Table S1. BDEs calculated using six functionals with three different basis sets for ten representative bonds. In all cases, the MP2/6-31G(d) geometry was used and zero-point energy and enthalpy corrections were derived from HF/6-31G(d) geometry/frequency calculations. All values are in kcal/mol.

		CH_3-H	NH_2-H	HO-H	HS-H	H_3C-CH_3	H_3C-NH_2	H_3C-OH	H_2N-NH_2	HO-OH	HS-SH	MAE
Experiment		104.8	108.6	118.8	90.1	89.7	84.9	92.0	68.2	50.4	66.0	--
G3MP2		104.1	106.6	117.8	90.6	88.5	85.6	90.2	63.7	47.5	62.2	1.9
B3LYP	**6-31G***	104.0	101.0	108.7	86.1	87.9	80.7	88.3	61.3	48.7	54.6	5.2
	6-311G**	102.8	103.3	112.2	87.7	84.7	79.0	86.0	61.3	46.5	52.3	5.8
	6-311G(2d,2p)	103.1	103.6	113.6	88.7	84.6	78.6	86.8	60.4	48.1	57.2	4.9
B3P86	**6-31G***	106.5	104.7	112.8	89.3	91.5	85.1	92.2	66.6	52.8	59.5	2.5
	6-311G**	105.2	106.9	116.3	91.1	88.6	83.4	90.2	66.4	50.4	57.7	2.0
	6-311G(2d,2p)	105.5	107.1	117.7	92.2	88.6	83.0	91.0	65.4	52.2	62.9	1.7
B3PW91	**6-31G***	102.9	100.9	108.7	86.0	88.9	82.2	89.0	63.5	49.4	57.2	4.5
	6-311G**	101.7	103.0	112.1	87.7	86.0	80.6	87.1	63.3	47.1	55.6	4.9
	6-311G(2d,2p)	101.9	103.2	113.5	88.7	86.0	80.1	87.9	62.3	48.9	60.8	4.0
BHandHLYP	**6-31G***	102.1	98.2	103.9	83.7	85.4	76.9	81.9	55.7	34.7	49.7	10.1
	6-311G**	100.8	100.4	107.4	85.6	82.1	75.1	79.9	55.6	32.7	48.0	10.6
	6-311G(2d,2p)	101.1	100.7	108.8	86.5	82.1	74.7	80.6	54.6	34.4	52.7	9.7
mPW1PW91	**6-31G***	102.1	99.9	107.3	85.2	89.4	82.4	88.7	63.5	47.8	57.4	5.0
	6-311G**	100.8	101.9	110.7	86.8	86.5	80.8	86.9	63.2	45.5	55.8	5.5
	6-311G(2d,2p)	101.0	102.1	112.1	87.9	86.5	80.4	87.7	62.3	47.4	60.9	4.5
PBE1PBE	**6-31G***	102.4	100.3	107.7	85.4	91.1	84.1	90.2	65.2	49.4	58.7	4.2
	6-311G**	101.1	102.4	111.1	87.1	88.2	82.5	88.4	65.0	47.0	57.0	4.4
	6-311G(2d,2p)	101.4	102.6	112.5	88.1	88.2	82.1	89.2	64.0	49.0	62.3	3.4

Table S2. BDEs calculated using B3P86/Basis//B3P86/6-31G(d) for the purpose of determining the optimal basis set for the model chemistries presented in this work. Experimental values are also shown. Overall MAEs are given at the bottom of the Table. All values are in kcal/mol.

Bond	Basis				Expt
	6-31G(d)	6-311G(d,p)	6-311G(2d,2p)	6-311++G(3df,3pd)	
HO-H	113.5	116.9	118.4	120.0	118.8
HS-H	89.8	91.6	92.7	92.9	90.1
H2N-H	105.4	107.5	107.7	108.3	108.6
H_3C-H	107.4	106.2	106.5	105.7	104.8
C_2H_5O-H	99.8	103.6	104.2	105.0	104.6
CH_3NH-H	97.2	99.0	99.1	99.5	100.0
C_2H_5-H	102.6	101.5	101.7	100.9	100.5
HOO-H	80.3	83.9	84.6	85.6	87.8
H_2NNH-H	79.2	80.7	81.3	81.6	82.2
H_3C-NO_2	60.4	58.6	59.1	59.2	62.0
H_3C-Br	77.1	73.2	73.3	73.5	69.8
H_3C-SH	75.1	73.2	74.1	74.0	73.6
H_3C-Cl	84.9	83.3	84.9	85.1	83.8
H_3C-NH_2	86.2	84.5	84.1	83.8	84.9
H_3C-CH_3	92.9	89.9	89.9	88.6	89.7
H_3C-OH	93.3	91.4	92.2	92.2	92.0
H_3C-CF_3	102.2	100.8	100.3	99.3	101.4
H_3C-F	111.3	109.0	111.1	112.4	109.8
H_3C-CN	127.6	126.6	126.3	126.6	121.8
HO-OH	53.6	51.3	53.1	50.8	50.4
HS-SH	60.0	58.3	63.4	64.6	66.0
H_2N-NH_2	67.5	67.3	66.4	66.1	68.2
H_3C-SC_2H_5	71.6	69.8	70.8	70.7	72.7
H_3C-OC_2H_5	83.6	81.5	81.8	81.6	82.5
H_3C-$NHCH_3$	81.5	79.6	79.2	78.8	82.2
H_3C-C_2H_5	89.7	87.0	86.9	85.8	88.2
MAE	**2.7**	**1.8**	**1.6**	**1.6**	---

Table S3. Calculated C-H BDEs using two different basis sets to illustrate basis set independence in these systems. Geometry optimizations and scaled frequencies were obtained from HF/3-21G(d) and B3P86/6-31G(d) calculations and single-point energies are calculated using B3P86 with the indicated basis set. The MAEs are computed for the small basis set BDEs relative to those calculated with the larger basis set. All values are in kcal/mol.

	B3P86/Basis//HF/3-21G(d)		B3P86/Basis//B3P86/6-31G(d)	
	6-31G*	6-311G(2d,2p)	6-31G*	6-311G(2d,2p)
C_6H_5-H	111.9	112.9	113.0	113.3
H_2CCH-H	111.5	111.6	111.6	111.2
F_3C-H	104.8	106.0	105.0	106.0
$(CH_2)_2CH$-H	109.6	109.5	108.9	108.7
H_3C-H	107.5	106.6	107.4	106.5
H_3CCH_2-H	102.9	102.1	102.6	101.7
$H_3CCH_2CH_2$-H	103.2	102.4	102.9	101.9
$HOCH_2$-H	97.0	96.5	96.8	96.0
Cl_3C-H	93.2	93.9	93.0	93.6
$HCOCH_2$-H	97.9	98.2	95.3	95.3
$NCCH_2$-H	94.8	95.2	95.8	95.7
H_2NCH_2-H	93.9	92.7	93.9	92.8
OCH-H	90.1	89.0	89.8	88.7
$C_6H_5CH_2$-H	89.1	89.1	90.6	90.0
$C_4H_5CH_2$-H	80.1	80.2	81.6	81.2
$(H_3C_2)_2CH$-H	71.0	71.8	72.5	72.8
MAE		**0.6**		**0.8**

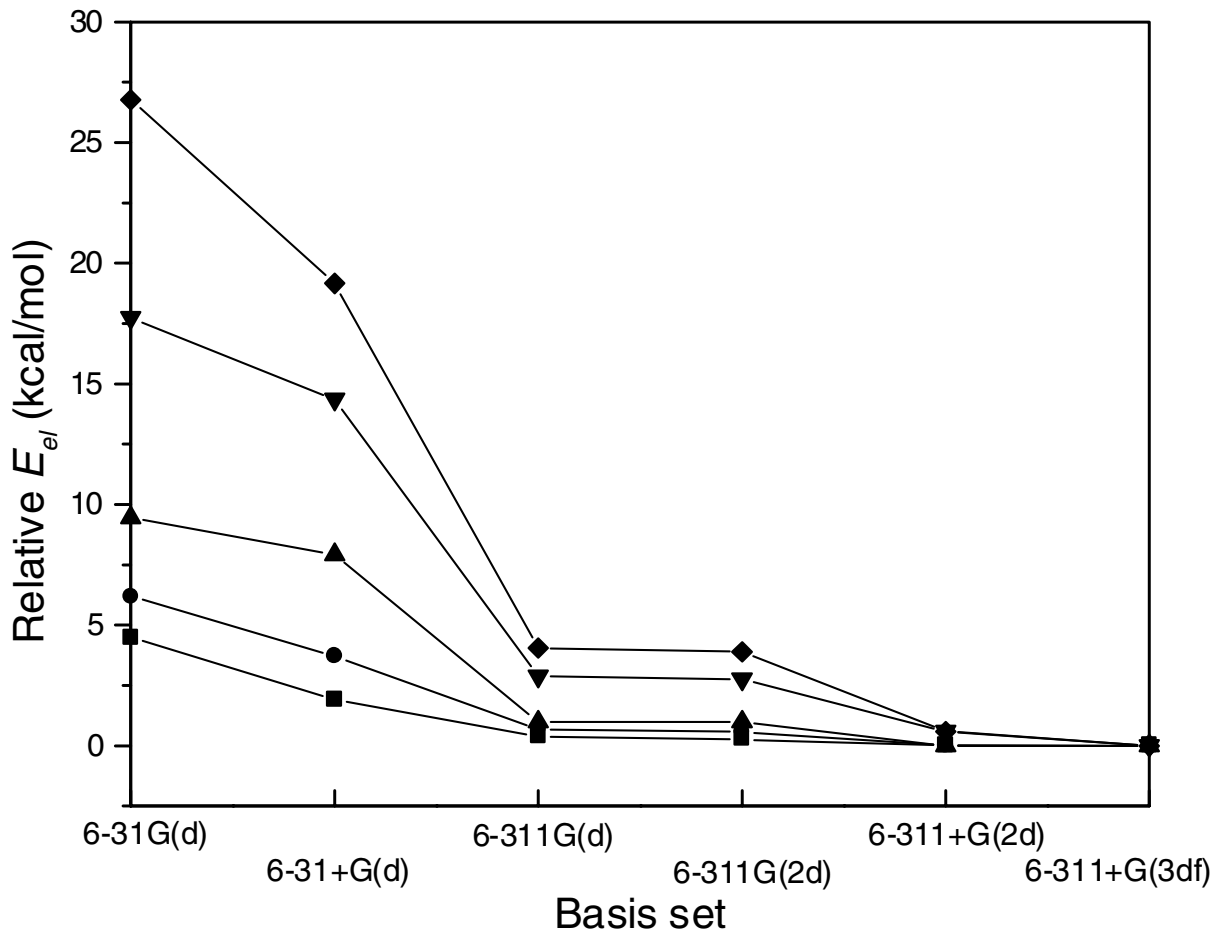

Figure S1. B3P86 electronic energy as a function of basis set for main group elements of the first row (■ = boron, ● = carbon, ▲= nitrogen, ▼= oxygen, ♦ = fluorine).

