39.84362	-39.84038
CH ₄	115.6	10.0	-40.52300	-40.51953
C ₂ H	42.8	9.0	-76.62941	-76.62380
C ₂ H ₂	70.3	9.8	-77.35200	-77.34609
NH ₃	89.4	10.0	-56.58637	-56.58224
C ₂	9.3	8.7	-75.93890	-75.93387
N ₂	14.1	8.7	-109.58573	-109.57958
CO	13.5	8.7	-113.37795	-113.37166
CN	12.8	8.7	-92.75157	-92.74627
NO	11.8	8.7	-129.96513	-129.95862
O ₂	10.3	8.7	-150.41429	-150.40737
OF	7.1	8.7	-175.00609	-174.99940
F ₂	6.4	8.8	-199.68441	-199.67775
PH ₃	64.4	10.1	-343.83483	-343.82197
HS	15.8	8.7	-399.70547	-399.69015
H ₂ S	39.1	10.0	-400.35849	-400.34268
HCl	17.7	8.7	-462.10589	-462.08621
SO	7.1	8.7	-474.37723	-474.35917
ClO	5.0	8.9	-536.64836	-536.62633
CIF	4.7	8.9	-561.34586	-561.32312
P ₂	4.4	8.9	-684.08395	-684.05993
S ₂	4.3	9.0	-798.29614	-798.26636
Cl ₂	3.6	9.1	-922.96361	-922.92537
Be ₂	1.4	10.0	-29.32989	-29.32796
B ₂	5.6	8.8	-49.41261	-49.40941
BH	14.0	8.7	-25.28925	-25.28734
BH ₃	69.0	10.1	-26.60225	-26.59970
BN singlet	10.5	8.7	-79.43324	-79.42879
BF	8.3	8.7	-124.75654	-124.75070
NH	19.9	8.7	-55.24354	-55.24038
NH ₂	49.9	9.9	-55.90215	-55.89859
HCN	42.5	9.2	-93.46309	-93.45715
HOF	37.3	10.0	-175.67527	-175.66785
AlH	10.8	8.7	-243.26106	-243.26674
AlH ₃	44.5	10.7	-244.48320	-244.48842
AlF	4.7	8.9	-342.71618	-342.71792
AlCl	2.8	9.3	-704.27391	-704.25970
SiH	11.5	8.7	-290.45078	-290.44649
SiH ₄	84.7	10.6	-292.35022	-292.34478
SiO	7.3	8.7	-365.25050	-365.24303
SiF	4.7	8.9	-389.87210	-389.86401
CS	7.6	8.7	-437.19169	-437.17442
BN triplet	9.7	8.7	-79.43237	-79.42779
CF	7.9	8.7	-137.87594	-137.86984

BeF ₂	18.5	10.9	-214.77976	-214.76989
CH ₂ C	60.9	11.2	-77.27896	-77.27342
CH ₂ CH	94.2	10.7	-77.91646	-77.91053
C ₂ H ₄	131.4	10.5	-78.60489	-78.59865
CH ₂ NH	103.8	10.2	-94.66432	-94.65786
HCO	34.2	10.0	-113.90916	-113.90276
H ₂ CO	69.4	10.0	-114.56113	-114.55437
CO ₂	31.3	9.3	-188.69702	-188.68679
HNO	37.3	9.9	-130.54997	-130.54309
NO ₂	23.0	10.2	-205.19511	-205.18479
N ₂ O	28.7	9.5	-184.76401	-184.75396
O ₃	20.8	10.2	-225.56442	-225.55419
HO ₂	38.0	10.0	-151.00154	-150.99422
H ₂ O ₂	70.6	10.9	-151.65147	-151.64344
F ₂ O	15.4	10.7	-274.88262	-274.87247
HOCl	34.9	10.2	-537.31054	-537.28739
S ₂ H	24.1	10.5	-798.89320	-798.86274

DBH24

H	0.0	6.2	-0.49999	-0.49997
N ₂ O	28.7	9.5	-184.76388	-184.75385
HCl	17.7	8.7	-462.10568	-462.08600
CH ₃	76.8	10.5	-39.84345	-39.84022
FCI	4.7	8.9	-561.34584	-561.32310
Cl•CH ₃ Cl	101.4	15.8	-963.00519	-962.96173
F•CH ₃ Cl	97.1	16.5	-601.38112	-601.35435
OH ⁻	22.7	8.7	-75.84940	-75.84493
CH ₃ F	101.9	10.1	-139.83872	-139.83151
N ₂	14.1	8.7	-109.58572	-109.57958
C ₂ H ₄	131.4	10.5	-78.60473	-78.59850
HCN	42.5	9.2	-93.46306	-93.45708
OH	22.3	8.7	-75.78229	-75.77841
CH ₄	115.6	10.0	-40.52279	-40.51934
H ₂ S	39.1	10.0	-400.35832	-400.34252
Cl	0.0	6.2	-461.43475	-461.41581
FCH ₃ •Cl	104.1	15.5	-601.42349	-601.39557
CH ₃ OH	133.1	11.4	-115.78270	-115.77516
F ⁻	0.0	6.2	-99.93746	-99.93359
HN ₂	35.4	10.0	-110.07986	-110.07348
CH ₃ CH ₂	153.1	12.9	-79.16840	-79.16211
HNC	42.1	9.6	-93.43913	-93.43295
H ₂ O	56.2	9.9	-76.48302	-76.47834
O	0.0	6.2	-75.11132	-75.10807
H ₂	26.3	8.7	-1.17459	-1.17418
HS	15.8	8.7	-399.70536	-399.69005
DBH24-1 TS	30.5	11.4	-185.23637	-185.22637
DBH24-2 TS	14.9	10.9	-462.57779	-462.55817

DBH24-3 TS	86.8	16.6	-601.17914	-601.15324
DBH24-4 TS	96.5	14.8	-962.98385	-962.94063
DBH24-5 TS	97.5	14.1	-601.37605	-601.34905
DBH24-6 TS	128.1	15.5	-215.69215	-215.68066
DBH24-7 TS	16.8	10.2	-110.06326	-110.05709
DBH24-8 TS	135.4	12.4	-79.10157	-79.09536
DBH24-9 TS	28.6	9.9	-93.38675	-93.38104
DBH24-10 TS	131.6	14.7	-116.29489	-116.28753
DBH24-11 TS	18.7	9.3	-76.26490	-76.26114
DBH24-12 TS	37.2	11.6	-400.85259	-400.83683

HB16

HCl	17.7	8.7	-462.10568	-462.08600
NH ₃	89.4	10.0	-56.58627	-56.58214
CO	13.5	8.7	-113.37798	-113.37166
HF	24.5	8.7	-100.53778	-100.53350
H ₂ O	56.2	9.9	-76.48302	-76.47834
HCN	42.5	9.2	-93.46306	-93.45708
H ₃ O ⁺	89.2	10.2	-76.75635	-76.75129
NH ₄ ⁺	128.9	10.0	-56.92403	-56.91954
HCC ⁻	38.4	9.5	-76.73878	-76.73302
CN ⁻	12.8	8.7	-92.89451	-92.88889
OH ⁻	22.7	8.7	-75.84940	-75.84493
ClH•NH ₃	115.1	14.8	-518.70508	-518.68109
CO•HF	42.2	17.3	-213.91853	-213.90791
FH•NH ₃	126.4	13.8	-157.14396	-157.13556
H ₂ O•H ₂ O	120.9	18.0	-152.97402	-152.96470
HCl•HCl	41.1	15.3	-924.21447	-924.17510
HF•H ₂ O	91.4	14.4	-177.03468	-177.02574
HF•HF	56.5	14.1	-201.08284	-201.07430
HF•HCN	75.0	15.5	-194.01278	-194.00246
NH ₃ •NH ₃	185.5	19.7	-113.17745	-113.16923
NH ₃ •H ₂ O	154.8	18.0	-133.07954	-133.07078
OC•HF	44.1	16.0	-213.92145	-213.91086
H ₃ O•H ₂ O ⁺	147.6	15.4	-153.29329	-153.28356
NH ₄ •H ₂ O ⁺	192.1	17.5	-133.43964	-133.43052
HCC•H ₂ O ⁻	100.3	17.1	-153.25099	-153.24068
CN•H ₂ O ⁻	76.0	16.0	-169.40245	-169.39222
OH•H ₂ O ⁻	82.5	13.7	-152.37538	-152.36664

WI9/04

He	0.0	6.2	-2.90380	-2.90362
Ne	0.0	6.2	-129.00494	-129.06088
Ar	0.0	6.2	-528.64782	-529.20487
CH ₄	115.6	10.0	-40.52279	-40.51934
C ₆ H ₆	259.5	14.3	-232.29976	-232.28279
C ₂ H ₂	70.3	9.8	-77.35197	-77.34604
C ₂ H ₄	131.4	10.5	-78.60473	-78.59850

He•Ne	0.3	10.9	-131.90878	-131.96454
He•Ar	0.1	11.0	-531.55162	-532.10850
Ne•Ne	0.1	11.0	-258.00989	-258.12177
Ne•Ar	0.2	11.0	-657.65281	-658.26580
CH ₄ •Ne	116.9	16.1	-169.52780	-169.58028
C ₆ H ₆ •Ne	259.5	21.5	-361.30483	-361.34378
CH ₄ •CH ₄	232.2	16.1	-81.04564	-81.03874
C ₂ H ₂ •C ₂ H ₂	142.6	20.3	-154.70631	-154.69453
C ₂ H ₄ •C ₂ H ₄	267.9	19.7	-157.21172	-157.19931

G2/09' neutrals

LiH	8.3	8.7	-8.06464	-8.06441
BeH	12.1	8.7	-15.24427	-15.24291
CH ₂ (¹ A ₁)	42.8	9.9	-39.14162	-39.13886
SiH ₂ (¹ A ₁)	30.0	10.0	-291.07822	-291.07357
SiH ₂ (³ B ₁)	30.9	10.1	-291.04435	-291.03978
SiH ₃	54.7	10.4	-291.69596	-291.69094
PH ₂	34.5	10.0	-343.19520	-343.18271
Li ₂	2.0	9.7	-14.98291	-14.98310
LiF	5.4	8.8	-107.50614	-107.50187
H ₃ COH	132.0	11.3	-115.78285	-115.77532
Na ₂	0.9	10.3	-324.76546	-324.71995
Si ₂	2.9	9.3	-579.78728	-579.77930
NaCl	2.1	9.6	-623.96116	-623.91690
CH ₃ Cl	97.3	10.5	-501.41871	-501.39600
H ₃ CSH	118.6	12.0	-439.67586	-439.65714
BCl ₃	19.4	14.1	-1409.47525	-1409.41517
CF ₄	43.6	12.9	-437.86283	-437.84451
CCl ₄	23.6	17.6	-1884.09331	-1884.01393
COF ₂	36.3	11.2	-313.25787	-313.24364
SiF ₄	32.3	15.6	-689.99862	-689.97822
SiCl ₄	18.5	19.7	-2136.19068	-2136.10737
CINO	16.9	11.3	-591.46083	-591.43491
NF ₃	26.4	11.9	-354.37359	-354.35991
PF ₃	21.8	13.1	-641.96607	-641.94195
ClF ₃	17.8	14.0	-761.07192	-761.04236
C ₂ F ₄	55.6	16.3	-475.89290	-475.87165
C ₂ Cl ₄	39.4	19.7	-1922.19658	-1922.11426
CF ₃ CN	58.3	16.0	-430.77467	-430.75476
CH ₃ CCH (propyne)	143.5	12.9	-116.68313	-116.67420
CH ₂ =C=CH ₂ (allene)	142.1	12.5	-116.68081	-116.67186
C ₃ H ₄ (cyclopropene)	144.4	11.3	-116.64571	-116.63693
CH ₃ CH=CH ₂ (propylene)	205.4	13.3	-117.93188	-117.92262
C ₃ H ₆ (cyclopropane)	209.7	11.4	-117.91998	-117.91091
C ₃ H ₈ (propane)	266.4	14.5	-119.16520	-119.15567
CH ₂ CHCHCH ₂ (butadiene)	219.7	14.8	-156.02647	-156.01457

C ₄ H ₆ (2-butyne)	216.9	17.6	-156.01275	-156.00082
C ₄ H ₆ (methylene cyclopropane)	219.5	13.8	-155.99506	-155.98338
C ₄ H ₆ (bicyclobutane)	222.7	12.4	-155.98411	-155.97257
C ₄ H ₆ (cyclobutene)	222.9	12.6	-156.00848	-155.99672
C ₄ H ₈ (cyclobutane)	285.6	13.5	-157.24558	-157.23353
C ₄ H ₈ (isobutene)	277.8	16.6	-157.26014	-157.24793
C ₄ H ₁₀ (trans butane)	339.9	17.9	-158.48806	-158.47556
C ₄ H ₁₀ (isobutane)	338.7	17.7	-158.49036	-158.47791
C ₅ H ₈ (spiro pentane)	296.5	15.5	-195.31382	-195.29931
C ₆ H ₆ (benzene)	259.6	14.1	-232.30033	-232.28327
CH ₂ F ₂	84.5	10.7	-239.17444	-239.16354
CHF ₃	65.0	11.6	-338.52063	-338.50605
CH ₂ Cl ₂	75.6	12.0	-962.31431	-962.27259
CHCl ₃	50.9	14.4	-1423.20679	-1423.14620
CH ₃ CN (methyl cyanide)	116.8	12.0	-132.79918	-132.79022
CH ₃ NO ₂ (nitromethane)	128.3	11.7	-245.14505	-245.13115
CH ₃ ONO (methyl nitrite)	124.6	14.2	-245.14060	-245.12703
CH ₃ SiH ₃ (methyl silane)	157.3	13.6	-331.68849	-331.68011
HCOOH (formic acid)	87.2	10.8	-189.87537	-189.86456
HCOOCH ₃ (methyl formate)	159.7	14.6	-229.18225	-229.16861
CH ₃ CONH ₂ (acetamide)	189.0	16.6	-209.31276	-209.29922
C ₂ H ₄ NH (aziridine)	181.1	11.1	-133.96527	-133.95588
(CH ₃) ₂ NH (dimethylamine)	237.8	14.2	-135.20462	-135.19460
CH ₃ CH ₂ NH ₂ (trans ethylamine)	238.8	14.2	-135.21790	-135.20778
CH ₂ CO (ketene)	81.5	11.8	-152.66700	-152.65744
C ₂ H ₄ O (oxirane)	147.9	10.8	-153.85550	-153.84580
CH ₃ CHO (acetaldehyde)	142.8	12.8	-153.89732	-153.88750
HCOCOH (glyoxal)	95.3	13.6	-227.94001	-227.92692
CH ₃ CH ₂ OH (ethanol)	206.0	13.9	-155.11040	-155.09983
CH ₃ OCH ₃ (dimethylether)	205.1	14.0	-155.09038	-155.08008
C ₂ H ₄ S (thiirane)	141.9	11.4	-477.76996	-477.74891
(CH ₃) ₂ SO (dimethyl sulfoxide)	204.2	17.4	-554.24847	-554.22347
C ₂ H ₅ SH (ethanethiol)	192.8	15.1	-478.99939	-478.97772
CH ₃ SCH ₃ (dimethyl sulfide)	194.7	15.5	-478.99751	-478.97585
CH ₂ =CHF (vinyl fluoride)	113.6	11.3	-177.93218	-177.92220
C ₂ H ₅ Cl (ethyl chloride)	171.6	13.2	-540.74481	-540.71914
CH ₂ =CHCl (vinyl chloride)	110.1	11.8	-539.50779	-539.48243
CH ₂ =CHCN (acrylonitrile)	131.1	13.4	-170.88529	-170.87367
CH ₃ COCH ₃ (acetone)	215.2	16.8	-193.23127	-193.21847
CH ₃ COOH (acetic acid)	159.2	14.6	-229.20971	-229.19588
CH ₃ COF (acetyl fluoride)	126.1	13.9	-253.25533	-253.24179
CH ₃ COCl (acetyl chloride)	121.8	14.8	-614.81786	-614.78877

