Quantification of Lewis Acid Induced Brønsted Acidity of Protic Lewis Bases

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Supporting Information

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1) Sample Calculation of pK_a of H_2-B(C_6F_5)$_3$

A 1.0 mL CD_3CN solution containing 20 mg (0.032 mmol) [2,6-lutidinium][HB(C_6F_5)$_3$],[1] and 10 mg (0.035 mmol) 1,3,5-tris(trifluoromethyl)benzene (internal standard) was treated with 25 µL (0.010 mmol) aliquots of a 0.4 M [Ph_2NH_2][BF_4] in CD_3CN solution. The solution was allowed to stand for 20 hr to allow for equilibration, before an NMR spectrum was obtained and the next aliquot was added. Protonations with triflic acid were complete within 30 minutes.

NMR data of [2,6-lutidinium][HB(C_6F_5)$_3$]. ^{1}H (400 MHz, CD_3CN) δ 2.65 (s, 6H, -C*H*$_3$ of lutidinium), 3.58 (br q, 1H, $^1J_{BH}$ = 88 Hz, B*H*), 7.57 (d, 2H, $^3J_{HH}$ = 8 Hz, lutidinium phenyl protons), 8.23 (t, 2H, $^3J_{HH}$ = 8 Hz, lutidinium phenyl protons), 12.99 (t, J = 66 Hz, *H*N of lutidinium). ^{11}B (128 MHz, CD_3CN) δ -25.56 (d, $^1J_{BH}$ = 88 Hz, [HB(C_6F_5)$_3$]$^-$). ^{19}F (377 MHz, CD_3CN) δ -134.66 (br d, $^3J_{FF}$ = 24 Hz, *o*-F of [HB(C_6F_5)$_3$]$^-$), -164.96 (t, $^3J_{FF}$ = 19 Hz, $^5J_{FF}$ = 7 Hz, *p*-F of [HB(C_6F_5)$_3$]$^-$), -168.29 (m, 6F, *m*-F of [HB(C_6F_5)$_3$]$^-$).

NMR data of CD_3CN-B(C_6F_5)$_3$. ^{11}B (128 MHz, CD_3CN) δ -11.22 (br s, CD_3CN-B(C_6F_5)$_3$). ^{19}F (377 MHz, CD_3CN) δ -134.66 (dd, $^3J_{FF}$ = 20 Hz, $^5J_{FF}$ = 7 Hz, *o*-F of CD_3CN-B(C_6F_5)$_3$), -158.66 (t, $^3J_{FF}$ = 21 Hz, *p*-F of CD_3CN-B(C_6F_5)$_3$), -165.76 (m, 6F, *m*-F of CD_3CN-B(C_6F_5)$_3$).

Integrals taken from ^{19}F NMR spectra were found to be the most reproducible, and were integrated with respect to 1,3,5-tris(trifluoromethyl)benzene, which was used as an internal standard. [CD_3CN-B(C_6F_5)$_3$] was assumed to be equal to the concentration of [H_2-B(C_6F_5)$_3$]. The effect of the binding of CD_3CN to B(C_6F_5)$_3$ was assumed to be negligible in the case of the stability of [2,6-lutidinium][HB(C_6F_5)$_3$], as CD_3CN solutions were found to be stable on the order of weeks with no measurable loss of H_2. The pK_a of H_2-B(C_6F_5)$_3$ was calculated according to the following equilibrium:

$$[HB(C_6F_5)_3]^- + HA \rightleftharpoons H_2\text{-}B(C_6F_5)_3 + A^- \quad \text{(S1)}$$

Equation S1 can be written as the sum of the acid dissociation constant of H_2-$B(C_6F_5)_3$ (K_{aH2}) and the acid dissociation constant of the acid HA (K_a):

$$\begin{array}{llll} [HB(C_6F_5)_3]^- + H^+ \rightleftharpoons & H_2\text{-}B(C_6F_5)_3 & 1/K_{aH2} \\ HA \rightleftharpoons H^+ + A^- & & K_a \\ \hline [HB(C_6F_5)_3]^- + HA \rightleftharpoons & H_2\text{-}B(C_6F_5)_3 + A^- & K_{eq} \end{array}$$

where

$$K_{eq} = \frac{K_a}{K_{aH2}} \quad \text{(S2)}$$

Solving Equation S2 for K_{aH2}, results in:

$$K_{aH2} = \frac{K_a}{K_{eq}} \quad \text{(S3)}$$

Inserting the experimental values for the protonation with $Ph_2NH_2BF_4$ (pK_a = 5.97 in MeCN)[2] :

$$K_{aH2} = \frac{(1.07 \times 10^{-6})}{(0.402)} = 2.66 \times 10^{-6}$$

where:

$$pK_{aH2} = -\log(K_{aH2}) = -\log(2.66 \times 10^{-6}) = 5.57$$

Repeating the addition of $Ph_2NH_2BF_4$ to CD_3CN solutions of [2,6-Lutidinium][$HB(C_6F_5)_3$] resulted in six pK_{aH2} values with the average value being 5.75 with a standard deviation of 0.23 pK_a units.

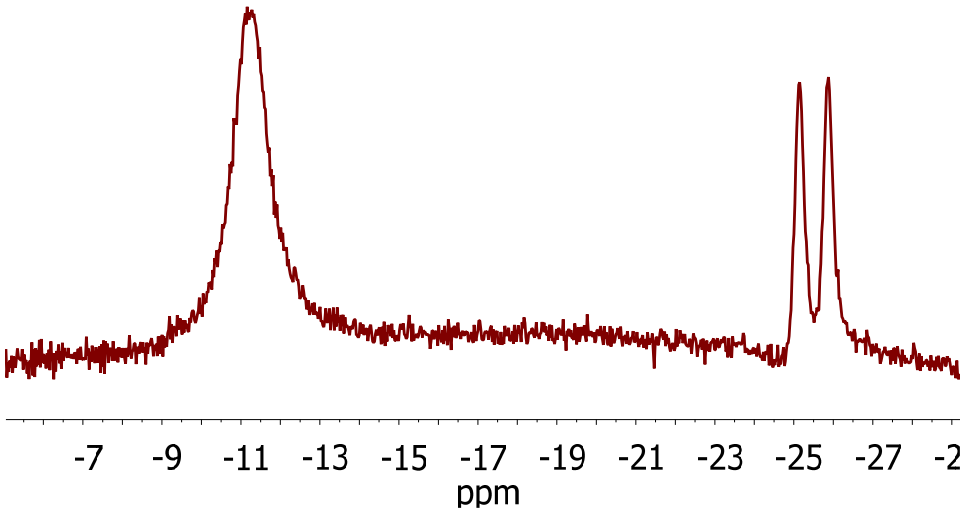


Figure S1. ^{11}B NMR spectrum in CD_3CN of the addition of four equivalents of $[Ph_2NH_2]BF_4$ to [lutidinium][$HB(C_6F_5)_3$]. The resonances at -11 ppm and -26 are MeCN-$B(C_6F_5)_3$ and $[HB(C_6F_5)_3]^-$, respectively.

2) Sample Calculation of computed pK_a for H_2O-$B(C_6F_5)_3$

Experimental pK_a of pyridine is 12.33 in acetonitrile[3]

Free energy for H_2O-$B(C_6F_5)_3$ in acetonitrile: -1433564.998 kcal/mol

Free energy for H_2O-$B(C_6F_5)_3$ in acetonitrile: -1433308.167 kcal/mol

Free energy for Pyridine in acetonitrile: -155734.5131 kcal/mol

Free energy for Pyridinium in acetonitrile: -156001.9376 kcal/mol

$$\text{Pyridine} + H_2O{-}B(C_6F_5)_3 \xrightleftharpoons[\text{MeCN}]{\Delta G_{eq}} \left[HO{-}B(C_6F_5)_3\right]^- + [H\text{Pyridine}]^+ \qquad \text{(S1)}$$

ΔG_{eq} = Products – Reactants = (-1433308.167 + -156001.9376) – (-1433564.998 + -155734.5131)

ΔG_{eq} = -10.5935 kcal/mol

$$\boldsymbol{\Delta G_{eq} = -RT\,ln(K_{eq}) = -10,593.5\,cal/mol = -\left(1.9781\frac{cal}{mol\,K}\right)(298\,K)\left(ln(K_{eq})\right)}$$

Solve for K_{eq}

$$\boldsymbol{K_{eq} = e^{(17.89)} = 5.89 \times 10^7}$$

Convert K_{eq} to a pK_{eq}

$$\boldsymbol{pK_{eq} = -log\left(5.89 \times 10^7\right) = -7.77}$$

$$\text{Pyridine} + H_2O{-}B(C_6F_5)_3 \rightleftharpoons \left[HO{-}B(C_6F_5)_3\right]^- + [H\text{Pyridine}]^+ \qquad K_{eq}$$

$$[H\text{Pyridine}]^+ \rightleftharpoons \text{Pyridine} + H^+ \qquad K_a(py)$$

$$H_2O{-}B(C_6F_5)_3 \rightleftharpoons \left[HO{-}B(C_6F_5)_3\right]^- + H^+ \qquad K_a = (K_{eq})(K_a(py))$$

Using the properties of logarithms:

pK_a = pK_{eq} + pK_a(py) = -7.77 + 12.33 = 4.56

The computed pK_a for H_2O-$B(C_6F_5)_3$ is 4.56 in acetonitrile. A similar approach was taken for Lewis acid-Lewis base adducts that include homoconjugation, except that H_2O-$B(C_6F_5)_3$ and OH-$B(C_6F_5)_3$ were replaced in Equation S1 by $(H_2O)_2$-$B(C_6F_5)_3$ and (H_2O-OH)-$B(C_6F_5)_3$, respectively.

3) Plots of Hydride Aceptor Ability versus pK_a of Lewis Acid-Substrate Adducts

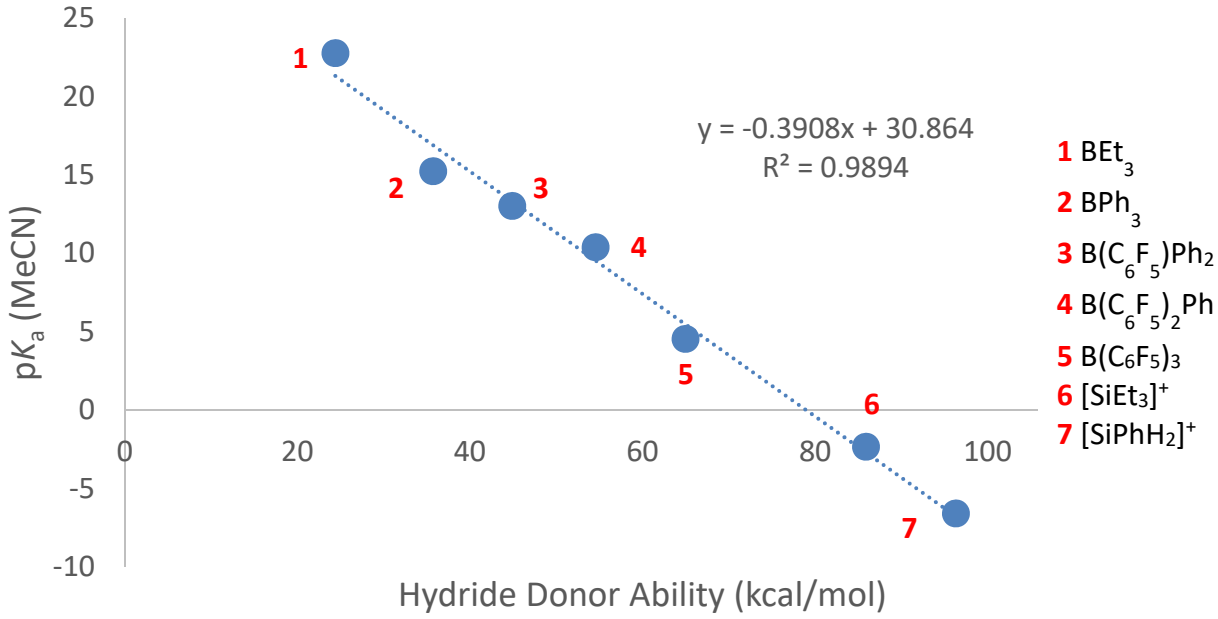


Figure S2. Plot showing the effect of Lewis acid strength on the resulting pK_a of the water-Lewis acid adduct, without taking into consideration homoconjugation.

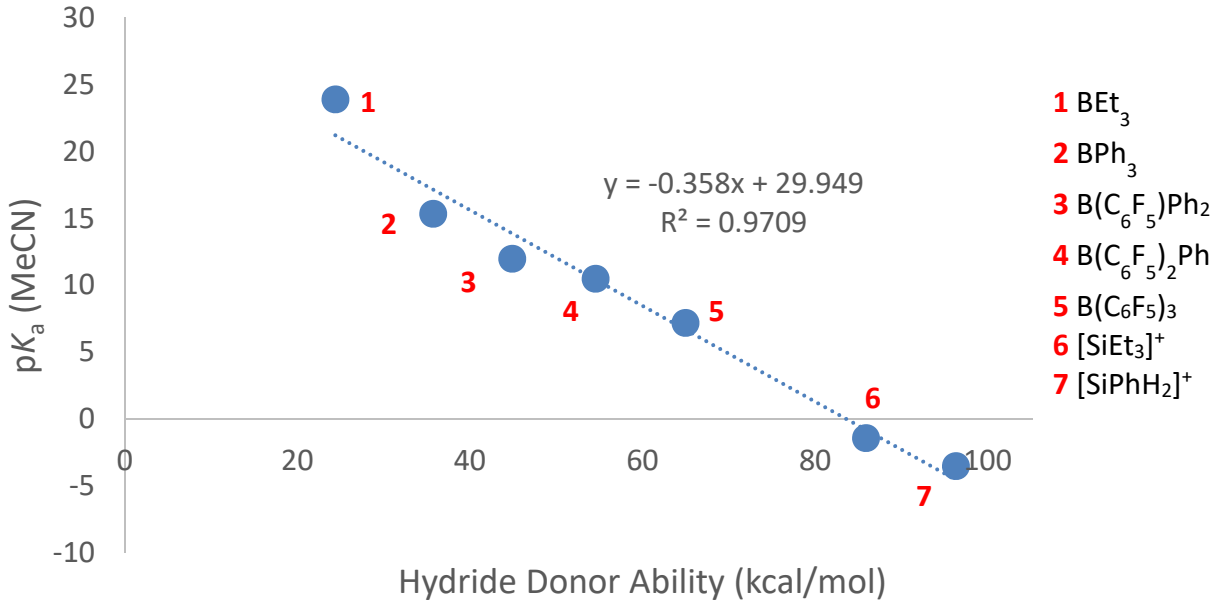


Figure S3. Plot showing the effect of Lewis acid strength on the resulting pK_a of the phenylethanol-Lewis acid adduct.

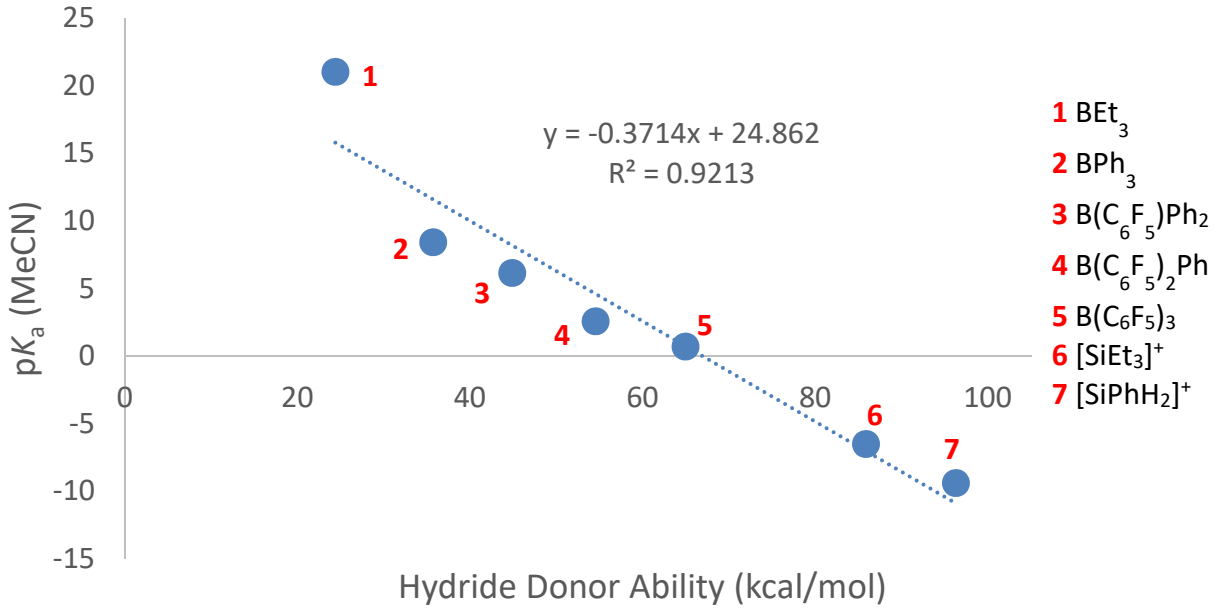


Figure S4. Plot showing the effect of Lewis acid strength on the resulting pK_a of the phenol-Lewis acid adduct.

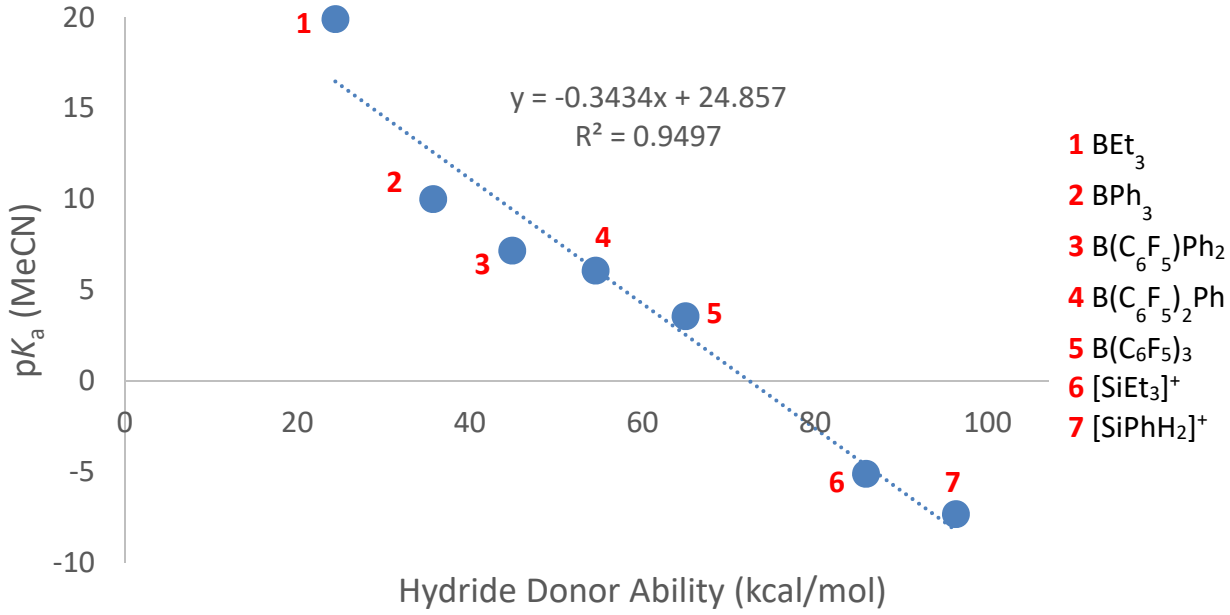


Figure S5. Plot showing the effect of Lewis acid strength on the resulting pK_a of the thiophenol-Lewis acid adduct.

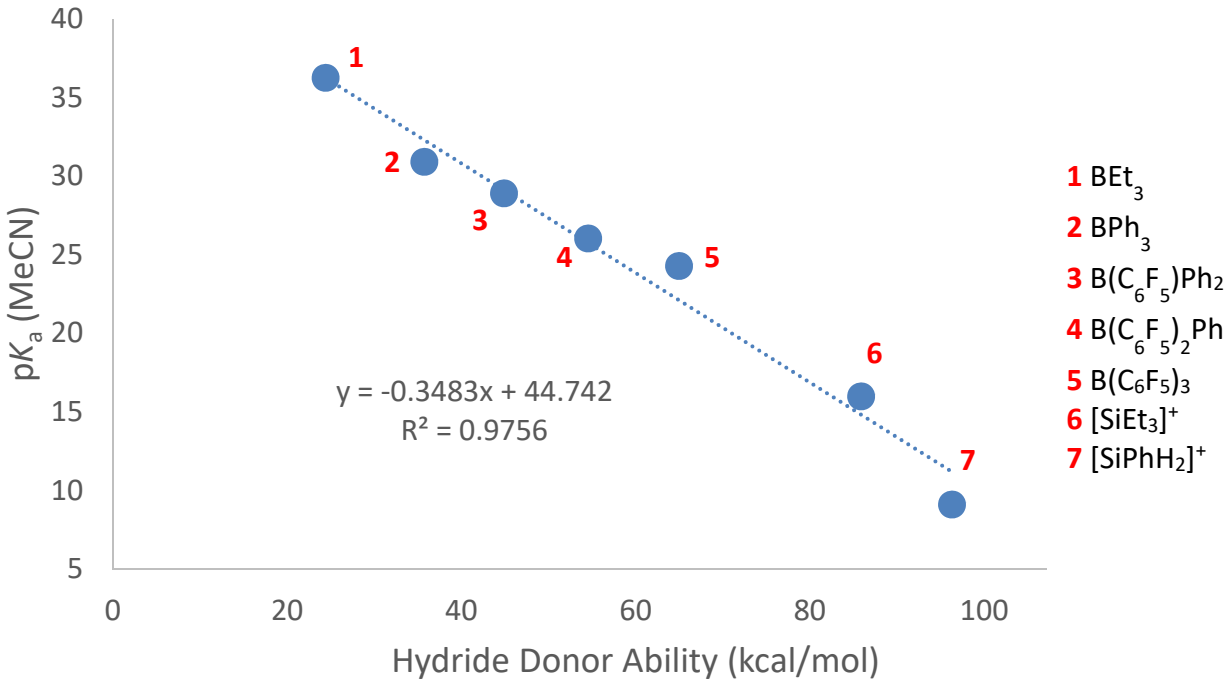


Figure S6. Plot showing the effect of Lewis acid strength on the resulting pK_a of the ammonia-Lewis acid adduct.

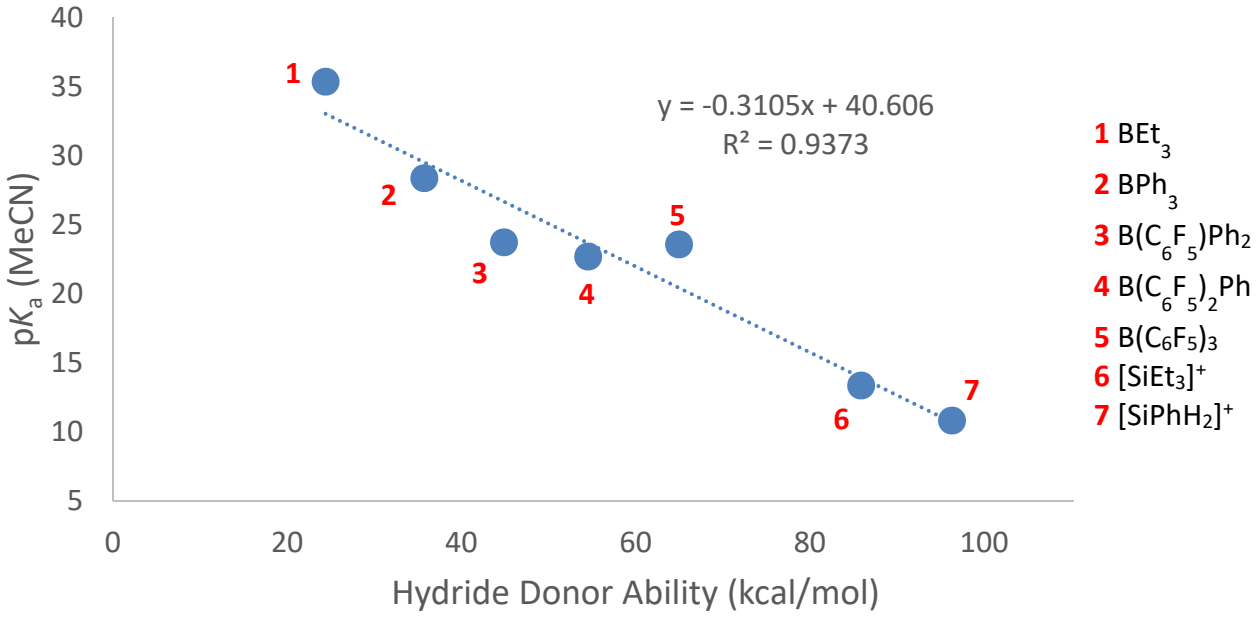


Figure S7. Plot showing the effect of Lewis acid strength on the resulting pK_a of the hydrazine-Lewis acid adduct.

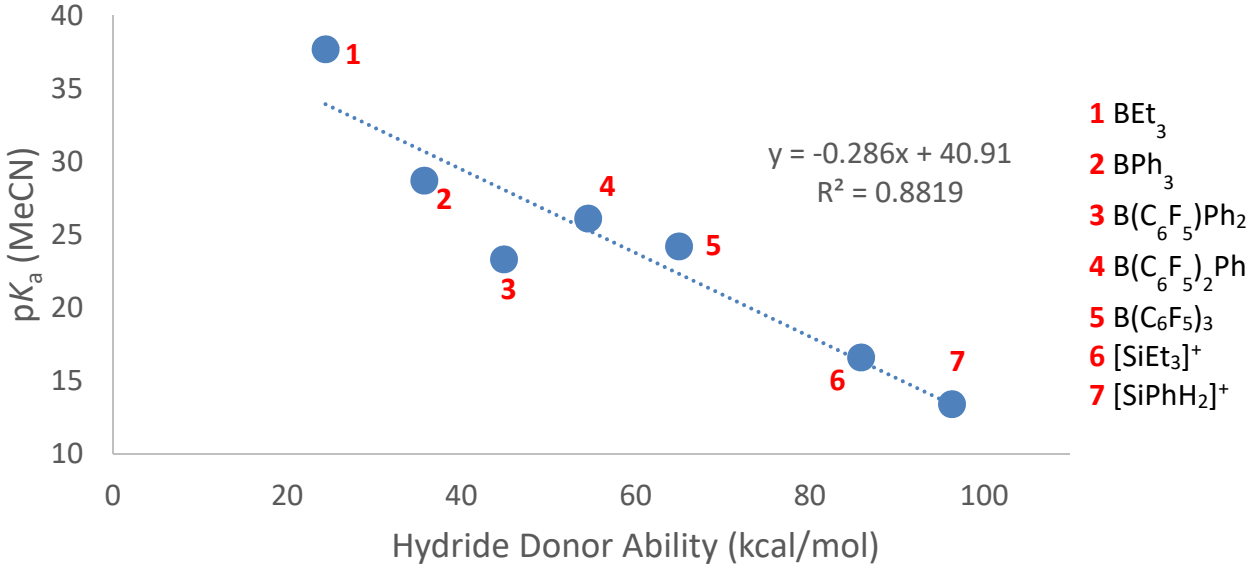


Figure S8. Plot showing the effect of Lewis acid strength on the resulting pK_a of the N-benzyl-2-methylpropan-2-amine-Lewis acid adduct.

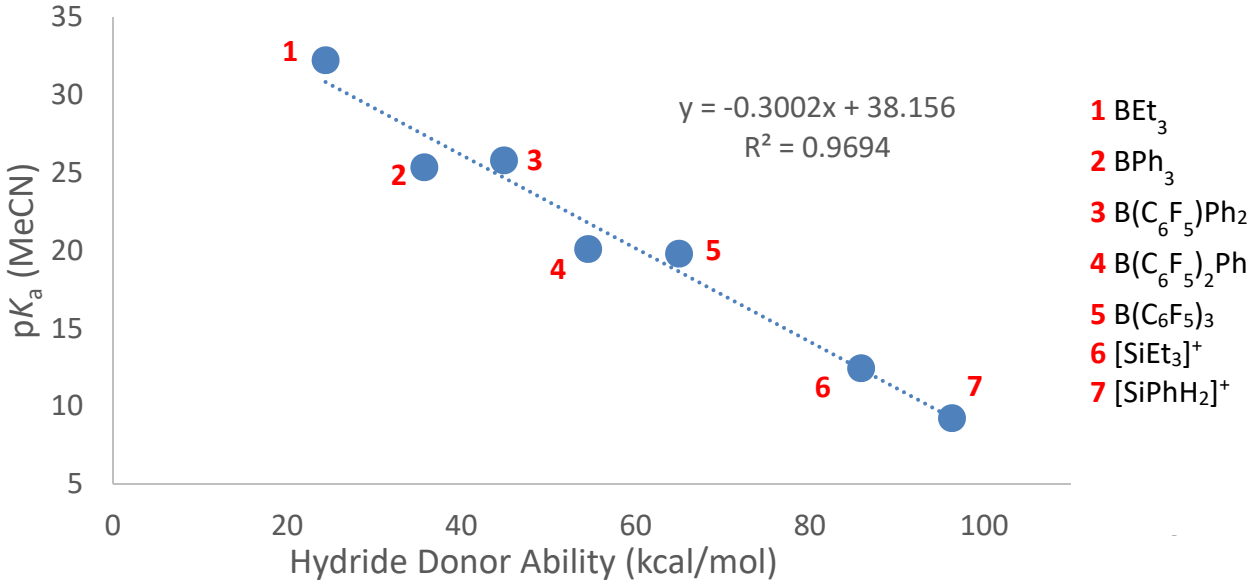


Figure S9. Plot showing the effect of Lewis acid strength on the resulting pK_a of the *N*-(1-phenylethyl)aniline-Lewis acid adduct.

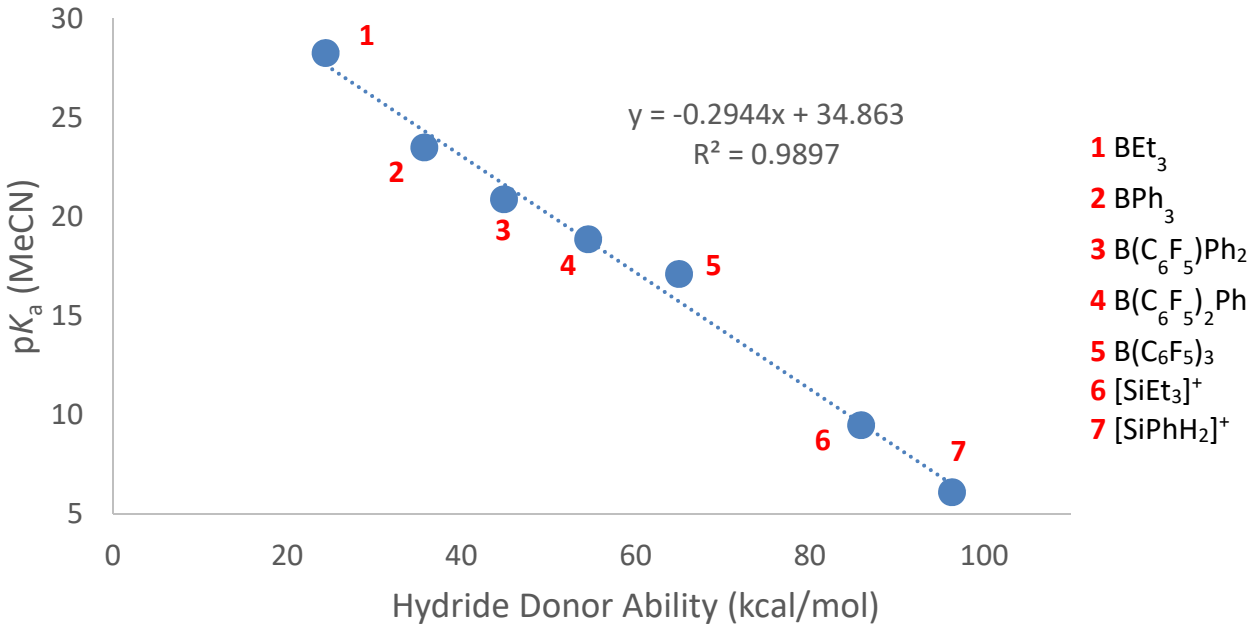


Figure S10. Plot showing the effect of Lewis acid strength on the resulting pK_a of the aniline - Lewis acid adduct.

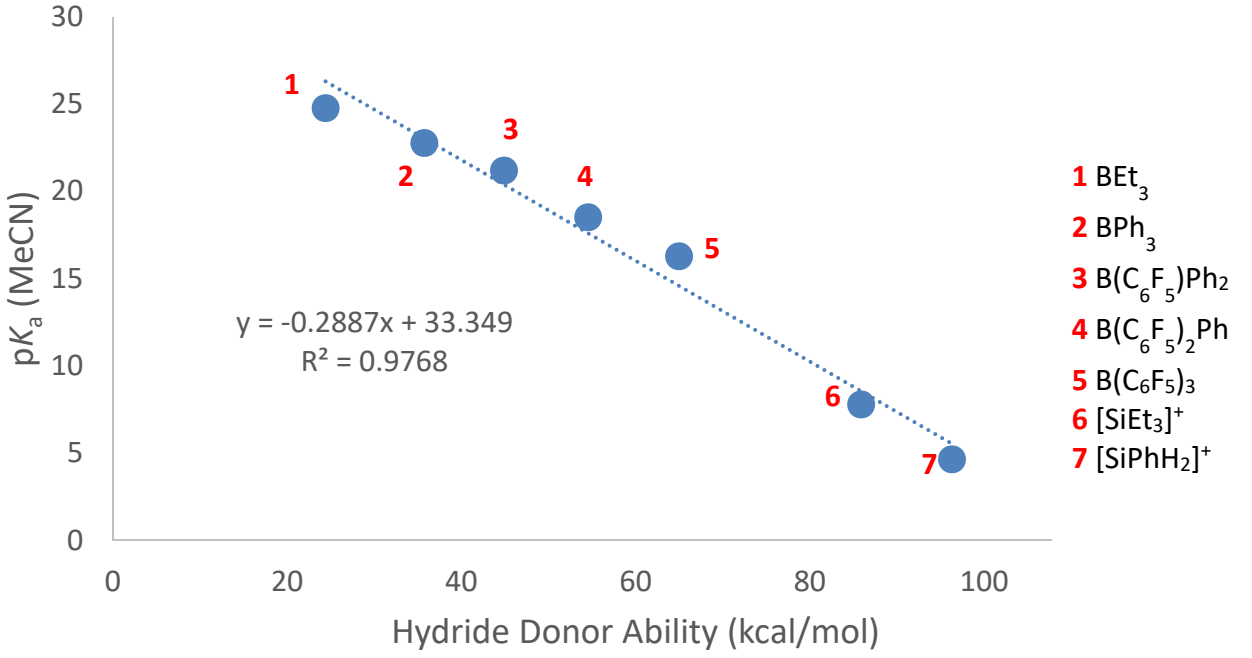


Figure S11. Plot showing the effect of Lewis acid strength on the resulting pK_a of the phenylphosphine-Lewis acid adduct.

4) Plots of Hydride Aceptor Ability versus pK_a of Lewis Acid-Substrate Adducts Accounting for Homoconjugation

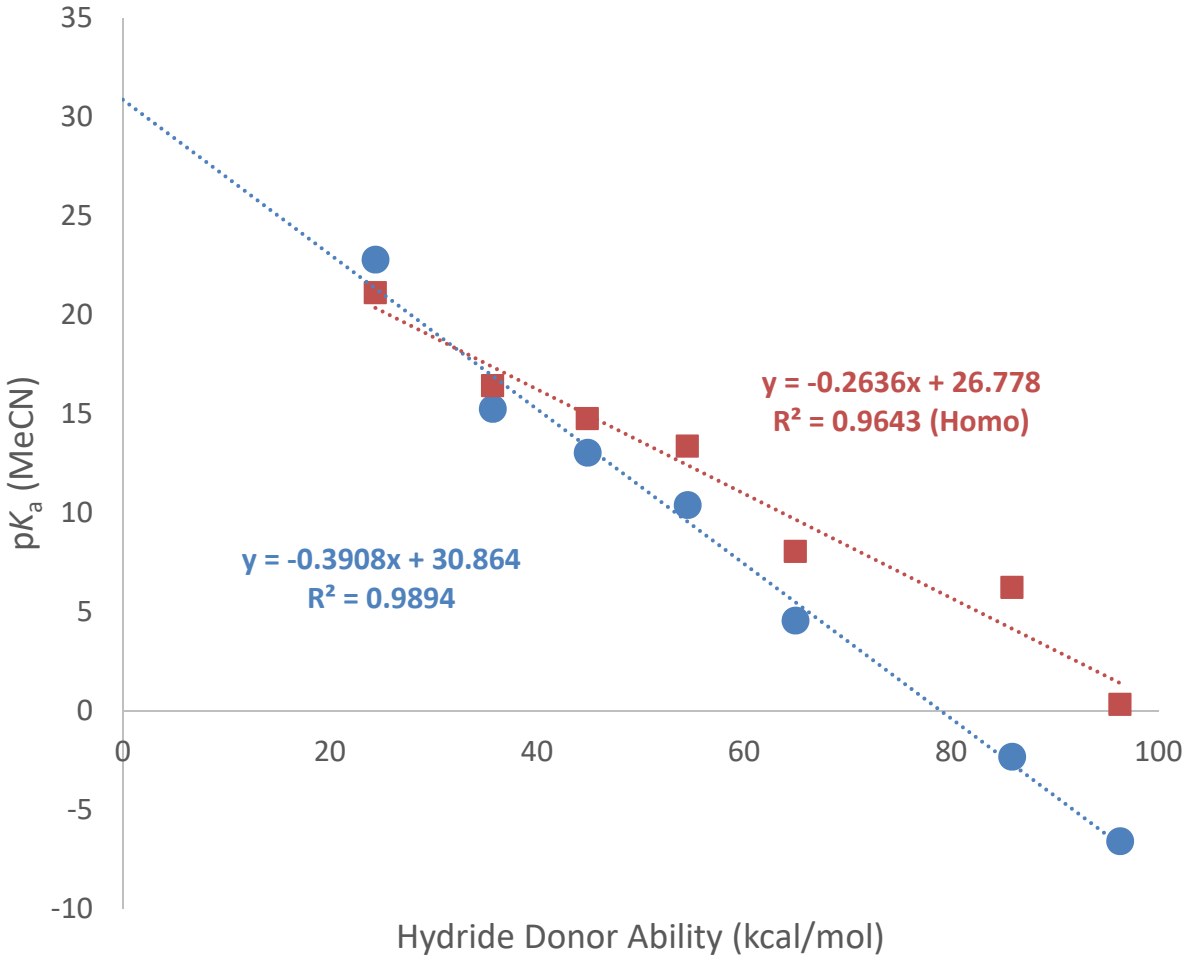


Figure S12. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the water-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

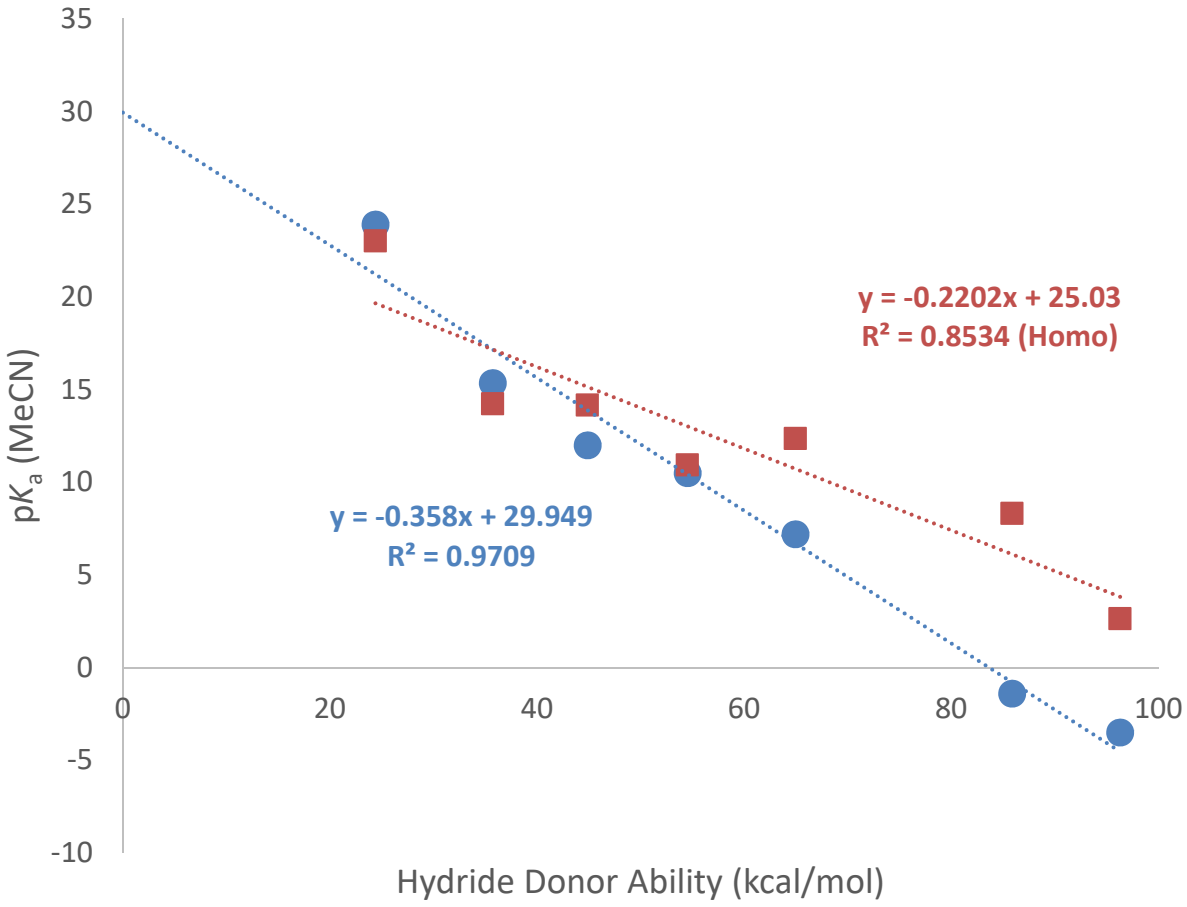


Figure S13. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the phenylethanol-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