Table S4. BDEs for 15 X-H, X-X, and X-Y bonds calculated using mB3LYP/6-311+G(3df,2p) electronic energies. For the two DFT methods, the B3P86/6-31G(d) geometries and scaled frequencies were used. All values are in kcal/mol.

Bond	B3P86/6-311G(2d,2p)	mB3LYP/6-11+G(3df,2p)	G3(MP2)
H_3C-H	106.5	104.6	104.1
H_2N-H	107.7	106.9	106.6
HO-H	118.4	116.6	117.8
SiH_3-H	91.3	91.5	90.9
HS-H	92.7	90.8	90.6
H_3C-CH_3	89.9	90.4	88.5
H_3C-NH_2	84.1	85.3	85.6
H_3C-OH	92.2	91.6	90.2
H_3C-SH	74.1	73.8	73.1
H_3C-F	111.1	112.7	109.5
H_3C-Cl	84.9	87.1	82.8
H_3C-Br	73.1	75.4	----
HO-OH	53.1	42.3	47.5
HS-SH	63.4	62.0	62.2
H_2N-NH_2	66.4	66.3	63.7
MAE	**1.2**	**2.0**	**1.6**
RMSE	**1.5**	**2.9**	**1.9**
MaxE	**3.3**	**8.1**	**4.5**

Table S5. BDEs of phenolic antioxidants using the MLM2 approach of reference 7 and the B3P86/6-31G(d) model of this work, along with experimental values. Relative BDEs are given in brackets. All data are in kcal/mol.

Antioxidant	MLM2 (ref. 6)	B3P86/6-31G(d) model (this work)	Experiment
Phenolic antioxidants[a]			
Phenol	87.5 (0.0)	87.8 (0.0)	88.3 (0.0)
p-methylphenol	85.2 (-2.3)	85.8 (-2.0)	86.2 (-2.1)
p-methoxyphenol	81.3 (-6.2)	82.1 (-5.7)	82.8 (-5.5)
2,4,6-trimethylphenol	80.7 (-6.8)	81.3 (-6.5)	82.7 (-5.6)
2,3,5,6-tetramethyl-4-methoxyphenol	79.5 (-8.0)	79.8 (-8.0)	81.8 (-6.5)
2,4,6-trimethoxyphenol	78.0 (-9.5)	78.6 (-9.2)	80.0 (-8.3)
2,3,6-trimethyl-4-methoxyphenol	76.9 (-10.6)	77.5 (-10.3)	79.2 (-9.1)
2,2,5,7,8-pentamethyl-6-hydroxychroman	74.9 (-12.6)	76.1 (-11.7)	78.3 (-10.1)
Pyrimidinolic antioxidants[b]			
5-pyrimidinol	89.6 (0.0)	89.8 (0.0)	91.1 (0.0)
2,4,6-trimethyl-5-pyrimidinol	83.0 (-6.6)	83.6 (-6.2)	85.2 (-5.9)
2-N,N-dimethyl-4,6-dimethyl-5-pyrimidinol	73.7 (-15.9)	74.7 (-15.1)	78.2 (-12.9)
MAE	2.1 (1.4)	1.5 (1.0)	---

[a] Experimental data taken from: Lucarini, M.; Pedrelli, P.; Pedulli, G. F.; Cabiddu, S.; Fattuoni, C. *J. Org. Chem.* **1996**, *61*, 9259-9263. Note that the value for phenol is different than that used in Table 1. We believe the value in Table 1 to be closer to the true value but use 88.3 kcal/mol in this Table in order to have consistent relative BDE data for substituted phenols.

[b] Reference 5b.

Table S6: Sum of zero-point vibrational energies (E_{ZP}), vibrational enthalpy corrections ($H_{298,vib}$), and B3P86/6-311G(2d,2p) electronic energies (E_{el}) obtained at the AM1 optimized geometries. All values are in hartree.

Species	$E_{ZP}+H_{298,vib}$	E_{el}
H	0.00236	-0.51852
F	0.00236	-99.90560
Cl	0.00236	-460.48351
Br	0.00236	-2574.90518
C_6H_6	0.10507	-233.06787
C_6H_5	0.09206	-232.35774
H_2CCH_2	0.05358	-78.90089
H_2CCH	0.03933	-78.18829
F_3CH	0.02953	-338.93208
F_3C	0.01736	-338.23607
c-C_3H_6	0.08458	-118.36858
c-C_3H_5	0.07082	-117.66314
CH_4	0.04702	-40.71518
CH_3	0.03320	-40.01568
H_3CCH_3	0.07678	-80.18363
H_3CCH_2	0.06321	-79.49126
$H_3CCH_2CH_3$	0.10620	-119.65486
$H_3CCH_2CH_2$	0.09262	-118.96237
$HOCH_3$	0.05416	-116.08285
$HOCH_2$	0.04073	-115.40072
Cl_3CH	0.02446	-1420.47984
Cl_3C	0.01304	-1419.79990
$HCOCH_3$	0.05984	-154.30484
$HCOCH_2$	0.04678	-153.62531
$NCCH_3$	0.04906	-133.18172
$NCCH_2$	0.03573	-132.50040
OCH_2	0.03047	-114.81779
OCH	0.01772	-114.14005
$PhCH_3$	0.13387	-272.54216
$PhCH_2$	0.12001	-271.87012
$C_4H_5CH_3$	0.11865	-196.05467
C_5H7	0.10451	-195.39686
$(H_3C_2)_2CH_2$	0.11852	-196.04002
NH_3	0.03735	-56.75925
NH_2	0.02282	-56.05511
H_3CNH_2	0.06646	-96.21622
H_3CNH	0.05228	-95.52526
$PhNH_2$	0.12344	-288.58875
PhNH	0.10902	-287.91138

H_2NNH_2	0.05752	-112.22111
H_2NNH	0.04347	-111.56810
H_2O	0.02367	-76.62985
OH	0.01132	-75.91129
CH_3CH_2OH	0.08314	-155.56007
CH_3CH_2O	0.06996	-154.86515
PhOH	0.11070	-308.45599
PhO	0.09703	-307.78669
HOOH	0.03064	-151.90071
HOO	0.01836	-151.22949
F_3SiH	0.02335	-590.68040
F_3Si	0.01470	-589.99681
$(CH_3)_3SiH$	0.12377	-410.70318
$(CH_3)_3Si$	0.11500	-410.01747
Cl_3SiH	0.01865	-1672.19753
Cl_3Si	0.01059	-1671.52195
$(CH_3)_2SiH$	0.09374	-371.21374
$(CH_3)_2Si$	0.08472	-370.53462
CH_3SiH_3	0.06346	-331.72771
CH_3SiH_2	0.05435	-331.05305
SiH_4	0.03310	-292.24246
SiH_3	0.02392	-291.57059
$PhSiH_3$	0.12130	-524.07643
$PhSiH_2$	0.11130	-523.40305
SiH_3SiH_3	0.05131	-583.26177
SiH_3SiH_2	0.04260	-582.59457
SH_2	0.01821	-399.76173
SH	0.00923	-399.08953
PhSH	0.10630	-631.58465
PhS	0.09599	-630.93095
CN	0.05777	-378.41672
H_3CCF_3	0.00860	-92.95858
$PhCH_2CH_3$	0.16327	0.01354
H_3CNHCH_3	0.09501	-135.67879
$PhCH_2NH_2$	0.15303	-328.04836
$PhNHCH_3$	0.15205	-328.04896
H_3CNO_2	0.05482	-245.65371
NO_2	0.01438	-205.53570
$CH_3OC_2H_5$	0.11265	-195.01820
$PhCH_2OH$	0.14012	-347.91626
$PhOCH_3$	0.14012	-347.91021
H_3CSH	0.04898	-439.22524
$H_3CSC_2H_5$	0.10848	-518.16595
SC_2H_5	0.06883	-478.03199
C_2F_6	0.03837	-676.61774

H_3CF	0.04201	-140.10385
$PhCH_2F$	0.12816	-371.93810
H_3CCl	0.03984	-500.63823
C_2F_5Cl	0.03676	-1037.12665
$PhCH_2Cl$	0.12635	-732.46902
H_3CBr	0.03914	-2615.04142
C_2F_5Br	0.03641	-3151.52332
$PhCH_2Br$	0.12578	-2846.87251
HSSH	0.02206	-798.27326

Table S7: Sum of zero-point vibrational energies (E_{ZP}), vibrational enthalpy corrections ($H_{298,vib}$), and B3P86/6-311G(2d,2p) electronic energies (E_{el}) obtained at the PM3 optimized geometries. All values are in hartree.