CH ₃ CH ₂ CH ₂ Cl (propyl chloride)	245.0	16.7	-580.06773	-580.03910
(CH ₃) ₂ CHOH (isopropanol)	278.0	17.0	-194.43896	-194.42550
C ₂ H ₅ OCH ₃ (methyl ethyl ether)	278.4	17.3	-194.41810	-194.40478
(CH ₃) ₃ N (trimethylamine)	309.4	17.0	-174.52140	-174.50857
C ₄ H ₄ O (furan)	180.7	12.3	-230.10932	-230.09418
C ₄ H ₄ S (thiophene)	172.2	13.3	-554.01566	-553.98921
C ₄ H ₅ N (pyrrole)	213.1	13.0	-210.23335	-210.21837
C ₅ H ₅ N (pyridine)	229.2	13.8	-248.35095	-248.33375
C ₂ H ₃ (² A')	94.1	10.7	-77.91638	-77.91042
CH ₃ CO (² A')	111.2	12.9	-153.24509	-153.23562
H ₂ COH (² A)	96.0	11.4	-115.11792	-115.11067
CH ₃ O CS (² A')	93.4	10.5	-115.10229	-115.09543
CH ₃ CH ₂ O (² A'')	164.8	12.5	-154.42952	-154.41964
CH ₃ S (² A')	91.4	10.9	-439.02875	-439.01046
C ₂ H ₅ (² A')	152.7	13.0	-79.16872	-79.16240
(CH ₃) ₂ CH (² A')	226.4	16.2	-118.49577	-118.48643
(CH ₃) ₃ C (t-butyl radical)	300.0	19.3	-157.82397	-157.81166
PO	7.4	8.7	-417.28885	-417.27361
PH	13.8	8.7	-342.56641	-342.55432
SiH	11.8	8.7	-290.45108	-290.44682
B ₂ F ₄	49.7	18.3	-449.66916	-449.64921
CF ₂	17.8	10.4	-237.88836	-237.87842
C ₆ H ₅ CH ₃ (toluene)	329.9	19.0	-271.62646	-271.60653
CH ₃ F	101.1	10.1	-139.83887	-139.83166
CH ₂ S	63.7	10.2	-438.43812	-438.42003
CH ₂ SH	80.7	13.4	-439.01250	-438.99407
CH ₃ OF	109.5	12.3	-214.99026	-214.97998
C ₆ H ₅ OH (phenol)	270.4	17.1	-307.57681	-307.55581
C ₆ H ₅ NH ₂ (aniline)	302.3	17.9	-287.68640	-287.66584
B ₂ H ₄	103.9	11.4	-52.02893	-52.02414
N ₂ H ₂	73.2	10.0	-110.69456	-110.68777
N ₂ H ₃	101.9	10.8	-111.27807	-111.27082
HOF	36.1	10.0	-175.67525	-175.66784
Si ₂ H ₂	40.3	10.8	-581.03961	-581.03090
Si ₂ H ₄	80.2	14.4	-582.26052	-582.25118
Si ₂ H ₅	101.8	15.6	-582.86959	-582.85996
C ₂ (1)	11.1	8.7	-75.93885	-75.93383
C ₂ O (3) CCO	23.0	10.5	-151.31837	-151.30973
NCO (2)	25.9	9.7	-168.08065	-168.07147
OF (2)	6.6	8.7	-175.00610	-174.99940
S ₂ O	13.4	11.2	-873.57187	-873.53848
H ₂ C=C=C (¹ A ₁)	80.1	12.6	-115.35578	-115.34755

H ₂ C=C=CH	105.9	13.2	-116.02461	-116.01595
CH ₂ CHCH ₂	170.7	12.6	-117.28076	-117.27172
HCF (1) ¹ A'	31.8	10.0	-138.50377	-138.49738
CH ₂ CN	80.1	12.0	-132.13316	-132.12449
CH ₂ NC	79.1	12.6	-132.09463	-132.08589
CHCO	48.5	11.7	-151.98681	-151.97766
CH ₂ CHO	109.6	11.8	-153.23394	-153.22441
CH ₃ CH ₂ S	166.5	13.8	-478.35289	-478.33162
HNO	35.8	9.9	-130.54984	-130.54292
HO ₂ (2) HOO ² A''	36.5	10.0	-151.00160	-150.99419

G2/97 cations

CH ₄ ⁺	92.5	11.9	-40.04789	-40.04464
NH ₃ ⁺	84.2	10.1	-56.21048	-56.20651
OH ⁺	17.9	8.7	-75.30278	-75.29901
OH ₂ ⁺	48.0	9.9	-76.01655	-76.01230
FH ⁺	17.7	8.7	-99.94541	-99.94160
SiH ₄ ⁺	73.4	12.5	-291.94299	-291.93780
PH ⁺	13.8	8.7	-342.19328	-342.18081
PH ₂ ⁺	34.7	10.0	-342.83432	-342.82155
PH ₃ ⁺	60.9	10.3	-343.47170	-343.45873
SH ⁺	14.9	8.7	-399.32317	-399.30796
SH ₂ ⁺ (² B ₁)	37.3	10.0	-399.97328	-399.95768
SH ₂ ⁺ (² A ₁)	35.0	10.0	-399.88785	-399.87215
CIH ⁺	15.4	8.7	-461.63672	-461.61809
C ₂ H ₂ ⁺	67.3	9.8	-76.93192	-76.92626
C ₂ H ₄ ⁺	125.6	10.9	-78.21597	-78.20996
CO ⁺	13.5	8.7	-112.86285	-112.85659
N ₂ ⁺ (² Sig)	13.7	8.7	-109.01117	-109.00489
N ₂ ⁺ (² Pi)	11.7	8.7	-108.97050	-108.96447
O ₂ ⁺	12.1	8.7	-149.97103	-149.96386
P ₂ ⁺ ² -Pi	4.1	9.0	-683.69752	-683.67318
S ₂ ⁺	4.9	8.9	-797.95203	-797.92251
Cl ₂ ⁺	3.7	9.1	-922.54069	-922.50407
ClF ⁺	5.5	8.8	-560.88061	-560.85895
CS ⁺	8.3	8.7	-436.77502	-436.75770
BF ₃ ⁺	26.1	12.9	-324.25927	-324.24560
BCl ₃ ⁺	16.2	15.4	-1409.03999	-1408.98157
B ₂ F ₄ ⁺	47.6	20.1	-449.23722	-449.21727
CO ₂ ⁺	22.7	9.8	-188.18625	-188.17640
CF ₂ ⁺	21.7	10.3	-237.46982	-237.45973
COS ⁺	22.0	10.4	-512.15182	-512.13068
CS ₂ ⁺	15.4	11.0	-836.05709	-836.02490

CH ₂ ⁺	42.0	10.1	-38.77471	-38.77193
CH ₃ ⁺	80.7	10.0	-39.48350	-39.48039
C ₂ H ₅ ⁺	156.2	10.9	-78.87143	-78.86517
C ₃ H ₄ ⁺ (cyclopropene ⁺)	133.6	12.3	-116.28710	-116.27851
CH ₂ =C=CH ₂ ⁺	135.5	12.9	-116.32159	-116.31290
sec-C ₃ H ₇ ⁺	227.1	15.4	-118.22232	-118.21302
C ₆ H ₆ ⁺	252.7	16.3	-231.95724	-231.94034
C ₆ H ₅ CH ₃ ⁺	324.7	17.8	-271.29942	-271.27961
CN ⁺	12.2	8.7	-92.24168	-92.23630
CHO ⁺	42.5	9.0	-113.61304	-113.60634
CH ₂ OH ⁺	104.7	10.2	-114.84394	-114.83671
CH ₃ O ⁺	85.6	10.5	-114.70510	-114.69842
CH ₃ OH ⁺	121.4	11.5	-115.37875	-115.37154
CH ₃ F ⁺	85.0	10.5	-139.37103	-139.36420
CH ₂ S ⁺	61.0	10.4	-438.09202	-438.07413
HSCH ₂ ⁺	90.6	10.5	-438.73835	-438.72003
CH ₃ SH ⁺	115.1	12.2	-439.32720	-439.30861
CH ₃ Cl ⁺	84.9	11.8	-500.99920	-500.97730
C ₂ H ₅ OH ⁺	199.3	14.8	-154.72542	-154.71509
CH ₃ CHO ⁺	136.5	13.3	-153.51790	-153.50827
CH ₃ OF ⁺	102.5	13.4	-214.56933	-214.55928
C ₂ H ₄ S ⁺ (thiirane ⁺)	139.3	11.8	-477.43582	-477.41494
NCCN ⁺	38.3	13.0	-185.23200	-185.22090
C ₄ H ₄ O ⁺ (furan ⁺)	178.4	12.7	-229.78150	-229.76655
C ₄ H ₅ N ⁺ (pyrrole ⁺)	211.8	13.1	-209.93058	-209.91574
C ₆ H ₅ OH ⁺	270.6	17.2	-307.26344	-307.24264
C ₆ H ₅ NH ₂ ⁺	304.1	17.6	-287.40274	-287.38225
B ₂ H ₄ ⁺	103.8	11.8	-51.67708	-51.67236
NH ⁺	17.5	8.7	-54.74786	-54.74461
NH ₂ ⁺	43.3	10.3	-55.48935	-55.48577
N ₂ H ₂ ⁺	68.0	10.2	-110.33979	-110.33289
N ₂ H ₃ ⁺	108.9	10.1	-111.00085	-110.99353
HOF ⁺	34.3	10.0	-175.20669	-175.19961
SiH ₂ ⁺	30.9	10.1	-290.74292	-290.73816
SiH ₃ ⁺	57.0	10.4	-291.39867	-291.39358
Si ₂ H ₂ ⁺	39.4	11.1	-580.73811	-580.72903
Si ₂ H ₄ ⁺	80.9	14.5	-581.96452	-581.95516
Si ₂ H ₅ ⁺	102.2	16.3	-582.58822	-582.57848
Si ₂ H ₆ ⁺	120.3	19.0	-583.16197	-583.15187
G2/97 anions				
CH ⁻	14.6	8.7	-38.53056	-38.52742

CH ₂ ⁻	39.0	9.9	-39.17837	-39.17524
CH ₃ ⁻	72.4	10.1	-39.84301	-39.83974
NH ⁻	17.6	8.7	-55.25573	-55.25193
NH ₂ ⁻	46.4	9.9	-55.92891	-55.92505
OH ⁻	21.1	8.7	-75.84933	-75.84489
SiH ⁻	10.6	8.7	-290.49632	-290.49186
SiH ₂ ⁻	27.3	10.0	-291.11687	-291.11210
SiH ₃ ⁻	49.6	10.3	-291.74536	-291.74033
PH ⁻	12.9	8.7	-342.60360	-342.59067
PH ₂ ⁻	32.7	10.0	-343.24082	-343.22776
SH ⁻	15.3	8.7	-399.79146	-399.77474
O ₂ ⁻	6.9	8.7	-150.42949	-150.42232
NO ⁻	8.5	8.7	-129.96534	-129.95860
CN ⁻	12.6	8.7	-92.89443	-92.88880
PO ⁻	6.1	8.8	-417.32858	-417.31284
S ₂ ⁻	3.3	9.2	-798.35809	-798.32700
Cl ₂ ⁻	1.2	10.1	-923.05113	-923.01142
CC ⁻ (2)	11.0	8.7	-76.05862	-76.05343
C ₂ O ⁻ (2) CCO	24.3	10.0	-151.40357	-151.39461
CF ₂ ⁻ (2) ² B ₁	12.1	11.0	-237.89208	-237.88209
NCO ⁻ (1)	28.1	9.5	-168.21495	-168.20534
NO ₂ ⁻ (1) ONO	20.4	10.2	-205.27829	-205.26790
O ₃ ⁻	15.1	10.6	-225.64265	-225.63221
OF ⁻ (2)	4.7	8.9	-175.08997	-175.08278
SO ₂ ⁻	15.0	10.8	-549.74103	-549.71868
S ₂ O ⁻	11.2	11.6	-873.64096	-873.60677
C ₂ H ⁻	37.7	9.6	-76.73871	-76.73293
C ₂ H ₃ ⁻	90.9	10.4	-77.93991	-77.93402
H ₂ C=C=C ⁻	76.3	12.4	-115.42114	-115.41268
H ₂ C=C=CH ⁻	104.5	12.6	-116.05742	-116.04876
CH ₂ CHCH ₂ ⁻	162.3	14.3	-117.29542	-117.28629
HCO ⁻	23.6	10.1	-113.91593	-113.90943
HCF ⁻ (2) ² A"	26.5	10.2	-138.52157	-138.51499
CH ₃ O ⁻	88.9	10.1	-115.15780	-115.15058
CH ₃ S ⁻	91.9	10.6	-439.09771	-439.07848
CH ₂ S ⁻	56.1	11.7	-438.45383	-438.43510
CH ₂ CN ⁻	78.5	12.2	-132.18936	-132.18052
CH ₂ NC ⁻	78.1	12.0	-132.13593	-132.12721
CHCO ⁻	49.1	11.6	-152.07316	-152.06361
CH ₂ CHO ⁻	107.6	11.7	-153.30053	-153.29068
CH ₃ CO ⁻	103.0	13.3	-153.25655	-153.24704