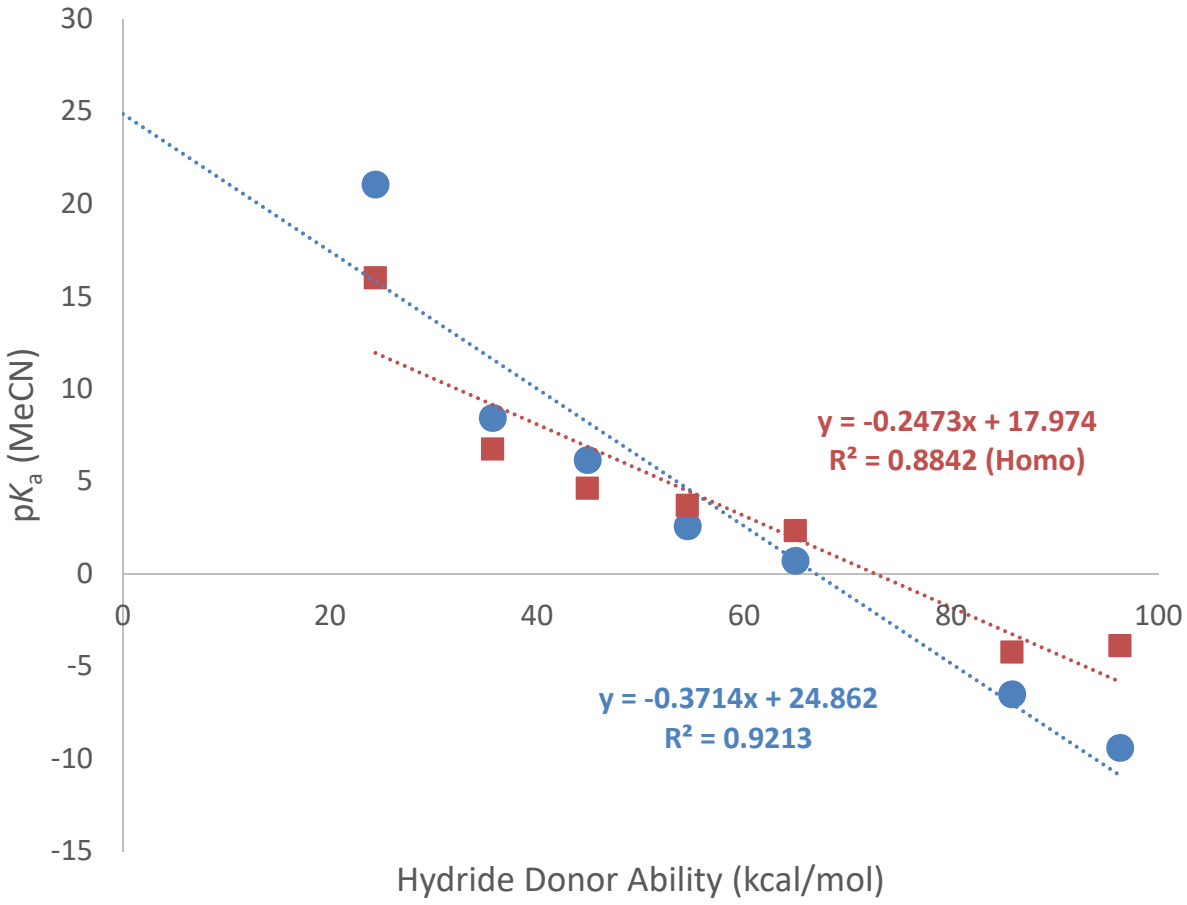


Figure S14. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the phenol-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

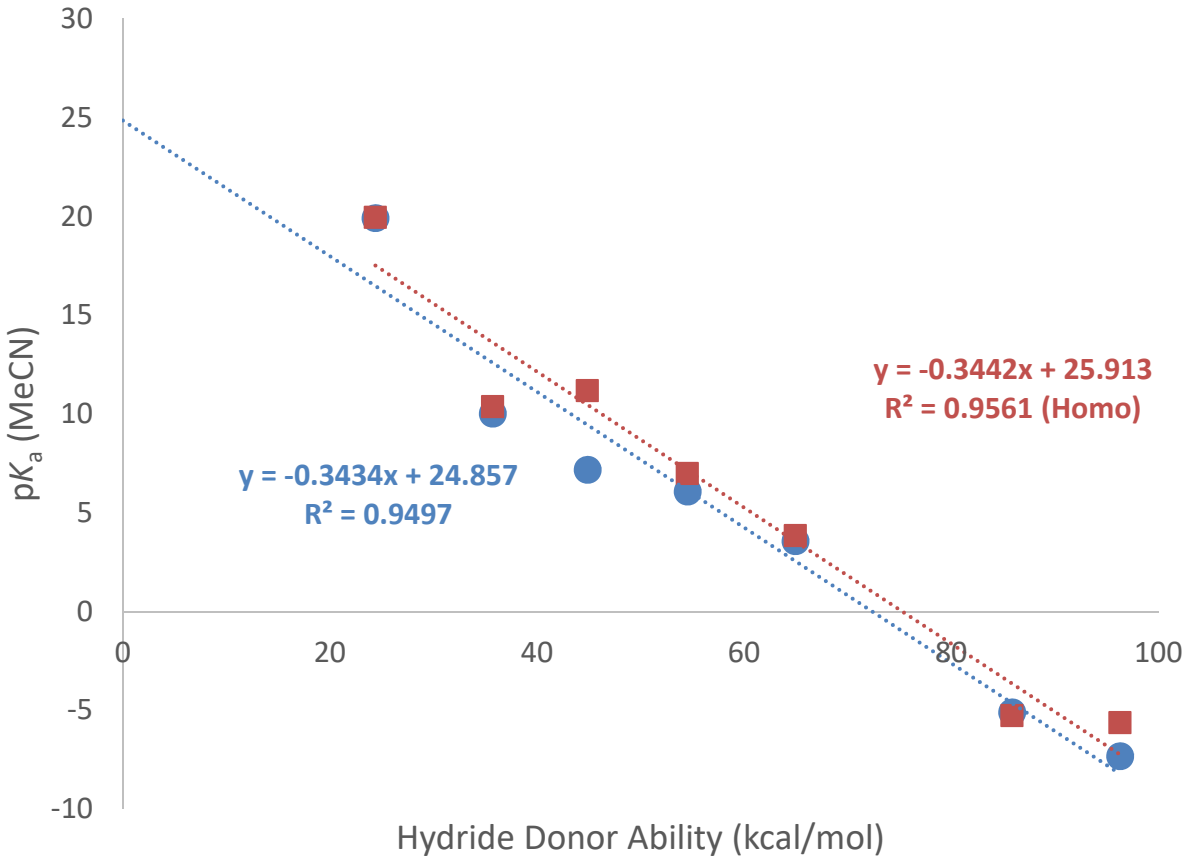


Figure S15. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the thiophenol-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

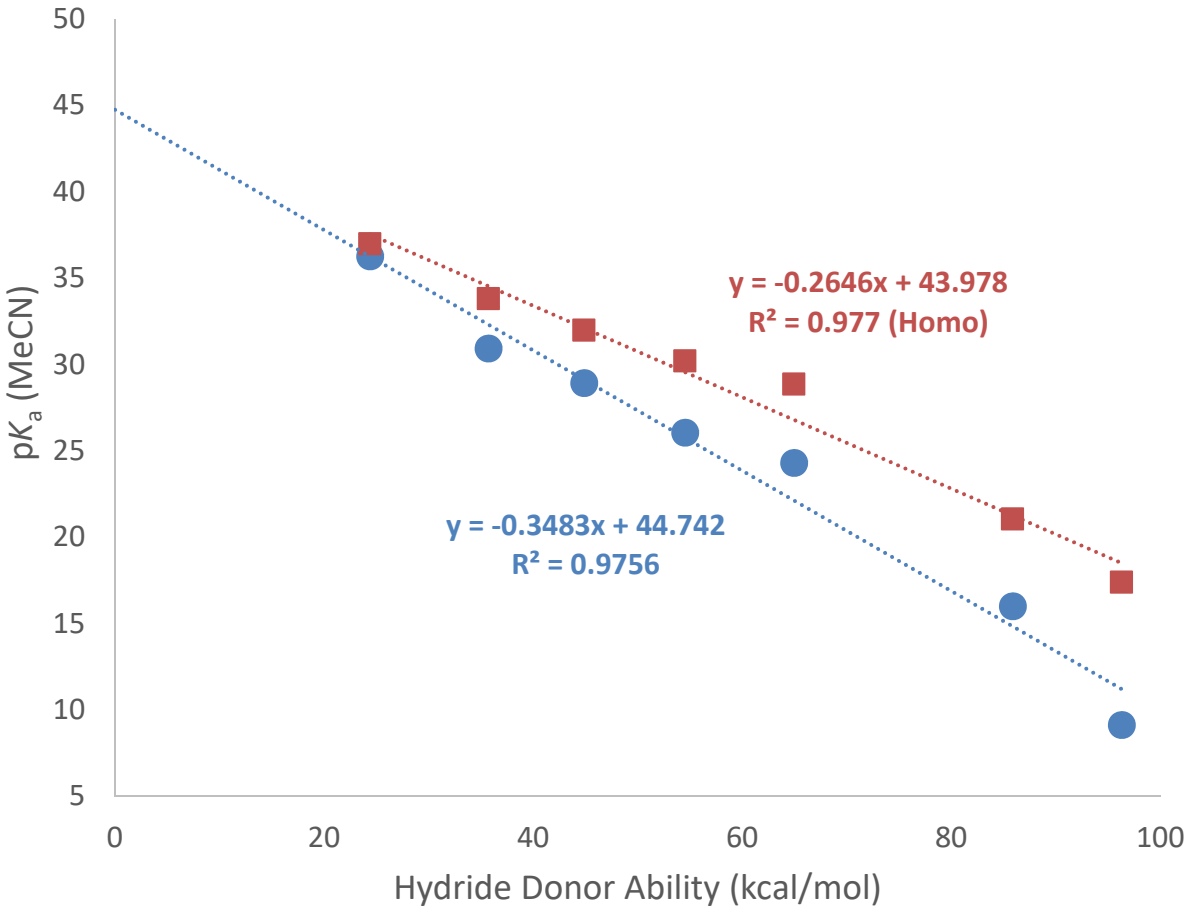


Figure S16. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the ammonia-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

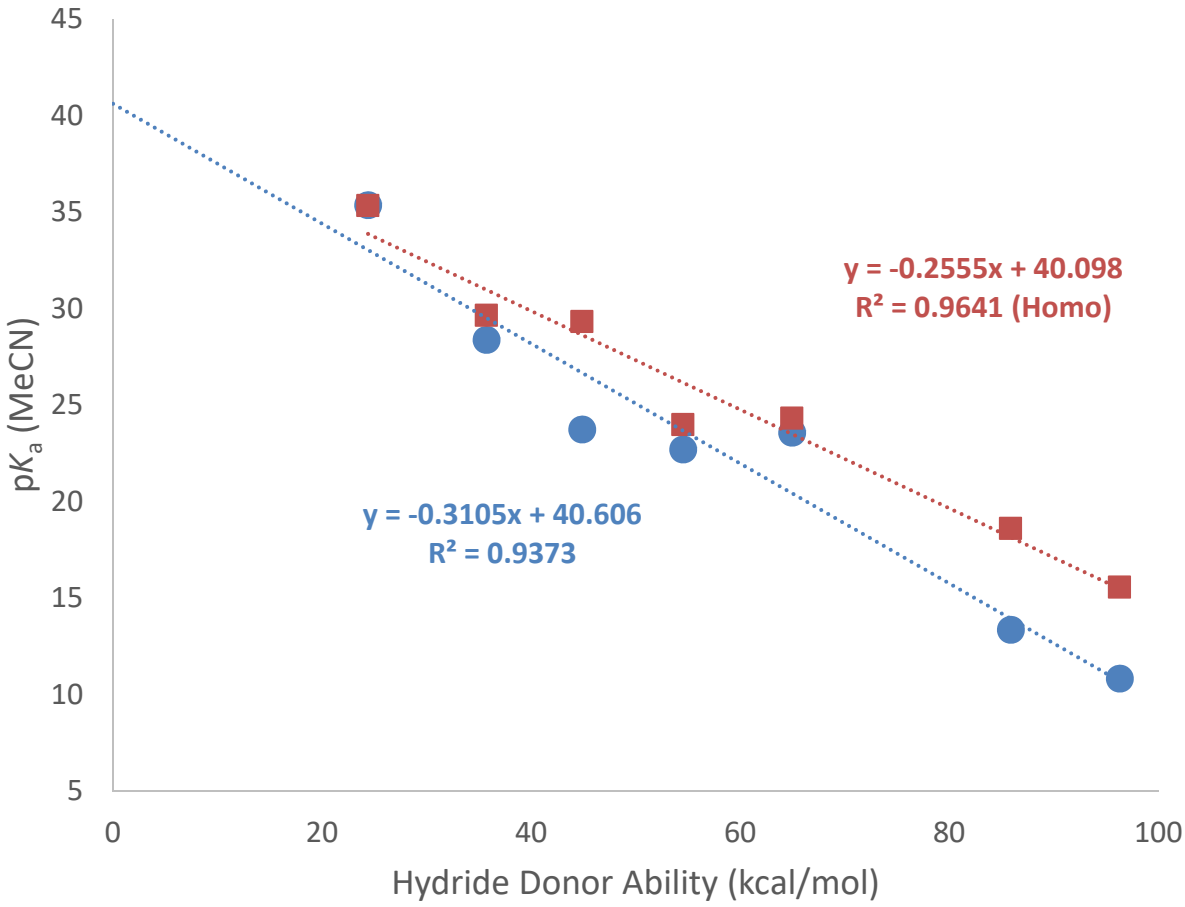


Figure S17. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the hydrazine-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

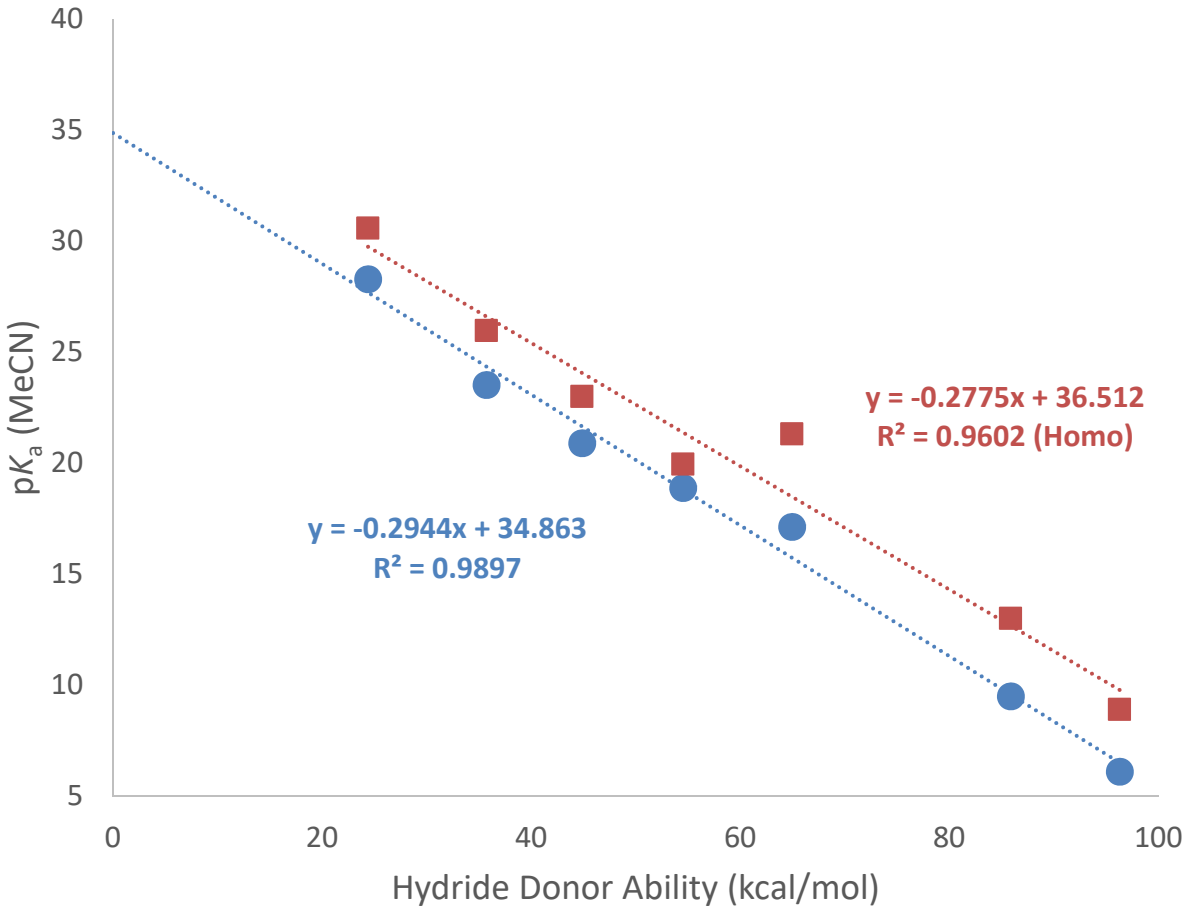


Figure S18. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the aniline-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

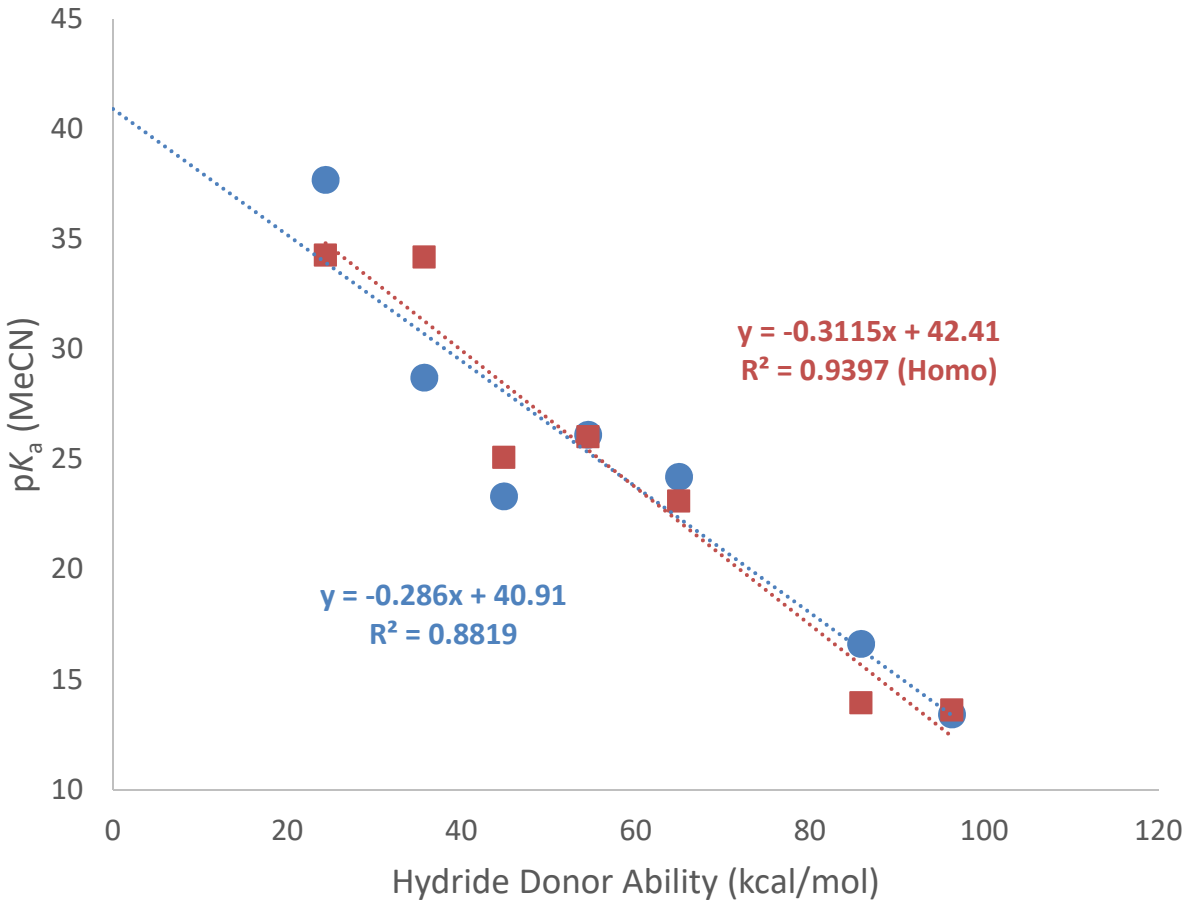


Figure S19. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the *N*-benzyl-2-methylpropan-2-amine-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

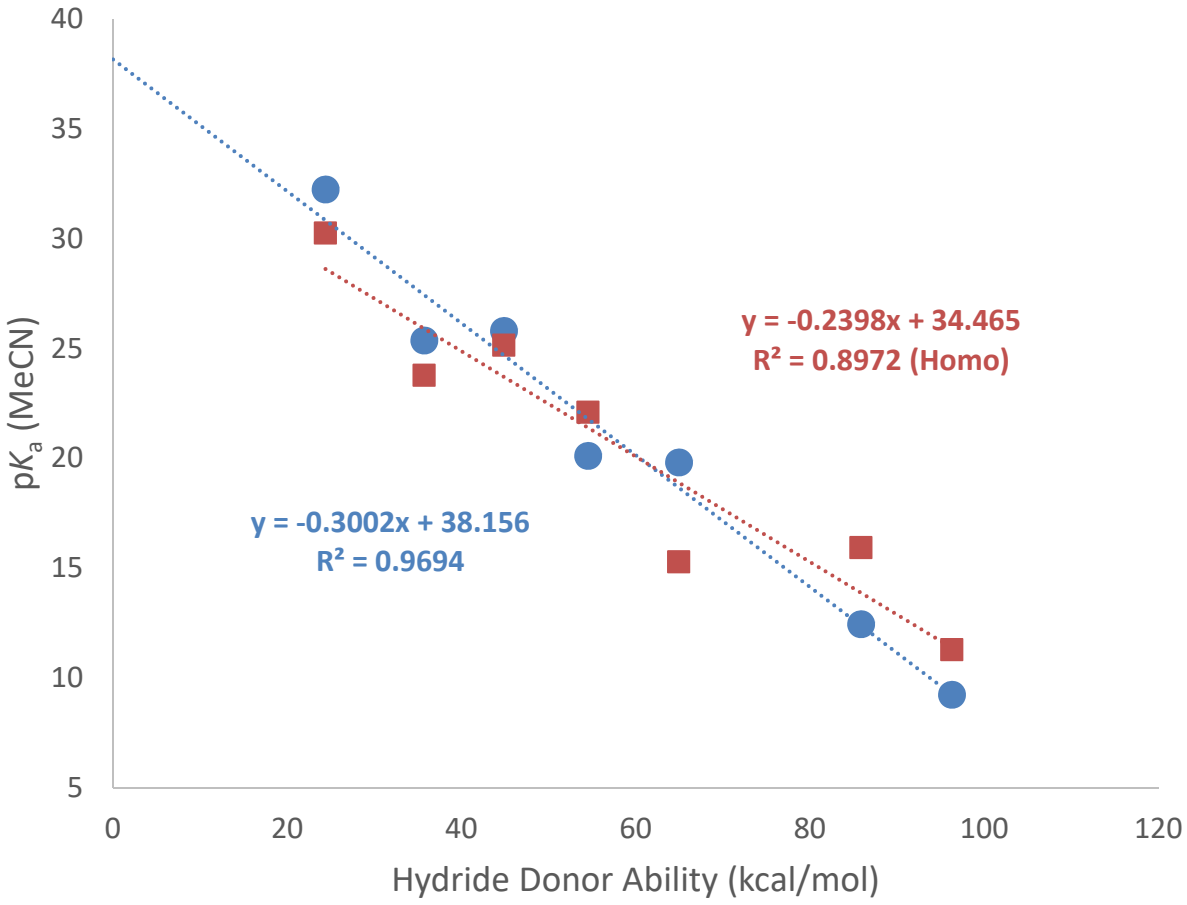


Figure S20. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the *N*-(1-phenylethyl)aniline-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

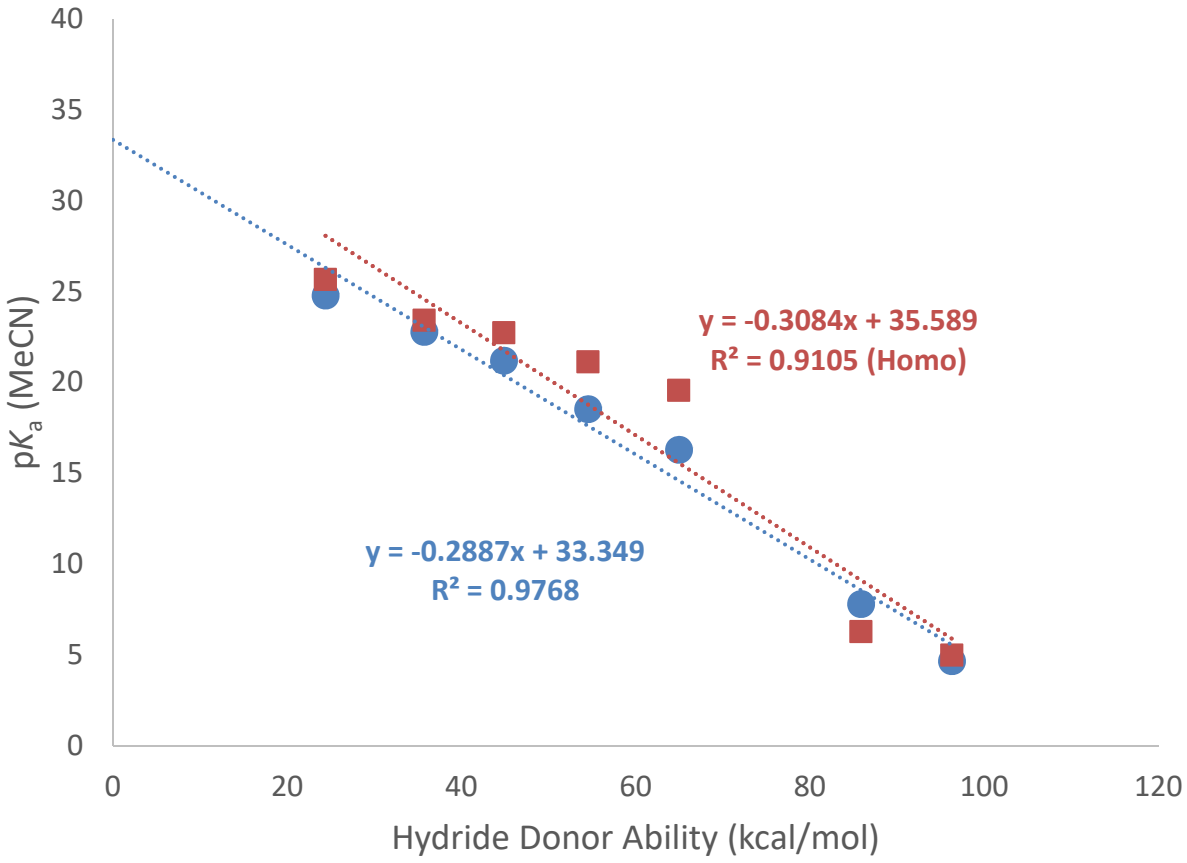


Figure S21. Plot showing the effect of homoconjugation and Lewis acid strength on the resulting pK_a of the phenylphosphine-Lewis acid adduct. The blue circles do not account for homoconjugation and the red squares include homoconjugation.

5) Plot of the Average Change in Lewis Acid-Lewis Base Adduct pK_a Not Accounting for Homoconjugation

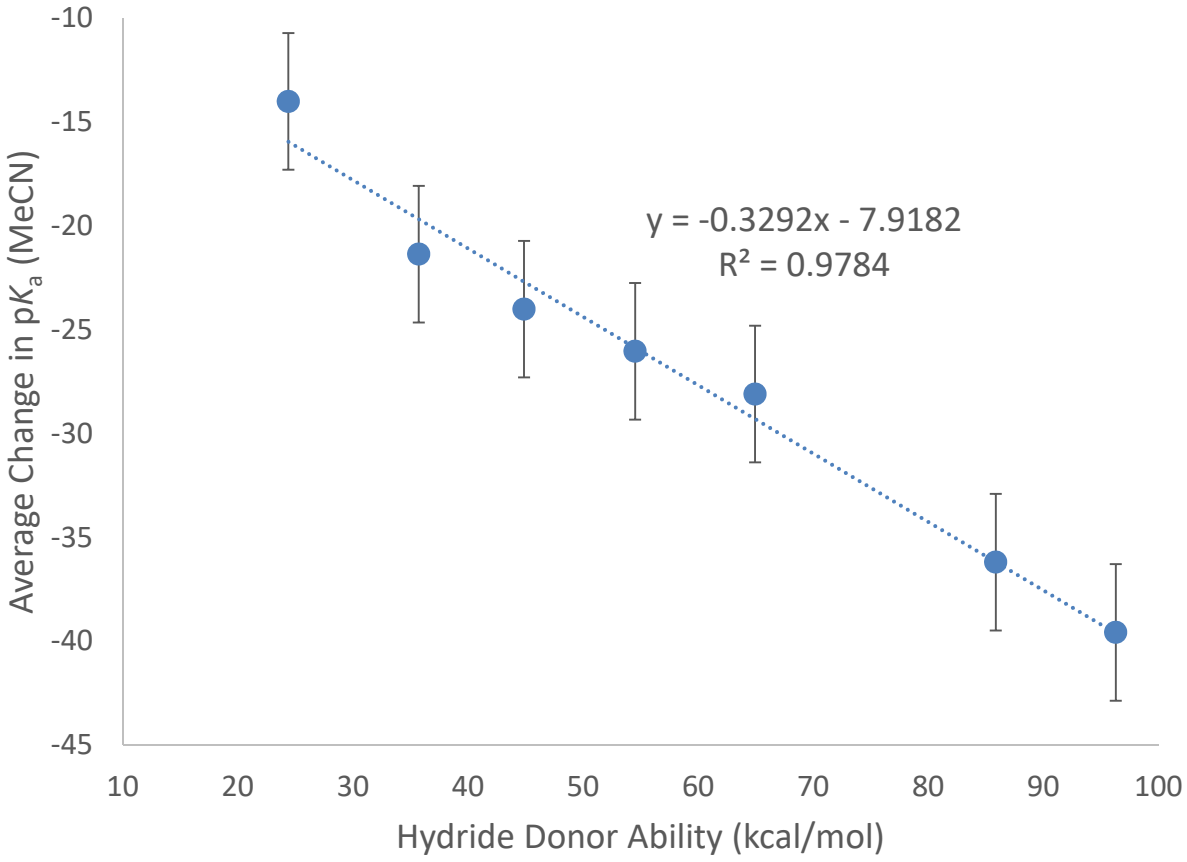


Figure S22. Linear correlation between the hydride donor ability and the average change of the pK_a of the substrate once bound to the Lewis acid. Homoconjugation was not accounted for in this plot.

6) Table of pK_a Change for Every Substrate-Lewis Acid Adduct

Table S1. pK_a differences of the parent Lewis base before and after coordintion to a Lewis acid.

	Change in pK_a after the addition of Lewis acid							
	H_2O	**Phenyl-ethanol**	**Phenol**	**Thiophenol**	**NH_3**	**N_2H_4**	**1-phenyl-1-ethylaniline**	**Benzyl-2-methyl propanamine**
BEt_3	-20.7	-17.8	-7.2	-2.6	-19.4	-20.3	-9.5	-19.6
BPh_3	-28.2	-26.3	-19.8	-12.5	-24.8	-27.3	-16.3	-28.6
$B(C_6F_5)Ph_2$	-30.4	-29.7	-22.1	-15.4	-26.7	-32.0	-15.9	-34.0
$B(C_6F_5)_2Ph$	-33.0	-31.2	-25.7	-16.5	-29.6	-33.0	-21.6	-31.2
$B(C_6F_5)_3$	-38.9	-33.5	-27.6	-19.0	-31.4	-32.1	-21.9	-34.5
$SiEt_3$	-45.8	-43.1	-34.8	-27.7	-39.7	-42.3	-29.2	-43.1
$SiPhH_2$	-50.0	-45.2	-37.7	-29.9	-46.6	-44.9	-36.9	-43.9

Table S1 Continued.

	Aniline	Phenyl-phosphine	Average ± Std. Dev
BEt_3	-14.5	-8.5	-14.0 ± 6.5
BPh_3	-19.3	-10.5	-21.4 ± 6.7
$B(C_6F_5)Ph_2$	-21.9	-12.1	-24.0 ± 7.7
$B(C_6F_5)_2Ph$	-23.9	-14.7	-26.0 ± 6.7
$B(C_6F_5)_3$	-25.7	-17.0	-28.1 ± 7.1
$SiEt_3$	-33.3	-25.5	-36.2 ± 7.1
$SiPhH_2$	-36.7	-28.6	-39.6 ± 7.6

7) Table of pK_a Change for Every Substrate-Lewis Acid Adduct Accounting for Homoconjugation

Table S2. pK_a differences of the parent Lewis base before and after coordintion to a Lewis acid.

	Change in pK_a after the addition of Lewis acid							
	H_2O	**Phenyl-ethanol**	**Phenol**	**Thiophenol**	**NH_3**	**N_2H_4**	**1-phenyl-1-ethylaniline**	**Benzyl-2-methyl propanamine**
BEt_3	-20.7	-17.8	-7.2	-2.6	-18.7	-20.3	-9.5	-19.6
BPh_3	-27.0	-27.4	-19.8	-12.5	-21.9	-26.0	-16.3	-28.6
$B(C_6F_5)Ph_2$	-28.7	-27.5	-22.1	-15.4	-23.7	-26.4	-15.9	-34.0
$B(C_6F_5)_2Ph$	-30.1	-30.7	-25.7	-16.5	-25.5	-31.7	-21.6	-31.3
$B(C_6F_5)_3$	-35.4	-29.3	-25.9	-19.0	-26.9	-31.4	-26.4	-34.2
$SiEt_3$	-37.2	-33.4	-32.5	-27.7	-34.7	-37.1	-25.8	-43.4
$SiPhH_2$	-43.1	-39.0	-32.2	-29.9	-38.3	-40.1	-30.4	-43.7

Table S2 Continued.

	Aniline	Phenyl-phosphine	Average ± Std. Dev
BEt_3	-12.2	-8.5	-13.7 ± 6.5
BPh_3	-16.8	-10.5	-20.7 ± 6.5
$B(C_6F_5)Ph_2$	-19.8	-12.1	-22.5 ± 6.9
$B(C_6F_5)_2Ph$	-22.8	-14.7	-25.0 ± 6.1
$B(C_6F_5)_3$	-21.5	-17.0	-26.7 ± 6.2
$SiEt_3$	-29.8	-25.5	-32.7 ± 5.7
$SiPhH_2$	-33.9	-28.6	-35.9 ± 5.6

8) Sample Calculation for the Determination of *Any* Lewis Base with *Any* Lewis Acid

The pK_a of phenol coordinated to $B(OC_6F_5)_3$ (ΔG_{H^-} ($[HB(OC_6F_5)_3]^-$ = 44 kcal/mol) can be estimated using the correlation seen in Figure 10. Free phenol has a pK_a of 28.3 in MeCN.

Correlation from Figure 10: y = (-0.28)(x)-9.02; where y = the difference in pK_a and x = the hydride donor ability of the respective main group hydride.

Using the correlation in Figure 10: y = (-0.28)(44) -9.02 = -21.3 pK_a units

This result indicates that coordination of phenol to $B(OC_6F_5)_3$ acidifies the phenol by 21.3 pK_a units. To determine the final pK_a of the phenol-$B(OC_6F_5)_3$ adduct the change is pK_a is subtracted from the pK_a of the free phenol molecule.

Final pK_a (MeCN) for phenol-$B(OC_6F_5)_3$ = 28.3 – 21.3 = 7.0

9) Ladder Diagrams Showing the Effect of Lewis Acidity on the Brønsted Acidity of the Lewis Acid/Base Adduct

Figure S23. pK_a's of Lewis acid-protic Lewis base adducts in MeCN (homoconjugation contributions are included).

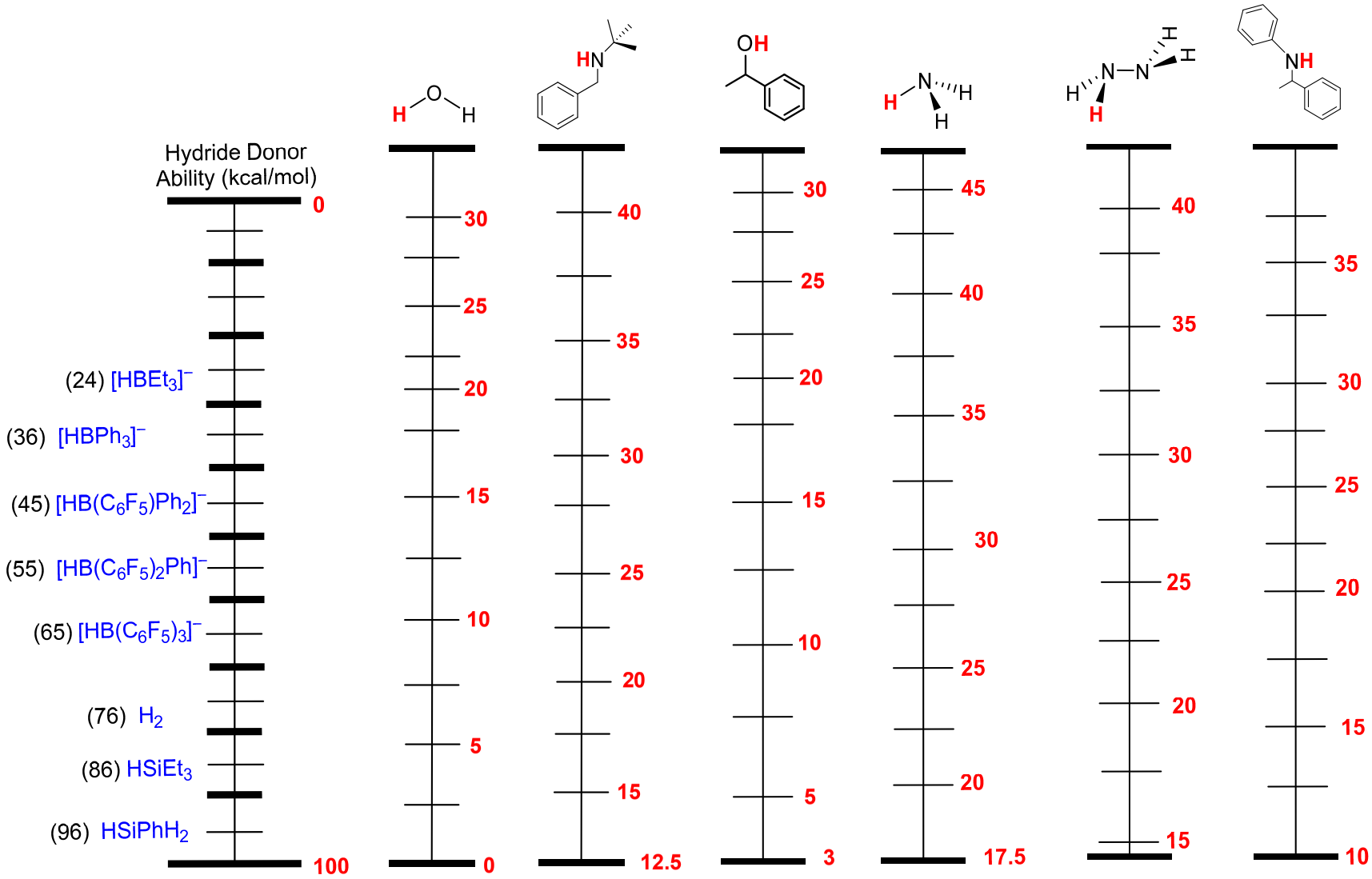
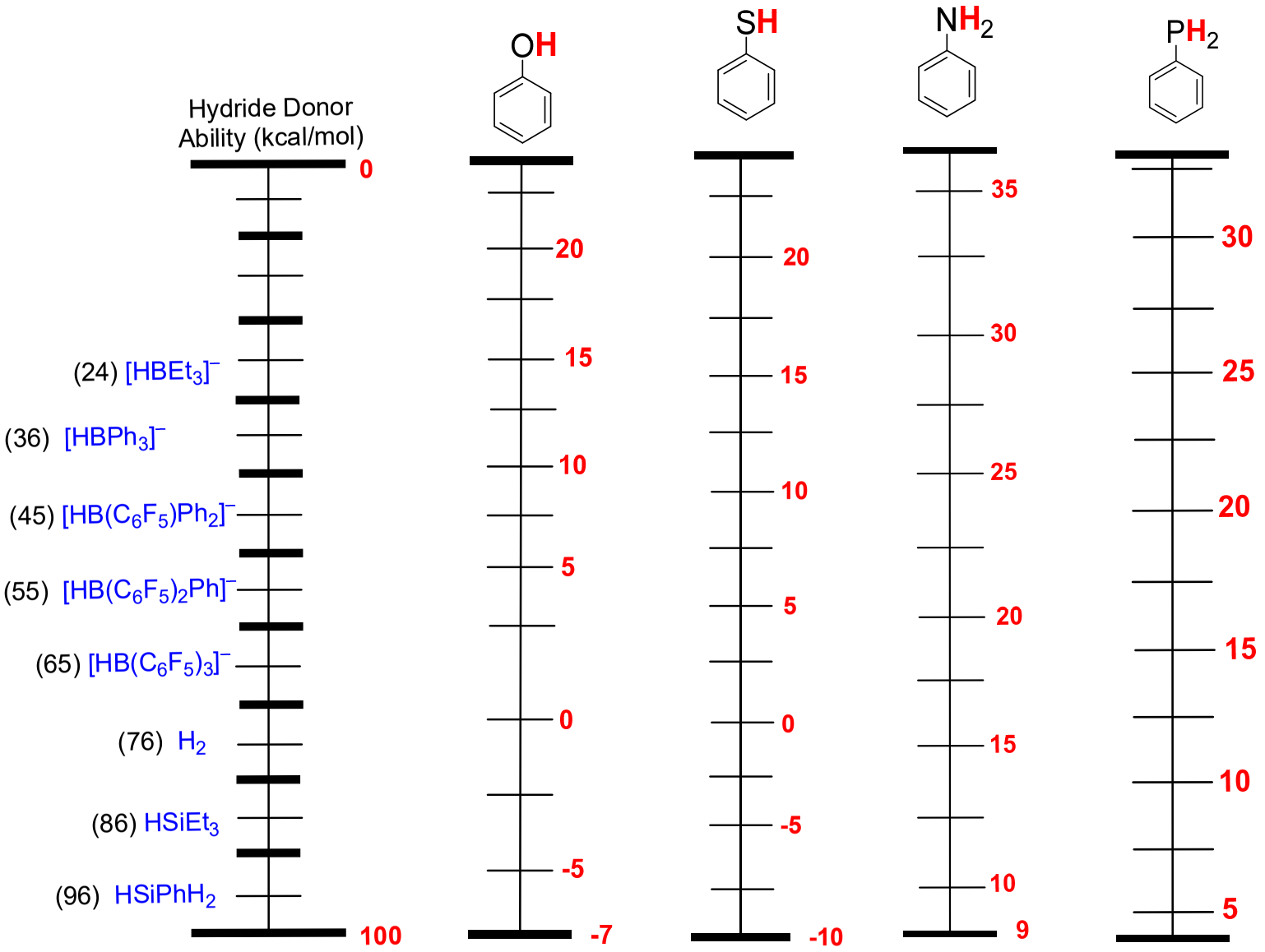


Figure S24. pK_a's of Lewis acid-protic Lewis base adducts in MeCN (homoconjugation contributions are included).



10) Energy Values for the Computed Substrates.