Species	$E_{ZP}+H_{298,vib}$	E_{el}
H	0.00236	-0.51852
F	0.00236	-99.90560
Cl	0.00236	-460.48351
Br	0.00236	-2574.90518
C_6H_6	0.10171	-233.06866
C_6H_5	0.08909	-232.35818
H_2CCH_2	0.05244	-78.90129
H_2CCH	0.03837	-78.19033
F_3CH	0.02846	-338.93503
F_3C	0.01792	-338.23736
c-C_3H_6	0.08314	-118.36864
c-C_3H_5	0.06933	-117.66328
CH_4	0.04798	-40.71658
CH_3	0.03250	-40.01574
H_3CCH_3	0.07657	-80.18626
H_3CCH_2	0.06221	-79.49272
$H_3CCH_2CH_3$	0.10513	-119.65809
$H_3CCH_2CH_2$	0.09083	-118.96452
$HOCH_3$	0.05335	-116.08388
$HOCH_2$	0.03962	-115.40011
Cl_3CH	0.02348	-1420.47825
Cl_3C	0.01134	-1419.79546
$HCOCH_3$	0.05869	-154.30691
$HCOCH_2$	0.04514	-153.62525
$NCCH_3$	0.04823	-133.18350
$NCCH_2$	0.03442	-132.50067
OCH_2	0.02922	-114.81897
OCH	0.01706	-114.14401
$PhCH_3$	0.13068	-272.54421
$PhCH_2$	0.11614	-271.87085

$C_4H_5CH_3$	0.11614	-196.05611
C_5H7	0.10125	-195.39692
$(H_3C_2)_2CH_2$	0.11533	-196.04165
NH_3	0.03814	-56.75958
NH_2	0.02314	-56.05330
H_3CNH_2	0.06551	-96.21810
H_3CNH	0.05139	-95.52576
$PhNH_2$	0.12019	-288.58870
PhNH	0.10545	-287.91091
H_2NNH_2	0.05576	-112.22422
H_2NNH	0.04281	-111.56844
H_2O	0.02506	-76.62946
OH	0.01214	-75.91065
CH_3CH_2OH	0.08180	-155.56156
CH_3CH_2O	0.06850	-154.86632
PhOH	0.10823	-308.45656
PhO	0.09366	-307.78688
HOOH	0.03105	-151.91196
HOO	0.01908	-151.24896
F_3SiH	0.02136	-590.68085
F_3Si	0.01333	-589.99771
$(CH_3)_3SiH$	0.12420	-410.70645
$(CH_3)_3Si$	0.11590	-410.02632
Cl_3SiH	0.01756	-1672.19662
Cl_3Si	0.01025	-1671.52582
$(CH_3)_2SiH$	0.09323	-371.21847
$(CH_3)_2Si$	0.08459	-370.54121
CH_3SiH_3	0.06200	-331.73054
CH_3SiH_2	0.05322	-331.05664
SiH_4	0.03058	-292.24287
SiH_3	0.02174	-291.57116
$PhSiH_3$	0.11647	-524.08130
$PhSiH_2$	0.10671	-523.40883
SiH_3SiH_3	0.04780	-583.26270
SiH_3SiH_2	0.03938	-582.59590
SH_2	0.01447	-399.76075
SH	0.00718	-399.08885
PhSH	0.10098	-631.58876
PhS	0.09264	-630.93613
CN	0.05802	-378.41912
H_3CCF_3	0.00826	-92.95883
$PhCH_2CH_3$	0.15926	-312.01223
H_3CNHCH_3	0.09283	-135.68102
$PhCH_2NH_2$	0.14835	-328.05058
$PhNHCH_3$	0.14774	-328.04654

H_3CNO_2	0.05328	-245.65337
NO_2	0.01351	-205.53823
$CH_3OC_2H_5$	0.10944	-195.02086
$PhCH_2OH$	0.13601	-347.91590
$PhOCH_3$	0.13552	-347.91186
H_3CSH	0.04676	-439.23018
$H_3CSC_2H_5$	0.10717	-518.17426
SC_2H_5	0.06755	-478.03830
C_2F_6	0.03941	-676.62628
H_3CF	0.04111	-140.10476
$PhCH_2F$	0.12405	-371.93947
H_3CCl	0.04001	-500.63993
C_2F_5Cl	0.03742	-1037.13446
$PhCH_2Cl$	0.12278	-732.47068
H_3CBr	0.03996	-2615.04297
C_2F_5Br	0.03769	-3151.53014
$PhCH_2Br$	0.12284	-2846.87253
HSSH	0.01740	-798.28209

Table S8: Sum of zero-point vibrational energies (E_{ZP}), vibrational enthalpy corrections ($H_{298,vib}$), and B3P86/6-311G(2d,2p) electronic energies (E_{el}) obtained at the HF/3-21G(d) optimized geometries. All values are in hartree.

Species	$E_{ZP}+H_{298,vib}$	E_{el}
H	0.00236	-0.51852
F	0.00236	-99.90560
Cl	0.00236	-460.48351
Br	0.00236	-2574.90518
C_6H_6	0.10217	-233.06886
C_6H_5	0.08758	-232.35829
H_2CCH_2	0.05300	-78.90145
H_2CCH	0.03852	-78.19291
F_3CH	0.02933	-338.93726
F_3C	0.01625	-338.23912
c-C_3H_6	0.08209	-118.37048
c-C_3H_5	0.06852	-117.66619
CH_4	0.04653	-40.71652
CH_3	0.03173	-40.01575
H_3CCH_3	0.07574	-80.18618
H_3CCH_2	0.06127	-79.49282
$H_3CCH_2CH_3$	0.10432	-119.65807
$H_3CCH_2CH_2$	0.08995	-118.96439
$HOCH_3$	0.05279	-116.08370

$HOCH_2$	0.03905	-115.40009
Cl_3CH	0.02460	-1420.48105
Cl_3C	0.01220	-1419.80286
$HCOCH_3$	0.05812	-154.30709
$HCOCH_2$	0.04472	-153.62107
$NCCH_3$	0.04841	-133.18359
$NCCH_2$	0.03356	-132.50086
OCH_2	0.02961	-114.81844
OCH	0.01629	-114.14709
$PhCH_3$	0.13008	-272.54457
$PhCH_2$	0.11455	-271.87096
$C_4H_5CH_3$	0.11596	-196.05667
C_5H7	0.10089	-195.39768
$(H_3C_2)_2CH_2$	0.11601	-196.04339
NH_3	0.03594	-56.75788
NH_2	0.02120	-56.05657
H_3CNH_2	0.06502	-96.21701
H_3CNH	0.05081	-95.52742
$PhNH_2$	0.11904	-288.58842
PhNH	0.10397	-287.91304
H_2NNH_2	0.05437	-112.22950
H_2NNH	0.04069	-111.56920
H_2O	0.02315	-76.62933
OH	0.01062	-75.91159
CH_3CH_2OH	0.08132	-155.56130
CH_3CH_2O	0.06776	-154.86315
PhOH	0.10700	-308.45659
PhO	0.09275	-307.78461
HOOH	0.02864	-151.91274
HOO	0.01623	-151.24286
F_3SiH	0.02328	-590.68282
F_3Si	0.01375	-589.99784
$(CH_3)_3SiH$	0.12191	-410.70640
$(CH_3)_3Si$	0.11316	-410.03213
Cl_3SiH	0.02001	-1672.19748
Cl_3Si	0.01104	-1671.52752
$(CH_3)_2SiH$	0.09284	-371.21849
$(CH_3)_2Si$	0.08386	-370.54508
CH_3SiH_3	0.06355	-331.73064
CH_3SiH_2	0.05429	-331.05817
SiH_4	0.03398	-292.24291
SiH_3	0.02443	-291.57127
$PhSiH_3$	0.11918	-524.08301
$PhSiH_2$	0.10881	-523.41470
SiH_3SiH_3	0.05319	-583.26320

SiH_3SiH_2	0.04410	-582.59641
SH_2	0.01837	-399.76307
SH	0.00914	-399.08990
PhSH	0.10333	-631.58885
PhS	0.09209	-630.93690
CN	0.05660	-378.42289
H_3CCF_3	0.00699	-92.95815
$PhCH_2CH_3$	0.15883	-312.01606
H_3CNHCH_3	0.09344	-135.68057
$PhCH_2NH_2$	0.14791	-328.04993
$PhNHCH_3$	0.14788	-328.05152
H_3CNO_2	0.05172	-245.65569
NO_2	0.01060	-205.53804
$CH_3OC_2H_5$	0.11008	-195.02025
$PhCH_2OH$	0.13562	-347.91754
$PhOCH_3$	0.13603	-347.91220
H_3CSH	0.04877	-439.23128
$H_3CSC_2H_5$	0.10727	-518.17480
SC_2H_5	0.06745	-478.03839
C_2F_6	0.03669	-676.63064
H_3CF	0.04148	-140.10483
$PhCH_2F$	0.12443	-371.94005
H_3CCl	0.04012	-500.64018
C_2F_5Cl	0.03501	-1037.13899
$PhCH_2Cl$	0.12313	-732.47203
H_3CBr	0.03966	-2615.04298
C_2F_5Br	0.03468	-3151.53850
$PhCH_2Br$	0.12275	-2846.87507
HSSH	0.02232	-798.28459

Table S9: Sum of zero-point vibrational energies (E_{ZP}), vibrational enthalpy corrections ($H_{298,vib}$), and B3P86/6-311G(2d,2p) electronic energies (E_{el}) obtained at the B3P86/3-21G(d) optimized geometries. All values are in hartree.