CH ₃ CH ₂ O ⁻	164.2	12.7	-154.49115	-154.48103
CH ₃ CH ₂ S ⁻	166.0	13.3	-478.42480	-478.40276
LiH ⁻	6.7	8.7	-8.07629	-8.07599
HNO ⁻	30.8	10.0	-130.56026	-130.55322
HO ₂ ⁻ (1) HOO ¹ A'	33.3	10.2	-151.04005	-151.03231
protonated species				
NH ₄ ⁺	127.8	10.0	-56.92412	-56.91961
OH ₃ ⁺	88.6	10.1	-76.75645	-76.75139
C ₂ H ₃ ⁺	88.1	11.3	-77.60279	-77.59685
SiH ₅ ⁺	98.7	13.6	-292.60014	-292.59459
PH ₄ ⁺	90.9	10.4	-344.14204	-344.12867
SH ₃ ⁺	66.7	10.1	-400.63614	-400.62013
CH ₂ ⁺	39.0	10.0	-462.32532	-462.30591
H ₃ ⁺	51.7	9.9	-1.34394	-1.34341
G3/99' neutrals				
C ₄ H ₆ (methyl allene)	217.0	15.7		-155.99417
C ₅ H ₈ (isoprene)	294.1	17.8		-195.33910
C ₅ H ₁₀ (cyclopentane)	361.5	14.1		-196.58494
C ₅ H ₁₂ (n-pentane)	411.9	21.8		-197.79471
C ₅ H ₁₂ (neo pentane)	405.0	23.0		-197.80082
C ₆ H ₈ (1,3 cyclohexadiene)	315.4	16.5		-233.45679
C ₆ H ₈ (1,4 cyclohexadiene)	315.1	16.7		-233.45679
C ₆ H ₁₂ (cyclohexane)	439.4	17.9		-235.91475
C ₆ H ₁₄ (n-hexane)	487.7	24.8		-237.11448
C ₆ H ₁₄ (3-methyl pentane)	484.4	25.2		-237.11502
C ₆ H ₅ CH ₃ (toluene)	330.3	18.9		-271.60596
C ₇ H ₁₆ (n-heptane)	558.2	29.0		-276.43425
C ₈ H ₈ (cyclooctatetraene)	342.6	20.2		-309.63693
C ₈ H ₁₈ (n-octane)	634.0	32.0		-315.75404
C ₁₀ H ₈ (naphthalene)	381.1	20.9		-385.95247
C ₁₀ H ₈ (azulene)	375.6	21.8		-385.89415
CH ₃ COOCH ₃ (acetic acid methyl ester)	234.0	18.2		-268.49899
(CH ₃) ₃ COH (t-butanol)	350.5	20.4		-233.75058
C ₆ H ₅ NH ₂ (aniline)	302.6	18.1		-287.66528
C ₆ H ₅ OH (phenol)	270.8	17.3		-307.55527
C ₄ H ₆ O (divinyl ether)	231.4	17.8		-231.26637
C ₄ H ₈ O (tetrahydrofuran)	301.0	15.8		-232.51976
C ₅ H ₈ O (cyclopentanone)	313.0	17.5		-270.65057
C ₆ H ₄ O ₂ (benzoquinone)	220.1	19.4		-381.58444
C ₄ H ₄ N ₂ (pyrimidine)	199.9	13.6		-264.38775
C ₂ H ₆ O ₂ S (dimethyl sulphone)	218.9	19.4		-629.51462
C ₆ H ₅ Cl (chlorobenzene)	235.0	17.2		-693.16644

N=C-CH ₂ -CH ₂ -C=N (butanedinitrile)	189.5	19.1	-264.37697
C ₄ H ₄ N ₂ (1,4-dipyridine) (pyrazine)	198.9	13.7	-264.38046
CH ₃ -C(=O)-CCH CH ₃ -CH=CH-CHO (crotonaldehyde)	169.1	17.5	-230.04761
CH ₃ -C(=O)-O-C(=O)-CH ₃ (Acetic anhydride)	231.6	18.0	-231.30202
255.2	23.8	-381.89347	
C ₄ H ₆ S (2,5-Dihydrothiophene)	231.3	15.5	-555.18514
(CH ₃) ₂ CH-CN	265.8	18.2	-211.43055
CH ₃ -CO-CH ₂ -CH ₃ (Methyl ethyl ketone)	291.3	19.4	-232.53832
(CH ₃) ₂ CH-CHO	290.8	19.4	-232.52778
C ₄ H ₈ O ₂ (cyc-CH ₂ -CH ₂ -O-CH ₂ -CH ₂ -O (para)) (1,4-Dioxane)	318.2	16.2	-307.77712
C ₄ H ₈ S (Tetrahydrothiophene)	293.5	16.3	-556.41504
(CH ₃) ₃ C-Cl (t-Butyl chloride)	317.8	19.5	-619.36814
CH ₃ -CH ₂ -CH ₂ -CH ₂ -Cl (n-Butyl chloride)	318.6	20.2	-619.35841
C ₄ H ₈ NH (Tetrahydropyrrole)	335.3	15.7	-212.63054
CH ₃ -CH ₂ -CH(CH ₃)-NO ₂ (Nitro-s-butane)	348.6	24.4	-363.10004
CH ₃ -CH ₂ -O-CH ₂ -CH ₃ (Diethyl ether)	351.6	20.9	-233.72887
CH ₃ -CH(OCH ₃) ₂ (acetaldehyde dimethyl acetal)	366.1	23.2	-308.98749
(CH ₃) ₃ C-SH (t-butanethiol)	338.2	21.4	-557.62419
CH ₃ -CH ₂ -S-S-CH ₂ -CH ₃ (Diethyl disulfide)	347.4	27.0	-956.77023
(CH ₃) ₃ C-NH ₂ (t-butylamine)	384.5	20.4	-213.85631
Si(CH ₃) ₄ (Tetramethylsilane)	377.4	28.0	-449.68945
C ₅ H ₆ S cyc-CH=CH-S-C(CH ₃)=CH- (2-methyl thiophene)	243.7	17.9	-593.31203
cyc-CH=CH-N(CH ₃)-CH=CH- (N-methyl pyrrole)	285.6	17.2	-249.53102
C ₅ H ₁₀ O (Tetrahydropyran)	378.4	17.1	-271.84700

CH ₃ -CH ₂ -CO-CH ₂ -CH ₃ (Diethyl ketone)	362.7	23.7	-271.85852
C ₅ H ₁₀ O ₂ CH ₃ -C(=O)-O- CH(CH ₃) ₂ (Isopropyl acetate)	377.3	25.5	-347.14830
C ₅ H ₁₀ S (Tetrahydrothiopyran)	369.0	18.6	-595.73823
cyc-C ₅ H ₁₀ NH (piperidine)	410.6	17.6	-251.95808
(CH ₃) ₃ C-O-CH ₃ (t-butyl methyl ether)	423.8	23.7	-273.05105
C ₆ H ₄ F ₂ (1,3- DiFluorobenzene)	218.3	18.3	-430.92829
C ₆ H ₄ F ₂ (1,4- DiFluorobenzene)	217.4	18.4	-430.92727
C ₆ H ₅ F (Fluorobenzene)	238.6	16.3	-331.60616
(CH ₃) ₂ CH-O-CH(CH ₃) ₂ (Di- isopropyl ether)	495.5	27.7	-312.37650
PF ₅	43.6	17.0	-841.86748
SF ₆	55.4	13.6	-998.66737
SCl ₂	7.8	12.4	-1322.08923
POCl ₃	25.5	17.9	-1801.86606
PCl ₅	22.9	23.6	-2649.51651
Cl ₂ O ₂ S	32.8	16.3	-1472.62804
PCl ₃	12.7	16.1	-1726.55629
Cl ₂ S ₂	12.5	16.5	-1721.25010
SiCl ₂	7.2	12.6	-1212.99126
CF ₃ Cl	40.0	13.9	-799.38154
C ₂ F ₆	78.1	20.2	-675.80976
CF ₃	32.4	11.5	-337.82539
C ₆ H ₅ (phenyl radical)	225.4	14.3	-231.59244

RR49

Me [•]	76.8	10.5	-39.84003
Et [•]	153.1	12.9	-79.16024
i-Pr [•]	226.3	16.5	-118.48243
CH ₂ =CH ₂	131.4	10.5	-78.59592
Me-CH ₂ CH ₂ [•]	228.0	15.2	-118.47805
Et-CH ₂ CH ₂ [•]	301.6	18.6	-157.79642
i-Pr-CH ₂ CH ₂ [•]	373.7	22.0	-197.11696
S=CH ₂	63.6	10.2	-438.41301
Me-SCH ₂ [•]	158.5	16.0	-478.30747
Et-SCH ₂ [•]	233.5	18.9	-517.62696
i-Pr-SCH ₂ [•]	304.5	22.8	-556.94809
O=CH ₂	69.4	10.0	-114.54457
Me-OCH ₂ [•]	170.4	14.3	-154.40584

Et-OCH ₂ [•]	243.8	17.4	-193.72902
i-Pr-OCH ₂ [•]	316.0	20.7	-233.05286
CH ₂ =CHMe	205.9	13.2	-117.91834
Me-CH ₂ C [•] HMe	300.4	19.5	-157.80041
CH ₂ =CMe ₂	277.3	16.8	-157.24203
Me-CH ₂ C [•] Me ₂	375.1	22.7	-197.12363
S=CHMe	138.2	13.1	-477.74057
Me-SC [•] HMe	233.1	19.6	-517.62823
S=CMe ₂	209.5	17.5	-517.06711
Me-SC [•] Me ₂	306.9	22.9	-556.94998
O=CHMe	143.5	12.7	-153.87607
Me-OC [•] HMe	244.4	17.7	-193.73076
O=CMe ₂	215.5	16.8	-193.20547
Me-OC [•] Me ₂	316.7	21.0	-233.05338
CH ₂ =CHCN	131.6	13.5	-170.86423
Me-CH ₂ C [•] HCN	229.3	18.7	-210.75894
CH ₂ =CHF	114.1	11.3	-177.90693
Me-CH ₂ C [•] HF	212.4	16.5	-217.79018
CH ₂ =CHOMe	220.7	15.1	-193.16588
Me-CH ₂ C [•] HOMe	318.4	20.9	-233.04863
CH ₂ =CHNH ₂	178.5	13.0	-133.97498
Me-CH ₂ C [•] HNH ₂	277.7	17.9	-173.86096
CH ₂ =CHCHO	158.8	14.1	-191.96263
Me-CH ₂ C [•] HCHO	258.6	18.8	-231.85719
CH ₂ =CF ₂	95.7	12.3	-277.22318
Me-CH ₂ C [•] F ₂	196.6	17.4	-317.11338
CH ₄	115.6	10.0	-40.51956
Me-CH ₂ CH ₃	265.3	14.8	-119.15225
Et-CH ₂ CH ₃	338.6	18.2	-158.47053
i-Pr-CH ₂ CH ₃	412.3	21.3	-197.79047
Me-SCH ₃	194.1	15.8	-478.96939
Et-SCH ₃	269.2	19.0	-518.28842
i-Pr-SCH ₃	341.0	22.6	-557.60949
Me-OCH ₃	206.3	13.9	-155.07073
Et-OCH ₃	280.2	17.0	-194.39383
i-Pr-OCH ₃	351.8	20.5	-233.71622
Me-CH ₂ CH ₂ CN	265.0	18.4	-211.41968
Me-CH ₂ CH ₂ F	248.7	16.1	-218.46086
Me-CH ₂ CH ₂ OMe	353.5	20.3	-233.71202
Me-CH ₂ CH ₂ NH ₂	313.8	17.6	-174.51963
Me-CH ₂ CH ₂ CHO	291.0	19.2	-232.51290
Me-CH ₂ CHF ₂	231.8	17.1	-317.78558
EtH	192.9	11.6	-79.83409

t-Bu [•]	299.5	20.0	-157.80597
t-BuH	340.0	17.5	-158.47298
F ₃ C [•]	32.4	11.5	-337.78796
F ₃ CH	66.7	11.6	-338.46896
Cl ₃ C [•]	19.2	14.3	-1422.46144
Cl ₃ CH	52.3	14.3	-1423.12200
MeO ₂ CCH ₂ [•]	198.5	17.6	-267.81030
MeO ₂ CCH ₃	234.0	18.2	-268.47917
NCC [•] Me ₂	227.3	19.7	-210.76563
NCCHMe ₂	265.8	18.2	-211.42072