Table S3. Computed energies for the optimized structures of the examined substrates. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Substrate	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$[H_3O]^+$	-76.653203	0.015477	0.038492
H_2O	-76.37986	0.004079	0.02549
$[OH]^-$	-75.703216	-0.008091	0.011493
H_2O-H_2O	-152.7806625	0.021168	0.053977
$[H_2O$-$OH]^-$	-152.1520687	0.006671	0.035571
$[NH_4]^+$	-56.8666485	0.030153	0.053605
NH_3	-56.504904	0.016769	0.038608
$[NH_2]^-$	-55.816974	0.000533	0.022032
$[N_2H_5]^+$	-112.1561667	0.045628	0.072878
N_2H_4	-111.8062109	0.030745	0.05828
$[N_2H_3]^-$	-111.1226805	0.01431	0.041064
1-pheny-l-ethyloxonium	-386.2541361	0.140652	0.184734
1-phenyl-1-ethanol	-385.800128	0.130251	0.172431
1-phenylethan-1-olate	-385.195774	0.114908	0.156327
(1-phenylethyl)benzenaminium	-597.4032343	0.231101	0.285653
(1-phenylethyl)aniline	-597.0270433	0.217462	0.271315
phenyl(1-phenylethyl)amide	-596.4307265	0.202882	0.255723
Benzyl-2-methylpropan-2-aminium	-484.3376386	0.235834	0.289075
1-benzyl-2-methyl-2-propanamine	-483.949135	0.221586	0.274231
Benzyl(tert-butyl)amide	-483.3085134	0.203594	0.256288
Phenol	-307.3415712	0.07695	0.112323
Phenoxide	-306.7576545	0.063025	0.09796
Thiophenol	-630.2978816	0.070081	0.107676
Thiophenoxide	-629.7442808	0.060844	0.097055
Aniline	-287.481028	0.0892	0.125016
Anilide	-286.8671637	0.074819	0.110059
Anilinium	-287.8326682	0.100318	0.139703
Phenylphosphine	-574.0470899	0.078529	0.116943
Phenylphosphide	-573.464655	0.068442	0.105425
Phenylphosphonium	-574.3839613	0.089461	0.128221

11) Energies for the Optimized Lewis Acid-H_2O Adducts.

Table S4. Computed energies for the optimized structures of the H_2O-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
H_2O-BEt_3	-338.607843	0.192972	0.242617
$[HO\text{-}BEt_3]^-$	-338.080071	0.178778	0.227613
$(H_2O)_2$-BEt_3	-415.2120272	0.216515	0.270786
$[(H_2O\text{-}HO)\text{-}BEt_3]^-$	-414.6742174	0.200932	0.256264
H_2O-BPh_3	-795.66901	0.259665	0.323808
$[HO\text{-}BPh_3]^-$	-795.164833	0.246039	0.309917
$(H_2O)_2$-BPh_3	-872.3439925	0.281625	0.352236
$[(H_2O\text{-}HO)\text{-}BPh_3]^-$	-871.8254283	0.269176	0.338621
H_2O-$B(C_6F_5)Ph_2$	-1291.716263	0.21416	0.288324
$[HO\text{-}B(C_6F_5)Ph_2]^-$	-1291.423964	0.200989	0.274324
$(H_2O)_2$-$B(C_6F_5)Ph_2$	-1368.346056	0.23689	0.316
$[(H_2O\text{-}HO)\text{-}B(C_6F_5)Ph_2]^-$	-1367.832947	0.223182	0.302936
H_2O-$B(C_6F_5)_2Ph$	-1787.76373	0.167817	0.251905
$[HO\text{-}B(C_6F_5)_2Ph]^-$	-1787.278444	0.155162	0.23832
$(H_2O)_2$-$B(C_6F_5)_2Ph$	-1864.343309	0.189692	0.279965
$[(H_2O\text{-}HO)\text{-}B(C_6F_5)_2Ph]^-$	-1863.843312	0.17888	0.267023
H_2O-$B(C_6F_5)_3$	-2283.804373	0.124689	0.216473
$[HO\text{-}B(C_6F_5)_3]^-$	-2283.334069	0.110152	0.202468
$(H_2O)_2$-$B(C_6F_5)_3$	-2360.342413	0.145385	0.243837
$[(H_2O\text{-}HO)\text{-}B(C_6F_5)_3]^-$	-2359.853692	0.133102	0.230961
$[H_2O\text{-}SiEt_3]^+$	-603.023596	0.185212	0.240183
HO-$SiEt_3$	-602.701292	0.176141	0.227486
$[(H_2O)_2\text{-}SiEt_3]^+$	-679.6371536	0.204721	0.267171
$(H_2O\text{-}HO)\text{-}SiEt_3$	-679.2788955	0.197046	0.255711
$[H_2O\text{-}SiPhH_2]^+$	-598.260904	0.100249	0.145036
HO-$SiPhH_2$	-597.949838	0.089747	0.132517
$[(H_2O)_2\text{-}SiPhH_2]^+$	-674.7948659	0.122603	0.171547
$(H_2O\text{-}HO)\text{-}SiPhH_2$	-674.4448756	0.111739	0.16108

12) Energies for the Optimized Lewis Acid-NH_3 Adducts.

Table S5. Computed energies for the optimized structures of the NH_3O-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
H_3N-BEt_3	-318.746701	0.209304	0.256863
$[H_2N$-$BEt_3]^-$	-318.183856	0.191536	0.240045
$(NH_3)_2$-BEt_3	-375.4977123	0.242776	0.297843
$[(NH_3$-$NH_2)$-$BEt_3]^-$	-374.919376	0.224767	0.28116
H_3N-BPh_3	-775.811046	0.2746	0.338358
$[H_2N$-$BPh_3]^-$	-775.270565	0.258943	0.322464
$(NH_3)_2$-BPh_3	-832.6334848	0.30882	0.379401
$[(NH_3$-$NH_2)$-$BPh_3]^-$	-832.0637864	0.29085	0.363257
H_3N-$B(C_6F_5)Ph_2$	-1271.860244	0.228421	0.302552
$[H_2N$-$B(C_6F_5)Ph_2]^-$	-1271.327213	0.212627	0.286679
$(NH_3)_2$-$B(C_6F_5)Ph_2$	-1328.635923	0.261691	0.34327
$[(NH_3$-$NH_2)$-$B(C_6F_5)Ph_2]^-$	-1328.076552	0.24568	0.327618
H_3N-$B(C_6F_5)_2Ph$	-1767.905723	0.183446	0.266593
$[H_2N$-$B(C_6F_5)_2Ph]^-$	-1767.381987	0.167851	0.250806
$(NH_3)_2$-$B(C_6F_5)_2Ph$	-1824.638013	0.215847	0.307319
$[(NH_3$-$NH_2)$-$B(C_6F_5)_2Ph]^-$	-1824.086275	0.200531	0.291658
H_3N-$B(C_6F_5)_3$	-2263.952594	0.137901	0.230699
$[H_2N$-$B(C_6F_5)_3]^-$	-2263.435934	0.121568	0.214883
$(NH_3)_2$-$B(C_6F_5)_3$	-2320.635588	0.170713	0.271346
$[(NH_3$-$NH_2)$-$B(C_6F_5)_3]^-$	-2320.093647	0.15598	0.255855
$[H_3N$-$SiEt_3]^+$	-583.170128	0.200867	0.254715
H_2N-$SiEt_3$	-582.807726	0.187154	0.239712
$[(NH_3)_2$-$SiEt_3]^+$	-639.9302236	0.232736	0.295137
$(NH_3$-$NH_2)$-$SiEt_3$	-639.5265505	0.217351	0.280654
$[H_3N$-$SiPhH_2]^+$	-578.402396	0.117869	0.158682
H_2N-$SiPhH_2$	-578.025990	0.102437	0.145018
$[(NH_3)_2$-$SiPhH_2]^+$	-635.0873073	0.146409	0.19989
$(NH_3$-$NH_2)$-$SiPhH_2$	-634.6942719	0.132218	0.186017

13) Energies for the Optimized Lewis Acid-Hydrazine Adducts.

Table S6. Computed energies for the optimized structures of the hydrazine-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
N_2H_4-BEt_3	-374.2509938	0.225032	0.275887
$[N_2H_3$-$BEt_3]^-$	-373.6769989	0.209268	0.259494
$(N_2H_4)_2$-BEt_3	-486.0802188	0.274277	0.33641
$[(N_2H_4$-$N_2H_3)$-$BEt_3]^-$	-485.5146998	0.25885	0.320568
N_2H_4-BPh_3	-831.380834	0.291875	0.357731
$[N_2H_3$-$BPh_3]^-$	-830.8273305	0.275912	0.341608
$(N_2H_4)_2$-BPh_3	-943.2147506	0.342501	0.418295
$[(N_2H_4$-$N_2H_3)$-$BPh_3]^-$	-942.6607126	0.325806	0.402776
N_2H_4-$B(C_6F_5)Ph_2$	-1327.379441	0.246555	0.321964
$[N_2H_3$-$B(C_6F_5)Ph_2]^-$	-1326.838288	0.229575	0.305578
$(N_2H_4)_2$-$B(C_6F_5)Ph_2$	-1439.222771	0.297751	0.382278
$[(N_2H_4$-$N_2H_3)$-$B(C_6F_5)Ph_2]^-$	-1438.670398	0.278911	0.366847
N_2H_4-$B(C_6F_5)_2Ph$	-1823.383673	0.200932	0.285724
$[N_2H_3$-$B(C_6F_5)_2Ph]^-$	-1822.848555	0.18437	0.27000
$(N_2H_4)_2$-$B(C_6F_5)_2Ph$	-1935.217408	0.251626	0.346129
$[(N_2H_4$-$N_2H_3)$-$B(C_6F_5)_2Ph]^-$	-1934.684349	0.235145	0.331002
N_2H_4-$B(C_6F_5)_3$	-2319.385093	0.155735	0.249713
$[N_2H_3$-$B(C_6F_5)_3]^-$	-2318.857278	0.139048	0.233977
$(N_2H_4)_2$-$B(C_6F_5)_3$	-2431.222563	0.206502	0.310501
$[(N_2H_4$-$N_2H_3)$-$B(C_6F_5)_3]^-$	-2430.685064	0.190004	0.294763
$[N_2H_4$-$SiEt_3]^+$	-638.6626334	0.219498	0.273782
N_2H_3-$SiEt_3$	-638.284859	0.203735	0.259005
$[(N_2H_4)_2$-$SiEt_3]^+$	-750.5144386	0.270721	0.334293
$(N_2H_4$-$N_2H_3)$-$SiEt_3$	-750.1103783	0.254308	0.319756
$[N_2H_4$-$SiPhH_2]^+$	-633.814985	0.131701	0.178492
N_2H_3-$SiPhH_2$	-633.4489462	0.118176	0.164154
$[(N_2H_4)_2$-$SiPhH_2]^+$	-745.6681436	0.182602	0.23839
$(N_2H_4$-$N_2H_3)$-$SiPhH_2$	-745.2751011	0.167622	0.225175

14) Energies for the Optimized Lewis Acid-*N*-benzyl-2-methylpropan-2-amine (HBMPA) Adducts.

Table S7. Computed energies for the optimized structures of the HBMPA-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
HBMPA-BEt_3	-746.3710895	0.422073	0.49288
$[BMPA\text{-}BEt_3]^-$	-745.8055042	0.405408	0.475765
$(HBMPA)_2\text{-}BEt_3$	-1230.33301	0.669178	0.769616
$[(HBMPA\text{-}BMPA)\text{-}BEt_3]^-$	-1229.77376	0.650072	0.751656
HBMPA-BPh_3	-1202.951338	0.489463	0.5742
$[BMPA\text{-}BPh_3]^-$	-1202.422266	0.47269	0.557368
$(HBMPA)_2\text{-}BPh_3$	-1687.463555	0.736041	0.850536
$[(HBMPA\text{-}BMPA)\text{-}BPh_3]^-$	-1686.906864	0.719108	0.833871
HBMPA-$B(C_6F_5)Ph_2$	-1699.052255	0.443491	0.538274
$[BMPA\text{-}B(C_6F_5)Ph_2]^-$	-1698.473998	0.426931	0.521528
$(HBMPA)_2\text{-}B(C_6F_5)Ph_2$	-2183.460055	0.689973	0.814355
$[(HBMPA\text{-}BMPA)\text{-}B(C_6F_5)Ph_2]^-$	-2182.926142	0.671323	0.797669
HBMPA -$B(C_6F_5)_2Ph$	-2195.101696	0.399093	0.501797
$[BMPA\text{ -}B(C_6F_5)_2Ph]^-$	-2194.515857	0.38157	0.485613
$(HBMPA)_2\text{-}B(C_6F_5)_2Ph$	-2679.468126	0.643319	0.778397
$[(HBMPA\text{-}BMPA)\text{-}B(C_6F_5)_2Ph]^-$	-2678.936063	0.625468	0.762137
HBMPA-$B(C_6F_5)_3$	-2691.506721	0.353994	0.466266
$[BMPA\text{ - }B(C_6F_5)_3]^-$	-2690.975533	0.336689	0.449928
$(HBMPA)_2\text{-}B(C_6F_5)_3$	-3175.477434	0.600485	0.742836
$[(HBMPA\text{-}BMPA)\text{-}B(C_6F_5)_3]^-$	-3174.953439	0.582978	0.726618
$[HBMPA\text{ -}SiEt_3]^+$	-1010.810112	0.416493	0.490712
BMPA -$SiEt_3$	-1010.412072	0.401682	0.475948
$[(HBMPA)_2\text{-}SiEt_3]^+$	-1494.786291	0.664219	0.767452
(HBMPA-BMPA)-$SiEt_3$	-1494.381721	0.646257	0.751753
$[HBMPA\text{ -}SiPhH_2]^+$	-1005.978045	0.327545	0.395082
BMPA -$SiPhH_2$	-1005.586889	0.312454	0.380556
$[(HBMPA)_2\text{-}SiPhH_2]^+$	-1489.952926	0.575447	0.672055
(HBMPA-BMPA)-$SiPhH_2$	-1489.552287	0.559005	0.656679

15) Energies for the Optimized Lewis Acid-*N*-(1-phenylethyl)aniline Adducts.

Table S8. Computed energies for the optimized structures of the *N*-(1-phenylethyl)aniline-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
PhNHMeBn-BEt_3	-859.4495853	0.414462	0.489243
$[PhNMeBn\text{-}BEt_3]^-$	-858.8940551	0.400033	0.473257
$(PhNHMeBn)_2\text{-}BEt_3$	-1456.49751	0.656603	0.763016
$[(PhNHMeBn\text{-}PhNMeBn)\text{-}BEt_3]^-$	-1455.948031	0.638992	0.747417
PhNHMeBn-BPh_3	-1316.096077	0.482124	0.570925
$[PhNMeBn\text{-}BPh_3]^-$	-1315.513585	0.46811	0.555436
$(PhNHMeBn)_2\text{-}BPh_3$	-1913.623399	0.726117	0.845009
$[(PhNHMeBn\text{-}PhNMeBn)\text{-}BPh_3]^-$	-1913.094446	0.707016	0.828346
PhNHMeBn-$B(C_6F_5)Ph_2$	-1812.577828	0.437137	0.534056
$[PhNMeBn\text{-}B(C_6F_5)Ph_2]^-$	-1812.044523	0.42045	0.518581
$(PhNHMeBn)_2\text{-}B(C_6F_5)Ph_2$	-2409.620867	0.680059	0.808598
$[(PhNHMeBn\text{-}PhNMeBn)\text{-}B(C_6F_5)Ph_2]^-$	-2409.088542	0.66486	0.792936
PhNHMeBn-$B(C_6F_5)_2Ph$	-2308.569408	0.391311	0.498018
$[PhNMeBn\text{-}B(C_6F_5)_2Ph]^-$	-2308.055857	0.376287	0.483287
$(PhNHMeBn)_2\text{-}B(C_6F_5)_2Ph$	-2905.617137	0.635937	0.772462
$[(PhNHMeBn\text{-}PhNMeBn)\text{-}B(C_6F_5)_2Ph]^-$	-2905.095926	0.619208	0.756375
PhNHMeBn-$B(C_6F_5)_3$	-2804.57404	0.347065	0.462402
$[PhNMeBn\text{-}B(C_6F_5)_3]^-$	-2804.059817	0.3297	0.446912
$(PhNHMeBn)_2\text{-}B(C_6F_5)_3$	-3401.621098	0.590221	0.736469
$[(PhNHMeBn\text{-}PhNMeBn)\text{-}B(C_6F_5)_3]^-$	-3401.115853	0.572125	0.72046
$[PhNHMeBn\text{-}SiEt_3]^+$	-1123.474979	0.408108	0.486898
PhNMeBn-$SiEt_3$	-1123.04689	0.395274	0.473066
$[(PhNHMeBn)_2\text{-}SiEt_3]^+$	-1720.941682	0.649854	0.760986
(PhNHMeBn-PhNMeBn)-$SiEt_3$	-1720.531952	0.635897	0.746592
$[PhNHMeBn\text{-}SiPhH_2]^+$	-1118.724641	0.321727	0.391433
PhNMeBn-$SiPhH_2$	-1118.303028	0.306894	0.377821
$[(PhNHMeBn)_2\text{-}SiPhH_2]^+$	-1716.10148	0.561839	0.665403
(PhNHMeBn-PhNMeBn)-$SiPhH_2$	-1715.706608	0.550173	0.651037

16) Energies for the Optimized Lewis Acid-Phenylethanol Adducts.

Table S9. Computed energies for the optimized structures of the phenylethanol-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
PhEtOH-BEt_3	-648.025171	0.321738	0.388796
$[PhEtO\text{-}BEt_3]^-$	-647.452763	0.309431	0.373813
$(PhEtOH)_2\text{-}BEt_3$	-1034.294847	0.475784	0.563866
$[(PhEtOH\text{-}PhEtO)\text{-}BEt_3]^-$	-1033.768783	0.460886	0.548399
PhEtOH-BPh_3	-1105.475575	0.389508	0.470462
$[PhEtO\text{-}BPh_3]^-$	-1104.965228	0.37604	0.455576
$(PhEtOH)_2\text{-}BPh_3$	-1491.426396	0.540826	0.645291
$[(PhEtOH\text{-}PhEtO)\text{-}BPh_3]^-$	-1490.922771	0.528294	0.63044
PhEtOH-$B(C_6F_5)Ph_2$	-1601.477752	0.345781	0.434152
$[PhEtO\text{-}B(C_6F_5)Ph_2]^-$	-1600.976631	0.330354	0.419656
$(PhEtOH)_2\text{-}B(C_6F_5)Ph_2$	-1987.437864	0.49667	0.608161
$[(PhEtOH\text{-}PhEtO)\text{-}B(C_6F_5)Ph_2]^-$	-1986.933066	0.483144	0.594182
PhEtOH-$B(C_6F_5)_2Ph$	-2097.479766	0.29916	0.397964
$[PhEtO\text{-}B(C_6F_5)_2Ph]^-$	-2096.986144	0.284752	0.38379
$(PhEtOH)_2\text{-}B(C_6F_5)_2Ph$	-2483.441873	0.456655	0.572706
$[(PhEtOH\text{-}PhEtO)\text{-}B(C_6F_5)_2Ph]^-$	-2482.946745	0.437271	0.558646
PhEtOH-$B(C_6F_5)_3$	-2593.483989	0.255444	0.362376
$[PhEtO\text{-}B(C_6F_5)_3]^-$	-2592.995545	0.239553	0.347912
$(PhEtOH)_2\text{-}B(C_6F_5)_3$	-2979.449315	0.408758	0.535978
$[(PhEtOH\text{-}PhEtO)\text{-}B(C_6F_5)_3]^-$	-2978.960243	0.396406	0.523039
$[PhEtOH\text{-}SiEt_3]^+$	-912.450885	0.318978	0.387049
PhEtO-$SiEt_3$	-912.065511	0.305678	0.37404
$[(PhEtOH)_2\text{-}SiEt_3]^+$	-1298.746623	0.466826	0.560156
(PhEtOH-PhEtO)-$SiEt_3$	-1298.36912	0.460026	0.549122
$[PhEtOH\text{-}SiPhH_2]^+$	-907.698872	0.228657	0.291522
PhEtO-$SiPhH_2$	-907.322346	0.220866	0.279052
$[(PhEtOH)_2\text{-}SiPhH_2]^+$	-1293.914803	0.387163	0.465141
(PhEtOH-PhEtO)-$SiPhH_2$	-1293.539073	0.372212	0.453435

17) Energies for the Optimized Lewis Acid-Phenol Adducts.

Table S10. Computed energies for the optimized structures of the phenol-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Phenol-BEt_3	-569.7587192	0.264872	0.327452
[Phenoxide-BEt_3]$^-$	-569.2356955	0.255108	0.31392
$(Phenol)_2$-BEt_3	-877.1154643	0.359678	0.442049
[(Phenol-Phenoxide)-BEt_3]$^-$	-876.6122327	0.350898	0.42839
Phenol-BPh_3	-1026.878189	0.334804	0.410167
[Phenoxide-BPh_3]$^-$	-1026.381673	0.321601	0.396059
$(Phenol)_2$-BPh_3	-1334.239931	0.431948	0.524772
[(Phenol-Phenoxide)-BPh_3]$^-$	-1333.749543	0.417534	0.510357
Phenol-$B(C_6F_5)Ph_2$	-1522.881707	0.289691	0.374282
[Phenoxide-$B(C_6F_5)Ph_2$]$^-$	-1522.390476	0.276537	0.36014
$(Phenol)_2$-$B(C_6F_5)Ph_2$	-1830.244011	0.383951	0.488922
[(Phenol-Phenoxide)-$B(C_6F_5)Ph_2$]$^-$	-1829.761236	0.372784	0.474857
Phenol-$B(C_6F_5)_2Ph$	-2018.88062	0.244546	0.338113
[Phenoxide-$B(C_6F_5)_2Ph$]$^-$	-2018.401257	0.231406	0.324351
$(Phenol)_2$-$B(C_6F_5)_2Ph$	-2326.238569	0.339896	0.452159
[(Phenol-Phenoxide)-$B(C_6F_5)_2Ph$]$^-$	-2325.762358	0.327726	0.43861
Phenol-$B(C_6F_5)_3$	-2514.879184	0.198147	0.301866
[Phenoxide-$B(C_6F_5)_3$]$^-$	-2514.407272	0.186052	0.288388
$(Phenol)_2$-$B(C_6F_5)_3$	-2822.248901	0.297983	0.415657
[(Phenol-Phenoxide)-$B(C_6F_5)_3$]$^-$	-2821.777042	0.284445	0.403218
[Phenol-$SiEt_3$]$^+$	-834.1702217	0.262079	0.326223
Phenoxide-$SiEt_3$	-833.8347832	0.250693	0.31383
[$(Phenol)_2$-$SiEt_3$]$^+$	-1141.55032	0.360424	0.440093
(Phenol-Phenoxide)-$SiEt_3$	-1141.193645	0.345663	0.428579
[Phenol-$SiPhH_2$]$^+$	-829.3223114	0.175516	0.231383
Phenoxide-$SiPhH_2$	-828.995148	0.164727	0.219047
[$(Phenol)_2$-$SiPhH_2$]$^+$	-1136.707417	0.273418	0.344687
(Phenol-Phenoxide)-$SiPhH_2$	-1136.355959	0.263085	0.333687

18) Energies for the Optimized Lewis Acid-Thiophenol Adducts.

Table S11. Computed energies for the optimized structures of the thiophenol-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
PhSH-BEt_3	-892.7114406	0.256848	0.322855
$[PhS\text{-}BEt_3]^-$	-892.1931003	0.251475	0.312455
$(PhSH)_2$-BEt_3	-1523.016592	0.342696	0.432429
$[(PhSH\text{-}PhS)\text{-}BEt_3]^-$	-1522.511648	0.340513	0.421819
PhSH-BPh_3	-1349.831853	0.328764	0.40545
$[PhS\text{-}BPh_3]^-$	-1349.331128	0.316535	0.393922
$(PhSH)_2$-BPh_3	-1980.144993	0.417722	0.514967
$[(PhSH\text{-}PhS)\text{-}BPh_3]^-$	-1979.650037	0.4061	0.503925
PhSH-$B(C_6F_5)Ph_2$	-1845.831346	0.284214	0.369588
$[PhS\text{-}B(C_6F_5)Ph_2]^-$	-1845.338198	0.273086	0.35786
$(PhSH)_2$-$B(C_6F_5)Ph_2$	-2476.149541	0.372771	0.479051
$[(PhSH\text{-}PhS)\text{-}B(C_6F_5)Ph_2]^-$	-2475.652945	0.361514	0.468028
PhSH-$B(C_6F_5)_2Ph$	-2341.829271	0.236366	0.333353
$[PhS\text{-}B(C_6F_5)_2Ph]^-$	-2341.345338	0.22653	0.321987
$(PhSH)_2$-$B(C_6F_5)_2Ph$	-2972.142637	0.325345	0.442698
$[(PhSH\text{-}PhS)\text{-}B(C_6F_5)_2Ph]^-$	-2971.664448	0.31724	0.431966
PhSH-$B(C_6F_5)_3$	-2837.827089	0.192977	0.297372
$[PhS\text{-}B(C_6F_5)_3]^-$	-2837.352132	0.181684	0.286064
$(PhSH)_2$-$B(C_6F_5)_3$	-3468.140835	0.283775	0.407079
$[(PhSH\text{-}PhS)\text{-}B(C_6F_5)_3]^-$	-3467.670856	0.274792	0.395895
$[PhSH\text{-}SiEt_3]^+$	-1157.120632	0.256873	0.321988
PhS-$SiEt_3$	-1156.782857	0.248242	0.312038
$[(PhSH)_2\text{-}SiEt_3]^+$	-1787.441624	0.34643	0.431008
(PhSH-PhS)-$SiEt_3$	-1787.091792	0.335817	0.42154
$[PhSH\text{-}SiPhH_2]^+$	-1152.274247	0.170026	0.226861
PhS-$SiPhH_2$	-1151.941671	0.159064	0.216813
$[(PhSH)_2\text{-}SiPhH_2]^+$	-1782.594921	0.260706	0.335788
(PhSH-PhS)-$SiPhH_2$	-1782.257085	0.254711	0.326705

19) Energies for the Optimized Lewis Acid-Aniline Adducts.

Table S12. Computed energies for the optimized structures of the aniline-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Aniline-BEt_3	-549.9127000	0.28374	0.342477
[Anilide-BEt_3]$^-$	-549.3613207	0.267473	0.326924
$(Aniline)_2$-BEt_3	-837.4138303	0.389769	0.469855
[(Aniline-Anilide)-BEt_3]$^-$	-836.8670859	0.377305	0.454387
Aniline-BPh_3	-1007.036964	0.349406	0.424494
[Anilide-BPh_3]$^-$	-1006.507575	0.333867	0.408679
$(Aniline)_2$-BPh_3	-1294.543488	0.462468	0.551463
[(Aniline-Anilide)-BPh_3]$^-$	-1294.009809	0.443475	0.536325
Aniline-$B(C_6F_5)Ph_2$	-1503.042251	0.304973	0.388663
[Anilide-$B(C_6F_5)Ph_2$]$^-$	-1502.517767	0.288797	0.37274
$(Aniline)_2$-$B(C_6F_5)Ph_2$	-1790.546382	0.415956	0.515791
[(Aniline-Anilide)-$B(C_6F_5)Ph_2$]$^-$	-1790.019093	0.397738	0.500184
Aniline-$B(C_6F_5)_2Ph$	-1999.043775	0.259504	0.352726
[Anilide-$B(C_6F_5)_2Ph$]$^-$	-1998.527768	0.243678	0.336945
$(Aniline)_2$-$B(C_6F_5)_2Ph$	-2286.546964	0.369692	0.47989
[(Aniline-Anilide)-$B(C_6F_5)_2Ph$]$^-$	-2286.031961	0.354511	0.46437
Aniline-$B(C_6F_5)_3$	-2495.043227	0.214123	0.316562
[Anilide-$B(C_6F_5)_3$]$^-$	-2494.533229	0.197545	0.300934
$(Aniline)_2$-$B(C_6F_5)_3$	-2782.553849	0.325817	0.443762
[(Aniline-Anilide)-$B(C_6F_5)_3$]$^-$	-2782.038765	0.308151	0.428664
[Aniline-$SiEt_3$]$^+$	-814.3336722	0.277883	0.340621
Anilide-$SiEt_3$	-813.9577233	0.262976	0.326544
[$(Aniline)_2$-$SiEt_3$]$^+$	-1101.849073	0.384846	0.467767
(Aniline-Anilide)-$SiEt_3$	-1101.452626	0.369634	0.453773
[Aniline-$SiPhH_2$]$^+$	-809.4881012	0.19067	0.245621
Anilide-$SiPhH_2$	-809.1231704	0.176656	0.231456
[$(Aniline)_2$-$SiPhH_2$]$^+$	-1097.006083	0.300044	0.372533
(Aniline-Anilide)-$SiPhH_2$	-1096.618387	0.285775	0.358497

20) Energies for the Optimized Lewis Acid-Phenylphosphine Adducts.

Table S13. Computed energies for the optimized structures of the phenylphosphine-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$PPhH_2$-BEt_3	-836.4637931	0.269714	0.333141
$[PPhH\text{-}BEt_3]^-$	-835.9236576	0.258543	0.321158
$(PPhH_2)_2$-BEt_3	-1410.522916	0.368187	0.452067
$[(PPhH_2\text{-}PPhH)\text{-}BEt_3]^-$	-1409.982886	0.35735	0.439977
$PPhH_2$-BPh_3	-1293.592657	0.338888	0.415304
$[PPhH\text{-}BPh_3]^-$	-1293.066581	0.326982	0.403318
$(PPhH_2)_2$-BPh_3	-1867.656838	0.439641	0.534193
$[(PPhH_2\text{-}PPhH)\text{-}BPh_3]^-$	-1867.127109	0.422655	0.5221
$PPhH_2$-$B(C_6F_5)Ph_2$	-1789.595302	0.293311	0.379242
$[PPhH\text{-}B(C_6F_5)Ph_2]^-$	-1789.075275	0.281513	0.36725
$(PPhH_2)_2$-$B(C_6F_5)Ph_2$	-2363.657839	0.393041	0.498075
$[(PPhH_2\text{-}PPhH)\text{-}B(C_6F_5)Ph_2]^-$	-2363.139016	0.381164	0.486135
$PPhH_2$-$B(C_6F_5)_2Ph$	-2285.593441	0.247561	0.343095
$[PPhH\text{-}B(C_6F_5)_2Ph]^-$	-2285.084536	0.236541	0.331297
$(PPhH_2)_2$-$B(C_6F_5)_2Ph$	-2859.658481	0.346935	0.462328
$[(PPhH_2\text{-}PPhH)\text{-}B(C_6F_5)_2Ph]^-$	-2859.142933	0.334773	0.450442
$PPhH_2$-$B(C_6F_5)_3$	-2781.590808	0.202218	0.307064
$[PPhH\text{-}B(C_6F_5)_3]^-$	-2781.091431	0.191069	0.295205
$(PPhH_2)_2$-$B(C_6F_5)_3$	-3355.657866	0.302176	0.426212
$[(PPhH_2\text{-}PPhH)\text{-}B(C_6F_5)_3]^-$	-3355.14955	0.289328	0.414122
$[PPhH_2\text{-}SiEt_3]^+$	-1100.880453	0.263447	0.331582
$PPhH\text{-}SiEt_3$	-1100.51407	0.255739	0.320873
$[(PPhH_2)_2\text{-}SiEt_3]^+$	-1674.949884	0.364367	0.450814
$(PPhH_2\text{-}PPhH)\text{-}SiEt_3$	-1674.573038	0.351714	0.439607
$[PPhH_2\text{-}SiPhH_2]^+$	-1096.037259	0.179295	0.236409
$PPhH\text{-}SiPhH_2$	-1095.679266	0.169838	0.225516
$[(PPhH_2)_2\text{-}SPhH_2]^+$	-1670.102127	0.275518	0.355066
$(PPhH_2\text{-}PPhH)\text{-}SiPhH_2$	-1669.738657	0.267364	0.344202

21) Computed pK_a values of Lewis Acid/Base Adducts.

Table S14. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	pK_a in MeCN
H_2O	43.4
NH_3	55.7
N_2H_4	55.7
(1-phenylethyl)aniline	46.7
phenylethanol	41.7
1-benzyl-2-methyl-2-propanamine	57.3
Phenol	28.3
Thiophenol	22.6
Aniline	42.8
Phenylphosphine	33.3
H_2O-BEt_3	22.8
H_2O-BPh_3	15.3
H_2O-$B(C_6F_5)Ph_2$	13.0
H_2O-$B(C_6F_5)_2Ph$	10.4
H_2O-$B(C_6F_5)_3$	4.6
$[H_2O$-$SiEt_3]^+$	-2.3
$[H_2O$-$SiPhH_2]^+$	-6.6
$(H_2O)_2$-BEt_3	21.1
$(H_2O)_2$-BPh_3	16.4
$(H_2O)_2$-$B(C_6F_5)Ph_2$	14.8
$(H_2O)_2$-$B(C_6F_5)_2Ph$	13.4
$(H_2O)_2$-$B(C_6F_5)_3$	8.1
$[(H_2O)_2$-$SiEt_3]^+$	6.2
$[(H_2O)_2$-$SiPhH_2]^+$	0.3
H_3N-BEt_3	36.3
H_3N-BPh_3	30.9
H_3N-$B(C_6F_5)Ph_2$	28.9
H_3N-$B(C_6F_5)_2Ph$	26.1
H_3N-$B(C_6F_5)_3$	24.3
$[H_3N$-$SiEt_3]^+$	16.0
$[H_3N$-$SiPhH_2]^+$	9.1
$(H_3N)_2$-BEt_3	37.0
$(H_3N)_2$-BPh_3	33.8
$(H_3N)_2$-$B(C_6F_5)Ph_2$	32.0
$(H_3N)_2$-$B(C_6F_5)_2Ph$	30.2

Complex	pK_a in MeCN
$(H_3N)_2$-$B(C_6F_5)_3$	28.9
$[(H_3N)_2$-$SiEt_3]^+$	21.1
$[(H_3N)_2$-$SiPhH_2]^+$	17.4
N_2H_4-BEt_3	35.4
N_2H_4-BPh_3	28.4
N_2H_4-$B(C_6F_5)Ph_2$	23.7
N_2H_4-$B(C_6F_5)_2Ph$	22.7
N_2H_4-$B(C_6F_5)_3$	23.6
$[N_2H_4$-$SiEt_3]^+$	13.4
$[N_2H_4$-$SiPhH_2]^+$	10.8
$(N_2H_4)_2$-BEt_3	35.33
$(N_2H_4)_2$-BPh_3	29.65
$(N_2H_4)_2$-$B(C_6F_5)Ph_2$	29.32
$(N_2H_4)_2$-$B(C_6F_5)_2Ph$	23.99
$(N_2H_4)_2$-$B(C_6F_5)_3$	24.3
$[(N_2H_4)_2$-$SiEt_3]^+$	18.6
$[(N_2H_4)_2$-$SiPhH_2]^+$	15.6
HBMPA-BEt_3	37.7
HBMPA-BPh_3	28.7
HBMPA-$B(C_6F_5)Ph_2$	23.3
HBMPA-$B(C_6F_5)_2Ph$	26.1
HBMPA-$B(C_6F_5)_3$	24.2
[HBMPA-$SiEt_3]^+$	16.6
[HBMPA-$SiPhH_2]^+$	13.4
$(HBMPA)_2$-BEt_3	34.3
$(HBMPA)_2$-BPh_3	34.2
$(HBMPA)_2$-$B(C_6F_5)Ph_2$	25.1
$(HBMPA)_2$-$B(C_6F_5)_2Ph$	26.0
$(HBMPA)_2$-$B(C_6F_5)_3$	23.1
$[(HBMPA)_2$-$SiEt_3]^+$	13.9
$[(HBMPA)_2$-$SiPhH_2]^+$	13.6
PhNHMeBn-BEt_3	32.2
PhNHMeBn-BPh_3	25.4
PhNHMeBn-$B(C_6F_5)Ph_2$	25.8
PhNHMeBn-$B(C_6F_5)_2Ph$	20.1
PhNHMeBn-$B(C_6F_5)_3$	19.8
[PhNHMeBn-$SiEt_3]^+$	12.4
[PhNHMeBn-$SiPhH_2]^+$	9.2

Complex	pK_a in MeCN
$(PhNHMeBn)_2$-BEt_3	30.3
$(PhNHMeBn)_2$-BPh_3	23.8
$(PhNHMeBn)_2$-$B(C_6F_5)Ph_2$	25.1
$(PhNHMeBn)_2$-$B(C_6F_5)_2Ph$	22.1
$(PhNHMeBn)_2$-$B(C_6F_5)_3$	15.3
$[(PhNHMeBn)_2$-$SiEt_3]^+$	15.9
$[(PhNHMeBn)_2$-$SiPhH_2]^+$	11.3
PhEtOH-BEt_3	23.9
PhEtOH-BPh_3	15.4
PhEtOH-$B(C_6F_5)Ph_2$	12.0
PhEtOH-$B(C_6F_5)_2Ph$	10.5
PhEtOH-$B(C_6F_5)_3$	7.2
$[PhEtOH$-$SiEt_3]^+$	-1.4
$[PhEtOH$-$SiPhH_2]^+$	-3.5
$(PhEtOH)_2$-BEt_3	23.0
$(PhEtOH)_2$-BPh_3	14.2
$(PhEtOH)_2$-$B(C_6F_5)Ph_2$	14.2
$(PhEtOH)_2$-$B(C_6F_5)_2Ph$	10.9
$(PhEtOH)_2$-$B(C_6F_5)_3$	12.4
$[(PhEtOH)_2$-$SiEt_3]^+$	8.3
$[(PhEtOH)_2$-$SiPhH_2]^+$	2.6
Phenol-BEt_3	21.1
Phenol-BPh_3	8.4
Phenol-$B(C_6F_5)Ph_2$	6.2
Phenol-$B(C_6F_5)_2Ph$	2.6
Phenol-$B(C_6F_5)_3$	0.7
$[Phenol$-$SiEt_3]^+$	-6.5
$[Phenol$-$SiPhH_2]^+$	-9.4
$(Phenol)_2$-BEt_3	16.0
$(Phenol)_2$-BPh_3	6.7
$(Phenol)_2$-$B(C_6F_5)Ph_2$	4.6
$(Phenol)_2$-$B(C_6F_5)_2Ph$	3.7
$(Phenol)_2$-$B(C_6F_5)_3$	2.3
$[(Phenol)_2$-$SiEt_3]^+$	-4.2
$[(Phenol)_2$-$SiPhH_2]^+$	-3.9
Thiophenol-BEt_3	19.9
Thiophenol-BPh_3	10.0
Thiophenol-$B(C_6F_5)Ph_2$	7.2
Thiophenol-$B(C_6F_5)_2Ph$	6.1

Complex	pK_a in MeCN
Thiophenol-B(C_6F_5)$_3$	3.6
[Thiophenol-SiEt$_3$]$^+$	-5.1
[Thiophenol-SiPhH$_2$]$^+$	-7.3
(Thiophenol)$_2$-BEt$_3$	20.0
(Thiophenol)$_2$-BPh$_3$	10.4
(Thiophenol)$_2$-B(C_6F_5)Ph$_2$	11.2
(Thiophenol)$_2$-B(C_6F_5)$_2$Ph	7.0
(Thiophenol)$_2$-B(C_6F_5)$_3$	3.8
[(Thiophenol)$_2$-SiEt$_3$]$^+$	-5.3
[(Thiophenol)$_2$-SiPhH$_2$]$^+$	-5.6
Aniline-BEt$_3$	28.3
Aniline-BPh$_3$	23.5
Aniline-B(C_6F_5)Ph$_2$	20.9
Aniline-B(C_6F_5)$_2$Ph	18.9
Aniline-B(C_6F_5)$_3$	17.1
[Aniline-SiEt$_3$]$^+$	9.5
[Aniline-SiPhH$_2$]$^+$	6.1
(Aniline)$_2$-BEt$_3$	30.6
(Aniline)$_2$-BPh$_3$	26.0
(Aniline)$_2$-B(C_6F_5)Ph$_2$	23.0
(Aniline)$_2$-B(C_6F_5)$_2$Ph	20.0
(Aniline)$_2$-B(C_6F_5)$_3$	21.3
[(Aniline)$_2$-SiEt$_3$]$^+$	13.0
[(Aniline)$_2$-SiPhH$_2$]$^+$	8.9
Phenylphosphine-BEt$_3$	24.8
Phenylphosphine-BPh$_3$	22.8
Phenylphosphine-B(C_6F_5)Ph$_2$	21.2
Phenylphosphine-B(C_6F_5)$_2$Ph	18.5
Phenylphosphine-B(C_6F_5)$_3$	16.3
[Phenylphosphine-SiEt$_3$]$^+$	7.8
[Phenylphosphine-SiPhH$_2$]$^+$	4.7
(Phenylphosphine)$_2$-BEt$_3$	25.7
(Phenylphosphine)$_2$-BPh$_3$	23.4
(Phenylphosphine)$_2$-B(C_6F_5)Ph$_2$	22.7
(Phenylphosphine)$_2$-B(C_6F_5)$_2$Ph	21.1
(Phenylphosphine)$_2$-B(C_6F_5)$_3$	19.6
[(Phenylphosphine)$_2$-SiEt$_3$]$^+$	6.3
[(Phenylphosphine)$_2$-SiPhH$_2$]$^+$	5.0

22) Calculated Binding Affinities of Lewis Acid/Base Adducts.

Table S15. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	Binding Affinity (kcal/mol)
H_2O-BEt_3	8.0
H_2O-BPh_3	8.2
H_2O-$B(C_6F_5)Ph_2$	3.3
H_2O-$B(C_6F_5)_2Ph$	-1.7
H_2O-$B(C_6F_5)_3$	-4.6
$[H_2O$-$SiEt_3]^+$	-24.6
$[H_2O$-$SiPhH_2]^+$	-27.9
H_3N-BEt_3	-4.5
H_3N-BPh_3	-7.3
H_3N-$B(C_6F_5)Ph_2$	-13.6
H_3N-$B(C_6F_5)_2Ph$	-17.8
H_3N-$B(C_6F_5)_3$	-24.5
$[H_3N$-$SiEt_3]^+$	-40.8
$[H_3N$-$SiPhH_2]^+$	-42.1
N_2H_4-BEt_3	-7.1
N_2H_4-BPh_3	-7.9
N_2H_4-$B(C_6F_5)Ph_2$	-10.3
N_2H_4-$B(C_6F_5)_2Ph$	-17.1
N_2H_4-$B(C_6F_5)_3$	-23.8
$[N_2H_4$-$SiEt_3]^+$	-37.3
$[N_2H_4$-$SiPhH_2]^+$	-43.9
N-benzyl-2-methylpropan-2-amine-BEt_3	7.3
N-benzyl-2-methylpropan-2-amine-BPh_3	9.2
N-benzyl-2-methylpropan-2-amine-$B(C_6F_5)Ph_2$	6.8
N-benzyl-2-methylpropan-2-amine-$B(C_6F_5)_2Ph$	-0.8
N-benzyl-2-methylpropan-2-amine-$B(C_6F_5)_3$	-9.6
[*N*-benzyl-2-methylpropan-2-amine-$SiEt_3]^+$	-31.0
[*N*-benzyl-2-methylpropan-2-amine-$SiPhH_2]^+$	-45.4

Complex	Binding Affinity (kcal/mol)
N-(1-phenylethyl)aniline-BEt_3	5.7
N-(1-phenylethyl)aniline-BPh_3	5.8
N-(1-phenylethyl)aniline-$B(C_6F_5)Ph_2$	2.4
N-(1-phenylethyl)aniline-$B(C_6F_5)_2Ph$	1.1
N-(1-phenylethyl)aniline-$B(C_6F_5)_3$	-4.4
[*N*-(1-phenylethyl)aniline-$SiEt_3$]$^+$	-30.0
[*N*-(1-phenylethyl)aniline-$SiPhH_2$]$^+$	-38.9
Phenylethanol-BEt_3	7.3
Phenylethanol-BPh_3	7.5
Phenylethanol-$B(C_6F_5)Ph_2$	1.9
Phenylethanol-$B(C_6F_5)_2Ph$	-4.1
Phenylethanol-$B(C_6F_5)_3$	-9.8
[Phenylethanol-$SiEt_3$]$^+$	-23.4
[Phenylethanol-$SiPhH_2$]$^+$	-31.2
Phenol-BEt_3	4.5
Phenol-BPh_3	11.9
Phenol-$B(C_6F_5)Ph_2$	8.0
Phenol-$B(C_6F_5)_2Ph$	4.9
Phenol-$B(C_6F_5)_3$	-1.0
[Phenol-$SiEt_3$]$^+$	-19.7
[Phenol-$SiPhH_2$]$^+$	-23.2
Thiophenol-BEt_3	3.8
Thiophenol-BPh_3	11.1
Thiophenol-$B(C_6F_5)Ph_2$	9.4
Thiophenol-$B(C_6F_5)_2Ph$	4.3
Thiophenol-$B(C_6F_5)_3$	0.1
[Thiophenol-$SiEt_3$]$^+$	-17.0
[Thiophenol-$SiPhH_2$]$^+$	-21.9
Aniline-BEt_3	-0.8
Aniline-BPh_3	-0.5
Aniline-$B(C_6F_5)Ph_2$	-4.9
Aniline-$B(C_6F_5)_2Ph$	-10.0

Complex	Binding Affinity (kcal/mol)
Aniline-$B(C_6F_5)_3$	-16.2
$[Aniline\text{-}SiEt_3]^+$	-32.9
$[Aniline\text{-}SiPhH_2]^+$	-39.3
Phenylphosphine-BEt_3	3.1
Phenylphosphine-BPh_3	3.4
Phenylphosphine-$B(C_6F_5)Ph_2$	-1.9
Phenylphosphine-$B(C_6F_5)_2Ph$	-5.7
Phenylphosphine-$B(C_6F_5)_3$	-11.1
$[Phenylphosphine\text{-}SiEt_3]^+$	-25.1
$[Phenylphosphine\text{-}SiPhH_2]^+$	-31.0

23) Calculated Free Energies for the Formation of Lewis Base-Lewis Acid Adducts Containg a Second Lewis Base (Homoconjugation).