Species	$E_{ZP}+H_{298,vib}$	E_{el}
H	0.00236	-0.51852
F	0.00236	-99.90560
Cl	0.00236	-460.48351
Br	0.00236	-2574.90518
C_6H_6	0.10596	-233.06906
C_6H_5	0.09278	-232.35934
H_2CCH_2	0.05504	-78.90165
H_2CCH	0.04066	-78.19402
F_3CH	0.02961	-338.93549

F_3C	0.01628	-338.23646
c-C_3H_6	0.08558	-118.37043
c-C_3H_5	0.07105	-117.66667
CH_4	0.04893	-40.71651
CH_3	0.03358	-40.01578
H_3CCH_3	0.07941	-80.18630
H_3CCH_2	0.06424	-79.49324
$H_3CCH_2CH_3$	0.10929	-119.65823
$H_3CCH_2CH_2$	0.09418	-118.96486
$HOCH_3$	0.05457	-116.08257
$HOCH_2$	0.04050	-115.39977
Cl_3CH	0.02504	-1420.48077
Cl_3C	0.01236	-1419.80284
$HCOCH_3$	0.06016	-154.30620
$HCOCH_2$	0.04677	-153.62450
$NCCH_3$	0.05021	-133.18340
$NCCH_2$	0.03578	-132.50055
OCH_2	0.03020	-114.81778
OCH	0.01650	-114.14653
$PhCH_3$	0.13509	-272.54484
$PhCH_2$	0.12107	-271.87160
$C_4H_5CH_3$	0.12032	-196.05739
C_5H7	0.10664	-195.39838
$(H_3C_2)_2CH_2$	0.12031	-196.04386
NH_3	0.03725	-56.75810
NH_2	0.02163	-56.05598
H_3CNH_2	0.06762	-96.21745
H_3CNH	0.05251	-95.52772
$PhNH_2$	0.12361	-288.58849
PhNH	0.10962	-287.91372
H_2NNH_2	0.05577	-112.22950
H_2NNH	0.04200	-111.56860
H_2O	0.02356	-76.62791
OH	0.01076	-75.91039
CH_3CH_2OH	0.08444	-155.56021
CH_3CH_2O	0.07088	-154.86351
PhOH	0.11073	-308.45641
PhO	0.09796	-307.78692
HOOH	0.02884	-151.90903
HOO	0.01691	-151.24450
F_3SiH	0.02395	-590.68287
F_3Si	0.01401	-589.99802
$(CH_3)_3SiH$	0.12765	-410.70626
$(CH_3)_3Si$	0.11842	-410.03202
Cl_3SiH	0.02041	-1672.19757

Cl_3Si	0.01116	-1671.52778
$(CH_3)_2SiH$	0.09710	-371.21840
$(CH_3)_2Si$	0.08762	-370.54504
CH_3SiH_3	0.06632	-331.73060
CH_3SiH_2	0.05654	-331.05817
SiH_4	0.03506	-292.24292
SiH_3	0.02517	-291.57129
$PhSiH_3$	0.12339	-524.08313
$PhSiH_2$	0.11360	-523.41513
SiH_3SiH_3	0.05505	-583.26314
SiH_3SiH_2	0.04545	-582.59639
SH_2	0.01889	-399.76330
SH	0.00937	-399.08997
PhSH	0.10680	-631.59008
PhS	0.09724	-630.93735
CN	0.05858	-378.42104
H_3CCF_3	0.00803	-92.95807
$PhCH_2CH_3$	0.16522	-312.01632
H_3CNHCH_3	0.09721	-135.68111
$PhCH_2NH_2$	0.15322	-328.05056
$PhNHCH_3$	0.15348	-328.05172
H_3CNO_2	0.05353	-245.64903
NO_2	0.01115	-205.53045
$CH_3OC_2H_5$	0.11434	-195.01970
$PhCH_2OH$	0.14010	-347.91661
$PhOCH_3$	0.14080	-347.91238
H_3CSH	0.05076	-439.23135
$H_3CSC_2H_5$	0.11188	-518.17490
SC_2H_5	0.07016	-478.03873
C_2F_6	0.03678	-676.62649
H_3CF	0.04293	-140.10424
$PhCH_2F$	0.12869	-371.93964
H_3CCl	0.04180	-500.64024
C_2F_5Cl	0.03510	-1037.13569
$PhCH_2Cl$	0.12752	-732.47228
H_3CBr	0.04128	-2615.04300
C_2F_5Br	0.03485	-3151.53520
$PhCH_2Br$	0.12708	-2846.87480
HSSH	0.02267	-798.28488

Table S10: Sum of zero-point vibrational energies (E_{ZP}), vibrational enthalpy corrections ($H_{298,vib}$), and B3P86/6-311G(2d,2p) electronic energies (E_{el}) obtained at the B3P86/6-31G(d) optimized geometries. All values are in hartree.

Species	$E_{ZP}+H_{298,vib}$	E_{el}
H	0.00236	-0.51852
F	0.00236	-99.90560
Cl	0.00236	-460.48351
Br	0.00236	-2574.90518
C_6H_6	0.10511	-233.06907
C_6H_5	0.09216	-232.35946
H_2CCH_2	0.05466	-78.90161
H_2CCH	0.04044	-78.19399
F_3CH	0.02982	-338.93793
F_3C	0.01659	-338.23959
c-C_3H_6	0.08529	-118.37087
c-C_3H_5	0.07096	-117.66719
CH_4	0.04853	-40.71651
CH_3	0.03360	-40.01578
H_3CCH_3	0.07885	-80.18646
H_3CCH_2	0.06397	-79.49332
$H_3CCH_2CH_3$	0.10849	-119.65855
$H_3CCH_2CH_2$	0.09372	-118.96515
$HOCH_3$	0.05529	-116.08450
$HOCH_2$	0.04145	-115.40148
Cl_3CH	0.02531	-1420.48114
Cl_3C	0.01262	-1419.80309
$HCOCH_3$	0.06011	-154.30755
$HCOCH_2$	0.04679	-153.62617
$NCCH_3$	0.04970	-133.18363
$NCCH_2$	0.03549	-132.50070
OCH_2	0.03039	-114.81917
OCH	0.01683	-114.14805
$PhCH_3$	0.13421	-272.54495
$PhCH_2$	0.12045	-271.87164
$C_4H_5CH_3$	0.11963	-196.05745
C_5H7	0.10608	-195.39834
$(H_3C_2)_2CH_2$	0.11963	-196.04400
NH_3	0.03810	-56.76012
NH_2	0.02267	-56.05686
H_3CNH_2	0.06821	-96.21861
H_3CNH	0.05304	-95.52933
$PhNH_2$	0.12308	-288.59055
PhNH	0.10939	-287.91436

H_2NNH_2	0.05740	-112.23152
H_2NNH	0.04350	-111.57185
H_2O	0.02489	-76.62977
OH	0.01161	-75.91171
CH_3CH_2OH	0.08481	-155.56226
CH_3CH_2O	0.07076	-154.86594
PhOH	0.11038	-308.45760
PhO	0.09716	-307.78830
HOOH	0.03047	-151.91524
HOO	0.01785	-151.25162
F_3SiH	0.02328	-590.68273
F_3Si	0.01359	-589.99783
$(CH_3)_3SiH$	0.12696	-410.70636
$(CH_3)_3Si$	0.11776	-410.03212
Cl_3SiH	0.02028	-1672.19763
Cl_3Si	0.01108	-1671.52784
$(CH_3)_2SiH$	0.09654	-371.21847
$(CH_3)_2Si$	0.08709	-370.54510
CH_3SiH_3	0.06590	-331.73063
CH_3SiH_2	0.05619	-331.05820
SiH_4	0.03493	-292.24292
SiH_3	0.02503	-291.57129
$PhSiH_3$	0.12246	-524.08318
$PhSiH_2$	0.11274	-523.41519
SiH_3SiH_3	0.05470	-583.26320
SiH_3SiH_2	0.04519	-582.59646
SH_2	0.01890	-399.76330
SH	0.00939	-399.08996
PhSH	0.10598	-631.59011
PhS	0.09649	-630.93734
CN	0.05818	-378.42315
H_3CCF_3	0.00820	-92.95860
$PhCH_2CH_3$	0.16415	-312.01664
H_3CNHCH_3	0.09741	-135.68206
$PhCH_2NH_2$	0.15326	-328.05208
$PhNHCH_3$	0.15269	-328.05277
H_3CNO_2	0.05514	-245.65759
NO_2	0.01279	-205.53881
$CH_3OC_2H_5$	0.11429	-195.02206
$PhCH_2OH$	0.14020	-347.91861
$PhOCH_3$	0.14021	-347.91380
H_3CSH	0.05054	-439.23138
$H_3CSC_2H_5$	0.11129	-518.17517
SC_2H_5	0.07007	-478.03899
C_2F_6	0.03717	-676.63168

H_3CF	0.04298	-140.10538
$PhCH_2F$	0.12803	-371.94103
H_3CCl	0.04171	-500.64035
C_2F_5Cl	0.03567	-1037.14038
$PhCH_2Cl$	0.12689	-732.47243
H_3CBr	0.04113	-2615.04304
C_2F_5Br	0.03524	-3151.54025
$PhCH_2Br$	0.12636	-2846.87528
HSSH	0.02268	-798.28487

Table S11: G3(MP2) enthalpies (H_{298}) in hartree.