PR10

Cyclobutene	223.3	12.8	-155.98965
cis-1,3,5-Hexatriene	308.3	20.2	-233.41916
o-Xylyene	341.5	20.6	-309.64127
1,3-Pentadiene	294.1	18.3	-195.32868
1,3-Cyclopentadiene	238.2	13.7	-194.12487
1,5-Hexadiene	366.0	22.2	-234.63870
1,3-Butadiene	220.8	14.8	-156.00797
Ethylene	131.4	10.5	-78.59592
cis-Triscyclopropencyclohexan	477.0	22.5	
1,3-Cyclohexadiene	315.4	16.5	-233.44599
Benzocyclobutane	347.3	18.7	-309.66179
Cyclohexene	377.4	17.3	-234.67474
Norbornene	394.4	16.7	-272.76767
Cyclopentadiene dimer	500.4	21.6	
Cyclonona-1,4,7-triene	476.8	24.4	
PR10-1 TS	216.2	12.6	-155.93450
PR10-2 TS	305.8	17.4	-233.37034
PR10-3 TS	336.9	19.0	-309.59666
PR10-4 TS	284.2	15.0	-195.26512
PR10-5 TS	231.3	12.7	-194.07955
PR10-6 TS	364.4	18.2	-234.58296
PR10-7 TS	360.2	19.9	-234.56922
PR10-8 TS	379.9	19.5	-272.69322
PR10-9 TS	485.1	23.6	
PR10-10 TS	474.9	21.8	

BDE261

H		-0.49999	-0.49997
H-H		-1.17459	-1.17417
H ₃ C		-39.84362	-39.84038
H ₃ C-H		-40.52300	-40.51953
H ₃ C-CH ₃		-79.84245	-79.83589
H ₃ C-NH ₂		-95.89236	-95.88523
H ₃ C-OH		-115.78284	-115.77532
H ₃ C-F		-139.83886	-139.83165
H ₃ C-SiH ₃		-331.68849	-331.68011
H ₃ C-PH ₂		-383.16126	-383.14536

H ₃ C-SH	-439.67587	-439.65715
H ₃ C-Cl	-501.41871	-501.39600
H ₂ N	-55.90212	-55.89857
H ₂ N-H	-56.58637	-56.58224
H ₂ N-NH ₂	-111.92117	-111.91340
H ₂ N-OH	-131.79601	-131.78807
H ₂ N-F	-155.83151	-155.82411
H ₂ N-SiH ₃	-347.77039	-347.76138
H ₂ N-PH ₂	-399.22788	-399.21130
H ₂ N-SH	-455.72213	-455.70287
H ₂ N-Cl	-517.44080	-517.41790
HO	-75.78226	-75.77839
HO-H	-76.48304	-76.47838
HO-OH	-151.65143	-151.64341
HO-F	-175.67525	-175.66784
HO-SiH ₃	-367.68284	-367.67338
HO-PH ₂	-419.12779	-419.11085
HO-SH	-475.60597	-475.58639
HO-Cl	-537.31045	-537.28732
F	-99.81155	-99.80826
F-H	-100.53774	-100.53347
F-F	-199.68434	-199.67766
F-SiH ₃	-391.75456	-391.74536
F-PH ₂	-443.18952	-443.17286
F-SH	-499.65286	-499.63358
F-Cl	-561.34577	-561.32304
H ₃ Si	-291.69596	-291.69094
H ₃ Si-H	-292.35020	-292.34476
H ₃ Si-SiH ₃	-583.51877	-583.50871
H ₃ Si-PH ₂	-635.01021	-634.99257
H ₃ Si-SH	-691.54725	-691.52641
H ₃ Si-Cl	-753.30956	-753.28451
H ₂ P	-343.19521	-343.18271
H ₂ P-H	-343.83481	-343.82195
H ₂ P-PH ₂	-686.48764	-686.46258
H ₂ P-SH	-743.01242	-742.98429
H ₂ P-Cl	-804.75884	-804.72661
HS	-399.70546	-399.69014
HS-H	-400.35847	-400.34266
HS-SH	-799.51771	-799.48682
HS-Cl	-861.24593	-861.21121
Cl	-461.43475	-461.41581
Cl-H	-462.10587	-462.08619
Cl-Cl	-922.96341	-922.92519
MeH ₂ C	-79.16872	-79.16240
MeH ₂ C-H	-79.84245	-79.83589

MeH ₂ C-CH ₃	-119.16519	-119.15566
MeH ₂ C-NH ₂	-135.21801	-135.20786
MeH ₂ C-OH	-155.11040	-155.09983
MeH ₂ C-F	-179.16758	-179.15735
MeH ₂ C-SiH ₃	-371.00680	-370.99548
MeH ₂ C-PH ₂	-422.48246	-422.46361
MeH ₂ C-SH	-478.99940	-478.97773
MeH ₂ C-Cl	-540.74482	-540.71914
MeHN	-95.22036	-95.21378
MeHN-H	-95.89236	-95.88523
MeHN-CH ₃	-135.20461	-135.19460
MeHN-NH ₂	-151.23634	-151.22571
MeHN-OH	-171.11226	-171.10142
MeHN-F	-195.15018	-195.13986
MeHN-SiH ₃	-387.07763	-387.06573
MeHN-PH ₂	-438.53644	-438.51698
MeHN-SH	-495.03323	-495.01111
MeHN-Cl	-556.75518	-556.72942
MeO	-115.10230	-115.09544
MeO-H	-115.78284	-115.77532
MeO-CH ₃	-155.09038	-155.08008
MeO-NH ₂	-171.10333	-171.09264
MeO-OH	-190.96249	-190.95166
MeO-F	-214.99025	-214.97997
MeO-SiH ₃	-406.98440	-406.97222
MeO-PH ₂	-458.43002	-458.41035
MeO-SH	-514.91241	-514.89009
MeO-Cl	-576.61968	-576.59376
MeH ₂ Si	-331.03296	-331.02498
MeH ₂ Si-H	-331.68849	-331.68011
MeH ₂ Si-CH ₃	-371.02747	-371.01611
MeH ₂ Si-NH ₂	-387.11108	-387.09908
MeH ₂ Si-OH	-407.02492	-407.01248
MeH ₂ Si-F	-431.09718	-431.08500
MeH ₂ Si-SiH ₃	-622.85644	-622.84348
MeH ₂ Si-PH ₂	-674.34934	-674.32878
MeH ₂ Si-SH	-730.88803	-730.86425
MeH ₂ Si-Cl	-792.65185	-792.62387
MeHP	-382.52377	-382.50826
MeHP-H	-383.16126	-383.14536
MeHP-CH ₃	-422.49095	-422.47204
MeHP-NH ₂	-438.56046	-438.54088
MeHP-OH	-458.46249	-458.44253
MeHP-F	-482.52504	-482.50534
MeHP-SiH ₃	-674.33595	-674.31535
MeHP-PH ₂	-725.81632	-725.78826

MeHP-SH	-782.34391	-782.31280
MeHP-Cl	-844.09284	-844.05761
MeS	-439.02876	-439.01046
MeS-H	-439.67587	-439.65715
MeS-CH ₃	-478.99751	-478.97585
MeS-NH ₂	-495.04697	-495.02478
MeS-OH	-514.93278	-514.91028
MeS-F	-538.98216	-538.95992
MeS-SiH ₃	-730.86508	-730.84140
MeS-PH ₂	-782.33197	-782.30096
MeS-SH	-838.84170	-838.80794
MeS-Cl	-900.57266	-900.53500
Me ₂ HC	-118.49577	-118.48643
Me ₂ HC-H	-119.16519	-119.15567
Me ₂ HC-CH ₃	-158.49036	-158.47791
Me ₂ HC-NH ₂	-174.54562	-174.53257
Me ₂ HC-OH	-194.43896	-194.42550
Me ₂ HC-F	-218.49727	-218.48412
Me ₂ HC-SiH ₃	-410.32855	-410.31436
Me ₂ HC-PH ₂	-461.80665	-461.78490
Me ₂ HC-SH	-518.32566	-518.30107
Me ₂ HC-Cl	-580.07222	-580.04362
Me ₂ N	-134.54185	-134.53236
Me ₂ N-H	-135.20462	-135.19460
Me ₂ N-CH ₃	-174.52140	-174.50858
Me ₂ N-NH ₂	-190.55046	-190.53715
Me ₂ N-OH	-210.43109	-210.41745
Me ₂ N-F	-234.47155	-234.45841
Me ₂ N-SiH ₃	-426.38990	-426.37525
Me ₂ N-PH ₂	-477.84425	-477.82214
Me ₂ N-SH	-534.34685	-534.32198
Me ₂ N-Cl	-596.07264	-596.04409
Me ₂ HSi	-370.37065	-370.35966
Me ₂ HSi-H	-371.02747	-371.01611
Me ₂ HSi-CH ₃	-410.36699	-410.35265
Me ₂ HSi-NH ₂	-426.45208	-426.43708
Me ₂ HSi-OH	-446.36625	-446.35080
Me ₂ HSi-F	-470.43965	-470.42446
Me ₂ HSi-SiH ₃	-662.19494	-662.17907
Me ₂ HSi-PH ₂	-713.68914	-713.66564
Me ₂ HSi-SH	-770.22931	-770.20263
Me ₂ HSi-Cl	-831.99415	-831.96323
Me ₂ P	-421.85509	-421.83658
Me ₂ P-H	-422.49095	-422.47204
Me ₂ P-CH ₃	-461.82378	-461.80190

Me ₂ P-NH ₂	-477.89468	-477.87217
Me ₂ P-OH	-497.79896	-497.77604
Me ₂ P-F	-521.86246	-521.83976
Me ₂ P-SiH ₃	-713.66487	-713.64134
Me ₂ P-PH ₂	-765.14812	-765.11711
Me ₂ P-SH	-821.67735	-821.64328
Me ₂ P-Cl	-883.42898	-883.39078
Me ₃ C	-157.82396	-157.81166
Me ₃ C-H	-158.49034	-158.47789
Me ₃ C-CH ₃	-197.81672	-197.80148
Me ₃ C-NH ₂	-213.87273	-213.85684
Me ₃ C-OH	-233.76747	-233.75116
Me ₃ C-F	-257.82691	-257.81092
Me ₃ C-SiH ₃	-449.65288	-449.63596
Me ₃ C-PH ₂	-501.13218	-501.10763
Me ₃ C-SH	-557.65211	-557.62473
Me ₃ C-Cl	-619.39985	-619.36843
Me ₃ Si	-409.70911	-409.69511
Me ₃ Si-H	-410.36699	-410.35265
Me ₃ Si-CH ₃	-449.70685	-449.68952
Me ₃ Si-NH ₂	-465.79225	-465.77424
Me ₃ Si-OH	-485.70730	-485.68884
Me ₃ Si-F	-509.78180	-509.76360
Me ₃ Si-SiH ₃	-701.53419	-701.51541
Me ₃ Si-PH ₂	-753.02936	-753.00296
Me ₃ Si-SH	-809.57047	-809.54088
Me ₃ Si-Cl	-871.33631	-871.30244
FH ₂ C	-139.16546	-139.15855
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FH ₂ C-CH ₃	-179.16758	-179.15735
FH ₂ C-NH ₂	-195.23168	-195.22085
FH ₂ C-OH	-215.12179	-215.11058
FH ₂ C-F	-239.17444	-239.16354
FH ₂ C-SiH ₃	-430.99815	-430.98614
FH ₂ C-PH ₂	-482.47648	-482.45696
FH ₂ C-SH	-538.99872	-538.97638
FH ₂ C-Cl	-600.74120	-600.71487
FHN	-155.17445	-155.16762
FHN-H	-155.83151	-155.82410
FHN-CH ₃	-195.15018	-195.13986
FHN-NH ₂	-211.19577	-211.18482
FHN-OH	-231.06556	-231.05443
FHN-F	-255.09609	-255.08548
FHN-SiH ₃	-447.00888	-446.99671
FHN-PH ₂	-498.47059	-498.45090

FHN-SH	-554.97527	-554.95297
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FO-H	-175.67525	-175.66784
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FO-NH ₂	-231.02233	-231.01147
FO-OH	-250.86769	-250.85688
FO-F	-274.88258	-274.87242
FO-SiH ₃	-466.87230	-466.86010
FO-PH ₂	-518.32203	-518.30236
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FH ₂ Si-H	-391.75457	-391.74537
FH ₂ Si-CH ₃	-431.09718	-431.08500
FH ₂ Si-NH ₂	-447.18748	-447.17470
FH ₂ Si-OH	-467.09919	-467.08597
FH ₂ Si-F	-491.16931	-491.15638
FH ₂ Si-SiH ₃	-682.91988	-682.90602
FH ₂ Si-PH ₂	-734.41482	-734.39338
FH ₂ Si-SH	-790.95672	-790.93213
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FHP-H	-443.18952	-443.17286
FHP-CH ₃	-482.52504	-482.50534
FHP-NH ₂	-498.60728	-498.58690
FHP-OH	-518.50701	-518.48630
FHP-F	-542.56735	-542.54694
FHP-SiH ₃	-734.35976	-734.33833
FHP-PH ₂	-785.84611	-785.81725
FHP-SH	-842.37994	-842.34804
FHP-Cl	-904.12688	-904.09089
FS	-499.01262	-498.99384
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FS-CH ₃	-538.98216	-538.95992
FS-NH ₂	-555.04988	-555.02703
FS-OH	-574.92840	-574.90533
FS-F	-598.97056	-598.94783
FS-SiH ₃	-790.84017	-790.81591
FS-PH ₂	-842.31297	-842.28137
FS-SH	-898.83095	-898.79662
FS-Cl	-960.55485	-960.51669
F ₂ HC	-238.50077	-238.49027
F ₂ HC-H	-239.17443	-239.16354
F ₂ HC-CH ₃	-278.50828	-278.49440
F ₂ HC-NH ₂	-294.56778	-294.55328