Table S16. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	Free Energy (kcal/mol)
$(H_2O)_2$-BEt_3	3.6
$(H_2O)_2$-BPh_3	0.3
$(H_2O)_2$-$B(C_6F_5)Ph_2$	0.7
$(H_2O)_2$-$B(C_6F_5)_2Ph$	0.3
$(H_2O)_2$-$B(C_6F_5)_3$	-1.1
$[(H_2O)_2\text{-}SiEt_3]^+$	-5.9
$[(H_2O)_2\text{-}SiPhH_2]^+$	-6.9
$(H_3N)_2$-BEt_3	4.9
$(H_3N)_2$-BPh_3	2.3
$(H_3N)_2$-$B(C_6F_5)Ph_2$	1.8
$(H_3N)_2$-$B(C_6F_5)_2Ph$	-0.1
$(H_3N)_2$-$B(C_6F_5)_3$	2.0
$[(H_3N)_2\text{-}SiEt_3]^+$	-1.3
$[(H_3N)_2\text{-}SiPhH_2]^+$	-6.2
$(N_2H_4)_2$-BEt_3	3.9
$(N_2H_4)_2$-BPh_3	2.9
$(N_2H_4)_2$-$B(C_6F_5)Ph_2$	-2.8
$(N_2H_4)_2$-$B(C_6F_5)_2Ph$	1.9
$(N_2H_4)_2$-$B(C_6F_5)_3$	1.4
$[(N_2H_4)_2\text{-}SiEt_3]^+$	2.0
$[(N_2H_4)_2\text{-}SiPhH_2]^+$	-0.8
(*N*-benzyl-2-methylpropan-2-amine)$_2$-BEt_3	11.8
(*N*-benzyl-2-methylpropan-2-amine)$_2$-BPh_3	8.0
(*N*-benzyl-2-methylpropan-2-amine)$_2$-$B(C_6F_5)Ph_2$	9.0
(*N*-benzyl-2-methylpropan-2-amine)$_2$-$B(C_6F_5)_2Ph$	7.7
(*N*-benzyl-2-methylpropan-2-amine)$_2$-$B(C_6F_5)_3$	9.3
[(*N*-benzyl-2-methylpropan-2-amine)$_2$-$SiEt_3$]$^+$	6.7
[(*N*-benzyl-2-methylpropan-2-amine)$_2$-$SiPhH_2$]$^+$	8.3

Complex	Free Energy (kcal/mol)
(*N*-(1-phenylethyl)aniline)$_2$-BEt_3	5.3
(*N*-(1-phenylethyl)aniline)$_2$-BPh_3	8.7
(*N*-(1-phenylethyl)aniline)$_2$-$B(C_6F_5)Ph_2$	8.6
(*N*-(1-phenylethyl)aniline)$_2$-$B(C_6F_5)_2Ph$	9.9
(*N*-(1-phenylethyl)aniline)$_2$-$B(C_6F_5)_3$	9.0
[(*N*-(1-phenylethyl)aniline)$_2$-$SiEt_3$]$^+$	4.9
[(*N*-(1-phenylethyl)aniline)$_2$-$SiPhH_2$]$^+$	5.3
(Phenylethanol)$_2$-BEt_3	7.8
(Phenylethanol)$_2$-BPh_3	5.3
(Phenylethanol)$_2$-$B(C_6F_5)Ph_2$	0.3
(Phenylethanol)$_2$-$B(C_6F_5)_2Ph$	2.8
(Phenylethanol)$_2$-$B(C_6F_5)_3$	-3.1
[(Phenylethanol)$_2$-$SiEt_3$]$^+$	-7.0
[(Phenylethanol)$_2$-$SiPhH_2$]$^+$	-4.9
(Phenol)$_2$-BEt_3	5.5
(Phenol)$_2$-BPh_3	4.4
(Phenol)$_2$-$B(C_6F_5)Ph_2$	3.1
(Phenol)$_2$-$B(C_6F_5)_2Ph$	4.7
(Phenol)$_2$-$B(C_6F_5)_3$	-0.3
[(Phenol)$_2$-$SiEt_3$]$^+$	0.9
[(Phenol)$_2$-$SiPhH_2$]$^+$	-2.1
(Thiophenol)$_2$-BEt_3	5.6
(Thiophenol)$_2$-BPh_3	4.4
(Thiophenol)$_2$-$B(C_6F_5)Ph_2$	0.9
(Thiophenol)$_2$-$B(C_6F_5)_2Ph$	4.0
(Thiophenol)$_2$-$B(C_6F_5)_3$	4.9
[(Thiophenol)$_2$-$SiEt_3$]$^+$	5.6
[(Thiophenol)$_2$-$SiPhH_2$]$^+$	4.9
(Aniline)$_2$-BEt_3	2.1
(Aniline)$_2$-BPh_3	3.3
(Aniline)$_2$-$B(C_6F_5)Ph_2$	3.7
(Aniline)$_2$-$B(C_6F_5)_2Ph$	3.8

Complex	Free Energy (kcal/mol)
$(Aniline)_2$-$B(C_6F_5)_3$	0.2
$[(Aniline)_2$-$SiEt_3]^+$	1.3
$[(Aniline)_2$-$SiPhH_2]^+$	2.0
$(Phenylphosphine)_2$-BEt_3	5.9
$(Phenylphosphine)_2$-BPh_3	4.9
$(Phenylphosphine)_2$-$B(C_6F_5)Ph_2$	5.0
$(Phenylphosphine)_2$-$B(C_6F_5)_2Ph$	4.8
$(Phenylphosphine)_2$-$B(C_6F_5)_3$	4.1
$[(Phenylphosphine)_2$-$SiEt_3]^+$	6.4
$[(Phenylphosphine)_2$-$SiPhH_2]^+$	4.6

24) References

(1) S. J. Geier; D. W. Stephan. *J. Am. Chem. Soc.,* **2009**, *131*, 3476-3477.
(2) I. Kaljurand; A. Kuett; L. Soovaeli; T. Rodima; V. Maeemets; I. Leito; I. A. Koppel. *J. Org. Chem.,* **2005**, *70*, 1019-1028.
(3) K. Izutsu *Acid-Base Dissociation Constants in Dipolar Aprotic Solvents*; Blackwell Scientific Publications: Oxford, 1990; Vol. 35,

25) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms,followed by the complex name, and the 3D coordinates.

4
$[H_3O]^+$
O -0.00000 -0.00000 -0.06707
H -0.82356 -0.47147 0.17885
H 0.00348 0.94897 0.17884
H 0.82012 -0.47748 0.17884

3
H_2O
O 0.00000 0.00000 0.11776
H 0.00000 -0.76008 -0.47105
H 0.00000 0.76008 -0.47105

2
[OH]-
O 0.00000 0.00000 0.10874
H 0.00000 0.00000 -0.86988

5
$[NH_4]^+$
N -0.00003 0.00000 0.00000
H 0.24219 -0.03356 0.99689
H 0.42208 0.83269 -0.42674
H 0.35630 -0.84171 -0.46714
H -1.02038 0.04256 -0.10303

4
NH_3
N 0.00000 0.00000 0.11687
H 0.00000 0.93757 -0.27270
H 0.81196 -0.46879 -0.27270
H -0.81196 -0.46879 -0.27270

3
$[NH_2]$-
N 0.00000 0.00000 0.15351
H 0.00000 0.78284 -0.53729
H 0.00000 -0.78284 -0.53729

7
$[N_2H_5]^+$
N 0.208927 0.714488 -0.231281
N -0.184535 -0.668061 -0.196351
H -0.548113 1.249911 -0.651764
H 0.348938 1.029605 0.726677
H -0.297128 -0.993427 -1.164451
H 0.591498 -1.211618 0.201274
H -1.044192 -0.890024 0.327570

6
N_2H_4
N 0.178121 0.690116 -0.266932
N -0.178121 -0.690116 -0.266932
H -0.656326 1.215837 -0.502654
H 0.488020 1.005664 0.649572
H 0.656326 -1.215837 -0.502654
H -0.488020 -1.005664 0.649572

5
$[N_2H_3]$-
N 0.274179 0.662821 -0.128755
N -0.232475 -0.686758 0.227020
H -0.453697 1.124017 -0.697860
H 0.240187 1.237600 0.727719
H 0.562454 -1.262664 -0.113006

20
1-pheny-l-ethyloxonium
C 1.56547 -0.31113 0.35841
C 0.10384 -0.10217 0.21021
O 2.12919 -0.73824 -1.09578
C 2.45668 0.82938 0.76491
C -0.42904 1.13712 -0.16942
C -1.80138 1.27651 -0.33227
C -2.64512 0.18601 -0.11893
C -2.12190 -1.04809 0.26100
C -0.74917 -1.19310 0.42446
H 1.80280 -1.23146 0.89360
H 1.53534 -1.39642 -1.50681
H 2.18021 0.03484 -1.69011
H 2.32979 1.70848 0.12817
H 2.17652 1.11746 1.78151
H 3.50470 0.52719 0.76888
H 0.21414 1.99858 -0.32198
H -2.21604 2.23661 -0.61813
H -3.71652 0.30272 -0.24169
H -2.78109 -1.89014 0.43918
H -0.33967 -2.14903 0.74326

19
1-phenyl-1-ethanol
C -1.65577 -0.29895 0.29190
C -0.15246 -0.13409 0.17016
O -2.28813 0.89546 0.71570
C -2.28167 -0.65932 -1.04866
C 0.39170 1.10214 -0.18125
C 1.76778 1.24745 -0.33311
C 2.61246 0.15744 -0.13835
C 2.07509 -1.07912 0.21115
C 0.69944 -1.22111 0.36698
H -1.85719 -1.11242 1.00749
H -1.87414 1.17135 1.54197
H -1.86430 -1.59489 -1.42806
H -3.36351 -0.76404 -0.93937
H -2.07501 0.13550 -1.77029
H -0.27684 1.94502 -0.32946
H 2.18225 2.21352 -0.60399
H 3.68537 0.27146 -0.25495
H 2.72857 -1.93116 0.36992
H 0.28032 -2.18470 0.64822

18
1-phenylethan-1-olate
C -1.74137 0.01804 -0.38174
C -0.19258 0.05400 -0.20756
O -2.25184 -1.19512 -0.36178
C -2.33350 0.94348 0.73400
C 0.43829 -1.15213 0.09555
C 1.81759 -1.21458 0.27887
C 2.59632 -0.06368 0.15532
C 1.97831 1.14764 -0.15741
C 0.59730 1.19989 -0.33720
H -1.89323 0.61879 -1.34095
H -2.12207 0.48443 1.70687
H -1.94697 1.97366 0.73454
H -3.42049 0.97103 0.60383
H -0.23321 -2.00626 0.15882
H 2.29687 -2.16364 0.51423
H 3.67416 -0.10899 0.29394
H 2.57800 2.05000 -0.26313
H 0.11956 2.14595 -0.59286

13
Phenol
C -1.150671 0.424570 -0.000028
C -1.135109 -0.967280 -0.000005
C 0.070645 -1.661212 0.000028
C 1.268104 -0.947117 0.000039

C	1.267025	0.441874	0.000017
C	0.052838	1.129111	-0.000017
O	0.105622	2.489224	-0.000038
H	-2.094333	0.964885	-0.000055
H	-2.075956	-1.508498	-0.000012
H	0.078385	-2.745436	0.000044
H	2.215619	-1.476710	0.000064
H	2.188389	1.013511	0.000026
H	-0.790557	2.843079	-0.000064

12
Phenoxide

C	-1.137578	0.432015	-0.000038
C	-1.125114	-0.951971	-0.000009
C	0.071104	-1.680566	0.000033
C	1.267330	-0.951982	0.000040
C	1.279809	0.432003	0.000009
C	0.071119	1.227495	-0.000030
O	0.071125	2.487160	-0.000051
H	-2.079510	0.977574	-0.000066
H	-2.075423	-1.489131	-0.000019
H	0.071100	-2.766933	0.000064
H	2.217634	-1.489152	0.000071
H	2.221746	0.977553	0.000014

13
Thiophenol

C	-0.126776	1.112830	-0.186779
C	-1.512244	1.177646	-0.075161
C	-2.266212	0.015342	0.054211
C	-1.622027	-1.219085	0.070204
C	-0.238557	-1.294202	-0.042808
C	0.516452	-0.125807	-0.171679
S	2.280736	-0.293785	-0.304912
H	0.450870	2.027086	-0.284656
H	-2.001503	2.146337	-0.088981
H	-3.345838	0.070596	0.141512
H	-2.198466	-2.133169	0.169826
H	0.257648	-2.259959	-0.032560
H	2.545497	1.010860	-0.461456

12
Thiophenoxide

C	-1.125411	0.398475	-0.000035
C	-1.125135	-0.990555	-0.000006
C	0.071105	-1.710364	0.000031
C	1.267352	-0.990567	0.000041
C	1.267641	0.398463	0.000014
C	0.071119	1.158574	-0.000026
S	0.071126	2.898014	-0.000065
H	-2.066129	0.942315	-0.000066
H	-2.075478	-1.522813	-0.000012
H	0.071099	-2.796937	0.000050
H	2.217690	-1.522833	0.000069
H	2.208364	0.942293	0.000023

15
Anilinium

C	0.156117	-1.229809	-0.028149
C	-1.236380	-1.211490	0.007285
C	-1.919074	0.001581	0.025907
C	-1.221309	1.208442	0.009895
C	0.169448	1.212435	-0.025399
C	0.817530	-0.013372	-0.042749
N	2.307543	-0.016169	-0.088514
H	0.695636	-2.172851	-0.042801
H	-1.781538	-2.148104	0.020959
H	-3.002834	0.008115	0.053984
H	-1.756790	2.150652	0.025720
H	0.721303	2.148100	-0.037963
H	2.658706	0.363049	-0.976026
H	2.674202	-0.969191	0.007308
H	2.706960	0.545262	0.672613

14
Aniline

C	-1.179663	0.371595	-0.041821
C	-1.140672	-1.017144	-0.041910
C	0.074707	-1.695972	-0.003342
C	1.256005	-0.959559	0.034094
C	1.228216	0.429544	0.034505
C	0.007125	1.114517	-0.002638
N	-0.024704	2.508257	-0.058194
H	-2.132786	0.892431	-0.077265
H	-2.072783	-1.573082	-0.070965
H	0.100696	-2.779900	-0.002259
H	2.213743	-1.469985	0.064895
H	2.155622	0.995487	0.058713
H	-0.881770	2.922674	0.279086
H	0.787867	2.962992	0.332906

13
Anilide

C	-1.129173	0.437137	0.000067
C	-1.122865	-0.946564	-0.000235
C	0.066529	-1.685033	-0.000216
C	1.266099	-0.952941	0.000122
C	1.285380	0.426247	0.000424
C	0.081876	1.228987	0.000432
N	0.160317	2.549671	0.000801
H	-2.081583	0.969334	0.000040
H	-2.079157	-1.473020	-0.000499
H	0.062000	-2.770801	-0.000449
H	2.217060	-1.488554	0.000136
H	2.229316	0.967263	0.000672
H	-0.802213	2.907651	0.000827

31
(1-phenylethyl)benzenaminium

C	-0.63385	1.65845	0.43254
N	0.47994	1.60239	-0.64086
C	-1.41050	2.95108	0.23703

C	-1.43483	0.38736	0.32712
C	1.49870	0.55830	-0.42583
C	2.59753	0.86858	0.36355
C	3.54545	-0.12336	0.59555
C	3.37656	-1.39192	0.04484
C	2.26069	-1.67918	-0.73799
C	1.30219	-0.69929	-0.97905
C	-2.33555	0.19772	-0.72631
C	-3.01885	-1.00762	-0.85109
C	-2.81313	-2.02482	0.07963
C	-1.92250	-1.83769	1.13295
C	-1.22972	-0.63628	1.25256
H	-0.08186	1.67704	1.37616
H	0.02388	1.45377	-1.54820
H	0.93781	2.51894	-0.69207
H	-1.88355	3.00211	-0.74717
H	-0.77067	3.82875	0.36585
H	-2.20220	2.99874	0.98636
H	2.72311	1.86279	0.78494
H	4.41625	0.09930	1.20138
H	4.12018	-2.16005	0.22525
H	2.13174	-2.66750	-1.16399
H	0.41844	-0.91687	-1.57257
H	-2.52443	0.98838	-1.44916
H	-3.71975	-1.14877	-1.66649
H	-3.35271	-2.96092	-0.01484
H	-1.76499	-2.62589	1.86083
H	-0.52400	-0.49452	2.06676

30
(1-phenylethyl)aniline

C	0.42993	0.75398	0.20863
N	-0.46882	-0.39007	0.32403
C	0.37069	1.61294	1.47842
C	1.84295	0.25805	-0.02184
C	-1.83273	-0.27073	0.06000
C	-2.47585	0.96256	-0.11368
C	-3.84819	1.01113	-0.35096
C	-4.60589	-0.15024	-0.42936
C	-3.96769	-1.38018	-0.26486
C	-2.60555	-1.44223	-0.02064
C	2.63285	0.79498	-1.03755
C	3.94116	0.35604	-1.22626
C	4.47152	-0.63165	-0.40191
C	3.68917	-1.17530	0.61469
C	2.38529	-0.73021	0.80595
H	0.14583	1.37386	-0.65717
H	-0.07136	-1.24702	-0.03738
H	0.99504	2.50326	1.36485
H	-0.65243	1.92319	1.70181
H	0.74062	1.03263	2.32742
H	-1.91345	1.88789	-0.07183
H	-4.32353	1.97862	-0.48141
H	-5.67292	-0.10260	-0.61578
H	-4.53837	-2.30186	-0.32496
H	-2.11760	-2.40356	0.11750
H	2.21793	1.56089	-1.68735
H	4.54355	0.78234	-2.02208
H	5.48927	-0.97750	-0.55056
H	4.09704	-1.94515	1.26203
H	1.77617	-1.14940	1.60295

29
phenyl(1-phenylethyl)amide

C	0.39172	0.64968	0.12794
N	-0.47663	-0.47724	0.27802
C	0.32786	1.59208	1.35431
C	1.83623	0.19072	-0.04778
C	-1.77510	-0.27062	0.06168
C	-2.41961	0.95389	-0.33504
C	-3.79040	1.02786	-0.55244
C	-4.63101	-0.07116	-0.39087
C	-4.03463	-1.28108	0.00415
C	-2.67828	-1.38099	0.22105
C	2.19201	-1.14157	0.16912
C	3.51669	-1.55332	0.03760
C	4.50944	-0.64325	-0.31892
C	4.16365	0.68784	-0.54539
C	2.83982	1.09556	-0.40786
H	0.16200	1.26708	-0.76787
H	0.63755	1.02935	2.24019
H	-0.70266	1.92599	1.50361
H	0.97549	2.47217	1.25239
H	-1.82652	1.85275	-0.47565
H	-4.21571	1.98534	-0.85532
H	-5.70102	0.00427	-0.55816
H	-4.65633	-2.16580	0.14249
H	-2.22912	-2.32454	0.52154
H	1.38482	-1.81945	0.42630
H	3.77726	-2.59502	0.20963
H	5.54137	-0.96721	-0.42567
H	4.92633	1.40722	-0.83330
H	2.57256	2.13486	-0.59163

30
Benzyl-2-methylpropan-2-aminium
Energy: -484.061991

N	1.03943	0.00005	-0.31661
C	0.15622	-0.00031	0.91569
C	2.56464	0.00003	-0.14854
C	3.12856	-0.00003	-1.56793
C	2.96149	1.26486	0.60462
C	2.96152	-1.26472	0.60473
C	-1.27987	-0.00017	0.47591
C	-1.93845	1.20944	0.24199
C	-3.24882	1.20841	-0.22515
C	-3.90162	0.00019	-0.46018
C	-3.24907	-1.20818	-0.22537
C	-1.93868	-1.20959	0.24177
H	0.77246	-0.81459	-0.88228

H	0.77245	0.81498	-0.88186
H	0.41423	-0.89131	1.48936
H	0.41423	0.89033	1.48992
H	2.82203	0.89117	-2.12478
H	2.82232	-0.89147	-2.12456
H	4.21921	0.00016	-1.51989
H	2.58989	2.16627	0.10641
H	2.61601	1.25725	1.64078
H	4.05157	1.32772	0.62514
H	2.61646	-1.25685	1.64102
H	4.05159	-1.32781	0.62482
H	2.58954	-2.16616	0.10684
H	-1.43588	2.15259	0.44529
H	-3.76283	2.14781	-0.39573
H	-4.92531	0.00034	-0.81830
H	-3.76325	-2.14747	-0.39611
H	-1.43632	-2.15288	0.44487

29

1-benzyl-2-methyl-2-propanamine

N	1.09062	-0.28055	-0.24619
C	2.53619	-0.07135	-0.06375
C	3.22825	-1.14276	-0.90871
C	3.00743	1.31983	-0.51497
C	2.89266	-0.28913	1.40956
C	0.19583	0.69522	0.35987
C	-1.25218	0.30166	0.15801
C	-1.63449	-1.04166	0.17813
C	-2.97120	-1.39647	0.02452
C	-3.94355	-0.41425	-0.14990
C	-3.56978	0.92631	-0.17397
C	-2.23114	1.27892	-0.02465
H	0.88921	-0.32202	-1.24385
H	4.31422	-1.08804	-0.79291
H	2.99629	-1.00817	-1.97137
H	2.88839	-2.13660	-0.60606
H	2.72403	1.50343	-1.55731
H	2.57238	2.11133	0.10250
H	4.09611	1.40242	-0.44011
H	2.50398	-1.25294	1.74898
H	3.97893	-0.28071	1.53885
H	2.48108	0.49650	2.04972
H	0.40519	0.72543	1.43642
H	0.33519	1.72424	-0.01218
H	-0.86624	-1.79733	0.30561
H	-3.25564	-2.44412	0.04065
H	-4.98562	-0.69241	-0.27098
H	-4.31924	1.69856	-0.31650
H	-1.94073	2.32633	-0.05299

28

Benzyl(tert-butyl)amide

N	1.08612	-0.39963	-0.06724
C	2.48204	-0.09741	-0.00044
C	3.21966	-1.43454	-0.16171
C	2.98195	0.85153	-1.12374
C	2.92258	0.51699	1.35837
C	0.24590	0.72944	-0.02672
C	-1.21986	0.32309	-0.01437
C	-1.56856	-1.02835	-0.01643
C	-2.90819	-1.41466	-0.00383
C	-3.92196	-0.45843	0.01158
C	-3.58266	0.89486	0.01324
C	-2.24324	1.27486	-0.00068
H	4.31206	-1.33073	-0.09772
H	2.95404	-1.87334	-1.12920
H	2.87582	-2.12153	0.61857
H	2.66663	0.44934	-2.09325
H	2.54105	1.84973	-1.01758
H	4.07520	0.96896	-1.12550
H	2.62035	-0.15873	2.16572
H	4.00774	0.68559	1.42251
H	2.42705	1.48027	1.52609
H	0.35311	1.41748	0.86290
H	0.32516	1.45918	-0.88575
H	-0.73354	-1.72276	-0.02707
H	-3.16731	-2.47164	-0.00613
H	-4.96621	-0.76151	0.02174
H	-4.36406	1.65161	0.02520
H	-1.97587	2.33121	-0.00143

15

Phenylphosphonium

C	-1.231160	-0.083356	-0.000176
C	-1.226390	-1.470860	-0.000639
C	-0.015890	-2.166187	-0.000722
C	1.198441	-1.484459	-0.000343
C	1.215594	-0.094149	0.000121
C	-0.003816	0.593961	0.000200
P	0.015328	2.372395	0.000775
H	-2.174863	0.454891	-0.000108
H	-2.166328	-2.010793	-0.000929
H	-0.021906	-3.250828	-0.001082
H	2.133991	-2.031861	-0.000405
H	2.163180	0.435856	0.000423
H	1.330089	2.841587	0.001358
H	-0.607772	2.947277	-1.111519
H	-0.608498	2.946527	1.113048

14

Phenylphosphine

C	-1.055703	0.375174	0.097930
C	-1.107165	-1.014124	0.098453
C	0.068359	-1.757351	0.000061
C	1.292047	-1.105586	-0.102795
C	1.340704	0.287607	-0.109139
C	0.170293	1.042628	-0.003925
P	0.324438	2.883004	-0.012222
H	-1.975674	0.947625	0.177710
H	-2.064901	-1.518972	0.176258
H	0.027027	-2.841865	0.000932

H	2.210197	-1.678605	-0.183366
H	2.297456	0.794345	-0.200040
H	-0.885652	3.161073	-0.696334
H	-0.249822	3.126902	1.262279

13
Phenylphosphide

C	-1.081258	0.404105	0.000009
C	-1.109311	-0.983773	-0.000301
C	0.068899	-1.733635	-0.000233
C	1.280980	-1.035346	0.000177
C	1.310508	0.349912	0.000510
C	0.130997	1.145126	0.000433
P	0.260959	2.943154	0.000811
H	-2.021298	0.951585	-0.000067
H	-2.072433	-1.493346	-0.000609
H	0.045231	-2.819579	-0.000486
H	2.220632	-1.586650	0.000247
H	2.272814	0.859318	0.000848
H	-1.153134	3.168508	0.000784

25
H_2O-BEt_3

B	-0.25925	0.03983	0.16286
O	0.51005	-0.26931	1.71841
C	-2.72433	0.02698	-0.65558
C	0.21569	1.54523	-0.14014
C	0.31506	-1.12781	-0.81518
C	-1.80891	-0.12376	0.56643
C	1.70837	1.76604	-0.40924
C	1.71842	-1.67843	-0.51471
H	0.10452	-1.07320	2.07343
H	1.44259	-0.47379	1.55208
H	-2.46494	-0.69896	-1.43376
H	-2.62587	1.02394	-1.09655
H	-3.77997	-0.11896	-0.40758
H	-0.10898	2.20558	0.67561
H	-0.34417	1.88143	-1.02519
H	0.32052	-0.71950	-1.83578
H	-0.37961	-1.97942	-0.85172
H	-2.10314	0.61133	1.32813
H	-1.99497	-1.11804	1.00851
H	2.04500	1.19331	-1.28000
H	2.32918	1.45598	0.44274
H	1.94805	2.81698	-0.59881
H	1.73552	-2.27020	0.41165
H	2.46565	-0.88163	-0.41458
H	2.08068	-2.34901	-1.29916

24
[HO-BEt_3]-

B	-0.17288	0.03218	0.36308
O	0.50199	-0.08393	1.69901
C	-2.64224	-0.00622	-0.71790
C	0.25456	1.50500	-0.23130
C	0.28366	-1.22920	-0.63477
C	-1.81584	-0.03022	0.57139
C	1.75778	1.68866	-0.45935
C	1.70694	-1.74922	-0.40044
H	0.19860	-0.91137	2.08717
H	-2.36043	-0.83950	-1.37384
H	-2.45455	0.91452	-1.28376
H	-3.72925	-0.07140	-0.55822
H	-0.08374	2.26850	0.48857
H	-0.27441	1.72655	-1.17306
H	0.17204	-0.95695	-1.69830
H	-0.40753	-2.08094	-0.49046
H	-2.13974	0.79975	1.22086
H	-2.07306	-0.95294	1.12505
H	2.10451	1.07300	-1.29885
H	2.31053	1.36233	0.42906
H	2.05382	2.72571	-0.68124
H	1.85717	-1.96411	0.66338
H	2.45776	-0.99523	-0.65980
H	1.94761	-2.66013	-0.96986

37
H_2O-BPh_3

B	0.00156	0.00502	0.36591
O	0.01047	0.09966	2.14483
C	1.18223	1.04780	0.04281
C	0.31235	-1.53949	0.09911
C	2.34245	0.67532	-0.64912
C	3.37119	1.58324	-0.89151
C	3.27161	2.89427	-0.43335
C	2.13114	3.29567	0.25753
C	1.10377	2.38243	0.48125
C	-1.50275	0.48187	0.05541
C	-2.58348	-0.22701	0.61124
C	-3.90436	0.16084	0.40316
C	-4.18143	1.26876	-0.39453
C	-3.13274	1.97455	-0.97747
C	-1.81360	1.58678	-0.74824
C	1.35083	-2.20037	0.77397
C	1.65859	-3.53259	0.51855
C	0.93389	-4.24194	-0.43810
C	-0.09499	-3.60890	-1.12773
C	-0.40090	-2.27617	-0.85513
H	0.51663	0.89839	2.36239
H	-0.90915	0.24962	2.41544
H	2.43816	-0.34802	-1.00163
H	4.25623	1.26553	-1.43452
H	4.07520	3.60062	-0.61714
H	2.03850	4.31854	0.61021
H	0.19975	2.72627	0.98669
H	-2.38316	-1.12600	1.19558
H	-4.71596	-0.40681	0.84844
H	-5.20883	1.57335	-0.56814
H	-3.34254	2.83143	-1.61071
H	-1.00616	2.15075	-1.20761
H	1.92949	-1.65578	1.51750
H	2.46338	-4.01929	1.06161

H	1.17172	-5.28130	-0.64320
H	-0.66353	-4.15356	-1.87569
H	-1.21400	-1.79649	-1.39458

36
[HO-BPh_3]-

O	0.01662	0.07658	2.26584
B	-0.00402	-0.01161	0.78336
C	0.13219	1.51580	0.21214
C	1.28251	-0.90868	0.26952
C	-1.42619	-0.65466	0.25255
C	-2.31308	-1.26123	1.15282
C	-3.51719	-1.83526	0.74677
C	-3.88251	-1.81521	-0.59680
C	-3.03315	-1.20318	-1.51726
C	-1.83590	-0.63195	-1.09119
C	2.50079	-0.75921	0.95559
C	3.65268	-1.45174	0.59338
C	3.62639	-2.33237	-0.48784
C	2.43552	-2.50641	-1.18666
C	1.28814	-1.80720	-0.80682
C	0.64341	1.83079	-1.05505
C	0.70101	3.14162	-1.52816
C	0.25281	4.19160	-0.73075
C	-0.24755	3.91043	0.54000
C	-0.30392	2.59531	0.99556
H	0.17503	-0.80789	2.60883
H	-2.04852	-1.25844	2.20803
H	-4.17678	-2.29532	1.48018
H	-4.81981	-2.26008	-0.92176
H	-3.31124	-1.16394	-2.56846
H	-1.20034	-0.13604	-1.82421
H	2.52228	-0.07593	1.80254
H	4.57581	-1.30650	1.15107
H	4.52158	-2.87687	-0.77831
H	2.39702	-3.19613	-2.02740
H	0.36490	-1.97669	-1.35727
H	1.02516	1.02474	-1.68136
H	1.10599	3.34615	-2.51719
H	0.29906	5.21638	-1.09143
H	-0.59352	4.72302	1.17608
H	-0.68514	2.37822	1.99036

37
H_2O-B(C_6F_5)Ph_2

B	0.83868	0.11669	0.45474
O	0.88162	0.39808	2.14252
C	1.47331	1.45998	-0.15546
C	1.70806	-1.22168	0.34116
C	-0.75580	-0.05620	0.20697
C	-1.28421	-1.00013	-0.67038
C	-2.64907	-1.13015	-0.91022
C	-3.54495	-0.29051	-0.26495
C	-3.06647	0.67718	0.60799
C	-1.69849	0.76930	0.80912
C	0.72962	2.40436	-0.87397
C	1.30011	3.58977	-1.33361
C	2.63843	3.86674	-1.07209
C	3.40420	2.94730	-0.35834
C	2.82503	1.76231	0.08478
C	2.67870	-1.39797	-0.65285
C	3.40757	-2.58086	-0.75561
C	3.18495	-3.61760	0.14563
C	2.22329	-3.46781	1.14249
C	1.49430	-2.28600	1.23035
F	-1.28763	1.75163	1.65673
F	-3.91135	1.49730	1.22976
F	-4.85051	-0.40540	-0.48403
F	-3.10315	-2.05091	-1.75668
F	-0.48446	-1.82607	-1.34573
H	1.80571	0.57024	2.37852
H	0.36006	1.20040	2.32136
H	-0.31753	2.20630	-1.08936
H	0.69852	4.29850	-1.89437
H	3.08493	4.79043	-1.42663
H	4.45174	3.15022	-0.15735
H	3.44838	1.03695	0.60826
H	2.86347	-0.59607	-1.36298
H	4.15084	-2.69244	-1.53923
H	3.75412	-4.53899	0.07036
H	2.03896	-4.27442	1.84573
H	0.73680	-2.18630	2.00527

36
[HO-B(C_6F_5)Ph_2]-

O	-0.95983	0.30685	2.29766
B	-0.88342	0.15759	0.84122
C	-1.55421	1.42886	0.05137
C	0.73670	0.05156	0.34978
C	-1.63467	-1.25786	0.50552
C	-1.45006	-2.33223	1.38829
C	-2.06395	-3.56708	1.19163
C	-2.89787	-3.76394	0.09273
C	-3.10632	-2.71203	-0.79581
C	-2.48225	-1.48318	-0.58578
C	1.78535	0.59625	1.08434
C	3.12699	0.50049	0.73069
C	3.47771	-0.16469	-0.43213
C	2.47506	-0.70602	-1.22045
C	1.14943	-0.58386	-0.81864
C	-1.35831	1.71028	-1.31013
C	-1.97102	2.79286	-1.93845
C	-2.80385	3.64314	-1.21351
C	-3.01803	3.38913	0.13896
C	-2.40278	2.29811	0.75098
F	0.24785	-1.10670	-1.66916
F	2.79879	-1.33568	-2.35912
F	4.76295	-0.26828	-0.79654
F	4.08446	1.04873	1.49378
F	1.55735	1.30249	2.21485
H	-0.46317	1.08368	2.56556
H	-0.81876	-2.17236	2.25907

H	-1.89691	-4.37808	1.89745
H	-3.38247	-4.72411	-0.06682
H	-3.76008	-2.84926	-1.65437
H	-2.65992	-0.67285	-1.29002
H	-0.71466	1.05761	-1.89735
H	-1.79576	2.97766	-2.99595
H	-3.27956	4.49226	-1.69767
H	-3.66771	4.04342	0.71654
H	-2.57546	2.09538	1.80551

37

H_2O-B(C_6F_5)$_2$Ph

O	-0.12458	0.81559	2.25493
B	-0.06674	0.69639	0.60604
C	1.37979	0.00432	0.36642
C	-0.21065	2.21910	0.14505
C	-1.32091	-0.25216	0.19465
C	-2.56386	-0.12466	0.80537
C	-3.68697	-0.85854	0.45779
C	-3.58620	-1.77745	-0.57843
C	-2.37502	-1.93389	-1.23691
C	-1.27610	-1.17561	-0.84617
C	-1.23192	2.66727	-0.69774
C	-1.33508	4.00834	-1.06450
C	-0.41519	4.93305	-0.58295
C	0.61024	4.51086	0.26246
C	0.70743	3.17049	0.61571
C	2.21203	0.34883	-0.69593
C	3.44001	-0.26311	-0.92204
C	3.87418	-1.27259	-0.07422
C	3.07149	-1.66494	0.98765
C	1.85489	-1.02597	1.16682
F	1.09780	-1.46987	2.21117
F	3.46534	-2.63671	1.80714
F	5.04597	-1.86263	-0.27919
F	4.20034	0.10473	-1.94912
F	1.84256	1.28201	-1.57251
F	-2.72721	0.77295	1.81373
F	-4.84213	-0.69080	1.09549
F	-4.64256	-2.49637	-0.93801
F	-2.27557	-2.80481	-2.23627
F	-0.14962	-1.36488	-1.54055
H	-1.01393	1.11850	2.50722
H	0.05776	-0.04910	2.66397
H	-1.95828	1.95709	-1.08558
H	-2.13437	4.32946	-1.72514
H	-0.49310	5.97836	-0.86506
H	1.33343	5.22731	0.63975
H	1.51580	2.84921	1.27005

36

[HO-B(C_6F_5)$_2$Ph]-

B	0.02733	0.71174	-0.84250
O	0.10054	0.86768	-2.28872
C	-0.30982	4.56331	-0.06991
C	-0.15251	3.34276	-0.72586
C	-0.11400	2.12915	-0.03200
C	-1.33299	-0.15943	-0.36785
C	1.42709	-0.08458	-0.45111
C	-1.41023	-0.96147	0.76599
C	-2.56115	-1.61448	1.18718
C	-3.73102	-1.46892	0.45739
C	-3.72014	-0.66669	-0.67102
C	-2.53938	-0.03542	-1.04619
C	1.56289	-1.46638	-0.54145
C	2.75093	-2.14902	-0.31487
C	3.89467	-1.43289	0.00169
C	3.82266	-0.05307	0.08253
C	2.60823	0.58681	-0.15177
C	-0.23388	2.19466	1.36398
C	-0.38227	3.40525	2.03424
C	-0.42576	4.60014	1.31662
F	4.92658	0.65041	0.37290
F	2.64844	1.92442	-0.08136
F	-0.32662	-1.14556	1.54557
F	-2.55971	-2.38052	2.28640
F	-4.85485	-2.08670	0.84261
F	-4.84600	-0.50247	-1.37936
F	-2.64367	0.75668	-2.13804
F	0.50857	-2.23734	-0.85650
F	2.81099	-3.48546	-0.40581
F	5.05342	-2.06768	0.22082
H	-0.72316	1.24185	-2.61157
H	-0.33730	5.48888	-0.64067
H	-0.03762	3.32049	-1.80739
H	-0.20362	1.26955	1.93850
H	-0.46703	3.42061	3.11835
H	-0.54647	5.54815	1.83431

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H_2O-B(C_6F_5)$_3$

B	0.07621	-0.09201	0.75638
O	0.08972	0.02462	2.37772
C	1.97144	-1.74173	-0.21906
C	1.58274	-0.59596	0.46494
C	-0.25977	1.40362	0.21724
C	-1.14969	-1.06256	0.36507
C	-1.34382	-1.33254	-0.98706
C	-2.40307	-2.08312	-1.47023
C	-3.34638	-2.57439	-0.57413
C	-3.21522	-2.30118	0.77853
C	-2.13178	-1.54759	1.21449
C	-1.32041	2.10767	0.77704
C	-1.73570	3.35851	0.35038
C	-1.06532	3.95200	-0.71191
C	-0.00838	3.28553	-1.31613
C	0.37499	2.03269	-0.84840
C	2.62992	0.18248	0.94699
C	3.97087	-0.10108	0.76329
C	4.31020	-1.24557	0.05140
C	3.30755	-2.06883	-0.43731
F	-0.46964	-0.83993	-1.87357

F	1.07312	-2.60705	-0.69450
F	3.62830	-3.17515	-1.10056
F	5.58577	-1.55489	-0.14308
F	4.91876	0.68907	1.25856
F	2.33233	1.29542	1.67006
F	1.39342	1.44411	-1.47973
F	0.63009	3.85138	-2.33512
F	-1.43541	5.14993	-1.14652
F	-2.75227	3.98434	0.93628
F	-2.01059	1.55207	1.80550
F	-2.08646	-1.28084	2.54007
F	-4.12343	-2.74668	1.64252
F	-4.37338	-3.29140	-1.01429
F	-2.53619	-2.32501	-2.77047
H	-0.79862	0.22351	2.72488
H	0.72095	0.72335	2.62426

36
$[HO\text{-}B(C_6F_5)_3]^-$

B	0.11559	-0.05479	1.00304
O	0.16848	-0.00826	2.44594
C	2.19532	-1.54512	0.11328
C	1.67339	-0.33508	0.54798
C	-0.48356	1.36875	0.34830
C	-0.95216	-1.17685	0.39698
C	-0.98537	-1.45999	-0.96506
C	-1.90058	-2.31463	-1.55901
C	-2.86749	-2.92088	-0.76754
C	-2.89243	-2.65750	0.59080
C	-1.94743	-1.79432	1.14081
C	-1.65516	1.88583	0.88932
C	-2.28139	3.04173	0.44388
C	-1.72648	3.73740	-0.61946
C	-0.56904	3.25659	-1.21037
C	0.01879	2.09171	-0.72675
C	2.62122	0.66694	0.73713
C	3.97848	0.50557	0.49965
C	4.44749	-0.72255	0.05682
C	3.54838	-1.75551	-0.14003
F	-0.08032	-0.88724	-1.77608
F	1.40667	-2.61503	-0.08617
F	3.99029	-2.94888	-0.55993
F	5.75275	-0.90437	-0.17664
F	4.84104	1.51247	0.69174
F	2.23878	1.88402	1.15050
F	1.12798	1.69824	-1.37054
F	-0.03330	3.91995	-2.24272
F	-2.30561	4.85515	-1.07297
F	-3.40889	3.48645	1.01380
F	-2.27327	1.23500	1.89953
F	-2.06700	-1.58423	2.46565
F	-3.82889	-3.22984	1.35896
F	-3.76756	-3.74646	-1.31451
F	-1.87484	-2.55951	-2.87510
H	-0.71823	0.06587	2.80719

40
$(H_2O)_2\text{-}B(C_6F_5)_3$

B	0.08367	-0.07221	0.67705
O	0.04518	-0.01249	2.25328
C	1.83786	-1.75719	-0.48758
C	1.55174	-0.70236	0.37063
C	-0.10019	1.46476	0.14263
C	-1.16887	-0.97634	0.18098
C	-1.48354	-0.96426	-1.17715
C	-2.54816	-1.65996	-1.72750
C	-3.36437	-2.41880	-0.89696
C	-3.08711	-2.47311	0.45884
C	-2.00228	-1.76283	0.96135
C	-1.24545	2.17316	0.48974
C	-1.52333	3.47017	0.08898
C	-0.60962	4.12447	-0.72521
C	0.54508	3.46315	-1.11598
C	0.77763	2.16064	-0.68477
C	2.66395	-0.14768	0.99527
C	3.96594	-0.57800	0.81869
C	4.19953	-1.63854	-0.04853
C	3.13096	-2.22852	-0.70367
F	-0.70524	-0.27537	-2.02018
F	0.87165	-2.38884	-1.16233
F	3.34508	-3.24603	-1.53316
F	5.43586	-2.08214	-0.24276
F	4.97827	0.00411	1.45621
F	2.48427	0.90780	1.83441
F	1.90697	1.59857	-1.12542
F	1.42289	4.07978	-1.90165
F	-0.84091	5.36850	-1.12658
F	-2.64274	4.08135	0.47287
F	-2.18455	1.57688	1.26579
F	-1.79787	-1.88691	2.29493
F	-3.85562	-3.19587	1.27323
F	-4.39448	-3.08965	-1.39953
F	-2.79499	-1.61163	-3.03308
H	-0.81736	0.19325	2.77664
H	0.78722	0.51962	2.58049
O	-2.00113	0.40897	3.65918
H	-2.57104	1.05730	3.22536
H	-2.46565	-0.43830	3.61928