Species	H_{298}
H	-0.49948
F	-99.63858
Cl	-459.68488
C_6H_6	-231.82430
C_6H_5	-231.14026
H_2CCH_2	-78.43076
H_2CCH	-77.75509
F_3CH	-337.91382
F_3C	-337.24440
c-C_3H_6	-117.65305
c-C_3H_5	-116.97983
CH_4	-40.41828
CH_3	-39.75287
H_3CCH_3	-79.64671
H_3CCH_2	-78.98616
$H_3CCH_2CH_3$	-118.87948
$H_3CCH_2CH_2$	-118.21840
$HOCH_3$	-115.54793
$HOCH_2$	-114.89522
Cl_3CH	-1417.87586
Cl_3C	-1417.22718
$HCOCH_3$	-153.59477
$HCOCH_2$	-152.94317
$NCCH_3$	-132.54151
$NCCH_2$	-131.88842
OCH_2	-114.34922
OCH	-113.70938
$PhCH_3$	-271.06162
$PhCH_2$	-270.41566
$C_4H_5CH_3$	-194.93071
C_5H7	-194.29971
$(H_3C_2)_2CH_2$	-194.92048

NH_3	-56.46633
NH_2	-55.79696
H_3CNH_2	-95.68177
H_3CNH	-95.02372
$PhNH_2$	-287.10687
PhNH	-286.45884
H_2NNH_2	-111.69540
H_2NNH	-111.06470
H_2O	-76.33863
OH	-75.65139
CH_3CH_2OH	-154.78565
CH_3CH_2O	-154.11764
PhOH	-306.97299
PhO	-306.33068
HOOH	-151.37838
HOO	-150.74087
F_3SiH	-589.15120
F_3Si	-588.49275
$(CH_3)_3SiH$	-409.17101
$(CH_3)_3Si$	-408.52208
Cl_3SiH	-1669.07174
Cl_3Si	-1668.42606
$(CH_3)_2SiH$	-369.92173
$(CH_3)_2Si$	-369.27419
CH_3SiH_3	-330.67355
CH_3SiH_2	-330.02763
SiH_4	-291.42663
SiH_3	-290.78231
$PhSiH_3$	-522.08221
$PhSiH_2$	-521.43592
SiH_3SiH_3	-581.68271
SiH_3SiH_2	-581.04261
SH_2	-398.94054
SH	-398.29660
PhSH	-629.58172
PhS	-628.95050
CN	-377.16065
H_3CCF_3	-92.59312
$PhCH_2CH_3$	-310.29491
H_3CNHCH_3	-134.90474
$PhCH_2NH_2$	-326.33094
$PhNHCH_3$	-326.32933
H_3CNO_2	-244.70021
NO_2	-204.85257
$CH_3OC_2H_5$	-194.00446

$PhCH_2OH$	-346.19777
$PhOCH_3$	-346.18985
H_3CSH	-438.16594
$H_3CSC_2H_5$	-516.63021
SC_2H_5	-476.76252
C_2F_6	-674.64553
H_3CF	-139.56600
$PhCH_2F$	-370.21585
H_3CCl	-499.56967
C_2F_5Cl	-1034.62855
$PhCH_2Cl$	-730.21925
HSSH	-796.69224

Table S12: B3P86/6-31G* Optimized geometries in Cartesian coordinates in Å.

C_6H_6

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.393183757256
C	1.206532525923	0.000000000000	2.089775635883
C	2.413065051846	0.000000000000	1.393183757256
C	2.413065051846	0.000000000000	0.000000000000
C	1.206532525923	0.000000000000	-0.696591878628
H	-0.941431409901	0.000000000000	-0.543535677930
H	-0.941431409901	0.000000000000	1.936719435186
H	1.206532525923	0.000000000000	3.176846991743
H	3.354496461747	0.000000000000	1.936719435186
H	3.354496461747	0.000000000000	-0.543535677930
H	1.206532525923	0.000000000000	-1.783663234488

C_6H_5

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.374746593789
C	1.252526288450	0.000000000000	2.001763351978
C	2.418867929700	0.000000000000	1.237900752616
C	2.356243205023	0.000000000000	-0.154908293405
C	1.115061754517	0.000000000000	-0.804092955291
H	-0.917768266222	0.000000000000	1.956344879698
H	1.311375157317	0.000000000000	3.087495564479
H	3.385882828787	0.000000000000	1.732788653138
H	3.271305248001	0.000000000000	-0.742223442307
H	1.049993040942	0.000000000000	-1.888676386461

H_2CCH_2

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.087057294795

H	0.973808843762	0.000000000000	-0.483104437961
C	-1.129226282536	0.000000000000	-0.700342211634
H	-1.129226282536	0.000000000000	-1.787399506429
H	-2.103035126298	0.000000000000	-0.217237773673

H_2CCH

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.089662261118
H	0.986204818694	0.000000000000	-0.475821710948
C	-1.107674473092	0.000000000000	-0.697067250592
H	-1.393874003036	0.000000000000	-1.741090469427

F_3CH

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.092392361015
F	1.252997156495	0.000000000000	-0.465014272375
F	-0.626498578248	-1.085127368395	-0.465014272375
F	-0.626498578248	1.085127368395	-0.465014272375

F_3C

C	0.000000000000	0.000000000000	0.000000000000
F	0.000000000000	0.000000000000	1.321132350526
F	1.231162344474	0.000000000000	-0.479197213219
F	-0.700730422511	1.012293234897	-0.479197213219

$c\text{-}C_3H_6$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.501896271448
C	1.300680324923	0.000000000000	0.750948135724
H	-0.295560483600	-0.910720762023	-0.512833061997
H	-0.295560483600	0.910720762023	-0.512833061997
H	-0.296346217790	-0.910720762023	2.014275689599
H	-0.296346217790	0.910720762023	2.014275689599
H	1.892587026313	0.910720762023	0.751401779570
H	1.892587026313	-0.910720762023	0.751401779570

$c\text{-}C_3H_5$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.528184742705
C	1.250103473732	0.000000000000	0.764010084308
H	-0.302938747957	-0.902545814357	-0.530856824245
H	-0.319450397247	0.918932487879	-0.491302433124
H	-0.302186314537	-0.902731673976	2.059110928819
H	-0.319500806581	0.919115687686	2.018985206178
H	2.095042956325	-0.676559747242	0.763618790445

CH_4

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.092624090154
H	1.030135871247	0.000000000000	-0.364208030051
H	-0.515067935624	-0.892123833850	-0.364208030051
H	-0.515067935624	0.892123833850	-0.364208030051

CH_3

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.082119030459
H	0.937142570296	0.000000000000	-0.541059515230
H	-0.937142570296	0.000000000000	-0.541059515230

H_3CCH_3

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.095435334224
H	1.044811212465	0.000000000000	-0.329162728410
H	-0.448812742043	-0.943502831089	-0.329162728410
C	-0.757571867338	1.199283617424	-0.555609053531
H	-0.308759125295	2.142786448513	-0.226446325122
H	-0.757571867338	1.199283617424	-1.651044387756
H	-1.802383079803	1.199283617424	-0.226446325122

H_3CCH_2

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.084866865340
H	0.962577131515	0.000000000000	-0.500381236056
C	-1.256276069383	-0.205721239937	-0.762822307872
H	-2.120847929220	0.231960211666	-0.250316674694
H	-1.200314671422	0.231960211666	-1.766323601743
H	-1.486990326841	-1.276320469375	-0.902914113028

$H_3CCH_2CH_3$

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.095492011219
H	1.044641568254	0.000000000000	-0.333365435320
H	-0.451000903922	-0.942270762989	-0.333365435320
C	-0.755213059532	1.198730526027	-0.563812244968
H	-0.303037578386	2.125929772928	-0.187953825908
H	-1.786767159328	1.191164258901	-0.187953825908
C	-0.769902695806	1.222047012938	-2.088419224788
H	-1.316278788715	2.089295921037	-2.475013641646
H	0.248931002486	1.263011190058	-2.491790457036
H	-1.246711469689	0.320740427069	-2.491790457036

$H_3CCH_2CH_2$

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.094987777552
H	1.041033873094	0.000000000000	-0.339668903017
H	-0.458214422655	-0.937943884776	-0.334098998817
C	-0.756776768798	1.204732845009	-0.557190772787
H	-0.301792740773	2.134708137765	-0.188182169649
H	-1.779641489035	1.204868448305	-0.136516806802
C	-0.817174194247	1.228747183154	-2.042056015915
H	-1.009490984954	2.150469003883	-2.581450031717
H	-0.828556980769	0.302647165298	-2.609400386264

$HOCH_3$

H	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	0.966101974968
C	1.344235254531	0.000000000000	1.393647501573
H	1.327400912945	0.000000000000	2.486241646522
H	1.896727701153	0.892562604906	1.062557225095
H	1.896727701153	-0.892562604906	1.062557225095

$HOCH_2$

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.082986762776
H	0.944340440919	0.000000000000	-0.540519809092
O	-1.056212469610	0.681741033674	-0.528145930586
H	-0.971207006686	0.691909187320	-1.490922785170

Cl_3CH

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.086731779136
Cl	1.691641687144	0.000000000000	-0.535073128717
Cl	-0.845820843572	1.465004675167	-0.535073128717
Cl	-0.845820843572	-1.465004675167	-0.535073128717

Cl_3C

C	0.000000000000	0.000000000000	0.000000000000
Cl	0.000000000000	0.000000000000	1.716194899011
Cl	1.526145285198	0.000000000000	-0.784987579429
Cl	-1.286507384653	0.820986102664	-0.784987579429

$HCOCH_3$

C	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.208392974740
H	0.960088617842	0.000000000000	-0.564239845264
C	-1.234336798203	0.000000000000	-0.854449796559
H	-1.232707870657	-0.879670584126	-1.510142373488
H	-2.130716542241	0.000000000000	-0.231465958473

H	-1.232707870657	0.879670584126	-1.510142373488

$HCOCH_2$

C	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.234803444034
H	0.955654507763	0.000000000000	-0.560084447046
C	-1.194591642330	0.000000000000	-0.774899161245
H	-2.154677077697	0.000000000000	-0.269151737845
H	-1.165183502931	0.000000000000	-1.859883148468

$NCCH_3$

C	1.109761	0.000000	-0.392343
H	1.638424	0.888478	-0.035169
H	1.638424	-0.888478	-0.035168
H	1.125481	0.000000	-1.486054
C	-0.262067	0.000000	0.092651
N	-1.355499	0.000000	0.479221

$NCCH_2$

C	1.034196	0.000000	0.597093
H	1.038595	0.000000	1.680603
H	1.974743	0.000000	0.059148
C	-0.160806	0.000000	-0.092841
N	-1.179097	0.000000	-0.680752

OCH_2

H	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.109404775237
O	1.018370917032	0.000000000000	1.751990844638
H	-1.001360514705	0.000000000000	1.586956945066

OCH

C	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.180424082832
H	0.936119770350	0.000000000000	-0.626114132380

$PhCH_3$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.397754591204
C	1.192982499398	0.000000000000	2.115154542649
C	2.412929160209	-0.002846948126	1.443778777072
C	2.427837226613	-0.007262798966	0.051377387832
C	1.231697807338	-0.007244231540	-0.660746494308
H	-0.948904292017	-0.001837256641	1.930026101105
H	1.169105365612	-0.002217858247	3.201749851739
H	3.345272275417	-0.006070184337	2.001654762002