F ₂ HC-OH	-314.46507	-314.45016
F ₂ HC-F	-338.52062	-338.50605
F ₂ HC-SiH ₃	-530.32921	-530.31355
F ₂ HC-PH ₂	-581.81102	-581.78786
F ₂ HC-SH	-638.33088	-638.30490
F ₂ HC-Cl	-700.07689	-700.04692
F ₂ N	-254.46568	-254.45562
F ₂ N-H	-255.09609	-255.08548
F ₂ N-CH ₃	-294.42253	-294.40909
F ₂ N-NH ₂	-310.46519	-310.45113
F ₂ N-OH	-330.33899	-330.32473
F ₂ N-F	-354.37357	-354.35989
F ₂ N-SiH ₃	-546.26730	-546.25206
F ₂ N-PH ₂	-597.73296	-597.71028
F ₂ N-SH	-654.23459	-654.20924
F ₂ N-Cl	-715.96009	-715.93107
F ₂ HSi	-490.50687	-490.49436
F ₂ HSi-H	-491.16931	-491.15638
F ₂ HSi-CH ₃	-530.51433	-530.49837
F ₂ HSi-NH ₂	-546.60388	-546.58733
F ₂ HSi-OH	-566.51816	-566.50119
F ₂ HSi-F	-590.58705	-590.57039
F ₂ HSi-SiH ₃	-782.33273	-782.31508
F ₂ HSi-PH ₂	-833.82943	-833.80422
F ₂ HSi-SH	-890.37005	-890.34171
F ₂ HSi-Cl	-952.13415	-952.10163
F ₂ P	-541.93943	-541.91953
F ₂ P-H	-542.56736	-542.54694
F ₂ P-CH ₃	-581.90981	-581.88635
F ₂ P-NH ₂	-597.99517	-597.97102
F ₂ P-OH	-617.90137	-617.87693
F ₂ P-F	-641.96607	-641.94195
F ₂ P-SiH ₃	-833.73066	-833.70550
F ₂ P-PH ₂	-885.22393	-885.19136
F ₂ P-SH	-941.75916	-941.72355
F ₂ P-Cl	-1003.51522	-1003.47552
F ₃ C	-337.83925	-337.82517
F ₃ C-H	-338.52061	-338.50604
F ₃ C-CH ₃	-377.85522	-377.83768
F ₃ C-NH ₂	-393.91611	-393.89793
F ₃ C-OH	-413.81104	-413.79242
F ₃ C-F	-437.86281	-437.84449
F ₃ C-SiH ₃	-629.67549	-629.65622
F ₃ C-PH ₂	-681.15478	-681.12801

F ₃ C-SH			-737.67214	-737.64255
F ₃ C-Cl			-799.41506	-799.38147
F ₃ Si			-589.91841	-589.90215
F ₃ Si-H			-590.58705	-590.57038
F ₃ Si-CH ₃			-629.93258	-629.91284
F ₃ Si-NH ₂			-646.01945	-645.99917
F ₃ Si-OH			-665.93109	-665.91041
F ₃ Si-F			-689.99859	-689.97820
F ₃ Si-SiH ₃			-881.75113	-881.72972
F ₃ Si-PH ₂			-933.24540	-933.21644
F ₃ Si-SH			-989.78379	-989.75173
F ₃ Si-Cl			-1051.54571	-1051.50950

MS14

C ₆ F ₆	133.8	28.0		-826.97580
C ₆ F ₅ Cl	130.2	28.8		-1186.97849
Dodecane	928.9	45.4		-472.43978
Hexadecane	1223.7	59.1		-629.51861
Adamantane	630.6	20.7		-390.29692
Diadamantane	813.9	26.3		-544.98175
Pyrene	535.2	29.2		-615.02739
Fuloranthene	533.5	29.9		-615.00512
Anthracene	501.2	27.6		-538.87861
Phenazine	439.8	26.8		-570.94168
trans-Azobenzene	492.7	31.3		-572.10132
Benzophenone	494.5	31.0		-575.97520
Dibenzothiophene	416.7	26.7		-859.33871
3,6-Diphenyl-1,2-dithiin	595.2	42.1		-1411.72758

HF clusters and TSs

			W1w	W2w
(HF) ₂			-201.08269	-201.08717
(HF) ₃			-301.63735	-301.64401
(HF) ₄			-402.19501	-402.20378
(HF) ₅			-502.74881	-502.75967
(HF) ₆			-603.30014	
(HF) ₂ TS			-201.01511	-201.01961
(HF) ₃ TS			-301.60426	-301.61077
(HF) ₄ TS			-402.17161	-402.18004
(HF) ₅ TS			-502.72563	-502.73591
(HF) ₆ TS			-603.27382	

298 K (ΔH_{298}) (kJ mol⁻¹), W1w, W1-F12, W1X-1 and W1X-2 Total Electronic Energies (har

<u>W1X-1</u>	<u>W1X-2</u>
-0.49997	-0.49991
-2.90363	-2.90363
-7.47090	-7.47090
-14.66217	-14.66217
-24.65211	-24.65097
-37.85023	-37.84818
-54.60718	-54.60365
-75.10621	-75.10054
-99.80479	-99.79640
-129.05377	-129.04278
-162.33690	-162.33690
-200.22557	-200.22557
-242.63799	-242.63687
-289.79648	-289.79410
-341.87884	-341.87417
-398.95968	-398.95097
-461.28099	-461.26775
-529.01397	-528.99463
<hr/>	
-2.00005	-2.00005
-7.27360	-7.27360
-14.31956	-14.31956
-24.34824	-24.34710
-37.43705	-37.43502
-54.07320	-54.06982
-74.60585	-74.60095
-99.16422	-99.15656
-128.26089	-128.25049
-162.19754	-162.19754
-199.99874	-199.99874
-242.41831	-242.41753
-289.49693	-289.49497
-341.49302	-341.48878
-398.57913	-398.57196
-460.80505	-460.79304
-528.43587	-528.41726
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-7.49375	-7.49375
-24.66056	-24.66040

-37.89553 -37.89422
-75.15930 -75.15352
-99.93036 -99.92152
-162.40639 -162.40639
-242.65308 -242.65249
-289.84723 -289.84522
-341.90490 -341.90048
-399.03501 -399.02662
-461.41292 -461.39983

-53.26883 -53.26653
-225.41432 -225.39683
-324.81393 -324.78846
-79.83494 -79.83074
-94.00386 -93.99795
-185.71313 -185.70155
-95.22467 -95.21873
-95.21251 -95.20660
-95.88410 -95.87826
-237.87095 -237.85226
-110.07223 -110.06455
-110.68655 -110.67881
-111.91217 -111.90451
-250.22795 -250.20864
-350.06275 -350.03545
-542.73062 -542.70392
-583.43971 -583.43475
-1367.97688 -1367.95581
-549.58195 -549.56227
-624.82262 -624.79722
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-836.21322 -836.19332
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-1197.14084 -1197.11459
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-934.38812 -934.38812
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-1626.97116 -1626.92909
-554.19112 -554.17195
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-611.68939 -611.66530
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-76.47694	-76.47115
-38.48398	-38.48172
-39.15315	-39.15114
-39.83975	-39.83759
-40.51900	-40.51696
-76.62270	-76.61841
-77.34508	-77.34074
-56.58159	-56.57772
-75.93383	-75.92941
-109.57815	-109.57050
-113.36964	-113.36167
-92.74519	-92.73937
-129.95634	-129.94688
-150.40431	-150.39301
-174.99411	-174.98017
-199.67069	-199.65420
-343.76248	-343.75745
-399.59785	-399.58895
-400.25051	-400.24160
-461.95040	-461.93709
-474.26505	-474.25131
-536.48867	-536.46926
-561.18343	-561.16182
-683.94226	-683.93205
-798.08240	-798.06484
-922.65372	-922.62718
-29.24112	-29.24112
-49.40954	-49.40716
-25.28711	-25.28586
-26.59899	-26.59782
-79.42797	-79.42286
-124.74683	-124.73729
-55.23936	-55.23556
-55.89775	-55.89383
-93.45589	-93.44990
-175.66283	-175.64889
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W1X-1	W1X-2
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tree)

Table S3. Deviations from Benchmark Values (kJ mol⁻¹)

Property	W1w	W1-F12	W1X-1	W1X-2
W4/08 TAE				
B ₂ H ₆	1.0	-4.0	-6.3	-5.3
BHF ₂	2.9	-2.7	-2.0	-0.6
BF ₃	5.2	-2.3	-0.6	1.6
C ₂ H ₆	3.0	-1.7	-1.7	-0.9
H ₂ CN	-1.7	-3.7	-3.0	-3.4
NCCN	-3.8	-6.3	-4.0	-5.1
CH ₂ NH ₂	0.7	-3.6	-2.4	-2.6
CH ₃ NH	-0.2	-3.6	-2.7	-2.9
CH ₃ NH ₂	2.3	-2.5	-1.2	-1.0
CF ₂	0.9	-1.9	1.0	1.3
N ₂ H	-2.3	-3.9	-1.4	-2.8
N ₂ H ₂	-0.7	-3.2	-0.6	-2.0
N ₂ H ₄	1.5	-3.6	-0.9	-1.7
FO ₂	-12.0	-13.3	-7.4	-6.3
F ₂ O ₂	-8.6	-10.2	-2.8	-0.7
AlF ₃	-2.6	-9.7	-11.3	-12.4
Si ₂ H ₆	-4.4	-9.6	-15.2	-14.6
P ₄	-3.3	-4.3	0.1	-6.2
SO ₂	-6.5	-7.2	-7.1	-6.2
SO ₃	-7.4	-9.1	-10.5	-9.7
OCS	-0.7	-3.3	-0.4	-0.9
CS ₂	-4.6	-6.1	-2.8	-3.9
S ₂ O	-8.0	-9.4	-7.7	-7.1
S ₃	-9.6	-11.5	-7.9	-8.2
S ₄	-16.8	-18.7	-11.6	-10.9
BeCl ₂	1.7	-3.3	1.7	1.7
CCl ₂	-3.3	-4.6	-0.8	-1.9
AlCl ₃	3.3	-6.0	-4.3	-7.5
CICN	-2.1	-3.5	-0.9	-1.8
OCIO	-5.7	-4.1	-2.2	-2.7
CIOO	-13.7	-14.3	-8.6	-7.3
Cl ₂ O	-2.6	-3.6	-0.4	-0.6
H ₂	0.0	-1.0	-1.0	-0.6
OH	-0.2	-1.7	-0.8	-1.0
HF	1.9	-0.7	0.9	0.8
H ₂ O	1.3	-2.4	-0.4	-0.4
CH	0.4	0.0	0.0	-0.4
CH ₂	0.6	-0.8	-1.6	-1.2
CH ₃	1.7	-0.5	-0.9	-0.7
CH ₄	1.3	-1.5	-1.6	-0.8
C ₂ H	-6.9	-9.4	-9.7	-10.0
C ₂ H ₂	-0.7	-4.0	-4.0	-4.3

NH ₃	1.2	-2.0	-0.6	-1.0
C ₂	-0.8	-1.8	0.6	-0.2
N ₂	-1.6	-2.7	-0.4	-1.9
CO	-0.3	-2.2	-0.4	-1.0
CN	-3.9	-4.2	-2.7	-3.3
NO	-2.5	-3.5	-0.7	-1.3
O ₂	-2.6	-3.7	0.0	0.0
OF	-5.2	-5.6	-3.0	-2.7
F ₂	-3.3	-3.5	-0.6	0.2
PH ₃	-3.8	-6.9	-8.2	-8.7
HS	-2.1	-3.4	-3.2	-3.5
H ₂ S	0.4	-2.1	-1.6	-1.8
HCl	0.5	-1.4	-0.5	-0.5
SO	-3.0	-3.0	-1.8	-0.1
ClO	-6.2	-5.8	-3.9	-5.2
CIF	-0.7	-2.0	-0.6	-0.5
P ₂	-4.8	-6.8	-6.0	-8.3
S ₂	-3.6	-4.1	-2.1	-2.5
Cl ₂	-2.4	-3.3	-1.6	-1.7
Be ₂	-2.9	-2.3	-2.9	-2.9
B ₂	-5.4	-5.4	-4.6	-4.8
BH	0.6	-0.1	-0.5	-0.5
BH ₃	0.5	-1.8	-3.4	-3.0
BN singlet	1.8	1.9	3.0	1.9
BF	1.6	-0.8	0.0	-0.1
NH	-0.2	-0.9	-0.6	-1.1
NH ₂	0.3	-1.4	-0.6	-1.3
HCN	-1.4	-3.4	-2.3	-3.2
HOF	-1.9	-4.1	-0.8	-0.3
AlH	-0.3	-1.2	-2.0	-1.9
AlH ₃	5.0	3.0	-0.7	-0.3
AlF	0.7	-2.0	-2.3	-2.9
AlCl	0.8	-2.7	-1.4	-2.4
SiH	-0.3	-1.1	-1.9	-2.2
SiH ₄	-1.7	-5.4	-9.1	-8.4
SiO	-3.3	-4.0	-4.3	-4.4
SiF	0.3	-1.9	-2.0	-2.6
CS	-3.6	-3.9	-2.2	-2.9
BN triplet	-3.6	-3.9	-4.4	-5.6
CF	0.0	-1.3	0.3	0.1
BeF ₂	2.9	-2.9	2.9	2.9
CH ₂ C	-0.7	-2.9	-2.6	-3.6
CH ₂ CH	0.8	-2.4	-2.7	-2.9
C ₂ H ₄	2.1	-1.9	-2.0	-2.1
CH ₂ NH	0.4	-2.8	-1.6	-2.0
HCO	0.2	-1.9	-0.3	-0.4
H ₂ CO	0.6	-2.4	-0.9	-0.6

CO ₂	0.0	-3.6	-0.9	-0.9
HNO	-1.8	-3.8	-0.7	-1.2
NO ₂	-3.6	-6.1	-1.2	-0.5
N ₂ O	-2.2	-5.0	-0.6	-0.2
O ₃	-14.1	-15.3	-8.6	-8.1
HO ₂	-2.0	-4.1	-0.6	-0.4
H ₂ O ₂	-1.2	-5.1	-1.2	-0.9
F ₂ O	-4.6	-5.5	-0.7	0.4
HOCl	-0.7	-3.2	-0.8	-0.8
S ₂ H	-2.5	-4.7	-3.1	-3.9