39
$(H_2O)HO\text{-}B(C_6F_5)_3$

B	-0.09217	0.00305	0.87697
O	-0.15941	0.05254	2.33449
C	0.10616	-2.23838	-0.69442
C	0.56459	-1.43269	0.34112
C	0.93512	1.13298	0.23181
C	-1.65717	0.18924	0.40278
C	-2.23170	1.33277	-0.13151
C	-3.59007	1.46678	-0.40134
C	-4.44334	0.41425	-0.12176
C	-3.92315	-0.75186	0.42115
C	-2.56184	-0.83481	0.67291

C	1.88184	1.83938	0.96287
C	2.79305	2.71797	0.38172
C	2.78055	2.90625	-0.98986
C	1.86222	2.21080	-1.76565
C	0.97856	1.34399	-1.14240
C	1.74531	-1.87037	0.93039
C	2.42143	-3.02632	0.56610
C	1.91103	-3.80525	-0.46117
C	0.74615	-3.40649	-1.09699
F	-1.48612	2.41946	-0.42430
F	-1.00757	-1.92797	-1.37316
F	0.25258	-4.15052	-2.09362
F	2.53871	-4.92451	-0.83697
F	3.55380	-3.39129	1.17906
F	2.31874	-1.13633	1.90922
F	0.11568	0.68375	-1.93265
F	1.85076	2.38366	-3.09270
F	3.64935	3.74425	-1.56522
F	3.68730	3.37339	1.13022
F	1.99144	1.69111	2.29315
F	-2.12682	-1.99547	1.18277
F	-4.74060	-1.77645	0.69222
F	-5.75269	0.51777	-0.37126
F	-4.07798	2.59912	-0.92051
H	-0.63150	1.88123	2.57738
H	0.72480	-0.00661	2.70867
O	-0.79603	2.83118	2.44345
H	-0.80066	2.92141	1.48513

25
$[H_2O\text{-}SiEt_3]^+$

O	0.06133	-0.02954	1.70701
Si	-0.01192	0.01157	-0.19453
C	-1.34948	-1.22365	-0.56351
C	-2.74232	-0.80580	-0.06296
C	-0.43895	1.79862	-0.44908
C	0.69533	2.77004	-0.08410
C	1.73969	-0.51177	-0.52245
C	2.06622	-1.95610	-0.10657
H	0.64165	-0.66854	2.15256
H	-0.72150	0.15573	2.25078
H	-1.36965	-1.35932	-1.65290
H	-1.06393	-2.20017	-0.15431
H	-3.48478	-1.56712	-0.30700
H	-2.76836	-0.67822	1.02525
H	-3.06971	0.13215	-0.51810
H	-0.72164	1.91664	-1.50345
H	-1.35124	2.03153	0.11550
H	0.37451	3.80348	-0.22374
H	1.00356	2.65884	0.95949
H	1.57420	2.61008	-0.71345
H	1.91494	-0.38890	-1.59897
H	2.41634	0.20196	-0.03688
H	3.11016	-2.19097	-0.31960
H	1.92127	-2.13135	0.96663
H	1.44755	-2.67951	-0.64261

24
$HO\text{-}SiEt_3$

O	0.10479	-0.05456	1.76920
Si	0.00514	-0.00085	0.09662
C	-1.31326	-1.19594	-0.51896
C	-2.74492	-0.76647	-0.17239
C	-0.41080	1.74455	-0.47363
C	0.70969	2.75057	-0.17990
C	1.70904	-0.51397	-0.48756
C	2.02683	-1.98419	-0.18565
H	-0.69532	0.14753	2.26212
H	-1.10613	-2.18740	-0.09843
H	-1.20807	-1.29959	-1.60695
H	-3.48648	-1.49406	-0.51384
H	-2.99291	0.19584	-0.63075
H	-2.87836	-0.65681	0.90985
H	-1.34144	2.06801	0.01112
H	-0.63001	1.72069	-1.54936
H	0.43203	3.76892	-0.46645
H	1.62251	2.49234	-0.72531
H	0.95885	2.75984	0.88563
H	1.79827	-0.31577	-1.56340
H	2.44157	0.13651	0.00544
H	3.04595	-2.24904	-0.48137
H	1.92440	-2.19190	0.88333
H	1.34539	-2.65405	-0.71937

17
$[H_2O\text{-}SiPhH_2]^+$

Si	1.84468	-0.03806	0.64396
O	2.53328	0.07683	-1.09793
C	0.05784	-0.01461	0.30483
C	-0.62883	1.20918	0.19309
C	-1.98900	1.22090	-0.08756
C	-2.67359	0.01691	-0.25223
C	-2.00741	-1.20269	-0.13658
C	-0.64691	-1.22238	0.14337
H	2.45532	1.16466	1.21921
H	2.43005	-1.31263	1.07560
H	3.46685	-0.00006	-1.35566
H	1.93247	-0.01130	-1.85711
H	-0.10554	2.15132	0.33668
H	-2.51790	2.16391	-0.16910
H	-3.73746	0.02932	-0.46482
H	-2.55034	-2.13367	-0.25548
H	-0.13785	-2.17729	0.24909

16
$HO\text{-}SiPhH_2$

Si	-1.90960	0.54046	0.12687
O	-2.63924	-0.88636	-0.30710
C	-0.07878	0.21345	0.04495
C	0.41009	-1.09758	0.10446
C	1.77913	-1.34913	0.06595
C	2.67885	-0.29085	-0.03032

C	2.20876	1.01886	-0.09507
C	0.83966	1.26542	-0.06169
H	-2.34539	0.93680	1.49239
H	-2.25169	1.66138	-0.78589
H	-3.57259	-0.99067	-0.10608
H	-0.29224	-1.92423	0.16836
H	2.14456	-2.37042	0.10871
H	3.74630	-0.48613	-0.06041
H	2.90841	1.84458	-0.17805
H	0.48484	2.29208	-0.12805

6

$(H_2O)_2$

O	0.839634	0.126310	0.286657
H	0.201017	-0.382663	-0.229751
H	1.063726	-0.441856	1.030088
O	-1.840356	0.315898	-0.286652
H	-1.201587	0.824963	0.229476
H	-2.065165	0.884137	-1.029818

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$[H_2O\text{-}OH]^-$

O	0.437450	0.002426	-0.058983
H	-1.840642	1.444658	-0.506281
H	0.448261	-0.036805	0.905399
O	-1.938193	0.504604	-0.309950
H	-0.755487	0.209599	-0.222148

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$BEt_3\text{-}(H_2O)_2$

B	-0.350428	0.151331	0.278491
C	-2.771126	0.210209	-0.710925
C	0.217734	1.571604	-0.240237
C	0.161090	-1.159612	-0.560387
C	-1.939474	0.154691	0.575802
C	1.725694	1.671433	-0.500153
C	1.531038	-1.750351	-0.187653
H	-2.530518	-0.627843	-1.374856
H	-2.567443	1.129748	-1.268422
H	-3.848148	0.177669	-0.518080
H	-0.079487	2.359656	0.466224
H	-0.301500	1.813065	-1.178280
H	0.188030	-0.877462	-1.622346
H	-0.589440	-1.972239	-0.532474
H	-2.212746	1.001563	1.219927
H	-2.234205	-0.750540	1.134353
H	2.040339	0.980332	-1.289213
H	2.322756	1.430761	0.392021
H	2.032049	2.676589	-0.806724
H	1.539355	-2.176775	0.824305
H	2.319724	-0.991033	-0.221983
H	1.837310	-2.554710	-0.863310
O	0.313807	0.013556	1.815252
H	0.061860	-0.886388	2.156873
H	1.277828	0.041309	1.738380
O	-0.530916	-2.435460	2.292690
H	-0.672482	-2.613774	1.350964
H	-1.413319	-2.419958	2.682644

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$[BEt_3\text{-}(H_2O\text{-}OH)]^-$

B	-0.308214	-0.420250	0.226093
C	-2.697422	-0.138066	-0.966006
C	0.016812	1.181697	0.371473
C	0.340822	-1.093650	-1.149424
C	-1.937650	-0.688918	0.243693
C	1.504907	1.539922	0.327073
C	1.776280	-1.613164	-1.002997
H	-2.288452	-0.547393	-1.898034
H	-2.593787	0.951709	-1.029740
H	-3.773893	-0.361400	-0.955893
H	-0.390037	1.534079	1.333686
H	-0.508455	1.759529	-0.405866
H	0.306586	-0.373322	-1.984083
H	-0.286146	-1.939915	-1.484846
H	-2.384678	-0.282560	1.165969
H	-2.119588	-1.778148	0.296748
H	1.924231	1.343270	-0.667538
H	2.061067	0.921779	1.040850
H	1.712986	2.594007	0.561707
H	1.842951	-2.324892	-0.172835
H	2.472678	-0.804708	-0.758447
H	2.155322	-2.113838	-1.906094
O	0.304116	-1.072483	1.457851
H	0.037281	-1.997925	1.451247
O	-1.027875	0.081441	3.546151
H	-1.583825	0.644517	2.999098
H	-0.471221	-0.360161	2.860967

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$BPh_3\text{-}(H_2O)_2$

B	0.084652	0.118554	0.590612
O	-0.208957	0.332945	2.220094
C	1.873747	-1.333045	-0.626223
C	1.534800	-0.562334	0.495689
C	-0.001043	1.616945	-0.005334
C	-1.129400	-0.868500	0.170942
C	-2.242608	-0.455758	-0.575870
C	-3.347399	-1.290970	-0.767778
C	-3.360431	-2.569546	-0.216117
C	-2.251911	-3.017268	0.504059
C	-1.154270	-2.177995	0.682968
C	-1.027125	2.497490	0.379017
C	-1.118922	3.793640	-0.123049
C	-0.174545	4.246036	-1.040447
C	0.852128	3.395349	-1.442471
C	0.936481	2.104512	-0.925880
C	2.531511	-0.373330	1.461544
C	3.803118	-0.924419	1.321843
C	4.115095	-1.679692	0.194599
C	3.144452	-1.881412	-0.783275
H	-1.175407	0.143503	2.438471

H	-0.021768	1.255104	2.447860
H	1.120062	-1.510766	-1.391150
H	-2.249799	0.542390	-1.006796
H	-4.195724	-0.942949	-1.349892
H	-4.218991	-3.218371	-0.358559
H	-2.243465	-4.021989	0.917040
H	-0.290403	-2.536396	1.239834
H	-1.790148	2.161487	1.083886
H	-1.924999	4.446990	0.197679
H	-0.238161	5.254299	-1.437716
H	1.594923	3.742565	-2.154545
H	1.752416	1.456926	-1.236524
H	2.310636	0.210863	2.352230
H	4.551765	-0.764294	2.092358
H	5.105375	-2.109904	0.080791
H	3.375609	-2.472179	-1.664875
O	-2.729602	-0.229226	2.599943
H	-3.038948	-0.146632	1.682312
H	-2.723491	-1.187175	2.736518

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$[BPh_3\text{-}(H_2O\text{-}OH)]^-$

B	0.266298	-0.006772	0.747667
O	0.508096	0.046792	2.230635
C	0.372424	-1.887054	-1.149621
C	0.665306	-1.488276	0.165219
C	1.119781	1.195527	0.019964
C	-1.340499	0.209886	0.527702
C	-1.891138	0.886723	-0.569492
C	-3.269563	1.014423	-0.746209
C	-4.147081	0.471409	0.187989
C	-3.629554	-0.201690	1.294539
C	-2.251525	-0.330699	1.451588
C	1.021398	2.496782	0.549747
C	1.717045	3.571805	0.003404
C	2.544319	3.382878	-1.103718
C	2.664420	2.108200	-1.647389
C	1.963227	1.037758	-1.087946
C	1.309957	-2.436501	0.969651
C	1.662660	-3.700093	0.495312
C	1.373566	-4.058847	-0.818253
C	0.720774	-3.142179	-1.641965
H	1.443603	0.220712	2.372263
H	-0.153226	-1.189551	-1.801668
H	-1.217807	1.338508	-1.296316
H	-3.659528	1.549450	-1.609261
H	-5.221531	0.575426	0.060204
H	-4.304009	-0.625089	2.035370
H	-1.852728	-0.848460	2.321528
H	0.380109	2.659385	1.415371
H	1.614341	4.562550	0.440603
H	3.089039	4.219663	-1.534213
H	3.310473	1.943362	-2.507115
H	2.083216	0.047895	-1.522939
H	1.520949	-2.170563	2.003000
H	2.161249	-4.409297	1.152958
H	1.645066	-5.041813	-1.194811
H	0.477372	-3.412264	-2.667236
O	-1.107269	2.073784	3.226208
H	-0.491272	1.344340	3.004787
H	-1.767606	1.972899	2.530534

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$B(C_6F_5)Ph_2\text{-}(H_2O)_2$

B	-0.000278	-0.100081	0.702536
O	-0.279443	-0.184382	2.289245
C	1.874006	-1.747285	-0.190968
C	1.517470	-0.609310	0.540546
C	-0.131099	1.469611	0.250023
C	-1.167053	-1.041067	0.107534
C	-2.124763	-0.607993	-0.821210
C	-3.162326	-1.439320	-1.247675
C	-3.265752	-2.734680	-0.750462
C	-2.326888	-3.191824	0.172805
C	-1.298344	-2.353823	0.592830
C	-0.496198	2.555677	1.031305
C	-0.542243	3.867833	0.572548
C	-0.208350	4.131510	-0.745740
C	0.158181	3.080150	-1.578064
C	0.191731	1.789707	-1.069095
C	2.553892	0.101261	1.163950
C	3.880285	-0.312621	1.090500
C	4.205929	-1.455247	0.363556
C	3.199646	-2.167125	-0.282656
F	0.533498	0.811908	-1.913853
F	0.469828	3.324115	-2.848206
F	-0.246769	5.375402	-1.212963
F	-0.903735	4.860888	1.384751
F	-0.848499	2.385436	2.335434
H	-1.254970	0.060093	2.455768
H	0.302816	0.392802	2.801817
H	1.100300	-2.311692	-0.704563
H	-2.063827	0.400906	-1.223231
H	-3.885870	-1.074534	-1.970534
H	-4.071369	-3.383729	-1.078781
H	-2.400040	-4.200785	0.567170
H	-0.575228	-2.719112	1.318815
H	2.325988	1.021113	1.706366
H	4.658993	0.258299	1.587310
H	5.238747	-1.782260	0.294415
H	3.447752	-3.051721	-0.861563
O	-2.757952	0.363077	2.311649
H	-2.845927	1.315985	2.182968
H	-2.972890	-0.051732	1.459511

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$[B(C_6F_5)Ph_2\text{-}(H_2O\text{-}OH)]^-$

B	0.099004	0.001572	0.803085
O	0.187019	0.216913	2.269856
C	0.978295	-1.876763	-0.906816
C	0.696461	-1.474137	0.408548
C	0.982372	1.171930	-0.014075

C	-1.489212	0.136194	0.434260
C	-2.100572	1.376200	0.190358
C	-3.471963	1.498397	-0.024467
C	-4.284647	0.366834	-0.005404
C	-3.706487	-0.877342	0.230479
C	-2.332506	-0.982204	0.444392
C	2.005125	1.908802	0.574700
C	2.739321	2.890643	-0.080697
C	2.459824	3.178188	-1.406221
C	1.457316	2.470157	-2.049259
C	0.754032	1.497671	-1.348424
C	0.916253	-2.428646	1.411657
C	1.401144	-3.706340	1.130630
C	1.680610	-4.072199	-0.182336
C	1.462027	-3.148155	-1.203308
F	-0.190350	0.850689	-2.057353
F	1.182117	2.732637	-3.334623
F	3.156065	4.116725	-2.060097
F	3.717731	3.556097	0.547448
F	2.378542	1.686793	1.852397
H	1.107762	0.151517	2.542047
H	0.803352	-1.178619	-1.721488
H	-1.480572	2.271451	0.176392
H	-3.907338	2.476963	-0.213532
H	-5.354587	0.454283	-0.176074
H	-4.327763	-1.769940	0.245164
H	-1.896830	-1.962999	0.623316
H	0.688237	-2.153975	2.439044
H	1.559533	-4.417929	1.937971
H	2.060484	-5.064842	-0.409836
H	1.669786	-3.422025	-2.235104
O	-0.569465	2.858773	2.576433
H	-0.213133	1.946320	2.570583
H	-1.486639	2.701372	2.328442

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$B(C_6F_5)_2Ph\text{-}(H_2O)_2$

B	0.057703	0.091529	0.640466
O	-0.019288	0.200700	2.239374
C	1.716510	-1.780242	-0.237495
C	1.510130	-0.558325	0.410437
C	-0.095163	1.627505	0.128299
C	-1.162189	-0.866236	0.131063
C	-1.671188	-0.767135	-1.162966
C	-2.664370	-1.601776	-1.663759
C	-3.188578	-2.603003	-0.858383
C	-2.700016	-2.758901	0.430331
C	-1.700768	-1.906225	0.879405
C	-0.973933	2.523042	0.721391
C	-1.131864	3.843368	0.325919
C	-0.382387	4.313567	-0.742021
C	0.494262	3.453969	-1.389040
C	0.617203	2.139562	-0.954015
C	2.638514	0.096195	0.931240
C	3.914382	-0.443608	0.811125
C	4.093586	-1.660741	0.156061
C	2.991861	-2.327086	-0.370125
F	-1.195423	0.153183	-2.007282
F	1.446245	1.360936	-1.650333
F	1.202109	3.894582	-2.426825
F	-0.511195	5.572663	-1.148247
F	-1.991472	4.648074	0.950770
F	-1.753121	2.117386	1.753467
F	-1.261556	-2.141558	2.142912
F	-3.184807	-3.715507	1.221970
F	-4.142253	-3.405867	-1.316342
F	-3.113583	-1.451793	-2.906015
H	-0.945456	0.192874	2.665453
H	0.504472	-0.523490	2.611760
H	0.867155	-2.316364	-0.654183
H	2.511651	1.055330	1.431176
H	4.769924	0.085387	1.219812
H	5.087774	-2.084556	0.054971
H	3.124022	-3.274461	-0.883646
O	-2.336820	0.058022	3.297105
H	-2.928289	0.647485	2.812808
H	-2.664532	-0.843037	3.187150

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$[B(C_6F_5)_2Ph\text{-}(H_2O\text{-}OH)]^-$

B	-0.008654	0.021850	0.850696
O	-0.001066	0.207552	2.311455
C	0.814746	-1.801866	-0.927424
C	0.637580	-1.419117	0.410146
C	0.918309	1.178851	0.074539
C	-1.614557	0.124248	0.448841
C	-2.279957	1.268651	0.024018
C	-3.645314	1.333821	-0.228326
C	-4.424560	0.206144	-0.033488
C	-3.820997	-0.957278	0.415203
C	-2.451188	-0.972138	0.653445
C	2.006415	1.786886	0.691966
C	2.852293	2.693286	0.062577
C	2.626870	3.028486	-1.261910
C	1.562870	2.444194	-1.931756
C	0.749494	1.544694	-1.256841
C	1.071817	-2.325798	1.384645
C	1.663877	-3.542799	1.052424
C	1.830219	-3.895985	-0.283648
C	1.395771	-3.018749	-1.275158
F	-1.619185	2.429851	-0.173995
F	-0.259911	1.020369	-1.981158
F	1.335444	2.755277	-3.214510
F	3.430307	3.894853	-1.889812
F	3.886667	3.236524	0.715354
F	2.337101	1.493557	1.965381
F	-1.964732	-2.130506	1.114941
F	-4.567287	-2.049483	0.624116
F	-5.741231	0.241796	-0.266540
F	-4.214798	2.470424	-0.647804
H	0.906017	0.164332	2.630163
H	0.484661	-1.131981	-1.718068

H	0.917762	-2.074982	2.431544
H	1.990518	-4.220515	1.837639
H	2.289236	-4.844255	-0.550135
H	1.513315	-3.283451	-2.323207
O	-0.340649	2.995897	2.455462
H	-0.284865	2.029401	2.569014
H	-0.651989	3.078972	1.548304

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$B(C_6F_5)_3$-$(H_2O)_2$

B	0.083676	-0.072148	0.676991
O	0.045160	-0.012392	2.253243
C	1.837847	-1.757481	-0.487197
C	1.551751	-0.702360	0.370654
C	-0.100151	1.464803	0.142547
C	-1.168856	-0.976249	0.180902
C	-1.483628	-0.963943	-1.177211
C	-2.548231	-1.659648	-1.727604
C	-3.364313	-2.418699	-0.897151
C	-3.086992	-2.473192	0.458633
C	-2.002189	-1.762896	0.961203
C	-1.245276	2.173290	0.489936
C	-1.523158	3.470300	0.089219
C	-0.609604	4.124519	-0.725213
C	0.544942	3.463111	-1.116292
C	0.777514	2.160606	-0.685085
C	2.663970	-0.147460	0.995084
C	3.965944	-0.577819	0.818597
C	4.199523	-1.638666	-0.048277
C	3.130939	-2.228869	-0.703193
F	-0.705468	-0.274803	-2.020161
F	0.871604	-2.389356	-1.161695
F	3.345032	-3.246637	-1.532348
F	5.435862	-2.082293	-0.242406
F	4.978297	0.004532	1.455862
F	2.484318	0.908298	1.833868
F	1.906707	1.598444	-1.126027
F	1.422592	4.079676	-1.902189
F	-0.840931	5.368551	-1.126572
F	-2.642403	4.081603	0.473383
F	-2.184190	1.577073	1.266268
F	-1.797774	-1.887044	2.294766
F	-3.855404	-3.196130	1.272950
F	-4.394405	-3.089532	-1.399780
F	-2.795152	-1.611138	-3.033158
H	-0.817434	0.193035	2.776618
H	0.786994	0.520036	2.580405
O	-2.001144	0.408552	3.659262
H	-2.571285	1.056635	3.225382
H	-2.465434	-0.438857	3.619575

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$[B(C_6F_5)_3$-$(H_2O$-$OH)]^-$

B	-0.092213	0.002843	0.876854
O	-0.159391	0.052438	2.334456
C	0.106310	-2.238570	-0.694334
C	0.564669	-1.432796	0.341185
C	0.935062	1.132870	0.231744
C	-1.657198	0.189028	0.402629
C	-2.231627	1.332755	-0.131395
C	-3.589991	1.467074	-0.400984
C	-4.443432	0.414643	-0.121578
C	-3.923373	-0.751655	0.421031
C	-2.562029	-0.834935	0.672513
C	1.881728	1.839333	0.962779
C	2.792858	2.718021	0.381645
C	2.780425	2.906267	-0.989926
C	1.862110	2.210793	-1.765712
C	0.978538	1.343899	-1.142468
C	1.745462	-1.870332	0.930422
C	2.421628	-3.026280	0.566197
C	1.911245	-3.805324	-0.460984
C	0.746340	-3.406679	-1.096816
F	-1.485902	2.419362	-0.424084
F	-1.007399	-1.928243	-1.373121
F	0.252795	-4.150793	-2.093393
F	2.538980	-4.924578	-0.836710
F	3.554058	-3.391097	1.179127
F	2.318963	-1.136124	1.909067
F	0.115690	0.683674	-1.932747
F	1.850646	2.383639	-3.092758
F	3.649176	3.744327	-1.565255
F	3.687033	3.373494	1.130193
F	1.991321	1.691130	2.293081
F	-2.127248	-1.995884	1.181970
F	-4.740938	-1.776193	0.691931
F	-5.752778	0.518452	-0.370929
F	-4.077744	2.599600	-0.919919
H	-0.631845	1.880830	2.577169
H	0.724883	-0.006389	2.708537
O	-0.796416	2.830826	2.443468
H	-0.800046	2.921582	1.485204

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$[SiEt_3$-$(H_2O)_2]^+$

O	-0.103262	-0.474759	1.632044
Si	-0.069041	-0.147959	-0.163534
C	-1.472414	-1.204690	-0.775150
C	-2.852791	-0.783350	-0.244665
C	-0.329123	1.690886	-0.292004
C	0.813826	2.513055	0.323126
C	1.653938	-0.735099	-0.551162
C	1.858673	-2.243613	-0.343038
H	0.764593	-0.419149	2.217721
H	-0.931465	-0.450213	2.130796
H	-1.467334	-1.159732	-1.871399
H	-1.262998	-2.249939	-0.519258
H	-3.635143	-1.437700	-0.632924
H	-2.911725	-0.841790	0.848551
H	-3.103238	0.239333	-0.537680
H	-0.447047	1.941947	-1.353644
H	-1.286244	1.951041	0.176737

H	0.599622	3.582058	0.273566
H	0.966701	2.261543	1.378513
H	1.757301	2.340492	-0.201055
H	1.875514	-0.461690	-1.590165
H	2.361828	-0.160662	0.059472
H	2.894762	-2.528318	-0.535652
H	1.614803	-2.549248	0.680139
H	1.227128	-2.829099	-1.015635
O	2.024130	-0.352403	2.853798
H	2.499490	-1.149937	3.118874
H	2.289217	0.368350	3.438728

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$SiEt_3$-(H_2O-OH)

O	0.404096	0.478589	1.693379
Si	0.210210	0.153680	0.076245
C	-1.057559	-1.227975	-0.180392
C	-2.306888	-1.056327	0.693135
C	-0.403776	1.746651	-0.699015
C	0.497787	2.945717	-0.376387
C	1.846918	-0.370915	-0.703249
C	2.504884	-1.576496	-0.021118
H	0.498905	-0.310707	2.250640
H	-1.339540	-1.242123	-1.240950
H	-0.592730	-2.205193	0.008209
H	-3.026840	-1.868900	0.557059
H	-2.044483	-1.003968	1.755392
H	-2.820427	-0.119298	0.458266
H	-0.491234	1.612972	-1.784736
H	-1.419521	1.937754	-0.331341
H	0.102227	3.876409	-0.793291
H	0.596755	3.072420	0.704825
H	1.503974	2.805907	-0.784159
H	1.682396	-0.585803	-1.766985
H	2.532676	0.484011	-0.667381
H	3.467969	-1.834643	-0.470423
H	2.686228	-1.369613	1.039726
H	1.870941	-2.469378	-0.099515
O	0.474238	-2.195790	2.602617
H	-0.401755	-2.522294	2.366763
H	1.075751	-2.601066	1.967006

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$[SiPhH_2$-$(H_2O)_2]^+$

Si	1.667285	-0.324497	0.768189
O	2.474446	-0.386240	-0.839875
C	-0.104090	-0.112152	0.361187
C	-0.651790	1.174804	0.219785
C	-1.990919	1.333833	-0.116609
C	-2.795270	0.211814	-0.309080
C	-2.268494	-1.070554	-0.164180
C	-0.929865	-1.233995	0.172071
H	2.320607	0.829254	1.401833
H	2.038786	-1.620146	1.353491
H	3.520055	-0.499394	-1.000890
H	1.927245	-0.302490	-1.634300
H	-0.036045	2.055690	0.384704
H	-2.410088	2.328615	-0.219809
H	-3.841896	0.337720	-0.565691
H	-2.902746	-1.938911	-0.304261
H	-0.531630	-2.237712	0.299526
O	4.883862	-0.651603	-1.060265
H	5.314649	-1.486473	-1.282328
H	5.491295	0.074535	-1.249008

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$SiPhH_2$-(H_2O-OH)

Si	1.776680	-0.038572	0.344555
O	2.448740	-0.026944	-1.160646
C	-0.082359	-0.010338	0.184295
C	-0.783966	1.201966	0.145042
C	-2.169920	1.227360	0.018040
C	-2.880300	0.032473	-0.066272
C	-2.203264	-1.183733	-0.021401
C	-0.817214	-1.200858	0.105748
H	2.186396	1.154152	1.134785
H	2.152927	-1.263930	1.100798
H	3.421168	-0.040067	-1.200682
H	-0.239094	2.140467	0.217380
H	-2.696678	2.176158	-0.011255
H	-3.961592	0.048996	-0.162546
H	-2.756059	-2.116130	-0.081457
H	-0.298573	-2.155952	0.147158
O	5.237334	-0.066375	-1.276941
H	5.562789	0.701545	-1.758204
H	5.539060	-0.832378	-1.776376

26

H_3N-BEt_3

B	-0.59681	0.00028	-0.00014
N	-2.28339	0.00096	-0.00078
C	-0.23605	-1.00381	1.23212
C	-0.23484	-0.56498	-1.48550
C	-0.23449	1.56917	0.25327
C	1.17521	-1.60168	1.19169
C	1.17707	-0.23179	-1.98178
C	1.17705	1.83190	0.79121
H	-2.64216	-0.91478	-0.26736
H	-2.64227	0.22829	0.92544
H	-2.64145	0.68974	-0.66088
H	-0.38063	-0.49612	2.20007
H	-0.94362	-1.85182	1.24277
H	-0.37982	-1.65706	-1.52991
H	-0.94150	-0.14993	-2.22594
H	-0.37834	2.15355	-0.67054
H	-0.94166	2.00329	0.98218
H	1.37678	-2.25032	2.05074
H	1.31339	-2.20374	0.28735
H	1.94440	-0.82342	1.18072
H	1.37898	-0.65090	-2.97318
H	1.31614	0.85236	-2.05014
H	1.94549	-0.61255	-1.30203

H	1.37954	2.90005	0.92299
H	1.31487	1.35009	1.76502
H	1.94591	1.43239	0.12283

25
$[H_2N\text{-}BEt_3]^-$

B	0.17355	-0.18956	-0.00012
N	0.08550	-0.47902	1.54016
C	-1.30706	2.06759	-0.06346
C	-1.02648	-1.04201	-0.77230
C	1.62788	-0.74820	-0.54855
C	0.05883	1.43579	-0.34741
C	-2.31837	-1.24307	0.02968
C	2.86560	-0.04115	0.01307
H	0.78826	0.09288	2.01317
H	-0.79710	-0.10741	1.89744
H	-1.34050	3.15899	-0.20351
H	-1.61747	1.86762	0.97175
H	-2.07918	1.63554	-0.71227
H	-0.64617	-2.04416	-1.03135
H	-1.27432	-0.56944	-1.73890
H	1.70086	-1.82067	-0.30757
H	1.65987	-0.68486	-1.65006
H	0.81632	1.99316	0.23207
H	0.31049	1.62026	-1.40704
H	-2.78677	-0.28682	0.29603
H	-2.08896	-1.75616	0.97045
H	-3.08075	-1.83700	-0.49719
H	2.86663	1.02358	-0.25107
H	2.88004	-0.09635	1.10963
H	3.82007	-0.46186	-0.33827

38
$H_3N\text{-}BPh_3$

B	0.00016	0.00004	0.49350
C	-1.48473	-0.52974	0.11531
C	0.28384	1.55080	0.11494
C	1.20119	-1.02130	0.11548
C	-2.36322	0.18213	-0.71158
C	-3.63903	-0.29381	-1.01235
C	-4.07757	-1.50451	-0.48562
C	-3.22431	-2.24254	0.33179
C	-1.95123	-1.75751	0.61622
C	1.34160	1.95619	-0.70910
C	1.56718	3.29917	-1.00950
C	0.73571	4.28381	-0.48540
C	-0.33203	3.91332	0.32923
C	-0.54824	2.56819	0.61343
C	1.02334	-2.13859	-0.71052
C	2.07326	-3.00555	-1.01167
C	3.34147	-2.77947	-0.48629
C	3.55456	-1.67105	0.33034
C	2.49811	-0.81104	0.61524
N	0.00004	0.00092	2.17444
H	-2.03996	1.13121	-1.13064
H	-4.29234	0.28402	-1.65958
H	-5.07168	-1.87540	-0.71536
H	-3.54783	-3.19672	0.73741
H	-1.28627	-2.37860	1.21970
H	2.00354	1.20208	-1.12624
H	2.39582	3.57653	-1.65449
H	0.91136	5.33024	-0.71499
H	-0.99835	4.67019	0.73272
H	-1.41990	2.30217	1.21474
H	0.03945	-2.33353	-1.12862
H	1.89907	-3.86064	-1.65826
H	4.15963	-3.45491	-0.71645
H	4.54303	-1.47372	0.73486
H	2.70394	0.07575	1.21804
H	-0.59194	0.74981	2.53236
H	-0.35227	-0.88577	2.53366
H	0.94430	0.13960	2.53294

37
$[H_2N\text{-}BPh_3]^-$

B	0.02774	-0.00009	0.76850
N	-0.04230	-0.00001	2.32279
C	-1.69976	-1.99558	1.01727
C	1.60392	-0.00100	0.26473
C	-0.77057	-1.32127	0.21096
C	-0.76896	1.32205	0.21088
C	2.33975	1.18779	0.11699
C	3.70593	1.19737	-0.16015
C	4.39959	-0.00242	-0.30268
C	3.70465	-1.20146	-0.16053
C	2.33845	-1.19050	0.11664
C	-1.69715	1.99767	1.01721
C	-2.42395	3.09454	0.55524
C	-2.24669	3.55485	-0.74728
C	-1.33505	2.90218	-1.57556
C	-0.61493	1.80975	-1.09715
C	-0.61706	-1.80931	-1.09698
C	-1.33858	-2.90085	-1.57537
C	-2.25117	-3.55220	-0.74714
C	-2.42796	-3.09150	0.55534
H	0.47441	-0.80687	2.67271
H	0.47531	0.80629	2.67268
H	-1.84348	-1.63108	2.03196
H	1.81681	2.13767	0.21922
H	4.23228	2.14370	-0.26846
H	5.46431	-0.00295	-0.52284
H	4.22995	-2.14834	-0.26915
H	1.81454	-2.13988	0.21859
H	-1.84124	1.63348	2.03196
H	-3.13375	3.59306	1.21280
H	-2.81026	4.40971	-1.11329
H	-1.18457	3.24909	-2.59586
H	0.10227	1.32065	-1.75561
H	0.10089	-1.32125	-1.75541
H	-1.18842	-3.24806	-2.59561
H	-2.81590	-4.40632	-1.11311
H	-3.13851	-3.58902	1.21286

38
H_3N-B(C_6F_5)Ph_2

B	0.84547	0.03067	0.67228
N	1.00186	0.06203	2.32078
C	1.39481	1.47060	0.17639
C	1.72619	-1.25907	0.25431
C	-0.74291	-0.10701	0.32779
C	-1.80384	-0.12855	1.22051
C	-3.13920	-0.19667	0.84021
C	-3.45240	-0.24719	-0.50852
C	-2.42799	-0.22931	-1.44778
C	-1.11140	-0.15547	-1.01630
C	2.34143	1.61561	-0.84513
C	2.77982	2.87140	-1.26119
C	2.27810	4.02291	-0.66199
C	1.32115	3.91020	0.34372
C	0.88742	2.64981	0.74338
C	3.11523	-1.25075	0.46691
C	3.91080	-2.36162	0.20148
C	3.32945	-3.52622	-0.29430
C	1.95653	-3.56358	-0.51709
C	1.17203	-2.44478	-0.24248
F	-0.16107	-0.14152	-1.95677
F	-2.72213	-0.27952	-2.74511
F	-4.72116	-0.31462	-0.90154
F	-4.10874	-0.21291	1.75457
F	-1.57557	-0.07955	2.55797
H	0.60844	-0.77570	2.74745
H	1.99797	0.09702	2.53521
H	0.54601	0.86676	2.74884
H	2.73652	0.72639	-1.32865
H	3.51340	2.95052	-2.05791
H	2.62027	5.00169	-0.98328
H	0.90696	4.80164	0.80518
H	0.10194	2.59335	1.50007
H	3.59483	-0.33848	0.82415
H	4.98228	-2.31735	0.37236
H	3.94310	-4.39573	-0.50799
H	1.49425	-4.46580	-0.90612
H	0.10036	-2.50053	-0.41793

37
[H_2N-B(C_6F_5)Ph_2]-

B	0.88753	-0.17410	0.86555
N	1.07815	-0.38547	2.37228
C	1.62498	1.24814	0.51860
C	1.54137	-1.42663	0.03725
C	-0.74199	-0.06115	0.38387
C	-1.79804	-0.64455	1.07955
C	-3.13501	-0.55205	0.70414
C	-3.47632	0.15194	-0.43789
C	-2.46803	0.73827	-1.18556
C	-1.14797	0.61596	-0.76604
C	2.90267	1.32168	-0.05084
C	3.55958	2.53663	-0.24351
C	2.95177	3.73123	0.13356
C	1.68166	3.69184	0.70531
C	1.04062	2.46935	0.88901
C	2.34843	-2.36814	0.69136
C	2.93945	-3.43624	0.01575
C	2.74675	-3.59092	-1.35413
C	1.96120	-2.66213	-2.03513
C	1.37248	-1.60491	-1.34580
F	-0.24307	1.19067	-1.57974
F	-2.78165	1.41093	-2.30264
F	-4.75697	0.25404	-0.81920
F	-4.09843	-1.13804	1.43155
F	-1.58835	-1.37754	2.19331
H	0.50264	-1.14015	2.73164
H	0.81480	0.44669	2.89340
H	3.39325	0.39840	-0.35115
H	4.55087	2.55172	-0.69137
H	3.45898	4.68077	-0.01761
H	1.19056	4.61584	1.00285
H	0.04268	2.45963	1.32899
H	2.51321	-2.23578	1.75767
H	3.55559	-4.14941	0.55963
H	3.20496	-4.42073	-1.88659
H	1.80805	-2.76363	-3.10731
H	0.77434	-0.88506	-1.90044

38
H_3N-B(C_6F_5)$_2$Ph

B	0.06223	0.65642	0.64806
N	0.16268	1.01824	2.25071
C	0.07170	2.10032	-0.08464
C	-1.36789	-0.08259	0.40021
C	1.38607	-0.25481	0.34930
C	-2.29338	-0.46470	1.35880
C	-3.53545	-1.01688	1.06235
C	-3.88710	-1.20723	-0.26306
C	-2.99246	-0.84799	-1.26583
C	-1.77024	-0.29711	-0.91785
C	2.64633	0.22180	0.70991
C	3.83914	-0.44241	0.47004
C	3.80088	-1.67066	-0.17549
C	2.57666	-2.19748	-0.55526
C	1.40534	-1.49342	-0.28873
C	1.06532	2.52454	-0.97261
C	1.03422	3.79149	-1.55105
C	0.00213	4.67429	-1.24787
C	-1.00590	4.27555	-0.37383
C	-0.96691	3.00330	0.18851
F	-2.02227	-0.30958	2.67985
F	-4.37811	-1.35590	2.03724
F	-5.06649	-1.73376	-0.57631
F	-3.32136	-1.03796	-2.54095
F	-0.93147	0.01201	-1.91082
F	2.75223	1.41188	1.34811
F	5.00321	0.07858	0.85110
F	4.92455	-2.33509	-0.41881
F	2.52771	-3.37845	-1.16555

F	0.27694	-2.09487	-0.67725
H	0.11302	0.19470	2.84835
H	1.04556	1.50537	2.40770
H	-0.60074	1.63566	2.52534
H	1.87563	1.84842	-1.23282
H	1.81767	4.08918	-2.24116
H	-0.02243	5.66245	-1.69613
H	-1.82476	4.94946	-0.14114
H	-1.78915	2.69718	0.83797

37
$[H_2N\text{-}B(C_6F_5)2Ph]^-$

B	0.01254	0.69619	-0.86157
N	0.07615	0.80117	-2.38764
C	-0.47462	4.52873	0.01664
C	-0.31747	3.32954	-0.67901
C	-0.12507	2.10847	-0.02567
C	-1.33990	-0.16187	-0.39554
C	1.41989	-0.08761	-0.45271
C	-1.41332	-0.94860	0.75077
C	-2.56085	-1.59874	1.18538
C	-3.73477	-1.46291	0.46151
C	-3.72935	-0.67235	-0.67468
C	-2.55277	-0.04207	-1.06675
C	2.60181	0.59875	-0.19145
C	3.82572	-0.02223	0.04602
C	3.90801	-1.40270	0.00566
C	2.76547	-2.13571	-0.27736
C	1.56843	-1.47153	-0.51024
C	-0.10002	2.14754	1.37802
C	-0.24904	3.33465	2.08773
C	-0.43957	4.53737	1.40722
F	2.83714	-3.47338	-0.33253
F	0.52101	-2.26001	-0.79581
F	-0.32855	-1.12522	1.53135
F	-2.55014	-2.35222	2.29369
F	-4.85625	-2.07733	0.85993
F	-4.86059	-0.51396	-1.37658
F	-2.67089	0.73854	-2.15851
F	2.63461	1.94135	-0.17820
F	4.92725	0.70062	0.29573
F	5.07446	-2.02261	0.22721
H	-0.69725	1.33537	-2.77041
H	0.92538	1.29252	-2.65862
H	-0.62235	5.45858	-0.52819
H	-0.33621	3.33940	-1.76725
H	0.04389	1.21660	1.92493
H	-0.21832	3.32624	3.17486
H	-0.55895	5.46774	1.95621

38
$H_3N\text{-}B(C_6F_5)_3$

B	0.06003	-0.07138	0.83726
N	0.05349	0.03934	2.46939
C	-0.26258	1.43668	0.29957
C	1.56053	-0.60098	0.49119
C	-1.15740	-1.03724	0.37198
C	-2.08227	-1.66521	1.19035
C	-3.15254	-2.41184	0.71046
C	-3.32325	-2.54136	-0.65843
C	-2.42266	-1.92854	-1.52372
C	-1.37504	-1.19327	-0.99483
C	2.65011	0.15694	0.91435
C	3.97399	-0.16779	0.67590
C	4.25543	-1.32882	-0.03367
C	3.21138	-2.12598	-0.47458
C	1.89525	-1.75722	-0.20606
C	0.42374	2.09436	-0.71739
C	0.06268	3.35448	-1.18257
C	-1.03149	4.00561	-0.63170
C	-1.75706	3.38582	0.37628
C	-1.36086	2.12779	0.80313
F	-2.11647	1.55978	1.77494
F	-2.81340	3.99124	0.91312
F	-1.38343	5.20996	-1.06550
F	0.75730	3.93959	-2.15379
F	1.47938	1.53031	-1.31054
F	0.95767	-2.59844	-0.65314
F	3.47210	-3.24572	-1.14290
F	5.51375	-1.67485	-0.27585
F	4.96296	0.60597	1.11543
F	2.42226	1.29615	1.61046
F	-0.51911	-0.62347	-1.85250
F	-2.57964	-2.05312	-2.83826
F	-4.33735	-3.24913	-1.14271
F	-4.00604	-2.99299	1.55065
F	-1.97508	-1.57752	2.53769
H	0.20033	-0.87036	2.90398
H	0.80318	0.67194	2.75242
H	-0.84002	0.39948	2.80599

37
$[H_2N\text{-}B(C_6F_5)_3]^-$

B	0.05606	-0.02041	0.78619
N	0.14615	0.00294	2.31467
C	-0.18379	2.32556	-0.59369
C	-0.66473	1.39882	0.32232
C	1.62317	-0.12039	0.26589
C	-0.86709	-1.30515	0.23087
C	-0.62860	-2.57644	0.75262
C	-1.39214	-3.69830	0.47264
C	-2.47598	-3.58123	-0.38647
C	-2.75224	-2.34918	-0.94975
C	-1.94973	-1.25239	-0.63930
C	2.22504	-1.16393	-0.42580
C	3.59053	-1.22664	-0.70062
C	4.42070	-0.20579	-0.27834
C	3.86961	0.86932	0.40451
C	2.50648	0.88860	0.65862
C	-1.88001	1.75529	0.90018
C	-2.56132	2.93339	0.63415
C	-2.02349	3.83392	-0.27260