H	3.374047751254	-0.015186228474	-0.483306878324
H	1.252145110909	-0.014782730287	-1.748524399023
C	-1.290719338404	0.032449991822	-0.772412152437
H	-1.610237030920	1.064248522817	-0.967225665805
H	-1.190519444442	-0.464438109829	-1.742735793999
H	-2.099938652607	-0.459089360102	-0.222849653064

$PhCH_2$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.422484130379
C	1.183812569121	0.000000000000	2.137297697022
C	2.414217642359	-0.000632302929	1.471511222305
C	2.442161317929	-0.001267679800	0.072802024056
C	1.264341526763	-0.001273717016	-0.651843526106
H	-0.953474423498	0.000492895641	1.944896548388
H	1.156862580596	0.000494925691	3.223689951513
H	3.341540107659	-0.000895283542	2.036731780820
H	3.395426103355	-0.001760237483	-0.448984027601
H	1.291752181144	-0.001768980024	-1.738709140818
C	-1.199149430117	-0.001306529686	-0.730903216955
H	-1.195403675857	-0.001525600142	-1.815756198302
H	-2.161679111111	-0.000552159470	-0.230447310868

$C_4H_5CH_3$

H	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.085332207936
C	1.137784542991	0.000000000000	1.791347051627
H	-0.971459724808	0.000000000000	1.574453178497
H	2.092272181439	0.000000000000	1.263850419453
C	1.205226246379	0.000000000000	3.240611842790
C	2.348982717040	0.000000000000	3.941369464665
H	0.253402027323	0.000000000000	3.774388663135
H	3.293212936660	0.000000000000	3.394107554796
C	2.444505227637	0.000000000000	5.430626697894
H	2.992237242402	0.879281397140	5.794494932782
H	2.992237242402	-0.879281397140	5.794494932782
H	1.454478852753	0.000000000000	5.897152458229

C_5H_7

H	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.084606787033
C	1.160006812323	0.000000000000	1.800280188684
H	-0.967989021943	0.000000000000	1.578909066262
H	2.105185808882	0.000000000000	1.255695390786
C	1.237704019207	0.000000000000	3.208891350367
C	2.450677651230	0.000000000000	3.929250447480

H	0.305556481644	0.000000000000	3.773998185148
H	3.370656807073	0.000000000000	3.343098342263
C	2.548717122271	0.000000000000	5.288732880094
H	3.510355129641	0.000000000000	5.790354475779
H	1.662770189135	0.000000000000	5.918364138468

$(H_3C_2)_2CH_2$

H	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.098918888701
H	1.050850599116	0.000000000000	1.420377660989
C	-0.667724913979	-1.246670262827	1.610056529806
C	-0.684104473215	1.246670262827	1.587917169506
C	-0.086897914317	-2.157887643842	2.387715978663
H	-1.709938442086	-1.376187589162	1.317204405109
H	0.949307574101	-2.058649107258	2.704803511939
H	-0.620121132462	-3.038871943925	2.733574656356
C	-1.257842871925	2.157887643842	0.805013298154
H	-0.708933285240	1.376187589162	2.670208689939
H	-1.257946865196	2.058649107258	-0.278622391168
H	-1.744553115259	3.038871943925	1.213741036799

NH_3

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.017370437291
H	0.977817473541	0.000000000000	-0.280919196765
H	-0.372988304091	-0.903884249544	-0.280919196765

NH_2

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.031810810405
H	1.007905889382	0.000000000000	-0.220815005421

H_3CNH_2

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.016752217566
H	0.977476237623	0.000000000000	-0.279866533919
C	-0.654129290110	1.204634289186	-0.493125551889
H	-1.704087251935	1.196422074295	-0.182466637559
H	-0.215180771021	2.162150034115	-0.162217375173
H	-0.644477369950	1.196422074295	-1.588035376071

H_3CNH

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.029993794599
C	1.379399778375	0.000000000000	-0.399415276851
H	1.919397344676	-0.879728457023	-0.008564093197

H	1.462704784392	-0.000415339540	-1.490070940856
H	1.919464557880	0.880133918328	-0.009360926982

$PhNH_2$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.402136956760
C	1.197365755774	0.000000000000	2.107432901096
C	2.419562431167	0.000948471113	1.438821940792
C	2.423400451867	0.000115188550	0.045699259757
C	1.231949582663	0.000115744266	-0.669543320399
H	-0.947672324263	-0.005769534431	1.936356228497
H	1.171586308068	0.001653499661	3.194010928409
H	3.352600240084	0.002404293104	1.993664172231
H	3.365782556496	0.001859649034	-0.495809788329
H	1.248798097422	-0.005563171395	-1.757288800493
N	-1.195726977542	-0.058316124013	-0.711056680396
H	-2.002013122217	0.301535318201	-0.218397219195
H	-1.147897597200	0.301615564159	-1.654701360610

PhNH

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.430123313216
C	1.182788344778	0.000000000000	2.140471868529
C	2.411848679805	0.000000000000	1.466554520812
C	2.445156182568	0.000000000000	0.065163451677
C	1.270191334101	0.000000000000	-0.659037919250
H	-0.965891551260	0.000000000000	1.925184336077
H	1.163873537642	0.000000000000	3.226602368366
H	3.340210353969	0.000000000000	2.029982788731
H	3.400857205602	0.000000000000	-0.451534027888
H	1.292212135453	0.000000000000	-1.746773107806
N	-1.182055914983	0.000000000000	-0.622359119097
H	-1.022105818378	0.000000000000	-1.636766327307

H_2NNH_2

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.015494911226
H	0.974734888540	0.000000000000	-0.300241061522
N	-0.691114168977	1.173146885878	-0.418484713332
H	-0.062020739882	1.966057178249	-0.544133126311
H	-1.101264901456	0.970374099271	-1.325065922262

H_2NNH

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.026899009275
N	1.303356449510	0.000000000000	-0.351731698083

H	1.991954488981	-0.451744719163	0.246675722944
H	1.437107818470	-0.210714348328	-1.333073619358

H_2O

O	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	0.965692225250
H	0.937441244855	0.000000000000	-0.231873643073

OH

O	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	0.979750152367

CH_3CH_2OH

O	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	0.966699185984
C	1.348743645190	0.000000000000	-0.433843172403
H	1.886176478734	0.886992163744	-0.059719951703
H	1.886176478734	-0.886992163744	-0.059719951703
C	1.347187471840	0.000000000000	-1.946567159399
H	0.829201913091	0.886144081737	-2.326085400986
H	2.370641579684	0.000000000000	-2.335880687017
H	0.829201913091	-0.886144081737	-2.326085400986

CH_3CH_2O

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.363703324043
H	1.021648672849	0.000000000000	1.781224470981
H	-0.569574570024	0.848145518125	1.781224470981
C	-0.697906960123	-1.309357595577	1.795720873851
H	-0.150638797898	-2.173931318915	1.413530622879
H	-0.720049178281	-1.350899066266	2.888717511192
H	-1.720757950387	-1.337034593034	1.413530622879

PhOH

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.395833281394
C	1.208579003274	0.000000000000	2.081972883157
C	2.420750638134	0.000000000000	1.392954896652
C	2.411936058020	0.000000000000	0.001094606145
C	1.208506055789	0.000000000000	-0.698922197875
H	-0.950306555764	0.000000000000	1.919908897743
H	1.201636240543	0.000000000000	3.168597414127
H	3.361123205509	0.000000000000	1.935393093249
H	3.347920831580	0.000000000000	-0.550842385350
H	1.207007762626	0.000000000000	-1.787557297580
O	-1.209060194456	0.000000000000	-0.625838611630

H	-1.065292754182	0.000000000000	-1.582849350157

PhO

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.449039043305
C	1.180262465587	0.000000000000	2.154794828200
C	2.411437526494	0.000000000000	1.474315839483
C	2.455910144256	0.000000000000	0.068305216851
C	1.289745081036	0.000000000000	-0.660508724366
H	-0.967726793904	0.000000000000	1.941358954241
H	1.169889971551	0.000000000000	3.241390592494
H	3.338299413242	0.000000000000	2.040984951012
H	3.418327565453	0.000000000000	-0.436224912074
H	1.286829488963	0.000000000000	-1.746264471146
O	-1.069486161249	0.000000000000	-0.653867400799

HOOH

O	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	0.971035397473
O	1.418445853947	0.000000000000	-0.248829603255
H	1.507570580985	-0.848889701793	-0.711812108719

HOO

O	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.320496229393
H	0.946909329203	0.000000000000	1.579322121703

F_3SiH

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.464261652996
F	1.483878475550	0.000000000000	-0.561076019774
F	-0.741939237775	1.285076455955	-0.561076019774
F	-0.741939237775	-1.285076455955	-0.561076019774

F_3Si

Si	0.000000000000	0.000000000000	0.000000000000
F	0.000000000000	0.000000000000	1.596316079414
F	1.518014952374	0.000000000000	-0.493817405287
F	-0.679930255301	-1.357226673609	-0.493817405287

$(CH_3)_3SiH$

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.495318717883
C	1.788325500214	0.000000000000	-0.596518140430
H	1.840755703439	0.000000000000	-1.691314628849
H	2.326905127956	0.884172208667	-0.238472734318

H	2.326905127956	-0.884172208667	-0.238472734318
C	-0.894162750107	-1.548735313421	-0.596518140430
H	-1.929168158004	-1.573072848672	-0.238472734318
H	-0.920377851719	-1.594141201339	-1.691314628849
H	-0.397736969952	-2.457245057339	-0.238472734318
C	-0.894162750107	1.548735313421	-0.596518140430
H	-1.929168158004	1.573072848672	-0.238472734318
H	-0.397736969952	2.457245057339	-0.238472734318
H	-0.920377851719	1.594141201339	-1.691314628849