DBH24 barriers

DBH24-1 fwd	0.5	0.4	0.0	0.5
DBH24-2 fwd	0.1	-0.1	-0.9	-0.9
DBH24-3 fwd	-1.6	-1.8	-2.7	-3.9
DBH24-4 fwd	-0.1	-0.7	-1.4	-0.6
DBH24-5 fwd	-1.1	-0.5	-0.6	-0.7
DBH24-6 fwd	-0.4	-0.9	-1.4	-1.5
DBH24-7 fwd	-1.1	-1.1	-1.5	-1.2
DBH24-8 fwd	0.6	0.5	0.2	0.3
DBH24-9 fwd	-0.8	-1.5	-1.9	-1.6
DBH24-10 fwd	0.2	0.3	-0.7	-1.0
DBH24-11 fwd	0.6	0.2	0.2	-0.2
DBH24-12 fwd	-0.4	-0.6	-1.0	-0.7
DBH24-1 rev	0.5	0.5	-1.1	-2.6
DBH24-2 rev	0.1	-0.1	-0.9	-0.9
DBH24-3 rev	-3.4	-4.0	-5.0	-5.6
DBH24-4 rev	-0.1	-0.7	-1.4	-0.6
DBH24-5 rev	1.5	-1.0	-2.3	-1.3
DBH24-6 rev	-0.3	-0.1	-0.7	-1.1
DBH24-7 rev	-0.8	-1.4	-1.5	-1.1
DBH24-8 rev	0.4	0.2	-0.2	0.3
DBH24-9 rev	0.2	-1.0	-1.0	-0.4
DBH24-10 rev	2.3	0.9	0.7	0.1
DBH24-11 rev	0.1	0.3	-0.7	-0.5
DBH24-12 rev	-2.4	-2.4	-3.1	-2.5

HB16 binding energies

ClH•NH ₃	-0.3	-0.8	0.0	0.0
CO•HF	0.2	0.1	0.2	0.5
FH•NH ₃	0.2	0.2	0.3	0.9
H ₂ O•H ₂ O	0.1	0.2	0.3	0.7
HCl•HCl	-0.2	-0.2	0.2	0.1
HF•H ₂ O	0.1	0.1	0.1	0.7
HF•HF	0.0	0.1	0.1	0.6
HF•HCN	0.4	0.3	0.3	0.9
NH ₃ •NH ₃	-0.3	-0.1	-0.1	0.2
NH ₃ •H ₂ O	0.1	0.2	0.3	0.8
OC•HF	0.2	0.2	0.2	0.7
H ₃ O•H ₂ O ⁺	0.4	0.4	0.6	1.2

NH ₄ •H ₂ O ⁺	0.8	0.9	0.9	1.3
HCC•H ₂ O ⁻	0.3	0.6	0.7	1.1
CN•H ₂ O ⁻	0.9	1.0	1.2	1.6
OH•H ₂ O ⁻	2.5	3.6	3.7	4.0

WI9/04 binding energies

He•Ne	0.0	-0.1	-0.1	-0.1
He•Ar	-0.3	-0.2	-0.2	-0.2
Ne•Ne	-0.3	-0.3	-0.3	-0.2
Ne•Ar	-0.4	-0.4	-0.4	-0.3
CH ₄ •Ne	-0.8	-0.8	-0.8	-0.7
C ₆ H ₆ •Ne	-1.6	-1.7	-1.7	-1.5
CH ₄ •CH ₄	-2.0	-2.0	-2.0	-2.0
C ₂ H ₂ •C ₂ H ₂	0.6	0.8	0.9	0.9
C ₂ H ₄ •C ₂ H ₄	0.0	0.1	0.3	0.4

G2/97' ΔH_f

LiH	-1.8	-0.8	-0.6	-0.6
BeH	-3.5	-2.9	-1.0	-1.0
CH ₂ (¹ A ₁)	0.7	1.8	1.7	2.0
SiH ₂ (¹ A ₁)	-5.8	-4.2	-2.6	-2.3
SiH ₂ (³ B ₁)	-3.2	-1.8	2.3	1.3
SiH ₃	-5.1	-2.6	1.3	0.4
PH ₂	7.1	9.2	10.3	11.0
Li ₂	0.1	0.6	-0.3	-0.3
LiF	-1.7	1.4	1.3	1.3
H ₃ COH	-3.9	1.0	-0.8	-1.5
Na ₂	0.3	-4.8	-2.1	-2.1
Si ₂	-0.5	-0.4	-0.1	1.0
NaCl	0.0	4.2	-0.6	-0.6
CH ₃ Cl	-2.8	0.8	-0.6	-0.8
H ₃ CSH	-3.8	0.2	-0.7	-0.8
BCl ₃	2.8	7.2	3.0	4.7
CF ₄	-7.1	0.3	-4.0	-8.0
CCl ₄	5.4	8.8	2.1	1.7
COF ₂	13.6	19.1	15.5	13.4
SiF ₄	-5.2	3.3	6.1	6.1
SiCl ₄	-1.3	8.1	4.7	8.8
CINO	7.0	9.2	4.5	4.7
NF ₃	0.0	2.4	-2.9	-4.3
PF ₃	-0.9	5.9	6.7	7.3
ClF ₃	1.0	2.9	-0.5	-3.2
C ₂ F ₄	-20.8	-11.7	-16.1	-20.4
C ₂ Cl ₄	-7.0	-2.0	-9.4	-9.7
CF ₃ CN	-5.3	1.4	-3.0	-6.0
CH ₃ CCH (propyne)	-2.1	2.9	2.9	2.5
CH ₂ =C=CH ₂ (allene)	-3.2	1.8	1.6	1.5

C ₃ H ₄ (cyclopropene)	3.4	8.0	7.7	7.9
CH ₃ CH=CH ₂ (propylene)	-4.4	1.4	1.2	1.0
C ₃ H ₆ (cyclopropane)	-3.8	1.4	1.0	0.8
C ₃ H ₈ (propane)	-6.6	-0.3	-0.5	-1.4
CH ₂ CHCHCH ₂ (butadiene)	-2.7	3.9	3.7	3.7
C ₄ H ₆ (2-butyne)	-2.1	4.5	4.3	3.4
C ₄ H ₆ (methylene cyclopropane)	-11.8	-5.7	-6.2	-6.3
C ₄ H ₆ (bicyclobutane)	2.1	7.7	6.8	6.8
C ₄ H ₆ (cyclobutene)	-0.8	5.4	4.8	5.1
C ₄ H ₈ (cyclobutane)	-8.2	-1.4	-2.0	-2.6
C ₄ H ₈ (isobutene)	-5.9	1.3	1.0	0.4
C ₄ H ₁₀ (trans butane)	-8.7	-0.7	-1.1	-2.3
C ₄ H ₁₀ (isobutane)	-7.4	0.4	0.0	-1.3
C ₅ H ₈ (spiro pentane)	-7.0	0.2	-0.6	-0.8
C ₆ H ₆ (benzene)	-6.4	1.6	0.6	1.6
CH ₂ F ₂	-3.2	1.9	-0.4	-1.7
CHF ₃	-5.2	1.0	-2.4	-4.8
CH ₂ Cl ₂	0.2	4.0	1.0	1.0
CHCl ₃	3.3	7.1	2.2	2.2
CH ₃ CN (methyl cyanide)	-1.1	2.6	1.6	1.8
CH ₃ NO ₂ (nitromethane)	-2.5	3.2	-1.7	-3.6
CH ₃ ONO (methyl nitrite)	0.1	4.9	-0.2	-1.1
CH ₃ SiH ₃ (methyl silane)	-3.1	2.0	5.2	4.4
HCOOH (formic acid)	-2.4	2.7	-0.6	-1.4
HCOOCH ₃ (methyl formate)	-7.0	-0.6	-3.8	-5.2
CH ₃ CONH ₂ (acetamide)	-1.0	6.1	3.1	2.4
C ₂ H ₄ NH (aziridine)	-2.6	2.1	0.5	0.6
(CH ₃) ₂ NH (dimethylamine)	-2.8	3.4	2.1	1.4
CH ₃ CH ₂ NH ₂ (trans ethylamine)	-7.8	-1.3	-2.8	-3.3
CH ₂ CO (ketene)	-2.6	1.7	0.2	0.1
C ₂ H ₄ O (oxirane)	-3.3	1.3	-0.6	-1.0
CH ₃ CHO (acetaldehyde)	-2.8	2.1	0.4	-0.1
HCOCOH (glyoxal)	-3.4	1.6	-1.6	-2.2
CH ₃ CH ₂ OH (ethanol)	-5.3	1.4	-0.5	-1.5
CH ₃ OCH ₃ (dimethylether)	-4.6	1.4	-0.3	-1.6
C ₂ H ₄ S (thiirane)	-8.7	-4.7	-6.6	-6.1
(CH ₃) ₂ SO (dimethyl sulfoxide)	-4.0	1.8	1.1	-0.4
C ₂ H ₅ SH (ethanethiol)	-4.6	1.0	-0.1	-0.5
CH ₃ SCH ₃ (dimethyl sulfide)	-6.5	-0.9	-2.2	-2.6
CH ₂ =CHF (vinyl fluoride)	-7.2	-2.0	-3.1	-3.6
C ₂ H ₅ Cl (ethyl chloride)	-3.9	1.3	-0.3	-0.8
CH ₂ =CHCl (vinyl chloride)	-17.4	-12.9	-14.5	-14.4
CH ₂ =CHCN (acrylonitrile)	6.2	10.8	9.6	10.2
CH ₃ COCH ₃ (acetone)	-4.3	2.2	0.4	-0.6
CH ₃ COOH (acetic acid)	-2.6	4.3	0.9	-0.5

CH ₃ COF (acetyl fluoride)	-1.5	4.5	1.8	0.2
CH ₃ COCl (acetyl chloride)	-1.2	4.6	1.2	0.3
CH ₃ CH ₂ CH ₂ Cl (propyl chloride)	-7.1	-0.3	-2.2	-2.9
(CH ₃) ₂ CHOH (isopropanol)	-7.3	0.8	-1.3	-2.9
C ₂ H ₅ OCH ₃ (methyl ethyl ether)	-8.5	-0.7	-2.5	-4.2
(CH ₃) ₃ N (trimethylamine)	-6.8	0.6	-0.9	-2.2
C ₄ H ₄ O (furan)	-4.8	1.9	-0.4	-0.6
C ₄ H ₄ S (thiophene)	-6.1	-0.1	-2.1	-1.4
C ₄ H ₅ N (pyrrole)	-5.9	1.3	-0.7	0.0
C ₅ H ₅ N (pyridine)	-5.6	1.3	-0.7	0.3
C ₂ H ₃ (² A')	-3.6	-0.3	0.0	0.2
CH ₃ CO (² A')	-0.4	3.6	2.0	1.6
H ₂ COH (² A)	-1.7	2.6	1.0	0.5
CH ₃ O CS (² A')	0.6	3.9	2.9	2.4
CH ₃ CH ₂ O (² A'')	-4.5	0.5	-0.7	-1.5
CH ₃ S (² A')	-5.2	-2.3	-2.9	-2.9
C ₂ H ₅ (² A')	-1.4	2.8	2.9	2.6
(CH ₃) ₂ CH (² A')	-6.4	-0.5	-0.5	-1.1
(CH ₃) ₃ C (t-butyl radical)	-5.0	2.5	2.2	1.4

G2/97 IE

H	0.6	0.6	0.6	0.4
He	0.0	0.0	0.2	0.2
Li	-0.5	-0.8	-1.7	-1.7
Be	-0.1	-1.2	0.1	0.1
B	-1.8	-1.3	-2.8	-2.8
C	-1.1	-1.0	-1.6	-1.7
N	-0.6	-0.4	-0.3	-0.7
O	-1.8	-0.8	-0.2	-2.2
F	-0.9	-0.4	0.8	-1.2
Ne	-0.3	-0.7	1.0	-0.5
Na	0.3	-1.5	-0.8	-0.8
Mg	-0.6	1.1	-0.3	-0.3
Al	-2.3	-1.4	-0.8	-1.7
Si	-2.3	-0.8	0.0	-1.1
P	-1.5	0.2	1.2	0.1
S	-1.0	-1.0	-0.4	-4.5
Cl	-0.6	-2.6	-1.6	-4.8
Ar	-0.6	-4.2	-2.8	-4.7
CH ₄	7.9	7.4	7.4	7.9
NH ₃	0.3	-0.1	1.0	0.4
OH	-0.1	-0.5	0.6	-0.6
OH ₂	-0.1	-1.2	0.2	-0.7
FH	0.8	-0.5	1.3	0.0
SiH ₄	0.7	0.0	0.9	0.4
PH	0.5	1.5	2.5	1.8
PH ₂	-0.2	0.5	1.5	1.1

PH ₃	0.3	0.5	3.3	1.2
SH	-0.4	-0.3	0.9	-2.2
SH ₂ (² B ₁)	1.1	0.5	2.2	-0.1
SH ₂ (² A ₁)	0.6	0.3	1.3	0.5
ClH	0.0	-2.8	-1.3	-3.4
C ₂ H ₂	0.0	-0.7	0.0	-0.1
C ₂ H ₄	0.5	-0.1	0.7	0.7
CO	0.8	0.7	1.4	0.3
N ₂ (² Sig)	4.4	4.6	4.3	3.4
N ₂ (² Pi)	1.3	0.9	1.2	0.9
O ₂	1.8	2.4	2.6	1.8
P ₂ ² Pi	-5.5	-4.7	-3.2	-4.7
S ₂	1.2	0.6	1.5	-0.8
Cl ₂	2.7	-1.5	-0.9	-3.9
ClF	0.6	-2.2	-1.1	-3.7
CS	1.5	1.7	3.1	0.4
BF ₃	2.5	0.8	1.0	0.7
BCl ₃	20.4	16.0	15.9	13.1
B ₂ F ₄	-32.6	-32.6	-31.4	-31.7
CO ₂	4.2	3.1	3.5	3.0
CF ₂	1.0	1.3	2.9	1.6
COS	2.1	1.5	2.7	1.4
CS ₂	3.2	2.4	3.8	1.4
CH ₂	-2.2	-2.6	-2.4	-2.2
CH ₃	0.3	0.0	0.5	0.4
C ₂ H ₅	0.9	0.7	0.9	1.0
cyclopropene	-2.1	-2.6	-2.1	-1.9
CH ₂ =C=CH ₂	1.8	1.1	1.7	1.9
sec-C ₃ H ₇	7.6	7.5	7.8	8.0
C ₆ H ₆	2.0	1.6	2.4	2.3
C ₆ H ₅ CH ₃	1.7	1.3	2.1	2.1
CN	-15.7	-15.6	-17.4	-17.7
CHO	1.0	1.8	2.4	2.3
CH ₂ OH	-1.4	-1.5	-0.9	-1.2
CH ₃ O	0.8	0.3	0.4	-0.3
CH ₃ OH	3.4	2.6	3.2	2.9
CH ₃ F	2.3	1.3	1.2	1.3
CH ₂ S	1.3	0.8	2.0	0.2
HSCH ₂	2.6	2.2	3.2	1.5
CH ₃ SH	0.8	0.5	1.8	-0.1
CH ₃ Cl	2.1	0.0	0.9	-0.8
C ₂ H ₅ OH	-6.1	-6.7	-6.4	-6.9
CH ₃ CHO	3.1	2.5	3.3	3.1
CH ₃ OF	4.0	3.4	3.9	3.5
thiirane	1.4	0.9	1.9	0.4