C	-0.82624	3.52383	-0.89300
F	0.43156	-2.78379	1.55723
F	0.95538	2.11229	-1.27353
F	-0.30088	4.37836	-1.78060
F	-2.65723	4.97988	-0.54859
F	-3.73040	3.20707	1.22837
F	-2.49653	0.90977	1.75161
F	2.04852	1.98165	1.27859
F	4.66161	1.87496	0.79989
F	5.73404	-0.24628	-0.53246
F	4.10520	-2.26818	-1.36855
F	1.51576	-2.20418	-0.89799
F	-2.29671	-0.11290	-1.26473
F	-3.78683	-2.22309	-1.79128
F	-3.23309	-4.64721	-0.67152
F	-1.09819	-4.89026	1.00913
H	-0.77616	-0.00018	2.73857
H	0.62174	-0.82680	2.65453

26

$[H_3N\text{-}SiEt_3]^+$

Si	0.04434	-0.32891	0.15401
N	-0.80339	-1.63836	1.31198
C	0.01318	1.21949	1.19304
C	1.71782	-1.08915	-0.14909
C	-1.12004	-0.29027	-1.29967
C	2.65986	-0.10419	-0.87048
C	-2.55868	0.11688	-0.94042
C	0.19701	2.48074	0.32426
H	-0.79965	-2.57411	0.89704
H	-1.78012	-1.39561	1.49950
H	-0.33138	-1.70942	2.21725
H	-0.93878	1.28825	1.73473
H	0.80029	1.16806	1.95465
H	1.60051	-2.00007	-0.74849
H	2.16889	-1.39421	0.80327
H	-0.70054	0.42753	-2.01666
H	-1.10455	-1.25631	-1.81831
H	3.61022	-0.58660	-1.10414
H	2.87769	0.76576	-0.24553
H	2.23375	0.25137	-1.81332
H	-3.17104	0.21293	-1.83852
H	-3.05305	-0.62816	-0.30685
H	-2.59179	1.07717	-0.41751
H	0.20082	3.37635	0.94755
H	1.14022	2.46203	-0.22825
H	-0.61345	2.58732	-0.40220

25

$H_2N\text{-}SiEt_3$

Si	-0.17519	0.01223	0.39141
N	0.64729	-0.19774	1.91324
C	0.40422	-1.37482	-0.75365
C	-2.06111	-0.07206	0.50341
C	0.31521	1.71709	-0.24586
C	-2.75675	-0.06338	-0.86470
C	1.78631	1.82201	-0.66532
C	1.86217	-1.81204	-0.56228
H	0.54177	0.51194	2.62636
H	0.67066	-1.11565	2.33764
H	-0.26230	-2.23749	-0.61951
H	0.24402	-1.04428	-1.78881
H	-2.33455	-0.98235	1.05251
H	-2.42197	0.76658	1.11275
H	0.09811	2.44763	0.54537
H	-0.33646	1.98985	-1.08533
H	-2.51596	0.84243	-1.43050
H	-2.44465	-0.91866	-1.47274
H	-3.84585	-0.10855	-0.77179
H	1.99252	1.18037	-1.52802
H	2.44785	1.50404	0.14622
H	2.06096	2.84370	-0.94426
H	2.55339	-0.98025	-0.72121
H	2.03670	-2.17418	0.45445
H	2.13710	-2.61303	-1.25511

18

$[H_3N\text{-}SiPhH_2]^+$

Si	1.78921	-0.74385	0.00014
C	0.01834	-0.24974	0.00006
C	-0.40931	1.08590	0.00013
C	-1.76520	1.39397	0.00008
C	-2.70882	0.36999	-0.00004
C	-2.30009	-0.96173	-0.00012
C	-0.94529	-1.27205	-0.00007
N	2.76120	0.90918	-0.00023
H	2.32629	-1.36510	1.22063
H	2.32619	-1.36562	-1.22013
H	0.29943	1.91195	0.00022
H	-2.08439	2.43027	0.00013
H	-3.76631	0.61117	-0.00008
H	-3.03562	-1.75839	-0.00021
H	-0.64666	-2.31813	-0.00014
H	3.77314	0.74917	-0.00017
H	2.54642	1.47794	-0.82513
H	2.54638	1.47834	0.82438

17

$H_2N\text{-}SiPhH_2$

Si	1.90306	-0.53964	0.22649
C	0.06629	-0.21105	0.09196
C	-0.43338	1.09386	0.20171
C	-1.80021	1.34545	0.12240
C	-2.69140	0.29173	-0.06749
C	-2.21314	-1.01100	-0.18338
C	-0.84466	-1.25610	-0.10772
N	2.73396	0.82606	-0.43182
H	2.37264	-0.65494	1.62931
H	2.14830	-1.85588	-0.42878
H	0.26230	1.91759	0.34148
H	-2.17168	2.36200	0.20774

H	-3.75765	0.48632	-0.12973
H	-2.90534	-1.83270	-0.33868
H	-0.48023	-2.27565	-0.21344
H	3.69500	1.00008	-0.17523
H	2.55512	1.10831	-1.38568

8
$2NH_3$

N	1.34438	-0.01478	0.11207
N	-1.21794	-0.00787	-0.02131
H	0.27770	-0.01191	0.05654
H	1.68645	0.83042	-0.33689
H	1.81378	-0.73443	-0.40940
H	-1.42454	0.79153	0.56902
H	-1.64649	0.12926	-0.91817
H	-1.59200	-0.84629	0.40358

7
$[NH_3\text{-}NH_2]^-$

N	1.30393	-0.01027	-0.11750
N	-1.29930	0.01137	-0.11793
H	-0.01702	-0.01864	-0.11505
H	1.61946	0.82637	0.36915
H	1.57025	-0.76956	0.51515
H	-1.60652	0.79341	0.50696
H	-1.59856	-0.83928	0.37180

30
$BEt_3\text{-}(NH_3)_2$

B	0.09031	-0.45793	-0.01034
C	-0.36162	0.54269	1.20513
C	1.47162	-1.28557	0.26531
C	-0.02110	0.20091	-1.50164
C	0.76712	1.37610	1.82251
C	2.76864	-0.58325	-0.15207
C	0.56273	1.61173	-1.63804
H	-1.15244	1.23297	0.86583
H	-0.82137	-0.04311	2.02127
H	1.54596	-1.56858	1.32872
H	1.43533	-2.24352	-0.28288
H	0.45486	-0.45468	-2.24944
H	-1.08191	0.25304	-1.80603
H	0.41358	2.02956	2.62784
H	1.54247	0.72733	2.24327
H	1.25169	2.01177	1.07452
H	3.65772	-1.18509	0.06588
H	2.76808	-0.38054	-1.22857
H	2.89249	0.37820	0.35578
H	0.47160	2.00769	-2.65553
H	0.05021	2.31097	-0.96758
H	1.62385	1.63633	-1.37166
N	-1.08087	-1.63983	-0.01518
H	-1.00842	-2.21710	0.82100
H	-2.02521	-1.20723	-0.04422
H	-0.96640	-2.24998	-0.82264
N	-3.44754	0.05819	0.00959
H	-3.08872	0.78094	-0.60943
H	-3.41635	0.45264	0.94579
H	-4.42402	-0.08607	-0.22828

29
$[BEt_3\text{-}(NH_3\text{-}NH_2)]^-$

B	0.26211	-0.22903	-0.12493
N	-0.37987	0.04358	1.28737
C	2.78710	0.52288	0.46118
C	0.03914	1.11202	-1.07779
C	-0.54471	-1.49015	-0.81734
C	1.87345	-0.61525	-0.00324
C	0.04190	2.46448	-0.35312
C	-0.44134	-2.83001	-0.08216
H	-0.20041	-0.75409	1.89796
H	0.09927	0.82002	1.74469
H	3.83240	0.22244	0.62726
H	2.42354	0.95259	1.40507
H	2.79850	1.33862	-0.27213
H	-0.92629	1.02440	-1.60508
H	0.79856	1.13623	-1.87805
H	-1.60971	-1.21821	-0.89855
H	-0.19294	-1.63022	-1.85351
H	2.00028	-1.45899	0.69781
H	2.24884	-0.98546	-0.97320
H	0.98307	2.63612	0.18404
H	-0.75810	2.49672	0.39648
H	-0.10536	3.32348	-1.02411
H	0.60040	-3.16734	-0.01867
H	-0.80974	-2.73765	0.94806
H	-1.01608	-3.64167	-0.55201
N	-3.22280	0.80676	0.48173
H	-3.53967	-0.06414	0.05681
H	-2.93550	1.37058	-0.31822
H	-2.31621	0.54557	0.91108

42
$BPh_3\text{-}(NH_3)_2$

B	-0.16262	0.05218	0.42808
C	-0.04827	-1.51358	0.03002
C	-1.65082	0.64784	0.17426
C	1.04892	0.95046	-0.18125
C	-0.61759	-1.96356	-1.17232
C	-0.49834	-3.28316	-1.59666
C	0.19163	-4.20972	-0.81626
C	0.76044	-3.79789	0.38357
C	0.64197	-2.46832	0.79096
C	-1.91182	1.79735	-0.58183
C	-3.20777	2.28459	-0.75581
C	-4.28535	1.63030	-0.16860
C	-4.05884	0.47722	0.58136
C	-2.76228	-0.00149	0.73832
C	1.98531	0.43954	-1.09094
C	3.08554	1.18510	-1.51574
C	3.28401	2.47649	-1.03566
C	2.35983	3.02196	-0.14515

C	1.26232	2.26721	0.26305
H	-1.17296	-1.25500	-1.78326
H	-0.95092	-3.59403	-2.53383
H	0.28094	-5.24206	-1.14003
H	1.29693	-4.51017	1.00417
H	1.11082	-2.18168	1.73236
H	-1.08335	2.32116	-1.05192
H	-3.37473	3.17638	-1.35318
H	-5.29481	2.00774	-0.30055
H	-4.89398	-0.05145	1.03194
H	-2.61017	-0.92701	1.29467
H	1.85504	-0.57345	-1.46471
H	3.79191	0.75420	-2.21959
H	4.14224	3.05763	-1.35866
H	2.49294	4.03468	0.22472
H	0.54463	2.72484	0.94484
N	0.06768	0.13492	2.06274
H	-0.50211	-0.55755	2.54683
H	1.07934	-0.01295	2.28271
H	-0.20795	1.05295	2.40630
N	2.93381	-0.10962	2.02671
H	2.99479	-0.74433	1.23300
H	3.16487	0.80796	1.64818
H	3.66583	-0.36783	2.68155

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[BPh_3-(NH_3-NH_2)]-

B	-0.10319	-0.02113	0.66515
N	-0.00182	0.08820	2.20888
C	-2.69958	0.19917	1.11807
C	0.81706	-1.26884	0.07193
C	-1.68051	-0.28059	0.27999
C	0.32377	1.41726	0.00051
C	2.01405	-1.13331	-0.64987
C	2.79084	-2.23006	-1.03259
C	2.38844	-3.52105	-0.70781
C	1.20130	-3.69675	0.00384
C	0.44387	-2.59161	0.37848
C	0.52965	2.55821	0.79170
C	0.86966	3.79546	0.24110
C	1.00175	3.93591	-1.13730
C	0.78259	2.82611	-1.95332
C	0.44973	1.59837	-1.38756
C	-2.09619	-0.92509	-0.89547
C	-3.44245	-1.08109	-1.22311
C	-4.43010	-0.59588	-0.36914
C	-4.04941	0.04615	0.80795
H	-0.29861	-0.78716	2.63698
H	0.95941	0.22393	2.51874
H	-2.39983	0.70018	2.03583
H	2.35398	-0.13435	-0.91754
H	3.71205	-2.07339	-1.59014
H	2.98655	-4.37857	-1.00532
H	0.86795	-4.69947	0.26293
H	-0.48708	-2.75031	0.92272
H	0.40438	2.45712	1.86788
H	1.02610	4.65434	0.89055
H	1.26527	4.89659	-1.57256
H	0.87114	2.92188	-3.03341
H	0.27835	0.74399	-2.04184
H	-1.33957	-1.32900	-1.56705
H	-3.72295	-1.58807	-2.14413
H	-5.48184	-0.71818	-0.61653
H	-4.81059	0.42922	1.48497
N	3.32853	0.67312	1.82805
H	4.16367	0.74953	1.25133
H	2.68028	1.36260	1.44659
H	2.91347	-0.21878	1.56141

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$B(C_6F_5)Ph_2$-(NH_3)$_2$

B	-0.83573	0.07184	0.56721
C	-1.69179	-1.08363	-0.18651
C	-1.39029	1.58358	0.38201
C	0.76128	0.01020	0.21504
C	1.80677	-0.30754	1.07127
C	3.14692	-0.29943	0.69735
C	3.48376	0.04097	-0.60234
C	2.47641	0.36318	-1.50385
C	1.15504	0.34499	-1.08094
C	-3.06354	-1.21628	0.08624
C	-3.82763	-2.25739	-0.43438
C	-3.23362	-3.20620	-1.26420
C	-1.88072	-3.09035	-1.57115
C	-1.12903	-2.04333	-1.03825
C	-0.89768	2.61519	1.19579
C	-1.34945	3.92671	1.08364
C	-2.31397	4.24548	0.13062
C	-2.80712	3.24654	-0.70346
C	-2.34855	1.93658	-0.57584
F	0.22381	0.64880	-1.99173
F	2.79147	0.68347	-2.75753
F	4.75762	0.05282	-0.98644
F	4.10066	-0.61556	1.57462
F	1.56469	-0.65381	2.35836
H	-3.55712	-0.47143	0.71120
H	-4.88555	-2.32650	-0.19884
H	-3.82221	-4.02036	-1.67529
H	-1.40920	-3.81520	-2.22839
H	-0.07111	-1.98344	-1.28456
H	-0.11755	2.39847	1.92752
H	-0.94571	4.70018	1.73037
H	-2.67069	5.26625	0.03401
H	-3.54952	3.48820	-1.45839
H	-2.73812	1.16960	-1.24012
N	-1.01721	-0.28548	2.15223
H	-0.44309	0.29281	2.76159
H	-1.99271	-0.13741	2.40480
H	-0.77534	-1.29565	2.30419
N	-0.42746	-3.05185	1.96077
H	-0.21314	-3.74478	2.67143
H	-1.20813	-3.39824	1.40676

H	0.36566	-3.01737	1.32476

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$[B(C_6F_5)Ph_2\text{-}(NH_3\text{-}NH_2)]^-$

B	-0.96556	-0.13733	-0.87723
N	-1.12444	-0.38444	-2.38078
C	-1.99297	1.08222	-0.51023
C	-1.28811	-1.50336	-0.03659
C	0.61167	0.30880	-0.41141
C	1.75405	-0.12424	-1.07849
C	3.05692	0.19783	-0.71375
C	3.27101	1.00610	0.39027
C	2.17576	1.45137	1.11301
C	0.89453	1.09408	0.70610
C	-3.23841	0.87075	0.09389
C	-4.14663	1.90853	0.30270
C	-3.83295	3.20567	-0.09311
C	-2.60206	3.44864	-0.69987
C	-1.70799	2.40039	-0.89959
C	-1.74406	-2.65894	-0.68444
C	-1.98889	-3.84738	0.00648
C	-1.79425	-3.90888	1.38438
C	-1.36606	-2.76589	2.06036
C	-1.12012	-1.59013	1.35608
F	-0.09416	1.53899	1.50291
F	2.36904	2.21707	2.19595
F	4.51359	1.33782	0.76246
F	4.10322	-0.26263	-1.41223
F	1.67003	-0.96250	-2.13921
H	-0.38192	-0.95654	-2.76828
H	-1.11637	0.48952	-2.89876
H	-3.50125	-0.13678	0.40859
H	-5.10402	1.70390	0.77679
H	-4.53639	4.01808	0.07030
H	-2.33959	4.45704	-1.01202
H	-0.74532	2.61101	-1.36701
H	-1.90893	-2.60431	-1.75760
H	-2.33147	-4.72892	-0.53108
H	-1.97718	-4.83262	1.92686
H	-1.21975	-2.79636	3.13746
H	-0.78969	-0.70657	1.90012
N	1.68770	-3.22431	0.15144
H	1.63877	-2.42790	0.78471
H	0.74506	-3.61225	0.19067
H	1.74886	-2.80153	-0.77284

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$B(C_6F_5)_2Ph\text{-}(NH_3)_2$

B	-0.05018	0.68185	-0.64656
C	-0.21389	2.18375	-0.06223
C	1.41465	-0.00371	-0.39768
C	-1.20561	-0.34448	-0.12488
C	1.83979	-1.07781	-1.17438
C	3.04575	-1.74029	-1.00019
C	3.88972	-1.33159	0.02278
C	3.50556	-0.28183	0.84372
C	2.28611	0.35371	0.62940
C	-2.20776	-0.93599	-0.88177
C	-3.14709	-1.82027	-0.36210
C	-3.09938	-2.14514	0.98426
C	-2.11707	-1.57932	1.78796
C	-1.20057	-0.70453	1.22205
C	-1.28374	2.58594	0.74488
C	-1.46710	3.91952	1.11189
C	-0.57345	4.89297	0.67568
C	0.51170	4.51865	-0.11531
C	0.68159	3.18448	-0.46986
F	1.04635	-1.54129	-2.16861
F	3.39323	-2.75524	-1.79051
F	5.05279	-1.94556	0.21690
F	4.30656	0.10583	1.83431
F	1.98160	1.33641	1.47800
F	-2.32392	-0.66660	-2.20133
F	-4.08597	-2.35167	-1.14456
F	-3.98893	-2.98567	1.50378
F	-2.06717	-1.88160	3.08310
F	-0.27747	-0.17780	2.03603
H	-2.00148	1.84479	1.08985
H	-2.30728	4.19664	1.74177
H	-0.71239	5.93163	0.95838
H	1.22637	5.26578	-0.44712
H	1.55292	2.91183	-1.06717
N	-0.21275	0.88234	-2.24952
H	-0.21943	0.00216	-2.76024
H	-1.10635	1.41017	-2.42427
H	0.56068	1.44858	-2.59467
N	-2.56705	2.45058	-2.21219
H	-3.15005	1.95081	-1.54534
H	-2.25624	3.29294	-1.73226
H	-3.16603	2.72927	-2.98348

41
$[B(C_6F_5)_2Ph\text{-}(NH_3\text{-}NH_2)]^-$

B	0.11330	0.57455	-0.88946
N	0.17634	0.64970	-2.41648
C	-0.86114	4.33509	-0.10734
C	-0.51983	3.15679	-0.77371
C	-0.22871	1.97227	-0.09040
C	-1.12172	-0.44283	-0.41702
C	1.60287	-0.00861	-0.44872
C	-1.10084	-1.25750	0.71179
C	-2.17237	-2.03208	1.13910
C	-3.36175	-2.00465	0.42744
C	-3.45174	-1.18974	-0.68837
C	-2.34766	-0.43744	-1.07265
C	2.67449	0.82008	-0.13257
C	3.96321	0.35796	0.12519
C	4.22856	-0.99767	0.05046
C	3.20114	-1.86693	-0.28510
C	1.93356	-1.35935	-0.53602
C	-0.29717	2.02459	1.31187
C	-0.63440	3.18959	1.99346

C	-0.92197	4.35662	1.28344
F	3.45053	-3.18102	-0.37086
F	1.00398	-2.26737	-0.86796
F	-0.00178	-1.32581	1.48815
F	-2.07269	-2.80341	2.22937
F	-4.40697	-2.74048	0.82188
F	-4.60148	-1.11520	-1.36926
F	-2.56854	0.38588	-2.12138
F	2.52816	2.15401	-0.07866
F	4.95189	1.21128	0.42805
F	5.46047	-1.46424	0.29021
H	-0.64658	1.08665	-2.81894
H	0.97246	1.21497	-2.70244
H	-1.08294	5.23660	-0.67376
H	-0.47306	3.15396	-1.86104
H	-0.07769	1.12105	1.88030
H	-0.67808	3.19240	3.07979
H	-1.19108	5.26837	1.80945
N	-3.70135	2.11463	0.40295
H	-3.61889	1.81567	-0.56683
H	-3.21730	1.38919	0.92940
H	-3.07766	2.91819	0.47508

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$B(C_6F_5)_3$-$(NH_3)_2$

B	0.00975	-0.09954	0.77917
N	0.05074	0.16271	2.37784
C	-0.13161	1.37641	0.07964
C	1.41811	-0.85177	0.44039
C	-1.32592	-0.94471	0.38357
C	-2.32714	-1.39253	1.23148
C	-3.47574	-2.04325	0.79236
C	-3.64970	-2.26826	-0.56290
C	-2.67307	-1.84266	-1.45679
C	-1.55035	-1.19579	-0.96884
C	2.61663	-0.17572	0.65520
C	3.87176	-0.70752	0.41171
C	3.96478	-2.00407	-0.07692
C	2.80519	-2.72705	-0.30465
C	1.56563	-2.14869	-0.04222
C	0.55342	1.79931	-1.05619
C	0.37095	3.05392	-1.63085
C	-0.53453	3.94325	-1.07115
C	-1.25065	3.56351	0.05570
C	-1.04080	2.29953	0.58703
F	-1.76732	1.98818	1.68450
F	-2.12009	4.40541	0.61406
F	-0.71263	5.14716	-1.60440
F	1.06108	3.40910	-2.71139
F	1.44367	1.00631	-1.65768
F	0.50571	-2.93155	-0.27400
F	2.88278	-3.97438	-0.76201
F	5.15380	-2.54601	-0.31550
F	4.97516	0.00222	0.64215
F	2.58271	1.08876	1.12569
F	-0.62223	-0.81577	-1.85764
F	-2.82870	-2.06054	-2.76003
F	-4.73775	-2.88874	-1.00659
F	-4.39989	-2.44682	1.66240
F	-2.23122	-1.21854	2.57088
H	0.44023	-0.64042	2.86790
H	0.60073	1.03032	2.60652
H	-0.88720	0.31533	2.74342
N	1.11857	2.76918	2.83533
H	1.46461	3.00227	1.90781
H	1.87413	2.96119	3.48677
H	0.36611	3.41930	3.04621

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$[B(C_6F_5)_3$-$(NH_3$-$NH_2)]$-

B	-0.05622	-0.02920	0.90105
N	-0.02780	-0.06727	2.42283
C	1.18634	1.15769	-1.08258
C	0.97124	1.10976	0.29331
C	0.57349	-1.47502	0.37377
C	-1.61748	0.20492	0.33782
C	-2.59707	-0.69952	0.74820
C	-3.94794	-0.58304	0.46492
C	-4.39144	0.50437	-0.27572
C	-3.46880	1.43839	-0.70971
C	-2.12024	1.26732	-0.40228
C	-0.00155	-2.40107	-0.48959
C	0.59596	-3.60806	-0.84130
C	1.84480	-3.92514	-0.33685
C	2.47680	-3.02466	0.50631
C	1.84372	-1.83146	0.83354
C	1.75049	1.99520	1.02539
C	2.67132	2.86775	0.44915
C	2.84942	2.86726	-0.92299
C	2.09132	2.00442	-1.70262
F	-2.23939	-1.78758	1.45742
F	0.46354	0.36203	-1.88753
F	2.24585	2.00418	-3.03206
F	3.73136	3.69522	-1.49334
F	3.38920	3.70357	1.20983
F	1.64364	2.09247	2.36392
F	2.54968	-1.00334	1.61174
F	3.69586	-3.31064	0.98259
F	2.43773	-5.07907	-0.66451
F	-0.02119	-4.46236	-1.66840
F	-1.19960	-2.18171	-1.05600
F	-1.31738	2.25028	-0.86270
F	-3.87884	2.49559	-1.41985
F	-5.69058	0.64642	-0.55872
F	-4.82788	-1.49826	0.88935
H	-0.23248	0.83062	2.84585
H	-0.70312	-0.73569	2.77922
N	-1.22634	3.29689	2.08591
H	-0.30142	3.17154	2.49060
H	-1.72379	2.43050	2.28072
H	-1.07942	3.28585	1.07888

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$[SiEt_3\text{-}(NH_3)_2]^+$

Si	0.17193	-0.00992	-0.30215
N	-1.08021	1.29456	-0.86182
C	-0.00570	0.00084	1.56032
C	-0.43091	-1.56256	-1.14618
C	1.82462	0.62995	-0.88552
C	0.28937	-2.82162	-0.62947
C	2.17947	2.01977	-0.33283
C	1.22052	-0.60776	2.26601
H	-1.21714	1.29092	-1.87474
H	-0.78554	2.23954	-0.60575
H	-2.03624	1.10347	-0.38803
H	-0.15476	1.03096	1.90965
H	-0.91229	-0.55234	1.83617
H	-0.28250	-1.46487	-2.22862
H	-1.51246	-1.66521	-0.98999
H	2.58177	-0.09946	-0.57038
H	1.85792	0.62885	-1.98145
H	-0.03334	-3.70699	-1.18010
H	0.07465	-2.99565	0.42847
H	1.37453	-2.74340	-0.74486
H	3.18770	2.31393	-0.62983
H	1.50389	2.79526	-0.71026
H	2.14002	2.04517	0.76048
H	1.08162	-0.61645	3.34860
H	1.40140	-1.63879	1.95001
H	2.12659	-0.03320	2.05439
N	-3.47031	0.74199	0.43157
H	-3.76437	-0.22798	0.33673
H	-3.40056	0.92105	1.43141
H	-4.24849	1.30650	0.09595

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$SiEt_3\text{-}(NH_3\text{-}NH_2)$

Si	0.10509	0.12846	-0.18041
N	-0.34990	-1.02835	-1.38863
C	1.90745	0.61792	-0.48414
C	-0.92461	1.72096	-0.18610
C	-0.11628	-0.70808	1.49729
C	-0.40210	2.80038	0.77080
C	0.91198	-1.81302	1.76583
C	2.79772	-0.50087	-1.04027
H	-1.32776	-1.31227	-1.35116
H	-0.04476	-0.88144	-2.34176
H	1.92102	1.47606	-1.16990
H	2.32427	0.99412	0.45987
H	-0.94420	2.11124	-1.21194
H	-1.96638	1.47479	0.06048
H	-1.12839	-1.13422	1.51887
H	-0.08385	0.04198	2.29758
H	-0.38510	2.44323	1.80568
H	0.62095	3.09303	0.51325
H	-1.01596	3.70614	0.74891
H	1.92235	-1.39719	1.83827
H	0.91350	-2.54487	0.95239
H	0.71001	-2.34626	2.70002
H	2.83483	-1.35697	-0.36146
H	2.41529	-0.87431	-1.99431
H	3.82429	-0.15843	-1.20359
N	-3.36131	-1.08964	-0.53664
H	-3.79921	-0.33125	-1.05097
H	-3.99397	-1.88249	-0.58401
H	-3.33454	-0.79720	0.43580

22
$[SiPhH_2\text{-}(NH_3)_2]^+$

Si	1.814201	0.331235	-0.513596
C	-0.015321	0.214180	-0.434470
C	-0.795369	1.370105	-0.265287
C	-2.178888	1.275959	-0.167076
C	-2.796074	0.028653	-0.240971
C	-2.035966	-1.126184	-0.416281
C	-0.652253	-1.035269	-0.514820
N	2.488233	0.189766	1.236497
H	2.489585	-0.803759	-1.165369
H	2.343813	1.646771	-0.911132
H	-0.326216	2.350468	-0.225130
H	-2.776083	2.172577	-0.042551
H	-3.876302	-0.042956	-0.170199
H	-2.522283	-2.093053	-0.485083
H	-0.070870	-1.941161	-0.670329
H	3.582602	0.255893	1.226621
H	2.124055	0.930067	1.840769
H	2.220839	-0.696007	1.672069
N	5.225231	0.365978	1.105616
H	5.535598	1.246788	0.699693
H	5.676772	0.298254	2.015887
H	5.631579	-0.370555	0.531745

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$SiPhH_2\text{-}(NH_3\text{-}NH_2)$

Si	1.862884	-0.503078	-0.018803
C	0.027368	-0.175812	-0.215543
C	-0.562321	0.938643	0.395914
C	-1.920632	1.204595	0.243601
C	-2.713082	0.357096	-0.527044
C	-2.146004	-0.758297	-1.138794
C	-0.788191	-1.021281	-0.978176
N	2.395091	0.151057	1.477337
H	2.044948	-1.968048	-0.244155
H	2.664651	0.184139	-1.067945
H	0.056077	1.594233	1.004155
H	-2.362706	2.071111	0.726040
H	-3.772487	0.562521	-0.646824
H	-2.763096	-1.424580	-1.733800
H	-0.358317	-1.903765	-1.447693
H	3.382205	0.397444	1.548647
H	2.008006	-0.186965	2.347044
N	5.256441	0.934439	0.783915
H	4.967188	1.163912	-0.162497
H	5.682897	1.770812	1.169902

H	5.990618	0.238180	0.703693

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BEt_3-N_2H_4

C	-0.599425	-1.442353	-0.439620
B	0.079027	-0.100940	0.193574
C	1.102776	-0.462200	1.413559
C	-0.956830	1.102440	0.560573
C	2.316172	-1.327929	1.051435
C	-1.645385	-1.259896	-1.546475
C	-1.414359	2.008358	-0.593257
N	1.053893	0.463322	-1.043939
N	1.838815	1.607292	-0.695715
H	-1.078969	-1.972680	0.394796
H	0.171011	-2.143906	-0.801748
H	1.455681	0.438428	1.942648
H	0.507412	-0.991267	2.169847
H	-0.530929	1.748690	1.341770
H	-1.842663	0.645260	1.024858
H	2.920761	-1.600553	1.921875
H	2.013133	-2.259942	0.563038
H	2.996438	-0.805510	0.361036
H	-2.029958	-2.215298	-1.918175
H	-1.246530	-0.725160	-2.420291
H	-2.500770	-0.680750	-1.185701
H	-1.852595	1.438927	-1.420504
H	-2.170152	2.733621	-0.275508
H	-0.572086	2.586157	-0.993228
H	1.624126	-0.332978	-1.336353
H	0.448611	0.727118	-1.822324
H	2.743078	1.553326	-1.154796
H	1.986540	1.548912	0.308629

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$[BEt_3$-$N_2H_3]^-$

C	-0.503160	-1.433235	-0.479681
B	0.231031	-0.057563	0.064896
C	1.176094	-0.421053	1.369024
C	-0.887195	1.093599	0.542479
C	2.215609	-1.511021	1.095995
C	-1.632842	-1.262077	-1.501860
C	-1.420957	2.010131	-0.568132
N	1.166363	0.457230	-1.077297
N	1.829083	1.713786	-0.796635
H	-0.909850	-1.991015	0.381382
H	0.263396	-2.088779	-0.921428
H	1.701578	0.489135	1.708057
H	0.545301	-0.719708	2.223099
H	-0.465762	1.740181	1.333419
H	-1.740665	0.593287	1.030733
H	2.933374	-1.666231	1.915574
H	1.728276	-2.475151	0.906135
H	2.777037	-1.261502	0.187604
H	-2.038818	-2.215293	-1.872704
H	-1.297222	-0.696899	-2.381459
H	-2.471737	-0.702634	-1.069979
H	-1.927555	1.437292	-1.352936
H	-2.135048	2.766604	-0.209801
H	-0.599697	2.544676	-1.061864
H	0.634879	0.632318	-1.929109
H	2.704575	1.456596	-0.341498
H	1.304436	2.189749	-0.054099

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BPh_3-N_2H_4

B	0.270811	0.211033	-0.491388
C	0.362498	-1.331755	0.006400
N	1.784886	0.540298	-1.064218
N	2.042225	1.885529	-1.539130
C	-0.025347	-1.757676	1.283646
C	0.047774	-3.096783	1.664719
C	0.521738	-4.053878	0.773110
C	0.899506	-3.664135	-0.509816
C	0.807219	-2.326195	-0.880284
C	-0.374837	0.382497	-3.089158
C	-0.750008	0.342278	-1.739182
C	-1.312506	0.418776	-4.123195
C	-2.669473	0.410623	-3.828238
C	-3.076489	0.356574	-2.495055
C	-2.130894	0.320983	-1.477576
C	0.101401	1.324995	0.679451
C	0.911815	1.266003	1.828179
C	0.889830	2.257821	2.805395
C	0.044256	3.355163	2.660256
C	-0.763282	3.448973	1.531019
C	-0.725880	2.451420	0.556999
H	2.458244	0.358363	-0.317970
H	2.049228	-0.097800	-1.817173
H	1.842403	2.471520	-0.726056
H	1.264450	2.077821	-2.173479
H	-0.399578	-1.026544	1.995336
H	-0.266435	-3.392569	2.661401
H	0.584500	-5.096425	1.069064
H	1.250301	-4.404154	-1.223090
H	1.052339	-2.059412	-1.909949
H	0.678563	0.375808	-3.376606
H	-0.978157	0.451078	-5.155873
H	-3.404712	0.439849	-4.626036
H	-4.134699	0.338180	-2.251762
H	-2.465334	0.268759	-0.443172
H	1.566266	0.406327	1.973304
H	1.526818	2.172965	3.680874
H	0.017874	4.130385	3.419683
H	-1.421978	4.303134	1.404494
H	-1.358064	2.549713	-0.321906

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$[BPh_3$-$N_2H_3]^-$

B	0.396870	0.207886	-0.693851
C	0.473419	-1.339083	-0.148916
N	1.736089	0.495339	-1.412166
N	1.860288	1.766572	-2.068206

C	-0.652979	-2.149864	0.059097
C	-0.555750	-3.447169	0.559409
C	0.690197	-3.988386	0.868133
C	1.829561	-3.212229	0.669503
C	1.715522	-1.914649	0.171890
C	-0.791363	0.244563	-3.082933
C	-0.911637	0.381439	-1.691238
C	-1.884790	0.327678	-3.944375
C	-3.160760	0.549190	-3.432723
C	-3.319667	0.693833	-2.055763
C	-2.212115	0.619222	-1.212909
C	0.285438	1.269333	0.566136
C	0.737504	0.957229	1.857916
C	0.727886	1.884605	2.898564
C	0.261521	3.179186	2.681160
C	-0.195248	3.525390	1.412242
C	-0.182851	2.582158	0.385033
H	1.966515	-0.212008	-2.105751
H	2.084030	2.430813	-1.328688
H	0.933825	2.061094	-2.398637
H	-1.636476	-1.755646	-0.188334
H	-1.455512	-4.041419	0.704607
H	0.771621	-5.001026	1.255619
H	2.810792	-3.620086	0.904119
H	2.606780	-1.309876	0.020382
H	0.200218	0.074125	-3.501567
H	-1.742038	0.220002	-5.017558
H	-4.018837	0.613120	-4.097081
H	-4.309189	0.872009	-1.640109
H	-2.353686	0.754813	-0.141269
H	1.107519	-0.047274	2.051502
H	1.084073	1.596086	3.885316
H	0.250592	3.906034	3.489654
H	-0.566328	4.530589	1.223378
H	-0.565473	2.869099	-0.593826

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$B(C_6F_5)Ph_2$-N_2H_4

B	0.230930	0.214391	-0.559009
C	0.171499	-1.279482	0.071477
N	1.784139	0.298495	-1.127668
N	2.354621	1.586774	-1.459690
C	0.279021	-1.547664	1.442657
C	0.314669	-2.851058	1.935127
C	0.254280	-3.929754	1.058527
C	0.148190	-3.694697	-0.310348
C	0.102445	-2.388589	-0.788977
C	-0.284876	0.874603	-3.098621
C	-0.718555	0.375775	-1.862645
C	-1.127563	0.934713	-4.211305
C	-2.437445	0.486765	-4.115353
C	-2.894078	-0.028583	-2.901784
C	-2.045120	-0.085194	-1.805055
C	0.119792	1.392193	0.581070
C	1.161254	1.660306	1.467515
C	1.116773	2.598472	2.487260
C	-0.047306	3.331588	2.668754
C	-1.123742	3.103981	1.826437
C	-1.025613	2.152628	0.813854
F	2.334117	0.980624	1.357471
F	2.166812	2.797547	3.282359
F	-0.126565	4.237814	3.636988
F	-2.247206	3.797644	1.991319
F	-2.120289	1.999578	0.066826
H	2.388854	-0.152549	-0.441420
H	1.824496	-0.274544	-1.973517
H	2.862173	1.884419	-0.629509
H	1.560824	2.221324	-1.540037
H	0.320301	-0.723201	2.150151
H	0.387483	-3.023127	3.004781
H	0.282268	-4.946203	1.438585
H	0.090834	-4.528984	-1.003045
H	-0.014533	-2.222667	-1.858729
H	0.736513	1.229209	-3.233438
H	-0.752290	1.329505	-5.150642
H	-3.097107	0.529897	-4.976226
H	-3.913131	-0.393373	-2.815879
H	-2.414625	-0.502186	-0.871423

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$[B(C_6F_5)Ph_2$-$N_2H_3]$-

B	0.461968	0.296388	-0.605142
C	0.476848	-1.245679	-0.067401
N	1.797613	0.611372	-1.288134
N	1.984203	1.950816	-1.768390
C	-0.410766	-1.719277	0.910521
C	-0.441748	-3.054195	1.301379
C	0.427634	-3.973768	0.716146
C	1.314949	-3.535035	-0.262132
C	1.330590	-2.194346	-0.646326
C	-0.481455	0.177455	-3.057178
C	-0.755752	0.366708	-1.695764
C	-1.491291	0.126419	-4.017742
C	-2.824273	0.252211	-3.637567
C	-3.129113	0.424600	-2.287924
C	-2.108582	0.479247	-1.343547
C	0.226061	1.368584	0.675917
C	0.840519	1.162333	1.913034
C	0.750304	2.038385	2.988091
C	0.040245	3.220847	2.846669
C	-0.553888	3.502468	1.629453
C	-0.436765	2.590768	0.582431
F	1.597291	0.075170	2.129940
F	1.352809	1.767703	4.154830
F	-0.052171	4.083903	3.866435
F	-1.216698	4.656903	1.468564
F	-1.005756	2.986320	-0.570639
H	2.598458	0.396865	-0.701045
H	1.492569	2.602197	-1.147066
H	1.457383	2.003255	-2.639204
H	-1.094188	-1.015514	1.385545
H	-1.142786	-3.380970	2.066116

H	0.410395	-5.017668	1.018607
H	1.996686	-4.241484	-0.730924
H	2.016599	-1.860381	-1.421189
H	0.558996	0.047930	-3.351395
H	-1.237835	-0.017435	-5.065917
H	-3.616865	0.212699	-4.380357
H	-4.166230	0.518602	-1.974010
H	-2.369983	0.620381	-0.294813

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$B(C_6F_5)_2Ph\text{-}N_2H_4$

B	0.340625	0.297290	-0.545580
C	0.328154	-1.231327	-0.011880
N	1.866414	0.544734	-1.073834
N	2.246038	1.860783	-1.539103
C	-0.075964	-1.606518	1.273670
C	-0.080439	-2.939812	1.675697
C	0.329233	-3.937502	0.795950
C	0.724620	-3.594111	-0.494127
C	0.710346	-2.259182	-0.887192
C	-0.392188	0.386245	-3.145332
C	-0.699520	0.393953	-1.794706
C	-1.337526	0.322661	-4.163088
C	-2.678285	0.240018	-3.827298
C	-3.044774	0.218294	-2.485724
C	-2.060958	0.281174	-1.512764
C	0.169562	1.426433	0.626974
C	1.025100	1.381014	1.729503
C	0.961296	2.249435	2.808766
C	0.001416	3.252726	2.803235
C	-0.854239	3.368010	1.718693
C	-0.748077	2.475212	0.655662
F	0.906072	0.428414	-3.555888
F	-0.962078	0.329586	-5.440767
F	-3.606058	0.176523	-4.776251
F	-4.329633	0.125667	-2.155037
F	-2.458579	0.230566	-0.236503
F	2.005237	0.453863	1.768198
F	1.810107	2.141549	3.827238
F	-0.082801	4.104116	3.817988
F	-1.756633	4.344698	1.690680
F	-1.579592	2.698500	-0.367279
H	2.489855	0.314477	-0.295935
H	2.101097	-0.106750	-1.823648
H	1.799990	2.508838	-0.889969
H	1.769255	1.975536	-2.431090
H	-0.406313	-0.843790	1.974296
H	-0.404042	-3.200088	2.678732
H	0.330950	-4.976606	1.109235
H	1.030600	-4.364764	-1.194879
H	0.977568	-2.022270	-1.919047

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$[B(C_6F_5)_2Ph\text{-}N_2H_3]^-$

B	0.469741	0.250793	-0.635813
C	0.496004	-1.300696	-0.129011
C	-0.648761	-1.940905	0.367391
C	-0.632102	-3.270486	0.780774
C	0.544115	-4.012568	0.699501
C	1.697364	-3.400956	0.215942
C	1.668791	-2.065839	-0.182967
C	-0.701246	0.119894	-3.069185
C	-0.836452	0.350944	-1.702861
C	-1.763677	0.115720	-3.969347
C	-3.049425	0.341697	-3.510508
C	-3.246959	0.566497	-2.156699
C	-2.152771	0.565844	-1.302957
C	0.277918	1.322697	0.622150
C	0.828701	1.083119	1.879519
C	0.778871	1.992515	2.931884
C	0.174784	3.224954	2.746403
C	-0.367637	3.525661	1.508108
C	-0.295342	2.583916	0.488577
F	0.501217	-0.127168	-3.621011
F	-1.557352	-0.109540	-5.273945
F	-4.085967	0.337195	-4.357507
F	-4.486609	0.780113	-1.695301
F	-2.440575	0.784071	-0.003945
F	1.462107	-0.064174	2.151887
F	1.319333	1.696487	4.121907
F	0.123066	4.114451	3.745542
F	-0.941877	4.719938	1.306824
F	-0.838090	2.972965	-0.682745
H	-1.577276	-1.378521	0.442354
H	-1.539295	-3.730590	1.165064
H	0.561814	-5.052767	1.013984
H	2.625464	-3.964696	0.155773
H	2.584560	-1.589728	-0.523439
N	1.800445	0.621348	-1.277333
N	1.872865	1.914357	-1.898056
H	2.072020	-0.042385	-1.994261
H	2.112019	2.571745	-1.157987
H	0.937497	2.197454	-2.205056

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$B(C_6F_5)_3\text{-}N_2H_4$

B	0.373204	0.318115	-0.536499
C	0.360817	-1.226792	-0.003967
N	1.889472	0.587748	-1.064296
N	2.232830	1.919969	-1.506752
C	-0.203500	-1.661255	1.192349
C	-0.263992	-3.001920	1.557347
C	0.246798	-3.971766	0.706832
C	0.807365	-3.590384	-0.504490
C	0.840696	-2.242385	-0.826089
C	-0.380272	0.408316	-3.127579
C	-0.675857	0.386023	-1.774234
C	-1.339541	0.335948	-4.131304
C	-2.673490	0.210782	-3.778533
C	-3.024171	0.159787	-2.433422
C	-2.028522	0.235317	-1.473719
C	0.185078	1.436472	0.634344