$(CH_3)_3Si$

Si	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.892472642627
H	1.025498840807	0.000000000000	2.286038197279
H	-0.509402936327	0.884444078018	2.289010772510
H	-0.509402936327	-0.884444078018	2.289010772510
C	0.845226692815	-1.556273154677	-0.667126981075
H	0.828231564614	-1.578474665887	-1.761747200899
H	1.895257358413	-1.601442362751	-0.347851140695
H	0.347881607541	-2.462918743906	-0.307103636254
C	0.845226692815	1.556273154677	-0.667126981075
H	0.828231564614	1.578474665887	-1.761747200899
H	0.347881607541	2.462918743906	-0.307103636254
H	1.895257358413	1.601442362751	-0.347851140695

Cl_3SiH

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.469699112105
Cl	1.928262546122	0.000000000000	-0.674442940078
Cl	-0.964131273061	-1.669924350107	-0.674442940078
Cl	-0.964131273061	1.669924350107	-0.674442940078

Cl_3Si

Si	0.000000000000	0.000000000000	0.000000000000
Cl	0.000000000000	0.000000000000	2.059442071388
Cl	1.941496905082	0.000000000000	-0.686923211863
Cl	-0.973071657233	-1.680042196592	-0.686923211863

$(CH_3)_2SiH$

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.492159199822
H	1.426351072252	0.000000000000	-0.438248441298
C	-0.848478649600	-1.559675183270	-0.626928947991
H	-0.840575767367	-1.601056226388	-1.721419390734
H	-0.345225887747	-2.458201702288	-0.255082555968
H	-1.892378114846	-1.601056226388	-0.297921818487

C	-0.848478649600	1.559675183270	-0.626928947991
H	-0.345225887747	2.458201702288	-0.255082555968
H	-0.840575767367	1.601056226388	-1.721419390734
H	-1.892378114846	1.601056226388	-0.297921818487

$(CH_3)_2Si$

Si	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.889566086824
H	1.024748648187	0.000000000000	2.282443232628
H	-0.509857627305	0.885579546793	2.281584577567
H	-0.511244609481	-0.883992240197	2.284207839707
C	0.883776075148	-1.507954472001	-0.717964592333
H	0.877628833217	-1.481837349659	-1.812114736618
H	1.929832287262	-1.544310781269	-0.387954193209
H	0.399050691225	-2.437195487198	-0.401566295203
H	0.631696222532	1.256849955618	-0.512743536888

CH_3SiH_3

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.489116249381
H	1.416097789517	0.000000000000	-0.460580345539
H	-0.634131299429	1.266179467753	-0.460580345539
C	-0.923351828501	-1.495114102176	-0.670646133708
H	-0.923961830785	-1.496101832951	-1.765424240924
H	-1.964636424883	-1.496101832951	-0.332613789871
H	-0.457945756526	-2.426603111474	-0.332613789871

CH_3SiH_2

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.492627551244
H	1.410791505111	0.000000000000	-0.487339284128
C	-0.983895577898	1.448554595038	-0.701703950233
H	-0.993644531330	1.420763829991	-1.795394045951
H	-0.546093532818	2.404718300798	-0.390846966908
H	-2.020849544852	1.422283023852	-0.353506454338

SiH_4

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.485241336996
H	1.400298961451	0.000000000000	-0.495080445665
H	-0.700149480725	-1.212694473509	-0.495080445665
H	-0.700149480725	1.212694473509	-0.495080445665

SiH_3

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.487835178700

H	1.389558866388	0.000000000000	-0.531770322434
H	-0.772882887157	1.154783913075	-0.531770322434

$PhSiH_3$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.402537272509
C	1.237837377804	0.000000000000	2.061983575775
C	2.432710840521	-0.008775844949	1.347590401327
C	2.411076636253	-0.013982890625	-0.044865517778
C	1.192308749590	-0.008775844949	-0.718665461294
H	-0.943351948547	0.012050569778	-0.541986350693
H	1.272632180734	0.012050569778	3.149389399216
H	3.381442703282	-0.007109831488	1.877616875884
H	3.342791133005	-0.017605257036	-0.604186670027
H	1.170598908189	-0.007109831488	-1.805196129952
Si	-1.605642012423	-0.022199320522	2.366426472065
H	-2.672563809323	0.667229609408	1.591448384421
H	-2.070231115560	-1.409896642248	2.645325762990
H	-1.423315871053	0.667229609408	3.672439617174

$PhSiH_2$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.406320536101
C	1.241713544004	0.000000000000	2.066536353009
C	2.433570902341	-0.015609077010	1.350870653784
C	2.411724523551	-0.023691308871	-0.042805195919
C	1.191431702921	-0.015609077010	-0.716374101251
H	-0.944043593468	0.003962141469	-0.540352547597
H	1.275625133436	0.003962141469	3.153757207373
H	3.382508987641	-0.023845412590	1.880235855965
H	3.342894905761	-0.036032665586	-0.602314770325
H	1.169519196276	-0.023845412590	-1.802758402070
Si	-1.590849766933	0.071574332049	2.362209697790
H	-2.717631628777	-0.543927828514	1.605527324334
H	-1.451718225288	-0.543927828514	3.712338577786

SiH_3SiH_3

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.488440342872
H	1.412786120225	0.000000000000	-0.468497633705
H	-0.648945228304	-1.254924185823	-0.468497633705
Si	-1.138065994068	1.869743497793	-0.821612059025
H	-0.489120765765	3.124667683616	-0.353114425320
H	-1.138065994068	1.869743497793	-2.310052401897
H	-2.550852114294	1.869743497793	-0.353114425320

SiH_3SiH_2

Si	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.487645584016
H	1.409124746084	0.000000000000	-0.476924347895
H	-0.650323679534	-1.258141544040	-0.466456894668
Si	-1.077312205119	1.912345181837	-0.772722448223
H	-1.057383897384	2.069495489307	-2.254888112842
H	-2.474857455802	2.069495489307	-0.278678455121

SH_2

S	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.345803096064
H	1.344263461166	0.000000000000	-0.064356199000

SH

S	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.351222972244

PhSH

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.398036201428
C	1.203908306907	0.000000000000	2.094075332564
C	2.416928726649	0.000000000000	1.409858832269
C	2.415082001358	0.000000000000	0.017693076088
C	1.216075836282	0.000000000000	-0.688331378521
H	-0.941361503251	0.000000000000	1.940703594184
H	1.190572231257	0.000000000000	3.180454163374
H	3.355059347516	0.000000000000	1.956572533721
H	3.353982061025	0.000000000000	-0.529182958038
H	1.229567823969	0.000000000000	-1.775019238474
S	-1.572380605746	0.000000000000	-0.825907749149
H	-1.090175480360	0.000358762459	-2.082070263230

PhS

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.416939873174
C	1.192163240360	0.000000000000	2.121473864597
C	2.410395368037	0.000000000000	1.435848842236
C	2.433197805469	0.000000000000	0.038118096692
C	1.245981717831	0.000000000000	-0.674720803755
H	-0.954514440344	0.000000000000	1.934026287602
H	1.180911000844	0.000000000000	3.207873456530
H	3.343927479351	0.000000000000	1.991944750400
H	3.383161833726	0.000000000000	-0.489100104117
H	1.246157779311	0.000000000000	-1.760297215535
S	-1.475597639394	0.000000000000	-0.878999018263

CN

C	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.172165276368

H_3CCF_3

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.500915733422
H	1.028654776142	0.000000000000	1.866032069760
H	-0.514327388071	0.890841167864	1.866032069760
H	-0.514327388071	-0.890841167864	1.866032069760
F	0.625974872025	1.084220282609	-0.494777821176
F	-1.251949744051	0.000000000000	-0.494777821176
F	0.625974872025	-1.084220282609	-0.494777821176

$PhCH_2CH_3$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.397883172883
C	1.193127312046	0.000000000000	2.115181181767
C	2.412755038744	-0.000139826477	1.442700945657
C	2.428008469926	-0.001119721335	0.050124071585
C	1.231519247008	-0.001084835653	-0.661544152243
H	-0.949182393658	-0.004699632410	1.930028079762
H	1.170090368862	-0.004750666090	3.201733572996
H	3.345214892892	-0.003845551844	2.000265059708
H	3.374297630265	-0.006761536534	-0.484343888475
H	1.251184467996	-0.006700867800	-1.749542566179
C	-1.293398678933	0.042784339971	-0.773408373296
H	-2.072451894750	-0.490880616646	-0.215236426791
H	-1.170571062386	-0.491550369165	-1.723676613408
C	-1.762898740596	1.472968999050	-1.054942144160
H	-1.922766438032	2.022798953710	-0.121334675807
H	-1.015890107695	2.022255431401	-1.637653409685
H	-2.703108728101	1.475723853249	-1.617139901010

H_3CNHCH_3

N	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.016160305264
C	1.368103662696	0.000000000000	-0.477785053058
H	1.931726042030	0.925803188453	-0.252585008413
H	1.911420440564	-0.846225445413	-0.045634988032
H	1.370659532432	-0.126714697670	-1.566894043831
C	-0.754056763128	1.141536696678	-0.477785053058
H	-1.759601246332	1.128463140284	-0.045634988032
H	-0.861195390306	1.073828044040	-1.566894043831

H	-0.292224035272	2.122093814707	-0.252585008413

$PhCH_2NH_2$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.399370407123
C	1.191398057046	0.000000000000	2.115112866906
C	2.412441891878	0.000946314375	1.441167263711
C	2.425289139606	0.002097821992	0.050819966965
C	1.226454390801	0.001807712268	-0.661687435064
H	-0.949211307166	0.001109431483	1.932551183920
H	1.169374043330	0.001123487095	3.201707569009
H	3.345047132604	0.002114708749	1.998344945413
H	3.370585321290	0.003847620561	-0.485505887100
H	1.247828189705	0.005169118340	-1.748592400323
C	-1.325515579898	-0.006846161945	-0.746770940123
H	-1.942649613250	0.819799562712	-0.370967251944
H	-1.874038631330	-0.920236881372	-0.480978497593
N	-1.305870090051	0.083334575890	-2.195158595390
H	-0.817306543535	0.924795977069	-2.491235401230
H	-0.800558541250	-0.703338372600	-2.594970321361