NCCN	4.6	3.8	3.9	3.6
furan	-1.3	-1.8	-1.0	-1.1
pyrrole	1.7	1.3	2.2	2.1
C ₆ H ₅ OH	2.1	1.6	2.3	2.2
C ₆ H ₅ NH ₂	1.7	1.5	2.2	2.0
B ₂ H ₄	-12.3	-12.5	-11.8	-12.1
NH	-1.8	-1.6	-1.3	-1.4
NH ₂	3.1	3.2	4.2	3.1
N ₂ H ₂	1.0	1.3	1.7	0.8
N ₂ H ₃	0.5	0.7	1.2	0.6
HOF	2.1	1.2	1.7	0.9
SiH ₂	-1.6	-1.3	2.5	0.9
SiH ₃	-2.0	-1.9	-1.0	-0.6
Si ₂ H ₂	-0.6	0.4	0.6	-1.2
Si ₂ H ₄	-2.7	-2.7	0.2	-0.2
Si ₂ H ₅	5.9	6.2	7.2	7.3
Si ₂ H ₆	-9.0	-8.9	-6.7	-7.7

G2/97 EA

Li	0.1	0.4	0.4	0.4
B	-2.1	-4.6	-4.8	-2.2
C	-1.0	-3.1	-2.9	-1.0
O	-1.5	-3.1	-1.6	-1.9
F	0.8	-0.7	1.5	0.3
Na	-1.6	0.3	0.3	0.3
Al	-1.9	-2.5	-2.2	-0.8
Si	-1.1	-1.2	-0.8	0.2
P	-1.0	-3.6	-3.6	-3.0
S	0.3	-3.4	-2.6	-1.8
Cl	1.5	-3.5	-2.2	-1.8
CH	-3.1	-4.8	-4.4	-3.0
CH ₂	-1.0	-1.6	-0.2	-0.3
CH ₃	-5.0	-5.1	-3.8	-4.1
NH	-2.1	-3.8	-2.7	-2.6
NH ₂	-1.9	-2.7	-1.3	-2.0
OH	-0.4	-1.9	0.0	-0.6
SiH	-3.2	-3.7	-3.1	-2.2
SiH ₂	-4.2	-4.5	-3.7	-3.2
SiH ₃	-0.9	-0.9	1.8	0.9
PH	-0.7	-2.9	-2.1	-1.7
PH ₂	-1.0	-2.5	-1.2	-1.3
SH	0.4	-3.7	-2.4	-1.7
O ₂	-1.0	-1.6	-0.9	-1.1
NO	0.5	0.0	0.2	0.6
CN	2.8	2.0	2.1	1.5
PO	0.3	-1.0	1.6	2.3
S ₂	3.3	-0.2	0.4	0.3
Cl ₂	0.8	-3.2	-2.2	-1.7

CC	-1.2	-1.7	-3.0	-2.8
CCO	1.5	0.7	1.0	1.4
CF ₂ ² B ₁	-1.8	-1.9	-1.3	-2.1
NCO	2.1	1.0	1.8	2.2
ONO	1.3	1.2	1.9	1.0
O ₃	6.5	6.2	6.0	5.8
OF	2.9	1.6	2.7	1.9
SO ₂	3.4	1.4	2.9	3.1
S ₂ O	2.5	0.4	1.4	1.0
C ₂ H	-0.9	-1.2	-0.2	0.0
C ₂ H ₃	0.7	0.9	2.0	1.6
H ₂ C=C=C	2.3	1.7	1.9	2.4
H ₂ C=C=CH	1.5	1.4	2.3	1.9
CH ₂ CHCH ₂	0.5	0.2	1.2	1.0
HCO	-2.5	-2.7	-1.8	-2.8
HCF ² A''	-0.3	-0.8	-0.3	-0.4
CH ₃ O	-1.3	-2.2	-0.7	-1.1
CH ₃ S	1.0	-1.5	-0.4	-0.3
CH ₂ S	4.0	2.3	2.9	2.9
CH ₂ CN	0.3	-0.2	0.5	0.5
CH ₂ NC	7.4	7.4	8.1	8.0
CHCO	-0.6	-1.7	-1.0	-0.6
CH ₂ CHO	0.8	0.0	0.8	0.8
CH ₃ CO	-2.6	-2.7	-1.4	-2.4
CH ₃ CH ₂ O	-2.9	-3.5	-1.9	-2.4
CH ₃ CH ₂ S	0.9	-1.1	0.0	-0.2
LiH	-0.8	-0.9	-0.9	-0.9
HNO	-0.2	-0.5	0.2	-0.2
HOO ¹ A'	0.2	-0.7	0.3	-0.1
G2/97 PA				
NH ₃	0.2	-0.8	-1.3	-0.6
OH ₂	-1.0	-2.0	-2.6	-1.5
C ₂ H ₂	3.5	3.6	3.4	3.3
SiH ₄	1.4	1.1	0.8	0.5
PH ₃	-1.4	-2.8	-5.4	-3.6
SH ₂	2.3	1.8	0.3	2.4
ClH	2.6	3.3	2.5	4.0
H ₂	1.8	1.5	1.5	1.4
G3/99' ΔH_f				
methyl allene		3.4	3.1	2.6
isoprene		5.5	4.9	4.6
cyclopentane		-0.9	-1.8	-2.9
n-pentane		0.3	-0.3	-1.7
neo pentane		-0.2	-1.0	-2.8
1,3 cyclohexadiene		4.1	3.1	3.2
1,4 cyclohexadiene		5.3	4.4	4.8

cyclohexane	3.6	2.5	1.3
n-hexane	1.5	0.7	-0.9
3-methyl pentane	2.1	1.2	-0.7
toluene	3.7	2.3	2.8
n-heptane	-1.0	-1.9	-3.7
cyclooctatetraene	8.7	7.5	8.1
n-octane	0.8	-0.3	-2.4
naphthalene	1.5	-0.7	0.0
azulene	11.3	8.9	9.5
acetic acid methyl ester	7.7	4.5	2.5
t-butanol	4.4	2.1	-0.2
aniline	3.8	1.2	2.0
phenol	8.0	5.1	5.1
divinyl ether	8.2	6.4	5.6
tetrahydrofuran	4.6	2.4	0.7
cyclopentanone	1.1	-1.3	-2.6
benzoquinone	13.0	8.9	8.3
pyrimidine	-4.2	-7.2	-6.2
dimethyl sulphone	2.8	3.9	2.6
chlorobenzene	3.2	0.2	1.1
butanedinitrile	5.3	3.0	3.6
1,4-dipyridine pyrazine	13.7	10.6	11.7
CH ₃ -C(=O)-CCH	17.7	15.9	15.1
crotonaldehyde	2.1	0.2	-0.4
Acetic anhydride	4.8	-0.1	-2.9
2,5-Dihydrothiophene	-1.6	-3.6	-3.3
(CH ₃) ₂ CH-CN	10.6	9.1	8.7
Methyl ethyl ketone	4.4	2.4	1.2
(CH ₃) ₂ CH-CHO	8.6	6.6	5.3
1,4-Dioxane	5.3	1.6	-1.0
Tetrahydrothiophene	2.4	0.2	-0.2
t-Butyl chloride	3.3	0.8	-0.5
n-Butyl chloride	2.8	0.6	-0.3
Tetrahydropyrrole	2.8	0.8	0.1
Nitro-s-butane	6.5	1.1	-2.0
Diethyl ether	2.7	0.7	-1.3
acetaldehyde dimethyl acetal	5.0	1.5	-1.9
t-butanethiol	1.9	0.0	-1.2
Diethyl disulfide	5.3	2.1	1.9
t-butylamine	4.8	2.8	1.3
Tetramethylsilane	15.2	16.8	15.5
2-methyl thiophene	1.7	-0.6	-0.4
N-methyl pyrrole	4.1	2.1	2.0
Tetrahydropyran	5.0	2.6	0.7
Diethyl ketone	0.2	-1.9	-3.4
Isopropyl acetate	6.7	3.1	0.1
Tetrahydrothiopyran	2.7	0.3	-0.4
piperidine	5.4	3.3	2.1

t-butyl methyl ether	4.9	2.6	-0.4
1,3-DiFluorobenzene	7.0	3.7	2.3
1,4-DiFluorobenzene	6.3	3.0	1.7
Fluorobenzene	5.6	3.4	3.2
Di-isopropyl ether	3.5	1.0	-2.1
PF ₅	5.3	7.7	5.8
SF ₆	-3.8	-3.3	-9.2
SCl ₂	5.5	2.5	3.6
POCl ₃	8.7	7.0	9.9
PCl ₅	-2.2	-8.3	3.0
Cl ₂ O ₂ S	11.2	10.6	10.4
PCl ₃	9.2	5.8	9.1
Cl ₂ S ₂	-2.1	-6.2	-4.8
SiCl ₂	5.3	2.9	5.0
CF ₃ Cl	3.1	-1.6	-4.7
C ₂ F ₆	5.1	-1.4	-8.8
CF ₃	-0.5	-3.5	-5.9
phenyl radical	-0.3	-1.3	-0.2

RR49 ΔH

ADD1	2.0	0.1	-0.3
ADD2	0.5	-0.8	-1.3
ADD3	-0.3	-0.8	-1.5
ADD4	-0.9	-0.9	-0.9
ADD5	-0.7	-0.6	-0.7
ADD6	-1.0	-0.4	-0.7
ADD7	-1.6	-0.6	-1.2
ADD8	-2.4	-0.7	-1.5
ADD9	-3.4	-0.7	-1.9
ADD10	0.7	-1.7	-2.0
ADD11	1.9	-0.6	-1.0
ADD12	0.6	1.0	0.8
ADD13	3.0	3.5	3.4
ADD14	0.0	0.9	0.3
ADD15	-1.1	-0.6	-1.3
ADD16	0.5	-1.8	-2.2
ADD17	0.4	-1.6	-2.1
ADD18	2.1	-0.4	-0.9
ADD19	1.5	-0.9	-1.3
ADD20	1.1	-1.1	-1.3
ADD21	1.0	-1.3	-1.6
ABS1	-1.7	-1.8	-1.7
ABS2	-1.9	-2.1	-2.0
ABS3	0.3	0.1	0.2
ABS4	-1.0	0.5	0.3
ABS5	-1.6	0.2	0.1
ABS6	-2.3	-0.8	-1.0
ABS7	1.0	0.5	0.8
ABS8	1.3	0.7	1.0

ABS9	1.9	1.3	1.6
ABS10	-1.4	-1.0	-0.8
ABS11	-0.5	0.1	0.2
ABS12	-2.2	-0.5	-0.6
ABS13	-4.7	-3.1	-3.3
ABS14	0.1	0.0	0.3
ABS15	0.6	1.1	1.3
ABS16	0.2	0.1	0.4
ABS17	0.6	0.1	0.4
ABS18	0.1	0.0	0.3
ABS19	-0.1	0.2	0.4
ABS20	-0.1	0.2	0.4
ABS21	1.5	1.0	1.3
ABS22	-0.2	-0.2	-0.1
ABS23	-1.1	-0.6	-0.5
ABS24	0.8	1.7	1.7
ABS25	1.7	0.9	1.5
ABS26	-2.1	-0.6	-0.8
ABS27	0.4	0.2	0.3
ABS28	1.7	2.0	2.2

PR8 barriers

PR8-1	-3.1	-1.7	-1.4
PR8-2	-1.2	-1.6	-1.6
PR8-3	-1.3	-1.4	-1.5
PR8-4	1.4	-1.1	-0.6
PR8-5	1.1	0.3	-0.1
PR8-6	-2.8	-2.9	1.3
PR8-7	-1.6	-1.2	-1.2
PR8-8	-4.0	-3.0	-3.8

BDE261 BDEs

H-H	-1.0	-1.0	-0.6
H ₃ C-H	-0.5	-0.3	0.2
H ₃ C-CH ₃	-0.2	0.6	0.9
H ₃ C-NH ₂	-0.9	0.0	0.6
H ₃ C-OH	-1.1	0.1	0.8
H ₃ C-F	-1.8	-0.3	0.3
H ₃ C-SiH ₃	-0.3	0.8	0.4
H ₃ C-PH ₂	-0.4	0.0	0.1
H ₃ C-SH	-0.4	0.6	0.9
H ₃ C-Cl	-1.4	0.4	0.4
H ₂ N-H	-1.5	-0.9	-0.7
H ₂ N-NH ₂	-1.7	-0.6	-0.2
H ₂ N-OH	-1.4	0.1	0.9
H ₂ N-F	-1.5	0.4	0.9
H ₂ N-SiH ₃	-1.2	-0.7	-0.8
H ₂ N-PH ₂	-1.4	-1.7	-1.5
H ₂ N-SH	-1.0	-0.4	-0.1
H ₂ N-Cl	-1.1	0.4	0.5