C	1.021485	1.378133	1.748301
C	0.964861	2.256611	2.816543
C	0.026366	3.281440	2.786844
C	-0.817244	3.401628	1.693860
C	-0.718301	2.494943	0.641043
F	-0.730076	-0.792268	2.059743
F	-0.809874	-3.362103	2.714923
F	0.197279	-5.254106	1.045845
F	1.294597	-4.506469	-1.336917
F	1.374110	-1.923798	-2.030556
F	0.906357	0.509850	-3.548559
F	-0.984771	0.376600	-5.413079
F	-3.610536	0.137841	-4.716167
F	-4.300928	0.028164	-2.087776
F	-2.398972	0.157460	-0.189375
F	1.956305	0.405378	1.809573
F	1.792581	2.137599	3.850120
F	-0.049910	4.144837	3.791238
F	-1.702357	4.392759	1.646714
F	-1.544564	2.708213	-0.388547
H	2.528403	0.361221	-0.297939
H	2.117984	-0.049074	-1.829841
H	1.769232	2.549987	-0.852687
H	1.765673	2.033835	-2.403645

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$[B(C_6F_5)_3\text{-}N_2H_3]^-$

B	0.510795	0.314891	-0.546537
C	0.429809	-1.259630	-0.038062
N	1.920735	0.648338	-1.004125
N	2.097595	1.961463	-1.554801
C	-0.201126	-1.727072	1.111681
C	-0.280388	-3.073475	1.453020
C	0.267791	-4.029296	0.613922
C	0.879616	-3.620703	-0.560206
C	0.933566	-2.265583	-0.858937
C	-0.412205	0.338895	-3.103432
C	-0.663122	0.349269	-1.737715
C	-1.414402	0.244337	-4.067466
C	-2.736045	0.138717	-3.671420
C	-3.039493	0.131108	-2.316212
C	-2.007515	0.229191	-1.396362
C	0.199308	1.405849	0.654404
C	0.867787	1.296122	1.872598
C	0.778740	2.233897	2.891718
C	0.004415	3.370221	2.705888
C	-0.662516	3.540372	1.505883
C	-0.543584	2.570578	0.513550
F	-0.789326	-0.888043	1.975852
F	-0.889492	-3.458412	2.581100
F	0.198302	-5.327875	0.926694
F	1.393311	-4.532824	-1.394844
F	1.492595	-1.956752	-2.045484
F	0.838687	0.436342	-3.585164
F	-1.113543	0.250664	-5.372480
F	-3.711807	0.044237	-4.582012
F	-4.315525	0.022481	-1.925204
F	-2.355790	0.202129	-0.098340
F	1.638486	0.230520	2.125631
F	1.433395	2.063507	4.047394
F	-0.090221	4.290421	3.672470
F	-1.397610	4.641937	1.304110
F	-1.196267	2.844523	-0.631171
H	2.291069	0.004985	-1.690914
H	2.177732	2.596035	-0.763074
H	1.246596	2.249235	-2.048127

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$[SiEt_3\text{-}N_2H_4]^+$

C	-0.740383	-1.666065	-0.488599
Si	-0.003892	-0.155806	0.324178
C	1.262502	-0.522901	1.645206
C	-1.172927	1.267406	0.624830
C	2.438617	-1.393704	1.171607
C	-1.688012	-1.373720	-1.664169
C	-1.465422	2.138092	-0.610344
N	1.111866	0.526014	-1.105484
N	1.899430	1.629757	-0.631581
H	-1.284599	-2.208574	0.295271
H	0.063292	-2.345922	-0.798770
H	1.615652	0.414783	2.091229
H	0.731147	-1.036455	2.456328
H	-0.769637	1.890985	1.429238
H	-2.105844	0.837585	1.010675
H	3.127201	-1.600474	1.992551
H	2.097726	-2.356639	0.782278
H	3.028546	-0.908941	0.383018
H	-2.085220	-2.300873	-2.080850
H	-1.185518	-0.848083	-2.484370
H	-2.538769	-0.764014	-1.349213
H	-1.836434	1.550269	-1.456998
H	-2.232521	2.880064	-0.382360
H	-0.571681	2.690112	-0.918265
H	1.659350	-0.221024	-1.550837
H	0.472979	0.900485	-1.814892
H	2.491249	1.971889	-1.385529
H	2.498124	1.286245	0.115859

27

$SiEt_3\text{-}N_2H_3$

C	-0.590037	-1.584941	-0.616614
Si	0.177063	-0.037727	0.144641
C	1.222964	-0.524863	1.638438
C	-1.123704	1.218101	0.676274
C	2.246504	-1.621685	1.323970
C	-1.678806	-1.291238	-1.656508
C	-1.583467	2.160031	-0.442785
N	1.145668	0.663360	-1.126662
N	1.813567	1.862947	-0.770939
H	-0.998688	-2.203352	0.193116
H	0.209666	-2.186201	-1.069681
H	1.733089	0.378097	1.997760

H	0.563041	-0.842614	2.456009
H	-0.714318	1.806835	1.505614
H	-1.979322	0.668500	1.092010
H	2.893231	-1.844560	2.177732
H	1.751567	-2.554303	1.034673
H	2.893634	-1.326999	0.490015
H	-2.070566	-2.206282	-2.110785
H	-1.293881	-0.655830	-2.460193
H	-2.522290	-0.762804	-1.200947
H	-1.991491	1.607782	-1.294270
H	-2.354340	2.854308	-0.094454
H	-0.737914	2.746659	-0.810393
H	1.607352	0.091353	-1.826058
H	1.767447	2.518550	-1.545561
H	2.794556	1.689298	-0.564487

20
$[SiPhH_2\text{-}N_2H_4]^+$

Si	-0.333977	0.790746	-1.367580
C	-0.667224	0.144477	0.311015
N	1.377221	0.041105	-1.841400
N	1.818919	0.596054	-3.092335
C	-1.390123	-1.049556	0.479355
C	-1.604193	-1.564544	1.752478
C	-1.102365	-0.892504	2.865738
C	-0.389533	0.296227	2.714611
C	-0.173444	0.815466	1.443986
H	-1.159534	0.264764	-2.461371
H	0.014835	2.217769	-1.464685
H	2.050985	0.128889	-1.068754
H	1.235326	-0.962913	-1.990027
H	2.710011	0.178840	-3.352245
H	1.956933	1.595282	-2.960368
H	-1.802340	-1.571271	-0.381205
H	-2.168327	-2.481972	1.878506
H	-1.275912	-1.292738	3.859075
H	-0.013717	0.820434	3.586302
H	0.363834	1.755439	1.338912

19
$SiPhH_2\text{-}N_2H_3$

Si	0.023678	1.134469	-1.196898
C	-0.458829	0.318222	0.418896
N	1.155042	0.051860	-1.939002
N	1.622976	0.441963	-3.217697
C	-0.738598	-1.055521	0.466193
C	-1.097064	-1.674211	1.660240
C	-1.184608	-0.925373	2.831859
C	-0.909069	0.438994	2.806240
C	-0.546548	1.051452	1.609043
H	-1.119015	1.311975	-2.120965
H	0.558471	2.486529	-0.870611
H	1.791498	-0.502158	-1.375554
H	1.640526	-0.366050	-3.832176
H	2.564685	0.820343	-3.161091
H	-0.670037	-1.646427	-0.444334
H	-1.309682	-2.738679	1.678841
H	-1.465287	-1.405724	3.764085
H	-0.972453	1.023789	3.718642
H	-0.323279	2.115800	1.601912

12
$(N_2H_4)_2$

N	1.66180	-0.52826	0.41924
N	1.34173	0.63779	-0.34330
H	1.45099	-1.37122	-0.11157
H	1.04084	-0.53156	1.22349
H	0.64790	0.41296	-1.05625
H	2.19495	0.94420	-0.79694
N	-1.35415	-0.55057	-0.44917
N	-1.55517	0.61100	0.35602
H	-2.19737	-0.69126	-0.99562
H	-1.21646	-1.38833	0.11277
H	-0.64666	1.05537	0.47433
H	-1.93366	0.38016	1.27030

11
$[N_2H_4\text{-}N_2H_3]^-$

N	1.22085	0.59944	0.52847
N	1.64654	-0.51360	-0.33471
H	1.36095	0.20069	1.46619
H	2.26766	-0.10565	-1.04019
H	0.83190	-0.79713	-0.89941
N	-1.35528	0.65849	-0.38965
N	-1.51872	-0.65492	0.22440
H	-1.23961	0.45223	-1.38294
H	-0.35987	0.91703	-0.03608
H	-2.19283	-0.50759	0.97547
H	-0.62193	-0.78543	0.71737

34
$BEt_3\text{-}(N_2H_4)_2$

C	-0.61943	1.33319	-1.17953
B	-1.06025	0.42331	0.10448
C	-2.62620	-0.04321	-0.01622
C	-0.74021	1.05875	1.57246
C	-2.98065	-0.93633	-1.21141
C	0.75884	2.00344	-1.13659
C	0.70020	0.98137	2.09752
H	-1.37561	2.12274	-1.29196
H	-0.69211	0.75108	-2.11406
H	-2.98617	-0.53220	0.90426
H	-3.22396	0.87655	-0.07533
H	-1.38827	0.59097	2.32863
H	-1.05382	2.11308	1.55118
H	-4.05397	-1.13432	-1.29432
H	-2.66018	-0.48720	-2.15783
H	-2.49593	-1.92204	-1.13818
H	0.99344	2.54534	-2.05958
H	1.56586	1.27489	-0.97513
H	0.81800	2.72164	-0.31273
H	1.40507	1.49163	1.43182

H	0.80488	1.44035	3.08664
H	1.01808	-0.06447	2.19123
N	-0.17351	-0.96348	-0.06590
N	-0.40845	-1.92906	0.96906
H	-0.42275	-1.32837	-0.98820
H	0.84860	-0.77850	-0.06326
H	-0.33277	-2.86399	0.57831
H	-1.37153	-1.79435	1.26795
N	2.75159	-0.78989	0.10837
N	3.49201	-0.79475	-1.11082
H	3.01299	-1.61678	0.63610
H	2.94319	0.02370	0.69061
H	4.39549	-0.34177	-0.99580
H	2.96575	-0.24760	-1.78509

33

$[BEt_3\text{-}(N_2H_4\text{-}N_2H_3)]^-$

C	0.64529	1.31650	1.10852
B	0.76701	-0.19406	0.45924
C	0.19767	-1.30576	1.53514
C	2.35658	-0.56903	0.09830
C	-1.28474	-1.15833	1.89220
C	1.20771	2.47492	0.27627
C	2.84809	-0.14536	-1.29392
H	1.15766	1.31950	2.08482
H	-0.40802	1.54379	1.34017
H	0.35917	-2.32541	1.14430
H	0.79875	-1.26188	2.45810
H	2.53709	-1.65392	0.19834
H	3.01521	-0.11433	0.85643
H	-1.65344	-1.93234	2.58029
H	-1.47916	-0.18759	2.36503
H	-1.90657	-1.19304	0.98806
H	1.04024	3.46151	0.73094
H	0.75648	2.50843	-0.72459
H	2.28933	2.36575	0.13410
H	2.73808	0.93399	-1.44921
H	3.90329	-0.39189	-1.47901
H	2.26085	-0.62845	-2.08544
N	-0.14082	-0.25176	-0.82297
N	-0.13067	-1.53731	-1.49636
H	0.19226	0.40329	-1.52935
H	-0.81431	-2.10344	-0.99264
H	0.76019	-1.99764	-1.27886
N	-2.91639	1.18598	-0.27987
N	-3.16469	0.07513	-1.17118
H	-3.19496	0.85328	0.64105
H	-1.89761	1.26877	-0.21021
H	-2.25555	-0.37798	-1.30590
H	-3.38972	0.49803	-2.06896

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$BPh_3\text{-}(N_2H_4)_2$

B	-0.31310	-0.02039	0.17708
C	0.75060	0.90477	-0.64105
C	1.63873	0.41073	-1.60668
C	2.61649	1.21919	-2.18903
C	2.73421	2.55540	-1.81611
C	1.84599	3.08343	-0.87884
C	0.86710	2.26769	-0.31569
C	-2.44179	1.09705	1.37946
C	-1.77383	0.67948	0.22026
C	-3.69133	1.71976	1.33415
C	-4.31285	1.94321	0.11269
C	-3.67035	1.54750	-1.06079
C	-2.42472	0.93484	-0.99995
C	-0.31939	-1.58731	-0.24767
C	0.83407	-2.37476	-0.07301
C	0.86763	-3.72969	-0.39161
C	-0.26908	-4.34636	-0.90994
C	-1.42607	-3.59618	-1.09248
C	-1.44747	-2.24193	-0.75843
H	1.56664	-0.63160	-1.90705
H	3.28675	0.80445	-2.93661
H	3.49645	3.18545	-2.26411
H	1.90945	4.13135	-0.59964
H	0.15960	2.70520	0.38899
H	-1.99783	0.94603	2.36436
H	-4.17483	2.02830	2.25645
H	-5.28446	2.42532	0.07100
H	-4.14035	1.72630	-2.02345
H	-1.92772	0.64875	-1.92535
H	1.73906	-1.91346	0.32513
H	1.77770	-4.30257	-0.23898
H	-0.25194	-5.40151	-1.16453
H	-2.32027	-4.06768	-1.48969
H	-2.36822	-1.68111	-0.89433
N	0.28544	0.00564	1.70663
N	-0.25033	-0.94078	2.66283
H	1.32310	-0.09248	1.67863
H	0.13321	0.93477	2.10414
H	0.16834	-1.83295	2.39988
H	-1.23141	-1.04833	2.40004
N	3.16342	0.26728	1.20974
N	4.24782	0.16722	2.13376
H	3.05349	1.20630	0.81964
H	3.37634	-0.33250	0.41709
H	4.98718	0.82602	1.90156
H	3.89309	0.42164	3.04908

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$[BPh_3\text{-}(N_2H_4\text{-}N_2H_3)]^-$

B	-0.16725	-0.05661	0.26548
C	-0.10932	1.44124	-0.40509
C	0.55006	1.76003	-1.60047
C	0.56750	3.05623	-2.11759
C	-0.07749	4.08914	-1.44504
C	-0.75000	3.80559	-0.25721
C	-0.76600	2.50528	0.23842
C	-2.50860	-0.62767	1.44833
C	-1.75321	-0.50825	0.27297
C	-3.86893	-0.94353	1.43672

C	-4.52710	-1.14881	0.22916
C	-3.80941	-1.02668	-0.96135
C	-2.45498	-0.71078	-0.92923
C	0.78870	-1.14443	-0.51100
C	2.17194	-0.89055	-0.60637
C	3.05938	-1.80467	-1.16914
C	2.59289	-3.02413	-1.66037
C	1.23459	-3.30874	-1.57427
C	0.35672	-2.38242	-1.00614
H	1.06746	0.97130	-2.14161
H	1.09106	3.25986	-3.04896
H	-0.06268	5.10086	-1.84211
H	-1.26944	4.59873	0.27592
H	-1.32925	2.29945	1.14888
H	-2.01880	-0.46226	2.40789
H	-4.41494	-1.02753	2.37385
H	-5.58568	-1.39461	0.21186
H	-4.31264	-1.17215	-1.91464
H	-1.91189	-0.60589	-1.86818
H	2.56107	0.05357	-0.22725
H	4.11905	-1.56547	-1.22423
H	3.28111	-3.74190	-2.09965
H	0.85432	-4.25839	-1.94447
H	-0.69865	-2.63729	-0.93847
N	0.42791	0.07003	1.69735
N	0.49400	-1.15982	2.45165
H	-0.08000	0.73055	2.28137
H	1.29873	-1.65352	2.06469
H	-0.29801	-1.75372	2.18163
N	3.41529	0.36328	2.52655
N	3.18247	1.48338	1.65211
H	3.72594	-0.39051	1.91616
H	2.50961	0.04958	2.88187
H	2.19977	1.44835	1.36451
H	3.29187	2.31492	2.22597

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$B(C_6F_5)Ph_2$-$(N_2H_4)_2$

B	0.48539	0.13848	0.33959
C	1.17124	-1.10531	-0.45378
C	1.80844	-0.93762	-1.69198
C	2.43888	-1.99865	-2.34266
C	2.45378	-3.26579	-1.76465
C	1.80582	-3.46891	-0.54769
C	1.16611	-2.40357	0.08209
C	2.44987	1.81761	-0.04992
C	1.06110	1.59347	-0.07613
C	2.99699	3.06810	-0.32636
C	2.16387	4.13884	-0.64285
C	0.78630	3.94668	-0.67154
C	0.24966	2.69204	-0.38613
C	-1.14403	0.01161	0.22933
C	-1.71920	0.13963	-1.03585
C	-3.07714	0.00079	-1.28414
C	-3.93529	-0.29671	-0.23254
C	-3.41635	-0.44305	1.04327
C	-2.04816	-0.28936	1.23734
F	-0.94058	0.41965	-2.08803
F	-3.56603	0.14144	-2.51451
F	-5.23997	-0.43731	-0.44922
F	-4.22140	-0.73026	2.06578
F	-1.62353	-0.45318	2.51821
H	1.81899	0.04921	-2.14624
H	2.92503	-1.83288	-3.29935
H	2.95186	-4.09092	-2.26405
H	1.78801	-4.45792	-0.09874
H	0.64358	-2.60349	1.01859
H	3.12783	0.99679	0.18632
H	4.07395	3.20445	-0.29918
H	2.58575	5.11447	-0.86344
H	0.12676	4.77445	-0.91457
H	-0.83077	2.56961	-0.40483
N	0.94919	-0.05851	1.89026
N	0.77216	1.03605	2.81948
H	0.47752	-0.85356	2.31979
H	1.96317	-0.31524	1.89698
H	-0.23409	1.18962	2.86330
H	1.15311	1.84746	2.33181
N	3.62502	-1.22553	1.87148
N	4.34298	-1.14527	0.63892
H	4.23141	-0.86377	2.60152
H	3.38825	-2.18850	2.11193
H	3.65377	-1.19146	-0.10828
H	4.95584	-1.94983	0.52455

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$[B(C_6F_5)Ph_2$-$(N_2H_4$-$N_2H_3)]$-

B	-0.89020	0.03596	0.38822
C	-1.68769	1.31191	-0.26770
C	-2.37823	1.23013	-1.48499
C	-3.06693	2.31532	-2.02442
C	-3.10083	3.53036	-1.34628
C	-2.43118	3.64235	-0.13007
C	-1.73794	2.55205	0.38920
C	-2.70673	-1.81702	0.91954
C	-1.72749	-1.33564	0.03962
C	-3.49092	-2.93255	0.62782
C	-3.32166	-3.60872	-0.57674
C	-2.35518	-3.15849	-1.47427
C	-1.57486	-2.04895	-1.16032
C	0.67769	-0.10931	-0.18862
C	1.40984	0.93532	-0.75273
C	2.73568	0.82591	-1.16213
C	3.40483	-0.37594	-1.00549
C	2.73347	-1.44545	-0.43790
C	1.40943	-1.28865	-0.04258
F	0.87153	2.15128	-0.92372
F	3.37573	1.87170	-1.70288
F	4.67931	-0.50087	-1.39329
F	3.36909	-2.61291	-0.27150
F	0.85625	-2.38601	0.50588
H	-2.38946	0.28470	-2.02252

H	-3.58670	2.20888	-2.97379
H	-3.64223	4.37791	-1.75853
H	-2.44520	4.58477	0.41264
H	-1.19922	2.66269	1.32772
H	-2.85291	-1.30462	1.86972
H	-4.23541	-3.27506	1.34274
H	-3.92990	-4.47796	-0.81205
H	-2.20568	-3.67928	-2.41717
H	-0.81428	-1.72353	-1.87009
N	-0.76065	0.31075	1.90421
N	-0.24396	-0.74510	2.73263
H	-1.65211	0.58875	2.30722
H	0.77329	-0.66774	2.68300
H	-0.46400	-1.64377	2.29748
N	1.85006	1.45515	2.78112
N	1.06385	1.75258	3.95316
H	2.36239	2.30351	2.55803
H	1.19975	1.28728	2.00836
H	0.93193	0.85339	4.41181
H	0.12059	1.98195	3.63426

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$B(C_6F_5)_2Ph\text{-}(N_2H_4)_2$

B	0.06536	0.51041	0.20636
C	-0.17397	1.56186	-1.00591
C	0.73115	1.80904	-2.04262
C	0.45979	2.74460	-3.03946
C	-0.72987	3.46677	-3.01933
C	-1.65656	3.22928	-2.00659
C	-1.38005	2.27953	-1.02686
C	-2.24461	-0.70048	0.96535
C	-1.13678	-0.59182	0.14173
C	-3.29957	-1.58106	0.74797
C	-3.27053	-2.40386	-0.36400
C	-2.18849	-2.33006	-1.23485
C	-1.16726	-1.43262	-0.97208
C	1.58477	-0.10773	0.26714
C	2.66971	0.77011	0.31049
C	3.99966	0.37684	0.32708
C	4.29710	-0.97889	0.31630
C	3.26073	-1.89898	0.30063
C	1.94110	-1.45504	0.28933
F	-2.36769	0.08217	2.07166
F	-4.32903	-1.62697	1.59419
F	-4.26393	-3.25567	-0.59884
F	-2.15326	-3.11363	-2.30989
F	-0.15408	-1.39017	-1.84492
F	2.44788	2.10145	0.35711
F	4.98033	1.27614	0.36625
F	5.56053	-1.38829	0.33713
F	3.53395	-3.20135	0.31643
F	1.01416	-2.41889	0.32093
H	1.66476	1.25343	-2.08431
H	1.18102	2.91011	-3.83406
H	-0.93871	4.19879	-3.79320
H	-2.60116	3.76585	-1.98442
H	-2.13972	2.08529	-0.26988
N	-0.04433	1.41153	1.54833
N	0.22940	0.80968	2.83506
H	0.64104	2.16183	1.43797
H	-0.96005	1.91071	1.65340
H	1.05268	0.22480	2.69258
H	-0.54485	0.17025	2.99827
N	-2.38437	2.98320	2.20843
N	-2.89365	3.92702	1.26690
H	-3.12861	2.32654	2.42340
H	-2.09186	3.41826	3.08213
H	-2.11935	4.23514	0.68645
H	-3.28902	4.73906	1.73266

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$[B(C_6F_5)_2Ph\text{-}(N_2H_4\text{-}N_2H_3)]^-$

B	0.02161	0.66232	0.06452
C	-0.05934	1.43412	-1.37190
C	0.58035	0.98281	-2.53487
C	0.45335	1.64872	-3.75140
C	-0.32565	2.79986	-3.84074
C	-0.97197	3.27078	-2.70118
C	-0.84019	2.59390	-1.48991
C	-2.45621	-0.19956	0.79918
C	-1.27527	-0.37361	0.08713
C	-3.56852	-1.03050	0.67569
C	-3.53428	-2.09554	-0.20524
C	-2.38073	-2.31669	-0.94451
C	-1.30224	-1.46158	-0.78577
C	1.47454	-0.15573	0.21979
C	2.65405	0.55154	-0.01846
C	3.92757	0.01613	0.12199
C	4.06854	-1.29562	0.55041
C	2.93380	-2.03651	0.83094
C	1.67836	-1.45497	0.67215
F	-2.61275	0.79990	1.69274
F	-4.67138	-0.80611	1.40160
F	-4.59171	-2.90386	-0.33941
F	-2.32905	-3.34685	-1.79786
F	-0.21836	-1.74526	-1.52811
F	2.60452	1.83819	-0.39895
F	5.01875	0.74773	-0.13528
F	5.28446	-1.83160	0.70101
F	3.05719	-3.29633	1.26783
F	0.64280	-2.24665	1.00312
H	1.19451	0.08642	-2.48582
H	0.96665	1.27040	-4.63203
H	-0.42600	3.32403	-4.78744
H	-1.58135	4.16951	-2.75381
H	-1.34789	2.97720	-0.60736
N	-0.07180	1.70638	1.17844
N	0.10484	1.25761	2.52704
H	0.59715	2.45652	1.02512
H	0.73012	0.44650	2.54560
H	-0.80512	0.91633	2.82841
N	-0.91539	4.14552	3.11293

N	-2.01167	3.78627	2.25084
H	-0.37644	4.83739	2.60006
H	-0.30461	3.33311	3.22992
H	-2.76198	3.47502	2.86117
H	-1.73210	2.97784	1.68873

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$B(C_6F_5)_3$-$(N_2H_4)_2$

B	-0.02361	-0.03480	0.59461
C	-0.68143	1.35267	0.04180
C	-0.86381	1.48720	-1.33272
C	-1.45852	2.58995	-1.92486
C	-1.91463	3.62719	-1.11946
C	-1.76314	3.53827	0.25471
C	-1.15833	2.41102	0.80069
C	-2.30347	-1.26334	1.06251
C	-1.12929	-1.21030	0.31455
C	-3.33894	-2.15846	0.83515
C	-3.23130	-3.05180	-0.22004
C	-2.09813	-3.02280	-1.01970
C	-1.08522	-2.10963	-0.75027
C	1.47799	-0.33371	0.01253
C	2.32675	0.65022	-0.48335
C	3.63565	0.41982	-0.88867
C	4.15536	-0.86165	-0.81458
C	3.35685	-1.88464	-0.32393
C	2.05871	-1.60056	0.07411
F	-0.43647	0.51004	-2.14365
F	-1.59859	2.66690	-3.24574
F	-2.48862	4.69495	-1.66422
F	-2.19366	4.52403	1.04040
F	-1.04388	2.39908	2.14745
F	-2.49735	-0.38737	2.07609
F	-4.42565	-2.15551	1.60397
F	-4.20571	-3.92002	-0.46660
F	-1.99262	-3.86527	-2.04396
F	-0.04498	-2.13407	-1.58795
F	1.93722	1.94220	-0.53795
F	4.39321	1.42357	-1.32900
F	5.40537	-1.10512	-1.19163
F	3.84310	-3.11963	-0.22928
F	1.36153	-2.64175	0.56483
N	0.18533	0.10529	2.19095
N	0.82488	-0.99074	2.88368
H	0.77619	0.94502	2.38664
H	-0.70407	0.27217	2.65913
H	1.78546	-0.98611	2.53804
H	0.40335	-1.84310	2.51507
N	2.29873	1.96824	2.46714
N	3.22867	0.91377	2.73722
H	2.38641	2.22169	1.48645
H	2.47558	2.80417	3.02201
H	3.01703	0.56408	3.66784
H	4.18816	1.25531	2.75330

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$[B(C_6F_5)_3$-$(N_2H_4$-$N_2H_3)]$-

B	0.15704	-0.03501	0.64251
C	-0.40605	1.43989	0.14837
C	0.21091	2.31185	-0.74435
C	-0.35136	3.51686	-1.15384
C	-1.60191	3.88691	-0.68728
C	-2.27595	3.03784	0.17598
C	-1.67385	1.84589	0.55603
C	-1.86567	-1.81831	0.22667
C	-0.79952	-1.07739	-0.25935
C	-2.71664	-2.57359	-0.57684
C	-2.51786	-2.59389	-1.94589
C	-1.47028	-1.86054	-2.48868
C	-0.65278	-1.12694	-1.64360
C	1.76322	-0.27068	0.32521
C	2.68537	0.69458	0.72856
C	4.06072	0.53819	0.63246
C	4.57829	-0.64851	0.13222
C	3.70785	-1.64912	-0.26038
C	2.33475	-1.44444	-0.14721
F	1.40518	2.03097	-1.28347
F	0.29851	4.31990	-2.00439
F	-2.15621	5.04052	-1.07391
F	-3.49704	3.36593	0.61395
F	-2.41733	1.04694	1.34780
F	-2.13888	-1.86514	1.54855
F	-3.72321	-3.27528	-0.04067
F	-3.32351	-3.30900	-2.73821
F	-1.27466	-1.86999	-3.81244
F	0.33545	-0.42645	-2.22453
F	2.26290	1.86351	1.22530
F	4.89612	1.50968	1.02027
F	5.90103	-0.82267	0.03706
F	4.19235	-2.80773	-0.72626
F	1.57173	-2.49033	-0.51727
N	0.04818	-0.15892	2.14702
N	0.40214	-1.43037	2.69890
H	-0.82206	0.12579	2.58090
H	1.41696	-1.45233	2.77633
H	0.15696	-2.17869	2.04362
N	-2.66682	-0.40725	4.01633
N	-2.13608	-1.66484	4.45896
H	-3.51538	-0.23270	4.54481
H	-2.92100	-0.44241	3.03149
H	-1.14635	-1.64300	4.20557
H	-2.53364	-2.42132	3.90163

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$[SiEt_3$-$(N_2H_4)_2]^+$

C	-1.35192	-1.20645	1.44756
Si	-1.14400	-0.29494	-0.17180
C	-2.44368	1.00683	-0.50730
C	-0.67727	-1.37332	-1.62431
C	-2.52271	2.11122	0.55884
C	-0.22224	-2.20765	1.74183

C	0.82122	-1.69163	-1.75284
N	0.38983	0.75568	0.20035
N	0.74914	1.57834	-0.92741
H	-2.31329	-1.73339	1.40963
H	-1.45128	-0.48515	2.26873
H	-2.27755	1.43688	-1.50254
H	-3.40948	0.49139	-0.57642
H	-1.03150	-0.89560	-2.54357
H	-1.25275	-2.30254	-1.52415
H	-3.33180	2.81098	0.34195
H	-2.70649	1.70091	1.55602
H	-1.60123	2.70518	0.60790
H	-0.37319	-2.69697	2.70600
H	0.76130	-1.72381	1.77407
H	-0.17883	-2.99007	0.97920
H	1.23510	-2.11119	-0.82951
H	0.99380	-2.41850	-2.54891
H	1.37294	-0.78181	-2.00550
H	0.24745	1.29955	1.06082
H	1.24465	0.15530	0.36926
H	1.62522	2.04417	-0.67778
H	0.01848	2.27452	-1.05739
N	3.03421	-0.04750	0.32679
N	3.32678	1.33513	0.58742
H	3.15284	-0.19464	-0.67338
H	3.67923	-0.68075	0.79968
H	4.30483	1.54877	0.39609
H	3.18755	1.49051	1.58227

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$SiEt_3$-(N_2H_4-N_2H_3)

C	0.20624	0.68751	-1.60072
Si	-0.70910	-0.34529	-0.30676
C	-0.63473	-2.16842	-0.77092
C	-2.51966	0.19528	-0.19727
C	0.79578	-2.71126	-0.85569
C	0.00388	2.20159	-1.45292
C	-2.76393	1.35172	0.78018
N	0.16117	-0.10138	1.17757
N	-0.39891	-0.73660	2.31883
N	2.70089	1.45046	0.56521
N	3.17274	0.10560	0.47070
H	-0.12435	0.36361	-2.59596
H	1.27388	0.43455	-1.54755
H	-1.20314	-2.73153	-0.02127
H	-1.15841	-2.31261	-1.72502
H	-3.12685	-0.66825	0.09859
H	-2.86163	0.47110	-1.20419
H	0.82256	-3.76379	-1.15314
H	1.39533	-2.15120	-1.58263
H	1.29430	-2.62956	0.11555
H	0.58466	2.77044	-2.18704
H	0.29656	2.54519	-0.45488
H	-1.04782	2.46994	-1.59409
H	-2.14962	2.22489	0.53975
H	-3.80997	1.67291	0.78000
H	-2.51237	1.05031	1.80108
H	0.78093	0.69094	1.34129
H	-0.78544	-0.04184	2.95362
H	0.33640	-1.22777	2.82039
H	2.52563	1.86320	-0.34941
H	3.42717	1.99837	1.01434
H	2.35029	-0.49243	0.51776
H	3.64247	-0.06768	-0.41477

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$[SiPhH_2$-(N_2H_4)$_2]^+$

Si	0.171261	0.957273	-1.545371
C	-0.666398	0.146927	-0.118190
N	1.843470	0.102462	-1.726670
N	2.660762	0.854339	-2.640777
C	-1.770573	-0.702514	-0.293487
C	-2.390116	-1.287081	0.806194
C	-1.911556	-1.034922	2.090675
C	-0.821316	-0.188658	2.281930
C	-0.208398	0.405927	1.184288
H	-0.443332	0.821529	-2.869524
H	0.635951	2.327029	-1.247336
H	2.280637	-0.064346	-0.812284
H	1.686931	-0.850560	-2.221178
H	3.543136	0.366072	-2.772968
H	2.858893	1.763991	-2.230834
H	-2.145802	-0.900292	-1.293730
H	-3.250243	-1.932633	0.664446
H	-2.397128	-1.490919	2.947042
H	-0.460581	0.017689	3.283675
H	0.619917	1.092357	1.352091
N	1.173554	-2.055761	-3.214756
N	-0.156099	-2.143132	-2.689380
H	1.111599	-1.591152	-4.118850
H	1.608314	-2.966329	-3.367359
H	-0.095328	-2.522650	-1.747875
H	-0.727172	-2.784856	-3.236743

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$SiPhH_2$-(N_2H_4-N_2H_3)

Si	-0.215721	1.297142	-1.140324
C	-0.606708	0.351883	0.434006
N	1.327701	0.710138	-1.646594
N	1.819929	1.215083	-2.883338
C	-0.214409	-0.986217	0.582103
C	-0.502630	-1.697241	1.743502
C	-1.194549	-1.079242	2.782578
C	-1.590025	0.249799	2.657609
C	-1.293260	0.956213	1.494718
H	-1.197856	1.041335	-2.219431
H	-0.287335	2.749035	-0.809789
H	2.053246	0.427725	-0.989489
H	2.300176	0.451822	-3.357394
H	2.511351	1.939530	-2.703250
H	0.329129	-1.474645	-0.224310
H	-0.190519	-2.732767	1.840050

H	-1.422011	-1.631800	3.688929
H	-2.124241	0.736384	3.467792
H	-1.595438	1.997967	1.414457
N	3.603916	-1.179011	-1.380789
N	2.827953	-1.665249	-2.474440
H	4.552039	-1.040292	-1.713082
H	3.643524	-1.843313	-0.610444
H	1.864621	-1.389502	-2.292001
H	2.870148	-2.678051	-2.556803

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1S,2R-phenylethanol-BEt_3

B	-1.89485	0.11676	-0.09845
O	-0.24305	-0.28257	0.28518
C	-2.57741	-2.25254	0.91013
C	-1.72490	0.99728	-1.44098
C	-2.26876	0.92795	1.25317
C	-2.65538	-1.29450	-0.28381
C	-2.97149	1.83104	-1.76696
C	-3.77753	1.06654	1.50134
C	0.76428	-0.77504	-0.62856
C	2.09955	-0.18234	-0.21475
C	0.72138	-2.29075	-0.71072
C	3.28015	-0.92443	-0.22097
C	4.48825	-0.33140	0.14247
C	4.52578	1.00637	0.51822
C	3.34897	1.75343	0.52934
C	2.14514	1.16353	0.16501
H	-0.16208	-0.69971	1.15546
H	-3.14371	-3.17601	0.75397
H	-2.96119	-1.78286	1.82209
H	-1.54212	-2.55495	1.12058
H	-1.50537	0.36025	-2.31154
H	-0.87065	1.68604	-1.34237
H	-1.83826	0.42726	2.13773
H	-1.80933	1.92712	1.23821
H	-2.32020	-1.81066	-1.19579
H	-3.71365	-1.06183	-0.47519
H	-3.15259	2.58357	-0.99317
H	-3.86692	1.20248	-1.82692
H	-2.87742	2.35861	-2.72130
H	-3.99531	1.64770	2.40302
H	-4.28087	1.55901	0.66448
H	-4.24973	0.08584	1.62142
H	0.45770	-0.34471	-1.58579
H	1.38767	-2.64796	-1.49906
H	-0.29219	-2.61996	-0.94264
H	1.03716	-2.74472	0.23490
H	3.27015	-1.97063	-0.50809
H	5.39915	-0.92106	0.13408
H	5.46636	1.46648	0.80287
H	3.36988	2.79778	0.82331
H	1.22389	1.73873	0.18295

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[1-phenylethoxy-BEt_3]-

B	-1.44142	0.34980	0.09969
O	-0.80317	-0.13657	-1.21166
C	-1.65179	2.67224	-1.20051
C	-3.03488	-0.05960	-0.01827
C	-0.76319	-0.26849	1.47656
C	-1.30400	1.99985	0.13051
C	-3.30074	-1.56543	0.01555
C	-1.58697	0.04466	2.73317
C	0.30614	-0.94135	-1.37299
C	1.54255	-0.44513	-0.61751
C	0.01800	-2.43312	-1.15882
C	1.84265	0.91883	-0.70112
C	2.95407	1.44969	-0.06025
C	3.79726	0.62181	0.68249
C	3.51173	-0.73555	0.77156
C	2.39360	-1.26334	0.12425
H	-2.70448	2.50461	-1.45902
H	-1.06235	2.22793	-2.01114
H	-1.48421	3.75931	-1.20932
H	-3.61896	0.42859	0.77881
H	-3.43620	0.33789	-0.96364
H	0.24726	0.13945	1.62747
H	-0.62750	-1.36135	1.43569
H	-0.28014	2.29233	0.41792
H	-1.95392	2.42127	0.91457
H	-2.76536	-2.05521	-0.80511
H	-2.92979	-2.01374	0.94726
H	-4.36282	-1.83692	-0.07554
H	-2.57532	-0.42833	2.68868
H	-1.75885	1.12325	2.82916
H	-1.10487	-0.29257	3.66164
H	0.59676	-0.85716	-2.44007
H	0.87060	-3.05634	-1.45521
H	-0.83749	-2.70445	-1.78157
H	-0.23880	-2.64978	-0.11877
H	1.15922	1.55634	-1.25534
H	3.16077	2.51434	-0.12916
H	4.66381	1.03496	1.19135
H	4.15463	-1.38922	1.35551
H	2.17383	-2.32208	0.22289

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1R,2R-phenylethanol-BPh_3

C	-4.460423	-0.186621	0.158811
C	-5.027497	0.511375	-0.904003
C	-4.323673	0.651159	-2.097881
C	-3.057966	0.088034	-2.228439
C	-2.484232	-0.615656	-1.164385
C	-3.192344	-0.745019	0.031615
C	-1.089081	-1.183274	-1.280701
C	-0.811977	-1.941041	-2.566218
O	-0.123967	-0.075607	-1.181961
B	0.887112	0.082255	0.167953
C	1.444295	1.582578	-0.033456
C	2.031865	-1.021251	-0.064447
C	-0.103723	-0.123412	1.432308

C	2.758253	-1.540152	1.017552
C	3.819360	-2.423756	0.834459
C	4.187847	-2.816271	-0.449299
C	3.500578	-2.298145	-1.543581
C	2.447946	-1.407487	-1.347106
C	1.665477	2.140408	-1.302064
C	2.203325	3.416039	-1.461570
C	2.555839	4.166925	-0.344708
C	2.367398	3.629537	0.926590
C	1.816463	2.359955	1.073653
C	-0.941579	0.920727	1.858225
C	-1.883688	0.749584	2.869539
C	-2.014476	-0.487234	3.497331
C	-1.198918	-1.544206	3.100079
C	-0.264471	-1.358994	2.081080
H	-4.998358	-0.289607	1.095610
H	-6.015240	0.949220	-0.802595
H	-4.761377	1.194742	-2.928646
H	-2.519869	0.194741	-3.166820
H	-2.739499	-1.268228	0.869843
H	-0.878590	-1.815495	-0.415814
H	0.182897	-2.387144	-2.530121
H	-1.553529	-2.734738	-2.683847
H	-0.868391	-1.282284	-3.436530
H	-0.591587	0.770573	-1.275781
H	2.491389	-1.239295	2.028304
H	4.359691	-2.806053	1.695505
H	5.010004	-3.509766	-0.596275
H	3.791972	-2.579761	-2.551445
H	1.946643	-0.987262	-2.216088
H	1.429364	1.560686	-2.192978
H	2.356001	3.819301	-2.458448
H	2.978998	5.159575	-0.463143
H	2.646441	4.203513	1.805318
H	1.666841	1.959323	2.073761
H	-0.853034	1.895912	1.383906
H	-2.516056	1.580544	3.168053
H	-2.742500	-0.625176	4.291123
H	-1.290252	-2.513017	3.582485
H	0.356640	-2.199526	1.780231

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[1-phenylethoxy-BPh_3]-

C	-4.460640	-0.784813	-0.182637
C	-4.784330	0.535725	-0.479582
C	-3.849289	1.344192	-1.125385
C	-2.602648	0.833745	-1.468007
C	-2.273808	-0.492647	-1.179640
C	-3.213642	-1.295226	-0.537302
C	-0.902041	-1.024675	-1.582301
C	-0.933479	-1.456828	-3.050683
O	0.083080	-0.054556	-1.428452
B	0.782567	0.040388	-0.100593
C	1.457860	1.527779	-0.052235
C	1.988488	-1.075767	-0.048434
C	-0.290473	-0.159832	1.134506
C	2.641700	-1.451494	1.136722
C	3.703470	-2.353521	1.148235
C	4.152862	-2.919420	-0.043581
C	3.529138	-2.564125	-1.237007
C	2.470344	-1.657067	-1.229926
C	1.549777	2.324165	-1.202004
C	2.148449	3.583796	-1.183507
C	2.677722	4.090866	0.000458
C	2.596920	3.322951	1.161250
C	1.995900	2.067267	1.126133
C	-1.140842	0.893117	1.511250
C	-2.182829	0.724030	2.418313
C	-2.402262	-0.522038	3.004129
C	-1.566331	-1.583055	2.670882
C	-0.533050	-1.396188	1.751019
H	-5.172816	-1.414589	0.343583
H	-5.752726	0.938188	-0.195689
H	-4.088776	2.381404	-1.344288
H	-1.838798	1.462019	-1.918056
H	-2.947056	-2.316294	-0.273802
H	-0.690548	-1.915342	-0.964366
H	0.026276	-1.900883	-3.328605
H	-1.732156	-2.182398	-3.235997
H	-1.106521	-0.578599	-3.680822
H	2.296896	-1.031713	2.080979
H	4.181073	-2.619918	2.088708
H	4.978493	-3.626663	-0.040921
H	3.871853	-2.994287	-2.175903
H	1.995277	-1.369134	-2.165087
H	1.133546	1.932262	-2.126520
H	2.201177	4.174451	-2.095941
H	3.143904	5.072840	0.020919
H	2.999785	3.708105	2.095502
H	1.927127	1.487709	2.046018
H	-0.991133	1.868259	1.050892
H	-2.834220	1.560333	2.661036
H	-3.217161	-0.662592	3.710006
H	-1.723448	-2.560902	3.121404
H	0.100677	-2.243382	1.493528

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1S,2R-phenylethanol-B(C_6F_5)Ph_2

C	-4.618062	-1.987960	0.114383
C	-5.412257	-0.927896	-0.310663
C	-4.874807	0.052314	-1.143286
C	-3.547281	-0.029212	-1.545962
C	-2.745148	-1.085205	-1.109288
C	-3.286318	-2.066176	-0.283977
C	-1.309084	-1.181180	-1.559049
C	-1.185446	-1.570009	-3.024321
O	-0.686461	0.133612	-1.379142
B	0.079454	0.547581	0.036200
C	0.149441	2.152222	-0.057818
C	1.569575	-0.137347	-0.046411
C	-0.870967	-0.062480	1.182552
C	2.331747	-0.289263	1.112674