$PhNHCH_3$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.406347488141
C	1.191462175646	0.000000000000	2.115548028025
C	2.417797300934	-0.001608835965	1.450201821812
C	2.423906078723	0.000095010159	0.059442562773
C	1.235353466566	0.005738578514	-0.665723193199
H	-0.950132793005	-0.007194059626	1.937076880006
H	1.161234422118	0.001156114708	3.202104938709
H	3.349087920217	-0.002047812326	2.008106007242
H	3.368171237078	0.003085309761	-0.479153871473
H	1.270566338030	0.013518078510	-1.750167475462
N	-1.204356685252	-0.037093210261	-0.683570987164
C	-1.277569013221	0.250877548755	-2.094567206478
H	-0.839438846389	1.224627210516	-2.368019974405
H	-0.762686277128	-0.525067269237	-2.672354290157
H	-2.326208107958	0.243944876968	-2.401003976611
H	-1.994224745310	0.284154553269	-0.143138984544

H_3CNO_2

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.088212428253
H	1.003578328948	0.000000000000	-0.420757443985
H	-0.569101530340	-0.851831472419	-0.378495272389
N	-0.700157943252	1.227624059205	-0.465657632811

O	-0.370820134672	1.675359203034	-1.552988334771
O	-1.575584624302	1.675359203034	0.258482943109

NO_2

N	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.197647730057
O	0.861019062367	0.000000000000	-0.832469975165

$CH_3OC_2H_5$

O	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.402023031346
H	1.042684786333	0.000000000000	1.729031577745
H	-0.501484549144	0.892011346632	1.812149559037
H	-0.501484549144	-0.892011346632	1.812149559037
C	-1.303706644853	0.000000000000	-0.533647217439
H	-1.859271445138	-0.886551967605	-0.180186657878
H	-1.859271445138	0.886551967605	-0.180186657878
C	-1.205777850784	0.000000000000	-2.043353267532
H	-0.666808209547	-0.886243321731	-2.391283174932
H	-2.203347580126	0.000000000000	-2.494168713660
H	-0.666808209547	0.886243321731	-2.391283174932

$PhCH_2OH$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396606822756
C	1.197077018220	0.000000000000	2.105409350451
C	2.411791691159	0.009913054539	1.422906784897
C	2.417350788557	0.018338280452	0.030813507861
C	1.218425893420	0.010287801726	-0.678240754270
H	-0.946035893570	0.003286416966	1.934910285517
H	1.181336516520	0.001100964536	3.191967630019
H	3.347886399277	0.016313929308	1.974424054127
H	3.360714035963	0.031989395970	-0.508676021159
H	1.214432749844	0.023349572107	-1.762834474086
C	-1.304896663952	-0.048630739881	-0.750830198096
H	-2.048354096439	0.574192646720	-0.226857038428
H	-1.689942538874	-1.082688497284	-0.734757412842
O	-1.109751931856	0.391610231754	-2.079553742772
H	-1.922698991173	0.215198736843	-2.570521547779

$PhOCH_3$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.399555489768
C	1.200871530170	0.000000000000	2.093020775930
C	2.416927083842	0.000000000000	1.407292069572
C	2.410720929582	0.000000000000	0.017954084431

C	1.211139911728	0.000000000000	-0.694977917998
H	-0.954692544982	0.000000000000	1.916150969587
H	1.188002375573	0.000000000000	3.179568633661
H	3.355542783171	0.000000000000	1.952989511482
H	3.348962885755	0.000000000000	-0.530423436400
H	1.232504035690	0.000000000000	-1.779134074710
O	-1.225348202940	0.000000000000	-0.589280650822
C	-1.276299067025	0.000000000000	-1.998025474901
H	-0.799293836549	0.894115264330	-2.420574576043
H	-0.799134723718	-0.894207421151	-2.420439065084
H	-2.335004582785	-0.000176948725	-2.261704024680

H_3CSH

S	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.347157900567
C	1.807346036248	0.000000000000	-0.219419738484
H	2.264924171262	0.895125078445	0.207158687205
H	2.264924171262	-0.895125078445	0.207158687205
H	1.985615952261	0.000000000000	-1.296897495431

$H_3CSC_2H_5$

S	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.811940105049
H	1.043538394325	0.000000000000	2.136418087510
H	-0.488961993124	0.893716207373	2.211863965794
H	-0.488961993124	-0.893716207373	2.211863965794
C	-1.796636449166	0.000000000000	-0.304139336815
H	-2.237903066189	-0.886018177259	0.167013257754
H	-2.237903066189	0.886018177259	0.167013257754
C	-2.069498102496	0.000000000000	-1.800465318895
H	-1.641725857961	-0.885856953923	-2.280498827461
H	-3.148113538644	0.000000000000	-1.989371026700
H	-1.641725857961	0.885856953923	-2.280498827461

SC_2H_5

S	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.805266208418
H	1.054339558710	0.000000000000	2.115314897552
H	-0.386351876269	0.981051298006	2.115209142152
C	-0.772539271934	-1.134713530077	2.458481867669
H	-0.364651993382	-2.106245524116	2.164818126295
H	-0.718890976734	-1.056105164373	3.550881452743
H	-1.826060380434	-1.111284893556	2.165130151672

C_2F_6

C	0.000000000000	0.000000000000	0.000000000000

C	0.000000000000	0.000000000000	1.539783181397
F	1.253596333265	0.000000000000	-0.451791287239
F	-0.626798166632	1.085646270698	-0.451791287239
F	-0.626798166632	-1.085646270698	-0.451791287239
F	0.626798166632	1.085646270698	1.991574468636
F	-1.253596333265	0.000000000000	1.991574468636
F	0.626798166632	-1.085646270698	1.991574468636

H_3CF

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.095722244449
H	1.034212478130	0.000000000000	-0.361955504255
H	-0.510160625337	0.899628582403	-0.361955504255
F	-0.652059956312	-1.119377349801	-0.462632117356

$PhCH_2F$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396586257716
C	1.199671848330	0.000000000000	2.100458731411
C	2.412388991219	0.006169681228	1.413763400986
C	2.415118314400	0.011299682478	0.022003193059
C	1.214169648649	0.005965830181	-0.683682300602
H	-0.943813910301	0.002262720820	1.938721669522
H	1.187811099096	0.001136426692	3.186908090533
H	3.349765766951	0.010284701105	1.962775799263
H	3.356861398961	0.020013409604	-0.519981464056
H	1.210566216717	0.013905073010	-1.768257936884
C	-1.304477578634	-0.034892294636	-0.747873776476
H	-2.002367738741	0.712324135680	-0.349072199834
H	-1.778408595117	-1.021565562317	-0.657633543867
F	-1.120408272300	0.220714777073	-2.093341925931

H_3CCl

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.089993987452
H	1.022916175403	0.000000000000	-0.376469641248
H	-0.539710925955	0.868947419759	-0.376469641248
Cl	-0.822284397617	-1.478713044682	-0.573575774156

C_2F_5Cl

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.545101595364
F	1.247281059754	0.000000000000	2.008710857192
F	-0.643026842692	-1.068749980865	2.008710857192
F	-0.621794977265	1.099774484463	1.972181305643
F	-1.267196398517	0.033453438620	-0.422590892446

F	0.624629013029	1.103061394961	-0.422590892446
Cl	0.809520475694	-1.431806296882	-0.649767103642

$PhCH_2Cl$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396938341922
C	1.198504590081	0.000000000000	2.103335005659
C	2.411322786436	0.001547342826	1.418363697735
C	2.420643331468	0.002878871686	0.025101145782
C	1.221256828000	0.002240117124	-0.678931405395
H	-0.946442046406	0.002301365482	1.932328858203
H	1.185752200878	-0.002992898775	3.189545313383
H	3.347669175865	-0.000262431065	1.969127551943
H	3.363874770147	0.002120972160	-0.513717744548
H	1.228999048166	0.007057616735	-1.766270425059
C	-1.288180186312	-0.004783774972	-0.757829409597
H	-2.095783633585	-0.459672665364	-0.182313508143
H	-1.195724237288	-0.523223929469	-1.713466016985
Cl	-1.860475781418	1.672564609830	-1.165590857874

H_3CBr

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.088221676475
H	1.016075253952	0.000000000000	-0.389637646356
H	-0.566719468813	0.843349254675	-0.389637646356
Br	-0.870342500894	-1.633455546175	-0.598388130696

C_2F_5Br

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.542240938141
F	1.248251409369	0.000000000000	-0.461284478163
F	-0.622463569278	-1.098707055295	-0.432058028109
F	-0.641650227725	1.070708441292	-0.461284478163
F	0.628742820658	-1.096223892810	1.972936326168
F	-1.263502799032	-0.024187487195	1.972936326168
Br	0.893041482044	1.576302655158	2.228675257407

$PhCH_2Br$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.398707777616
C	1.197222020164	0.000000000000	2.103369114899
C	2.411862201847	-0.001951195658	1.418223002174
C	2.421293222147	-0.005935793881	0.026451500733
C	1.220585734858	-0.006939630991	-0.678317428779
H	-0.947562377116	-0.011527845354	1.931698450854
H	1.184959545668	0.001476191928	3.189611593331

H	3.347773492131	-0.001363485275	1.969666832596
H	3.364060116544	-0.008635574168	-0.513156901950
H	1.229325137165	-0.012592491512	-1.765655444850
C	-1.284411235687	0.024185522643	-0.754332421027
H	-2.017715169033	0.701982710439	-0.318282851325
H	-1.145450142911	0.258602364212	-1.808864025029
Br	-2.186159498396	-1.740406742021	-0.737256416721

HSSH

S	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.351866120615
S	2.050307872757	0.000000000000	-0.325396031509
H	2.256516031859	-1.335012368197	-0.377952476856