HO-H	-2.0	-1.0	-0.8
HO-OH	-0.7	1.3	2.0
HO-F	-0.7	1.7	2.4
HO-SiH ₃	-1.5	-1.1	-1.1
HO-PH ₂	-1.5	-1.8	-1.3
HO-SH	-1.0	-0.5	0.1
HO-Cl	-0.8	0.6	0.8
F-H	-2.5	-1.0	-1.0
F-F	-0.3	2.5	3.3
F-SiH ₃	-2.3	-1.9	-2.5
F-PH ₂	-2.3	-2.5	-2.3
F-SH	-1.8	-1.1	-0.7
F-Cl	-1.3	0.1	0.3
H ₃ Si-H	-1.1	-0.9	-1.1
H ₃ Si-SiH ₃	0.0	2.2	0.8
H ₃ Si-PH ₂	-0.4	1.2	0.2
H ₃ Si-SH	-1.3	0.3	-0.9
H ₃ Si-Cl	-2.9	-1.2	-2.5
H ₂ P-H	-0.9	-1.2	-0.9
H ₂ P-PH ₂	-0.2	0.6	0.3
H ₂ P-SH	-0.8	0.1	-0.2
H ₂ P-Cl	-2.1	-1.0	-1.6
HS-H	-1.2	-0.9	-0.7
HS-SH	-0.7	0.5	0.3
HS-Cl	-1.2	0.2	-0.1
Cl-H	-1.9	-1.0	-1.0
Cl-Cl	-0.9	0.8	0.7
MeH ₂ C-H	-0.6	-0.4	0.1
MeH ₂ C-CH ₃	0.1	0.9	1.2
MeH ₂ C-NH ₂	-0.7	0.1	0.8
MeH ₂ C-OH	-1.0	0.1	1.0
MeH ₂ C-F	-1.6	-0.2	0.6
MeH ₂ C-SiH ₃	0.1	1.2	1.1
MeH ₂ C-PH ₂	-0.1	0.4	0.7
MeH ₂ C-SH	-0.1	1.1	1.4
MeH ₂ C-Cl	-1.1	0.8	0.9
MeHN-H	-1.4	-1.0	-0.7
MeHN-CH ₃	-0.5	0.3	0.9
MeHN-NH ₂	-1.3	-0.2	0.5
MeHN-OH	-1.0	0.4	1.4
MeHN-F	-1.2	0.6	1.5
MeHN-SiH ₃	-0.8	-0.2	-0.3
MeHN-PH ₂	-1.0	-1.2	-0.8
MeHN-SH	-0.6	0.1	0.7
MeHN-Cl	-0.6	1.0	1.4
MeO-H	-1.7	-0.9	-0.6

MeO-CH ₃	-0.5	0.5	1.2
MeO-NH ₂	-0.7	0.5	1.5
MeO-OH	-0.3	1.5	2.5
MeO-F	-0.3	1.8	2.6
MeO-SiH ₃	-0.8	-0.5	-0.5
MeO-PH ₂	-0.8	-1.1	-0.6
MeO-SH	-0.4	0.2	0.9
MeO-Cl	-0.3	1.3	1.6
MeH ₂ Si-H	-1.0	-0.8	-1.0
MeH ₂ Si-CH ₃	-0.3	0.8	0.4
MeH ₂ Si-NH ₂	-1.2	-0.6	-0.8
MeH ₂ Si-OH	-1.5	-1.0	-1.0
MeH ₂ Si-F	-2.4	-1.8	-2.4
MeH ₂ Si-SiH ₃	0.1	2.4	1.2
MeH ₂ Si-PH ₂	-0.2	1.5	0.5
MeH ₂ Si-SH	-1.2	0.5	-0.6
MeH ₂ Si-Cl	-2.8	-0.9	-2.2
MeHP-H	-1.0	-1.4	-1.2
MeHP-CH ₃	-0.4	-0.1	0.1
MeHP-NH ₂	-1.4	-1.6	-1.4
MeHP-OH	-1.5	-1.8	-1.3
MeHP-F	-2.4	-2.6	-2.4
MeHP-SiH ₃	-0.2	1.4	0.4
MeHP-PH ₂	-0.1	0.7	0.3
MeHP-SH	-0.7	0.2	-0.1
MeHP-Cl	-2.0	-0.9	-1.6
MeS-H	-1.1	-0.9	-0.7
MeS-CH ₃	-0.3	0.6	0.8
MeS-NH ₂	-0.9	-0.5	-0.1
MeS-OH	-0.9	-0.4	0.3
MeS-F	-1.7	-1.1	-0.8
MeS-SiH ₃	-0.9	0.6	-0.6
MeS-PH ₂	-0.6	0.3	-0.1
MeS-SH	-0.4	0.7	0.5
MeS-Cl	-1.1	0.4	-0.1
Me ₂ HC-H	-0.4	-0.2	0.2
Me ₂ HC-CH ₃	0.4	1.2	1.7
Me ₂ HC-NH ₂	-0.4	0.4	1.4
Me ₂ HC-OH	-0.6	0.5	1.7
Me ₂ HC-F	-1.4	0.1	1.2
Me ₂ HC-SiH ₃	0.5	1.8	1.8
Me ₂ HC-PH ₂	0.2	0.9	1.4
Me ₂ HC-SH	0.2	1.5	2.0
Me ₂ HC-Cl	-0.8	1.2	1.5
Me ₂ N-H	-1.3	-1.0	-0.5
Me ₂ N-CH ₃	-0.2	0.6	1.5

Me ₂ N-NH ₂	-0.7	0.4	1.6
Me ₂ N-OH	-0.7	0.6	2.2
Me ₂ N-F	-0.9	0.8	2.5
Me ₂ N-SiH ₃	-0.4	0.3	0.5
Me ₂ N-PH ₂	-0.3	-0.1	0.7
Me ₂ N-SH	-0.2	0.7	1.6
Me ₂ N-Cl	-0.3	1.5	2.5
Me ₂ HSi-H	-0.9	-0.6	-0.9
Me ₂ HSi-CH ₃	-0.3	0.9	0.6
Me ₂ HSi-NH ₂	-1.2	-0.5	-0.7
Me ₂ HSi-OH	-1.5	-0.9	-0.9
Me ₂ HSi-F	-2.4	-1.7	-2.1
Me ₂ HSi-SiH ₃	0.4	2.8	1.8
Me ₂ HSi-PH ₂	0.0	1.8	1.0
Me ₂ HSi-SH	-1.0	0.9	0.0
Me ₂ HSi-Cl	-2.6	-0.5	-1.6
Me ₂ P-H	-1.0	-1.4	-1.3
Me ₂ P-CH ₃	-0.3	0.2	0.5
Me ₂ P-NH ₂	-1.2	-1.4	-0.9
Me ₂ P-OH	-1.4	-1.7	-1.0
Me ₂ P-F	-2.4	-2.5	-2.2
Me ₂ P-SiH ₃	0.0	1.6	0.8
Me ₂ P-PH ₂	0.0	0.9	0.7
Me ₂ P-SH	-0.6	0.4	0.3
Me ₂ P-Cl	-2.0	-0.6	-1.1
Me ₃ C-H	-0.3	-0.1	0.4
Me ₃ C-CH ₃	0.8	1.7	2.5
Me ₃ C-NH ₂	-0.1	0.8	2.2
Me ₃ C-OH	-0.4	0.8	2.5
Me ₃ C-F	-1.0	0.4	2.0
Me ₃ C-SiH ₃	1.1	2.6	3.0
Me ₃ C-PH ₂	0.7	1.6	2.4
Me ₃ C-SH	0.6	2.2	3.0
Me ₃ C-Cl	-0.4	1.8	2.3
Me ₃ Si-H	-0.8	-0.5	-0.9
Me ₃ Si-CH ₃	-0.2	1.0	0.7
Me ₃ Si-NH ₂	-1.2	-0.5	-0.6
Me ₃ Si-OH	-1.5	-0.9	-0.8
Me ₃ Si-F	-2.4	-1.7	-2.0
Me ₃ Si-SiH ₃	0.6	3.1	2.3
Me ₃ Si-PH ₂	0.2	2.2	1.5
Me ₃ Si-SH	-0.7	1.4	0.6
Me ₃ Si-Cl	-2.4	-0.1	-1.1
FH ₂ C-H	-0.7	-0.6	-0.2

FH ₂ C-CH ₃	-0.2	0.5	0.9
FH ₂ C-NH ₂	-1.0	-0.2	0.4
FH ₂ C-OH	-1.1	0.0	0.9
FH ₂ C-F	-1.8	-0.4	0.4
FH ₂ C-SiH ₃	-0.2	0.6	0.4
FH ₂ C-PH ₂	-0.3	0.0	0.4
FH ₂ C-SH	-0.3	0.7	1.2
FH ₂ C-Cl	-1.3	0.4	0.7
FHN-H	-1.4	-1.2	-0.9
FHN-CH ₃	-0.7	0.0	0.9
FHN-NH ₂	-1.5	-0.5	0.1
FHN-OH	-1.1	0.2	1.3
FHN-F	-1.3	0.4	1.3
FHN-SiH ₃	-0.8	-0.5	-0.5
FHN-PH ₂	-0.9	-1.2	-0.7
FHN-SH	-0.4	0.2	0.9
FHN-Cl	-0.6	0.7	1.1
FO-H	-1.8	-1.1	-1.0
FO-CH ₃	-0.9	0.0	0.7
FO-NH ₂	-1.6	0.0	0.8
FO-OH	-0.6	1.2	2.1
FO-F	-0.4	1.6	2.4
FO-SiH ₃	-1.3	-1.1	-1.2
FO-PH ₂	-1.3	-1.5	-1.0
FO-SH	-0.3	0.4	0.9
FO-Cl	-0.3	0.9	1.2
FH ₂ Si-H	-1.1	-0.6	-1.0
FH ₂ Si-CH ₃	-0.4	1.0	0.5
FH ₂ Si-NH ₂	-1.2	-0.3	-0.6
FH ₂ Si-OH	-1.5	-0.7	-0.8
FH ₂ Si-F	-2.3	-1.5	-2.2
FH ₂ Si-SiH ₃	-0.2	2.2	0.8
FH ₂ Si-PH ₂	-0.4	1.4	0.3
FH ₂ Si-SH	-1.3	0.6	-0.6
FH ₂ Si-Cl	-2.8	-0.8	-2.3
FHP-H	-1.1	-1.6	-1.5
FHP-CH ₃	-0.6	-0.4	-0.3
FHP-NH ₂	-1.6	-1.9	-1.9
FHP-OH	-1.6	-2.0	-1.6
FHP-F	-2.3	-2.7	-2.7
FHP-SiH ₃	-0.5	0.7	-0.2
FHP-PH ₂	-0.4	0.2	-0.1
FHP-SH	-0.9	-0.1	-0.5
FHP-Cl	-2.2	-1.2	-1.9
FS-H	-1.3	-1.2	-1.2
FS-CH ₃	-0.6	0.3	0.4

FS-NH ₂	-1.3	-1.0	-0.9
FS-OH	-1.1	-0.7	-0.3
FS-F	-1.7	-1.3	-1.2
FS-SiH ₃	-1.2	0.0	-1.1
FS-PH ₂	-0.9	-0.1	-0.5
FS-SH	-0.6	0.3	0.0
FS-Cl	-1.2	0.1	-0.4
F ₂ HC-H	-1.0	-0.7	-0.6
F ₂ HC-CH ₃	-0.4	0.4	1.1
F ₂ HC-NH ₂	-1.2	-0.3	0.4
F ₂ HC-OH	-1.4	-0.3	0.8
F ₂ HC-F	-2.1	-0.7	0.4
F ₂ HC-SiH ₃	-0.4	0.5	0.4
F ₂ HC-PH ₂	-0.4	0.0	0.5
F ₂ HC-SH	-0.4	0.6	1.4
F ₂ HC-Cl	-1.4	0.3	0.9
F ₂ N-H	-1.4	-1.2	-0.9
F ₂ N-CH ₃	-0.4	0.2	1.9
F ₂ N-NH ₂	-1.2	-0.3	0.5
F ₂ N-OH	-0.8	0.3	1.6
F ₂ N-F	-0.9	0.6	1.8
F ₂ N-SiH ₃	-0.4	-0.3	-0.1
F ₂ N-PH ₂	-0.3	-0.5	0.3
F ₂ N-SH	0.1	0.6	1.6
F ₂ N-Cl	-0.1	1.1	1.7
F ₂ HSi-H	-1.0	-0.4	-0.9
F ₂ HSi-CH ₃	-0.5	1.1	0.8
F ₂ HSi-NH ₂	-1.3	-0.2	-0.4
F ₂ HSi-OH	-1.5	-0.6	-0.6
F ₂ HSi-F	-2.3	-1.4	-2.0
F ₂ HSi-SiH ₃	-0.3	2.2	0.9
F ₂ HSi-PH ₂	-0.5	1.6	0.5
F ₂ HSi-SH	-1.3	0.8	-0.4
F ₂ HSi-Cl	-2.8	-0.6	-2.1
F ₂ P-H	-1.3	-2.1	-2.0
F ₂ P-CH ₃	-0.8	-0.8	-0.6
F ₂ P-NH ₂	-1.9	-2.3	-2.3
F ₂ P-OH	-1.8	-2.3	-1.9
F ₂ P-F	-2.4	-3.0	-2.9
F ₂ P-SiH ₃	-0.7	0.1	-0.6
F ₂ P-PH ₂	-0.5	-0.1	-0.3
F ₂ P-SH	-1.0	-0.5	-0.6
F ₂ P-Cl	-2.3	-1.5	-2.4
F ₃ C-H	-1.2	-0.9	-0.9
F ₃ C-CH ₃	-0.6	0.2	1.4

F_3C-NH_2	-1.4	-0.6	0.3
F_3C-OH	-1.7	-0.7	0.7
F_3C-F	-2.5	-1.2	0.4
F_3C-SiH_3	-0.4	0.5	0.5
F_3C-PH_2	-0.5	0.0	0.6
F_3C-SH	-0.5	0.6	1.6
F_3C-Cl	-1.5	0.2	0.9
F_3Si-H	-1.0	-0.3	-0.9
F_3Si-CH_3	-0.6	1.1	1.0
F_3Si-NH_2	-1.3	-0.1	-0.2
F_3Si-OH	-1.5	-0.6	-0.5
F_3Si-F	-2.2	-1.5	-1.9
$F_3Si-SiH_3$	-0.4	2.2	1.0
F_3Si-PH_2	-0.6	1.5	0.7
F_3Si-SH	-1.3	0.8	-0.1
F_3Si-Cl	-2.7	-0.6	-1.9