C	3.620384	-0.808768	1.129157
C	4.217107	-1.196562	-0.062428
C	3.516878	-1.041966	-1.248431
C	2.234077	-0.512461	-1.207298
C	-0.821810	2.901828	-0.737745
C	-0.778831	4.294089	-0.779418
C	0.243694	4.978322	-0.130281
C	1.215171	4.258584	0.561112
C	1.166002	2.868308	0.590369
C	-2.022741	0.629064	1.584161
C	-2.922948	0.084192	2.494815
C	-2.681367	-1.171134	3.048375
C	-1.536647	-1.873011	2.681970
C	-0.651680	-1.321876	1.757829
F	1.839626	0.105393	2.292623
F	4.289984	-0.929999	2.272600
F	5.448390	-1.696477	-0.068527
F	4.074255	-1.388328	-2.407357
F	1.641918	-0.358458	-2.425750
H	-5.027166	-2.746569	0.773627
H	-6.446935	-0.860742	0.009347
H	-5.490235	0.882039	-1.475387
H	-3.123288	0.739885	-2.186254
H	-2.655055	-2.871784	0.079847
H	-0.759823	-1.882467	-0.922714
H	-0.139251	-1.649942	-3.328937
H	-1.668035	-2.537565	-3.174422
H	-1.698295	-0.838356	-3.655800
H	-1.637214	2.385549	-1.239043
H	-1.545495	4.843884	-1.317473
H	0.282589	6.062728	-0.159984
H	2.014832	4.781872	1.076578
H	1.932001	2.330020	1.142338
H	-2.221127	1.613274	1.167348
H	-3.812771	0.639780	2.775186
H	-3.377862	-1.596512	3.764769
H	-1.332082	-2.847589	3.115771
H	0.233757	-1.891805	1.480775
H	-0.073784	0.309816	-2.111882

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[1-phenylethoxy-B(C_6F_5)Ph_2]-

C	3.908622	-0.459260	1.615224
C	4.138752	0.913949	1.619778
C	3.073343	1.789556	1.826198
C	1.788275	1.295424	2.023685
C	1.548233	-0.080394	2.011392
C	2.619255	-0.950811	1.811983
C	0.123903	-0.594803	2.203083
C	-0.168005	-0.755795	3.695910
O	-0.807498	0.292184	1.663627
B	-1.208874	0.114978	0.240572
C	-1.938907	1.493395	-0.231473
C	-2.318519	-1.080798	0.097000
C	0.165221	-0.176267	-0.674007
C	-2.673219	-1.670657	-1.125764
C	-3.696090	-2.607708	-1.228296
C	-4.408946	-2.991768	-0.092587
C	-4.084259	-2.420358	1.133747
C	-3.058890	-1.478137	1.216941
C	-2.356245	2.440065	0.712220
C	-3.031080	3.602126	0.340296
C	-3.309295	3.852935	-1.000637
C	-2.904618	2.926736	-1.960588
C	-2.234585	1.769689	-1.573526
C	1.041452	0.865423	-0.980927
C	2.297907	0.687539	-1.546425
C	2.731483	-0.592723	-1.851711
C	1.906263	-1.666329	-1.567270
C	0.664380	-1.439389	-0.980869
F	0.735647	2.131499	-0.666641
F	3.102621	1.731503	-1.783312
F	3.938283	-0.789004	-2.396089
F	2.326757	-2.912783	-1.830310
F	-0.012491	-2.556024	-0.657092
H	4.728990	-1.148363	1.435043
H	5.138628	1.300340	1.445870
H	3.242280	2.862358	1.808854
H	0.936818	1.962149	2.122421
H	2.432680	-2.022614	1.773855
H	0.050983	-1.587294	1.724272
H	-1.164849	-1.181721	3.836848
H	0.570920	-1.403878	4.177563
H	-0.136617	0.227534	4.175344
H	-2.119194	-1.397886	-2.023707
H	-3.937653	-3.046003	-2.193918
H	-5.206757	-3.726312	-0.165908
H	-4.633972	-2.706504	2.027861
H	-2.821952	-1.018100	2.173687
H	-2.134658	2.250142	1.759157
H	-3.339796	4.317518	1.099656
H	-3.832926	4.758591	-1.295829
H	-3.111041	3.110259	-3.012593
H	-1.921455	1.060868	-2.339598

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1S,2R-phenylethanol-B(C_6F_5)$_2$Ph

C	-5.341887	-0.955430	-0.030854
C	-5.759301	0.308713	-0.433984
C	-4.921138	1.099836	-1.218601
C	-3.672328	0.624933	-1.599220
C	-3.248006	-0.639479	-1.186100
C	-4.087135	-1.428565	-0.405616
C	-1.912142	-1.175946	-1.634310
C	-1.922834	-1.508247	-3.119257
O	-0.884244	-0.149490	-1.404690
B	-0.097139	-0.040119	0.029942
C	0.657301	1.399661	-0.078952
C	1.052611	-1.197290	0.073413
C	-1.247083	-0.187793	1.131653
C	1.779892	-1.327838	1.256841
C	2.820655	-2.230570	1.421512

C	3.191385	-3.042636	0.356486
C	2.518414	-2.931497	-0.849911
C	1.481641	-2.012830	-0.962346
C	1.324949	1.760653	-1.244838
C	2.053097	2.927491	-1.406017
C	2.155926	3.798207	-0.329076
C	1.538836	3.474508	0.869500
C	0.815735	2.289223	0.981439
C	-2.164267	0.852943	1.342244
C	-3.238466	0.714943	2.211056
C	-3.418954	-0.480326	2.907300
C	-2.521245	-1.525614	2.723434
C	-1.450943	-1.375164	1.841500
F	1.483368	-0.541829	2.296962
F	3.472724	-2.318629	2.577541
F	4.186535	-3.912562	0.491787
F	2.868718	-3.691951	-1.885336
F	0.889767	-1.943977	-2.179697
F	1.299356	0.920271	-2.313915
F	2.655183	3.210897	-2.559179
F	2.847278	4.926776	-0.446120
F	1.648265	4.297866	1.908886
F	0.282297	2.041479	2.177445
H	-5.983824	-1.569215	0.592553
H	-6.733141	0.681448	-0.133659
H	-5.241395	2.088497	-1.530970
H	-3.007811	1.247981	-2.191929
H	-3.745446	-2.400427	-0.060300
H	-1.627158	-2.046843	-1.034830
H	-0.974371	-1.935011	-3.448836
H	-2.715248	-2.235455	-3.306449
H	-2.150577	-0.611338	-3.702684
H	-2.040276	1.787651	0.798486
H	-3.938474	1.533981	2.344415
H	-4.255834	-0.592263	3.590063
H	-2.650070	-2.457103	3.266526
H	-0.762146	-2.206662	1.706070
H	-0.224291	-0.175118	-2.119782

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[1-phenylethoxy-B(C_6F_5)$_2$Ph]-

C	-4.489440	-0.532210	1.590110
C	-4.176953	-1.846535	1.925852
C	-2.875472	-2.167897	2.310598
C	-1.894338	-1.183361	2.352256
C	-2.197116	0.135007	2.003338
C	-3.503021	0.452059	1.632426
C	-1.094279	1.189440	2.027909
C	-0.963081	1.760332	3.440601
O	0.138688	0.642070	1.662331
B	0.526313	0.666841	0.234975
C	1.814458	-0.361876	0.072112
C	1.109133	2.118421	-0.228652
C	-0.792343	0.189070	-0.667796
C	1.363695	2.426807	-1.573329
C	1.942212	3.632724	-1.953050
C	2.291839	4.574776	-0.984624
C	2.063810	4.286899	0.357158
C	1.486012	3.070545	0.723336
C	2.794264	-0.446539	1.059419
C	3.932388	-1.239289	0.946417
C	4.143738	-1.978065	-0.205873
C	3.212449	-1.905951	-1.229094
C	2.089578	-1.103213	-1.071981
C	-1.198053	-1.143751	-0.686776
C	-2.412093	-1.585311	-1.190406
C	-3.292856	-0.663804	-1.736684
C	-2.940211	0.673157	-1.755515
C	-1.718337	1.069277	-1.216649
F	2.705876	0.265534	2.190497
F	4.836413	-1.287014	1.935145
F	5.235545	-2.743001	-0.333131
F	3.408457	-2.606431	-2.354803
F	1.249405	-1.077902	-2.123844
F	-0.420544	-2.092440	-0.140504
F	-2.753787	-2.878345	-1.138999
F	-4.475082	-1.061453	-2.220122
F	-3.794814	1.577468	-2.255334
F	-1.517859	2.398808	-1.196922
H	-5.495824	-0.276049	1.271058
H	-4.937949	-2.619222	1.872389
H	-2.621235	-3.194771	2.556664
H	-0.863535	-1.425132	2.592761
H	-3.738815	1.472782	1.336702
H	-1.385722	2.006764	1.345134
H	-0.216912	2.558747	3.455205
H	-1.919411	2.155140	3.797493
H	-0.635450	0.966384	4.118258
H	1.096488	1.697247	-2.337881
H	2.122238	3.843705	-3.004438
H	2.742172	5.519974	-1.276093
H	2.341534	5.009262	1.121292
H	1.332949	2.833105	1.773449

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1S,2R-phenylethanol-B(C_6F_5)$_3$

C	4.792109	-0.911673	1.345764
C	5.132118	0.410527	1.616160
C	4.168903	1.288553	2.111384
C	2.870441	0.846083	2.335323
C	2.520857	-0.473199	2.039617
C	3.486196	-1.351398	1.552316
C	1.115738	-0.964252	2.286132
C	0.840185	-1.143993	3.770698
O	0.166822	0.038184	1.768090
B	-0.315407	0.011088	0.219437
C	-1.119576	1.412412	0.039337
C	-1.403624	-1.184631	0.032586
C	1.059103	-0.139366	-0.610709
C	-1.838431	-1.464349	-1.261519
C	-2.832920	-2.382797	-1.554601
C	-3.458415	-3.060712	-0.513645

C	-3.075843	-2.804407	0.792712
C	-2.071646	-1.873053	1.032224
C	-2.054512	1.805311	0.989070
C	-2.843880	2.939646	0.891328
C	-2.719966	3.736793	-0.238416
C	-1.816732	3.380303	-1.229607
C	-1.043412	2.233904	-1.081122
C	1.964021	0.920780	-0.645892
C	3.226776	0.836051	-1.207301
C	3.624253	-0.356929	-1.796042
C	2.756665	-1.436646	-1.803687
C	1.506767	-1.313699	-1.206131
F	-1.269690	-0.820494	-2.288015
F	-3.200160	-2.617414	-2.810753
F	-4.415834	-3.944338	-0.771367
F	-3.667965	-3.437822	1.802838
F	-1.763842	-1.663640	2.336189
F	-2.235091	1.037825	2.097056
F	-3.710296	3.259455	1.849398
F	-3.461872	4.830417	-0.369105
F	-1.699482	4.137770	-2.316252
F	-0.206592	1.951252	-2.081900
F	1.646884	2.082187	-0.058857
F	4.068183	1.866552	-1.158566
F	4.840457	-0.470428	-2.317747
F	3.138741	-2.593941	-2.342264
F	0.761901	-2.428641	-1.186048
H	5.535301	-1.596656	0.950684
H	6.142299	0.760470	1.432398
H	4.428006	2.322434	2.312953
H	2.111707	1.537573	2.689693
H	3.211853	-2.375613	1.310436
H	0.924793	-1.889969	1.731136
H	-0.163327	-1.531591	3.953891
H	1.565594	-1.852631	4.174835
H	0.975978	-0.192870	4.293554
H	-0.628857	0.063737	2.331182

C	-2.927653	-2.961866	0.713120
C	-1.936401	-2.032671	1.024798
C	-2.150940	1.688569	1.063754
C	-2.989749	2.791047	0.956392
C	-2.872799	3.629654	-0.141252
C	-1.925830	3.344341	-1.110415
C	-1.104519	2.230679	-0.963020
C	1.966163	0.969387	-0.641049
C	3.222573	0.907952	-1.221669
C	3.629808	-0.272041	-1.826898
C	2.771256	-1.356081	-1.835376
C	1.525223	-1.249602	-1.222708
F	-1.333956	-0.592611	-2.196710
F	-3.240918	-2.368095	-2.836230
F	-4.324361	-3.962901	-0.908636
F	-3.457643	-3.741708	1.664523
F	-1.572783	-2.000639	2.316344
F	-2.364831	0.893078	2.120161
F	-3.919593	3.044494	1.886570
F	-3.672125	4.695082	-0.267347
F	-1.815702	4.140794	-2.181300
F	-0.236184	2.025394	-1.963817
F	1.651767	2.129324	-0.044572
F	4.054001	1.955388	-1.184896
F	4.843429	-0.363573	-2.380365
F	3.158368	-2.505799	-2.404916
F	0.794635	-2.380382	-1.227731
H	5.567535	-1.610824	0.982002
H	6.199471	0.751572	1.408154
H	4.487676	2.353928	2.226043
H	2.144425	1.590286	2.579424
H	3.232759	-2.357047	1.357862
H	0.949571	-1.839734	1.764034
H	-0.160097	-1.340219	3.942879
H	1.561884	-1.749869	4.190057
H	1.027174	-0.057670	4.249343

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[1-phenylethoxy-B(C_6F_5)$_3$]-

C	4.829354	-0.908312	1.358438
C	5.184233	0.415855	1.596326
C	4.221605	1.314699	2.056840
C	2.916388	0.890175	2.274273
C	2.548276	-0.434898	2.023838
C	3.517194	-1.329200	1.574014
C	1.103619	-0.863725	2.257977
C	0.866114	-1.022943	3.759705
O	0.195601	0.089134	1.776902
B	-0.257408	0.018386	0.387149
C	-1.161427	1.376771	0.132380
C	-1.341887	-1.205681	0.083449
C	1.068864	-0.095535	-0.600668
C	-1.832329	-1.358602	-1.211500
C	-2.815993	-2.265657	-1.570793
C	-3.371995	-3.078324	-0.591703

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[1R,2R-phenylethanol-$SiEt_3$]$^+$

Si	1.43741	0.06773	-0.04592
O	0.45590	1.37861	-0.93083
C	1.34115	-1.43588	-1.14155
C	3.08659	0.95261	-0.11168
C	0.71395	-0.12403	1.66568
C	4.13102	0.35940	0.85417
C	-0.03487	-1.44939	1.87375
C	2.53566	-2.37986	-0.90397
C	-0.98016	1.84487	-0.84151
C	-1.01490	3.06746	0.04666
C	-1.82296	0.66661	-0.43683
C	-2.56908	0.66153	0.74368
C	-3.38911	-0.42296	1.04561
C	-3.46107	-1.50937	0.17736
C	-2.71573	-1.51205	-1.00118
C	-1.90925	-0.42238	-1.31149

H	1.01611	2.07602	-1.30945
H	1.32198	-1.11638	-2.19032
H	0.39813	-1.95958	-0.95358
H	3.47184	0.91761	-1.13903
H	2.94323	2.01302	0.13600
H	0.05640	0.72547	1.88270
H	1.54444	-0.04299	2.37743
H	3.81968	0.47280	1.89528
H	4.30421	-0.70347	0.66917
H	5.08811	0.87163	0.74094
H	0.63520	-2.30536	1.75330
H	-0.85589	-1.56387	1.16145
H	-0.45591	-1.50020	2.87999
H	2.61969	-2.68019	0.14565
H	3.47936	-1.91188	-1.19672
H	2.42502	-3.29205	-1.49315
H	-1.20349	2.11067	-1.87857
H	-2.03226	3.46440	0.07290
H	-0.36606	3.85343	-0.34823
H	-0.70300	2.83350	1.06715
H	-2.53235	1.50477	1.42584
H	-3.97469	-0.41566	1.95828
H	-4.10407	-2.35034	0.41356
H	-2.78058	-2.35009	-1.68667
H	-1.35347	-0.40781	-2.24655

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1-phenylethoxy-$SiEt_3$

Si	1.57547	-0.14200	-0.03267
O	-0.09445	-0.27262	0.02064
C	2.14603	-1.85705	-0.55364
C	2.06468	1.17297	-1.29624
C	2.24790	0.29946	1.67757
C	3.50622	1.68141	-1.14853
C	3.67585	-0.19635	1.94810
C	3.53177	-1.91840	-1.21048
C	-1.02145	0.78717	-0.08760
C	-0.85704	1.78175	1.06287
C	-2.42821	0.22043	-0.10296
C	-2.69798	-1.05909	0.37756
C	-4.00568	-1.53946	0.39675
C	-5.05319	-0.74718	-0.06304
C	-4.78779	0.53205	-0.54744
C	-3.48221	1.01004	-0.56695
H	1.38877	-2.23770	-1.24903
H	2.11111	-2.52149	0.31892
H	1.90365	0.77074	-2.30456
H	1.37556	2.02257	-1.20160
H	1.56092	-0.13597	2.41420
H	2.19669	1.38541	1.82701
H	3.66384	2.13569	-0.16504
H	4.23544	0.87222	-1.25422
H	3.74651	2.43791	-1.90103
H	4.39514	0.23762	1.24608
H	3.74150	-1.28468	1.85143
H	4.00786	0.06338	2.95741
H	4.31787	-1.55797	-0.53944
H	3.56659	-1.30329	-2.11545
H	3.79372	-2.93996	-1.50056
H	-0.86183	1.31736	-1.03983
H	-1.61780	2.56464	1.00974
H	0.12883	2.25740	1.03283
H	-0.96519	1.25419	2.01490
H	-1.87354	-1.67269	0.72267
H	-4.20566	-2.53903	0.77027
H	-6.07062	-1.12461	-0.04953
H	-5.59740	1.15439	-0.91554
H	-3.27624	2.00626	-0.95320

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[1R,2R-phenylethanol-$SiPhH_2$]$^+$

Si	1.38570	1.67556	-0.13902
O	-0.18785	0.79337	0.05379
C	2.63377	0.34153	-0.05327
C	-1.54075	1.27422	-0.45777
C	-1.81362	2.59134	0.23167
C	-2.50883	0.16405	-0.18572
C	-2.80360	-0.21518	1.12971
C	-3.69903	-1.25075	1.36654
C	-4.31014	-1.90298	0.29573
C	-4.02013	-1.52759	-1.01291
C	-3.11314	-0.50004	-1.25497
C	3.21755	-0.00430	1.17792
C	4.14686	-1.03545	1.24691
C	4.50397	-1.72561	0.08977
C	3.93870	-1.38907	-1.13945
C	3.00941	-0.35868	-1.21351
H	1.36889	2.61322	0.99090
H	1.18943	2.30663	-1.45466
H	-0.15196	-0.18005	0.07963
H	-1.39366	1.40670	-1.53323
H	-2.78390	2.95811	-0.10979
H	-1.06428	3.34724	-0.02070
H	-1.85354	2.46852	1.31568
H	-2.33624	0.29612	1.96718
H	-3.92722	-1.54519	2.38490
H	-5.01478	-2.70571	0.48427
H	-4.49627	-2.03467	-1.84465
H	-2.88442	-0.20623	-2.27585
H	2.95501	0.53810	2.08280
H	4.59827	-1.29612	2.19777
H	5.23392	-2.52642	0.14474
H	4.22994	-1.92291	-2.03730
H	2.58761	-0.09108	-2.17948

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1-phenylethoxy-$SiPhH_2$

Si	-0.73102	1.95111	0.67290
O	-1.78026	1.57175	-0.56162
C	0.98145	1.24958	0.41061
C	-2.41850	0.30247	-0.71911
C	-3.67978	0.26083	0.13051

C	-1.43784	-0.83243	-0.46806
C	-0.40570	-1.02489	-1.39295
C	0.57511	-1.98271	-1.17798
C	0.53116	-2.77523	-0.03091
C	-0.49452	-2.60047	0.89061
C	-1.47364	-1.62993	0.67484
C	1.73788	1.61446	-0.71313
C	2.98353	1.04544	-0.95417
C	3.49925	0.10199	-0.06622
C	2.76748	-0.26610	1.05840
C	1.51748	0.30378	1.29136
H	-1.22428	1.45214	1.98468
H	-0.69039	3.42923	0.66230
H	-2.70893	0.25964	-1.77593
H	-4.21413	-0.68328	-0.00583
H	-4.33410	1.08431	-0.16109
H	-3.44211	0.37834	1.19181
H	-0.36396	-0.38881	-2.27382
H	1.38062	-2.10504	-1.89485
H	1.29810	-3.52343	0.14292
H	-0.53521	-3.21626	1.78365
H	-2.26585	-1.50065	1.40579
H	1.34281	2.34528	-1.41598
H	3.55499	1.33632	-1.83026
H	4.47167	-0.34376	-0.25220
H	3.16436	-1.00426	1.74873
H	0.94266	-0.01005	2.15965

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BEt_3-$(PhEtOH)_2$

B	0.32385	1.14702	0.09516
O	0.81956	-0.50518	0.15184
C	-0.35710	1.12632	-1.37065
C	-0.78385	1.28806	1.30021
C	1.62681	2.09211	0.23611
C	-0.93555	2.70628	1.86627
C	2.54315	2.19521	-0.98864
C	-1.14074	2.40432	-1.68426
C	1.83500	-1.13600	0.97010
C	1.70393	-0.77606	2.44030
C	3.18213	-0.86470	0.33670
C	4.18813	-0.14294	0.97335
C	5.39698	0.10251	0.32466
C	5.61130	-0.37967	-0.96181
C	4.61355	-1.11464	-1.60065
C	3.40859	-1.35383	-0.95266
H	-0.02362	-1.00733	0.28963
H	-1.05795	0.27853	-1.42762
H	0.39527	0.94938	-2.15109
H	-1.77205	0.97157	0.92115
H	-0.55329	0.62559	2.14924
H	2.22690	1.84378	1.12391
H	1.24547	3.10197	0.44756
H	-0.02078	3.02368	2.37669
H	-1.12580	3.43387	1.07040
H	-1.75888	2.78120	2.58463
H	2.00724	2.64455	-1.83184
H	2.90049	1.21647	-1.32212
H	3.42455	2.81579	-0.79307
H	-0.49974	3.29099	-1.60867
H	-1.96758	2.53904	-0.97698
H	-1.57308	2.39824	-2.69143
H	1.63499	-2.21055	0.86508
H	2.48592	-1.28283	3.01219
H	0.73501	-1.11290	2.81625
H	1.78308	0.30100	2.60135
H	4.02956	0.24847	1.97321
H	6.16913	0.67671	0.82625
H	6.55193	-0.18496	-1.46666
H	4.77451	-1.49480	-2.60427
H	2.61772	-1.90606	-1.45393
C	-4.27592	-0.85990	0.93673
C	-5.18009	0.19088	0.83164
C	-5.28228	0.89871	-0.36381
C	-4.48740	0.54166	-1.44860
C	-3.58015	-0.50994	-1.33921
C	-3.45634	-1.21254	-0.14088
C	-2.41071	-2.28645	0.09071
C	-1.73337	-2.83054	-1.15220
O	-1.36517	-1.76650	0.93992
H	-4.20095	-1.41720	1.86893
H	-5.80525	0.45511	1.67819
H	-5.98295	1.72257	-0.45035
H	-4.56376	1.08797	-2.38297
H	-2.96253	-0.76956	-2.19251
H	-2.88604	-3.11392	0.63460
H	-1.01330	-3.60055	-0.86541
H	-2.46590	-3.27340	-1.83091
H	-1.19402	-2.03672	-1.67788
H	-1.72496	-1.03049	1.45816

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$[BEt_3$-(PhEtOH-PhEtO)]-

B	0.50282	1.38741	-0.16046
O	0.61594	-0.09129	0.32413
C	-0.43416	1.23617	-1.49706
C	-0.32377	2.26338	0.99991
C	1.96033	2.05431	-0.54195
C	0.33887	3.52133	1.57516
C	2.63757	1.54020	-1.81864
C	-0.73156	2.56095	-2.20468
C	1.58152	-0.58049	1.21425
C	1.78508	0.27443	2.46374
C	2.86964	-0.93608	0.47685
C	4.12594	-0.42754	0.79749
C	5.25447	-0.79731	0.06449
C	5.14169	-1.69292	-0.99243
C	3.88883	-2.21349	-1.31894
C	2.76820	-1.83171	-0.59337
H	-1.39291	0.76808	-1.21837
H	0.03763	0.54190	-2.21107
H	-1.29672	2.57688	0.58469

H	-0.59052	1.59702	1.83393
H	2.68301	1.97870	0.28625
H	1.80702	3.13867	-0.66405
H	1.33203	3.30820	1.99013
H	0.48789	4.27823	0.79591
H	-0.25109	3.99185	2.37367
H	2.02152	1.75265	-2.70020
H	2.78429	0.45665	-1.79267
H	3.62169	1.99741	-1.99117
H	0.19112	3.03582	-2.56055
H	-1.20391	3.27367	-1.51670
H	-1.39959	2.45489	-3.06965
H	1.18147	-1.54496	1.57450
H	2.50405	-0.20089	3.14040
H	0.82966	0.36669	2.98463
H	2.13747	1.27846	2.21673
H	4.22644	0.28223	1.61327
H	6.22354	-0.37734	0.31961
H	6.02014	-1.98005	-1.56318
H	3.78794	-2.90728	-2.14893
H	1.77990	-2.19534	-0.86361
C	-3.56004	0.23932	0.43867
C	-4.68373	0.90380	-0.04864
C	-5.72039	0.19233	-0.64594
C	-5.62684	-1.19408	-0.75554
C	-4.49969	-1.85366	-0.27630
C	-3.45248	-1.14528	0.31877
C	-2.21003	-1.87285	0.82358
C	-1.41158	-2.45521	-0.34938
O	-1.41184	-1.05973	1.63141
H	-2.74955	0.78286	0.91373
H	-4.74497	1.98471	0.03920
H	-6.59627	0.71203	-1.02359
H	-6.43281	-1.76022	-1.21463
H	-4.43055	-2.93700	-0.36086
H	-2.56373	-2.71027	1.44770
H	-0.56093	-3.02444	0.03931
H	-2.02914	-3.11601	-0.96556
H	-1.02388	-1.64220	-0.97054
H	-0.72462	-0.60417	1.05949

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BPh_3-$(PhEtOH)_2$

C	1.68403	-4.32456	-1.07555
C	0.60795	-4.51005	-0.20791
C	-0.27524	-3.46113	0.02771
C	-0.08594	-2.23021	-0.59775
C	0.99544	-2.03649	-1.45548
C	1.87693	-3.09366	-1.69298
C	1.24481	-0.69903	-2.11574
C	0.85282	-0.70678	-3.59150
O	0.49389	0.28272	-1.39608
H	2.37914	-5.13722	-1.26201
H	0.46533	-5.46686	0.28400
H	-1.11054	-3.58280	0.71108
H	-0.76588	-1.41275	-0.38857
H	2.73250	-2.94171	-2.34784
H	2.31489	-0.46420	-2.01464
H	1.04003	0.27087	-4.04781
H	1.43831	-1.45427	-4.13295
H	-0.20853	-0.94346	-3.70154
H	0.68770	1.15859	-1.75799
B	1.46776	1.04936	1.11305
C	0.49191	0.11397	1.90544
C	0.99140	2.48994	0.68306
C	2.93039	0.57834	0.79117
C	0.04174	3.20279	1.43289
C	-0.42754	4.44803	1.02144
C	0.02834	5.00548	-0.17024
C	0.97746	4.32638	-0.93253
C	1.46038	3.09602	-0.49762
C	-0.89594	0.16479	1.68686
C	-1.77193	-0.70615	2.32528
C	-1.27388	-1.64405	3.22830
C	0.09416	-1.70368	3.48506
C	0.96225	-0.83905	2.82515
C	3.22652	-0.78410	0.60019
C	4.50860	-1.20958	0.26534
C	5.54068	-0.28089	0.14841
C	5.28270	1.07204	0.35890
C	3.99140	1.49236	0.66329
H	-0.33851	2.76742	2.35292
H	-1.15840	4.97832	1.62412
H	-0.34874	5.96797	-0.50180
H	1.34445	4.76052	-1.85750
H	2.22348	2.58615	-1.08481
H	-1.30139	0.88064	0.97659
H	-2.83488	-0.65095	2.11366
H	-1.95254	-2.32529	3.73354
H	0.48413	-2.42765	4.19384
H	2.02828	-0.90124	3.02657
H	2.43194	-1.51928	0.69405
H	4.69975	-2.26601	0.10153
H	6.54455	-0.61021	-0.10248
H	6.08630	1.79758	0.27936
H	3.80012	2.55136	0.81682
C	-4.50994	0.82808	0.09856
C	-5.21505	0.01442	0.98196
C	-5.08440	-1.37157	0.91641
C	-4.23756	-1.93316	-0.03496
C	-3.54246	-1.11783	-0.92551
C	-3.67029	0.27263	-0.87273
C	-2.97925	1.14004	-1.92264
C	-2.32980	2.40494	-1.36028
O	-2.03384	0.40386	-2.66803
H	-4.63625	1.90532	0.15619
H	-5.86939	0.46486	1.72197
H	-5.63568	-2.00546	1.60370
H	-4.12402	-3.01138	-0.09557
H	-2.90398	-1.55346	-1.68621
H	-3.74910	1.43772	-2.64690
H	-1.92544	2.99780	-2.18474

H	-3.03054	3.02990	-0.80191
H	-1.50059	2.14899	-0.69093
H	-1.26972	0.24102	-2.08802

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[BPh_3-(PhEtOH-PhEtO)]-

C	-2.41434	4.38364	-1.12000
C	-1.53915	4.87673	-0.15374
C	-0.51815	4.06022	0.32530
C	-0.36523	2.76299	-0.16078
C	-1.23290	2.26573	-1.13317
C	-2.26001	3.08807	-1.60209
C	-1.05164	0.86555	-1.70581
C	-0.35089	0.96039	-3.06559
O	-0.31565	0.03233	-0.85593
H	-3.22502	5.00608	-1.48874
H	-1.66153	5.88509	0.23105
H	0.15763	4.42733	1.09283
H	0.40454	2.10897	0.23557
H	-2.95777	2.69476	-2.33876
H	-2.05707	0.45083	-1.87402
H	-0.21917	-0.03662	-3.49437
H	-0.93955	1.57589	-3.75323
H	0.64123	1.40834	-2.96180
B	-0.98373	-0.81676	0.22798
C	-0.33005	-0.42447	1.67668
C	-0.61865	-2.37707	-0.13593
C	-2.61252	-0.59515	0.25221
C	-0.42084	-3.37306	0.83180
C	-0.11624	-4.68984	0.49047
C	-0.00837	-5.06002	-0.84853
C	-0.21028	-4.09690	-1.83473
C	-0.50458	-2.78291	-1.47491
C	0.97191	0.08908	1.76109
C	1.59368	0.37074	2.97544
C	0.91763	0.13540	4.17065
C	-0.37636	-0.37911	4.12537
C	-0.98320	-0.64920	2.89874
C	-3.16992	0.56889	0.81204
C	-4.53951	0.81952	0.79911
C	-5.41307	-0.10586	0.23016
C	-4.89635	-1.27547	-0.31849
C	-3.52016	-1.50824	-0.30399
H	-0.48496	-3.10234	1.88383
H	0.04326	-5.42972	1.27155
H	0.23266	-6.08474	-1.11949
H	-0.12471	-4.36669	-2.88470
H	-0.63482	-2.03705	-2.25653
H	1.51285	0.27783	0.83861
H	2.60454	0.77258	2.98144
H	1.39091	0.35131	5.12505
H	-0.91789	-0.56495	5.05025
H	-2.00022	-1.03818	2.88616
H	-2.50463	1.29970	1.26826
H	-4.92617	1.73820	1.23359
H	-6.48380	0.08184	0.21962
H	-5.56594	-2.01046	-0.75935
H	-3.13693	-2.42829	-0.73961
C	4.98052	0.01151	-0.18334
C	5.53677	1.12186	0.44397
C	4.85206	2.33603	0.45361
C	3.61530	2.42784	-0.17833
C	3.06936	1.31668	-0.81735
C	3.73668	0.09190	-0.81577
C	3.11431	-1.13823	-1.47203
C	2.85464	-2.24438	-0.44489
O	1.96213	-0.82530	-2.20660
H	5.51884	-0.93393	-0.18155
H	6.50409	1.03903	0.93161
H	5.28016	3.20111	0.95123
H	3.06383	3.36407	-0.17431
H	2.09855	1.38059	-1.29799
H	3.84154	-1.51366	-2.20747
H	2.39689	-3.10596	-0.93892
H	3.78308	-2.55752	0.04320
H	2.16363	-1.89487	0.32788
H	1.20613	-0.64794	-1.60355

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$B(C_6F_5)Ph_2$-$(PhEtOH)_2$

C	3.04881	-3.02079	-1.80213
C	2.11784	-4.00075	-1.46978
C	0.76557	-3.67336	-1.38681
C	0.34503	-2.37186	-1.63690
C	1.27807	-1.37987	-1.94943
C	2.62905	-1.71353	-2.03646
C	0.83596	0.04301	-2.21295
C	-0.01293	0.14985	-3.47101
O	0.06494	0.60494	-1.11643
H	4.10442	-3.26692	-1.85783
H	2.44475	-5.01472	-1.26465
H	0.03871	-4.43099	-1.11377
H	-0.70805	-2.12084	-1.53355
H	3.35837	-0.94049	-2.26592
H	1.71245	0.69408	-2.28101
H	-0.29710	1.18631	-3.66825
H	0.54661	-0.23580	-4.32585
H	-0.92120	-0.45419	-3.36625
H	-0.78099	0.09393	-0.91246
B	0.75991	1.27807	0.19117
C	-0.50633	1.55228	1.17291
C	1.37187	2.68830	-0.28815
C	1.80250	0.13786	0.73009
C	2.07071	3.47749	0.63951
C	2.52416	4.75148	0.32638
C	2.28235	5.28873	-0.93865
C	1.57479	4.54047	-1.87000
C	1.12275	3.26109	-1.53981
C	-1.53505	2.39758	0.72003
C	-2.68882	2.62381	1.46851
C	-2.83234	2.02919	2.72180
C	-1.80790	1.22647	3.21561

C	-0.66694	0.99285	2.44702
C	1.30049	-1.11933	1.07306
C	2.08215	-2.20944	1.41888
C	3.46202	-2.06544	1.43693
C	4.01862	-0.84162	1.10665
C	3.19263	0.22301	0.75227
F	-0.02343	-1.34724	1.00075
F	1.53108	-3.39191	1.69376
F	4.24034	-3.10040	1.74146
F	5.34483	-0.69917	1.09906
F	3.83344	1.33961	0.39012
H	2.26468	3.07726	1.63284
H	3.06517	5.33153	1.06801
H	2.63651	6.28401	-1.18836
H	1.36709	4.95041	-2.85419
H	0.54415	2.70982	-2.27775
H	-1.42492	2.88336	-0.24833
H	-3.47004	3.27238	1.08181
H	-3.72830	2.20097	3.30989
H	-1.89847	0.77348	4.19828
H	0.11247	0.35325	2.85199
C	-5.80829	-0.89028	-1.21254
C	-6.98751	-1.21348	-0.55276
C	-6.98319	-1.40991	0.82710
C	-5.79200	-1.29067	1.53350
C	-4.60724	-0.97304	0.87081
C	-4.60821	-0.76216	-0.50720
C	-3.35040	-0.36300	-1.25747
C	-3.47067	1.03438	-1.86190
O	-2.19641	-0.45441	-0.42166
H	-5.81805	-0.74269	-2.28986
H	-7.91037	-1.31369	-1.11489
H	-7.90300	-1.66071	1.34503
H	-5.77710	-1.45113	2.60668
H	-3.68326	-0.91017	1.43726
H	-3.16705	-1.09380	-2.05533
H	-2.52842	1.32552	-2.33596
H	-4.26594	1.06621	-2.61002
H	-3.70736	1.75889	-1.07841
H	-2.29526	0.15622	0.33076

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[B(C_6F_5)Ph_2-(PhEtOH-PhEtO)]-

C	3.51191	-2.82108	-1.67848
C	2.91477	-3.81216	-0.90383
C	1.59445	-3.65568	-0.48504
C	0.87814	-2.51639	-0.83708
C	1.47301	-1.51418	-1.60601
C	2.79205	-1.68020	-2.02732
C	0.67869	-0.26601	-1.97290
C	-0.09273	-0.51553	-3.26933
O	-0.22220	0.07314	-0.94923
H	4.54639	-2.92483	-1.99320
H	3.47965	-4.69298	-0.61403
H	1.12887	-4.41434	0.13701
H	-0.13067	-2.35664	-0.46774
H	3.26908	-0.88925	-2.60331
H	1.38690	0.56091	-2.14335
H	-0.67522	0.36587	-3.54694
H	0.59940	-0.76906	-4.07802
H	-0.78243	-1.35557	-3.13254
B	0.26130	0.98677	0.15031
C	-0.79637	0.82213	1.38566
C	0.24666	2.54387	-0.34835
C	1.80005	0.49316	0.59448
C	0.94522	3.56259	0.32019
C	0.84822	4.90000	-0.04951
C	0.04126	5.26965	-1.12450
C	-0.65883	4.28377	-1.81192
C	-0.55590	2.94761	-1.42350
C	-1.77543	-0.17885	1.37732
C	-2.71018	-0.32019	2.40079
C	-2.68086	0.54368	3.49122
C	-1.71071	1.54324	3.53662
C	-0.79483	1.67841	2.49623
C	1.99338	-0.62127	1.41197
C	3.23319	-1.18954	1.67857
C	4.37348	-0.62862	1.12702
C	4.24442	0.47439	0.30209
C	2.97919	0.99387	0.04506
F	0.95083	-1.27307	1.94214
F	3.33892	-2.28111	2.44605
F	5.57715	-1.15949	1.36923
F	5.33473	1.00536	-0.27005
F	2.96383	1.99188	-0.85706
H	1.60413	3.29534	1.14606
H	1.40913	5.65621	0.49452
H	-0.03663	6.31202	-1.42200
H	-1.29253	4.55376	-2.65327
H	-1.12725	2.20046	-1.96923
H	-1.80265	-0.87623	0.54387
H	-3.46888	-1.09752	2.33350
H	-3.40723	0.44347	4.29354
H	-1.67505	2.22748	4.38128
H	-0.06563	2.48427	2.54404
C	-4.78139	-2.25201	-0.16795
C	-5.74973	-2.32044	0.83008
C	-6.30057	-1.14880	1.34597
C	-5.86994	0.08414	0.86244
C	-4.89969	0.14942	-0.13373
C	-4.35146	-1.01855	-0.66080
C	-3.32112	-0.94701	-1.77982
C	-3.97309	-1.28991	-3.11918
O	-2.75486	0.33106	-1.89230
H	-4.34263	-3.16697	-0.56203
H	-6.06783	-3.28653	1.21153
H	-7.04986	-1.19800	2.13048
H	-6.27672	1.00141	1.27758
H	-4.52152	1.09952	-0.49517
H	-2.53769	-1.69479	-1.56746
H	-3.21897	-1.27602	-3.91064
H	-4.45491	-2.27158	-3.09205

H	-4.73127	-0.53497	-3.34738
H	-1.88858	0.32384	-1.42590

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$B(C_6F_5)_2Ph\text{-}(PhEtOH)_2$

C	5.18321	1.70108	0.49973
C	5.50452	1.37686	-0.81477
C	4.68925	1.81559	-1.85766
C	3.55953	2.57924	-1.58467
C	3.22694	2.90241	-0.26536
C	4.04465	2.45849	0.77259
C	2.00241	3.73842	0.02124
C	2.16391	5.18365	-0.43032
O	0.91370	3.12859	-0.69337
H	5.81011	1.35697	1.31580
H	6.38250	0.77626	-1.02835
H	4.93391	1.55838	-2.88297
H	2.92066	2.92383	-2.39384
H	3.78410	2.69890	1.80048
H	1.78577	3.70196	1.09580
H	1.26016	5.76263	-0.21538
H	2.99965	5.64904	0.09693
H	2.36287	5.22534	-1.50421
H	0.10162	3.64101	-0.57970
B	-0.77525	0.09298	0.44159
C	-2.25149	0.54788	-0.12179
C	-0.50723	0.88703	1.83592
C	-0.53256	-1.52380	0.50472
C	-1.52525	1.03526	2.78824
C	-1.32729	1.73298	3.97741
C	-0.09560	2.32068	4.24831
C	0.93759	2.17932	3.32643
C	0.73068	1.46776	2.14715
C	-2.48607	1.64907	-0.93367
C	-3.74611	2.08808	-1.32172
C	-4.86671	1.42000	-0.85766
C	-4.69759	0.33031	-0.01434
C	-3.41558	-0.06876	0.33446
C	-1.26400	-2.48516	-0.18977
C	-0.96373	-3.84194	-0.18804
C	0.13065	-4.29615	0.52880
C	0.90192	-3.38376	1.23070
C	0.55581	-2.03989	1.21147
F	-1.45364	2.38630	-1.41770
F	-3.87834	3.14911	-2.11909
F	-6.08558	1.82248	-1.20542
F	-5.76363	-0.31239	0.45777
F	-3.33193	-1.10324	1.18462
F	-2.29811	-2.13978	-0.97891
F	-1.70165	-4.70092	-0.89289
F	0.45906	-5.58507	0.51397
F	1.98499	-3.79715	1.88834
F	1.38683	-1.22647	1.87223
H	-2.49703	0.58432	2.61084
H	-2.13991	1.81948	4.69232
H	0.06093	2.87081	5.17084
H	1.91412	2.60982	3.53645
H	1.56957	1.33032	1.46817
C	1.57281	-2.34624	-2.08924
C	2.44924	-3.38697	-1.78483
C	3.51171	-3.17539	-0.91166
C	3.70554	-1.91293	-0.35273
C	2.83672	-0.87459	-0.66263
C	1.75601	-1.08566	-1.52289
C	0.82765	0.07924	-1.80195
C	-0.32732	-0.19099	-2.74622
O	0.36207	0.62898	-0.52798
H	0.73538	-2.53321	-2.75424
H	2.28656	-4.36922	-2.21733
H	4.18151	-3.99152	-0.66151
H	4.52890	-1.73636	0.33213
H	2.97853	0.10432	-0.21140
H	1.43335	0.89937	-2.20528
H	-0.87964	0.73174	-2.92379
H	0.06877	-0.54270	-3.70217
H	-1.01360	-0.94299	-2.35247
H	0.53411	1.62337	-0.50181

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$[B(C_6F_5)_2Ph\text{-}(PhEtOH\text{-}PhEtO)]^-$

C	3.44300	-3.72323	-1.22929
C	2.78516	-4.34094	-0.16915
C	1.53415	-3.87280	0.23143
C	0.94621	-2.78885	-0.41456
C	1.61127	-2.15375	-1.46578
C	2.85567	-2.63638	-1.87219
C	0.99369	-0.95069	-2.16724
C	0.07122	-1.41593	-3.29402
O	0.23119	-0.14269	-1.30140
H	4.42376	-4.07114	-1.53987
H	3.24731	-5.17583	0.34904
H	1.01871	-4.34701	1.06181
H	-0.02414	-2.41195	-0.10012
H	3.38536	-2.12644	-2.67341
H	1.81608	-0.35810	-2.59512
H	-0.32627	-0.54929	-3.82987
H	0.60938	-2.05951	-3.99622
H	-0.76945	-1.97405	-2.87124
B	0.89162	0.93843	-0.52205
C	-0.33001	1.80733	0.17467
C	1.65669	2.02914	-1.46040
C	1.89494	0.20191	0.58139
C	2.67481	2.86236	-0.97811
C	3.23782	3.86317	-1.76490
C	2.79204	4.05972	-3.07077
C	1.77334	3.25290	-3.57067
C	1.21338	2.25967	-2.76923
C	-1.56764	1.97410	-0.44046
C	-2.61432	2.70216	0.11670
C	-2.42722	3.35810	1.32116
C	-1.18947	3.27849	1.94273
C	-0.17983	2.52764	1.35666

C	1.46401	-0.30173	1.80541
C	2.22170	-1.13594	2.61632
C	3.48253	-1.53052	2.19757
C	3.96098	-1.06915	0.98400
C	3.17141	-0.21804	0.21915
F	-1.84495	1.40739	-1.62844
F	-3.80299	2.76257	-0.49877
F	-3.41790	4.06809	1.87116
F	-0.98532	3.92826	3.09486
F	0.99252	2.51173	2.01231
F	0.22769	-0.03502	2.26586
F	1.74118	-1.58625	3.78221
F	4.21821	-2.35565	2.94875
F	5.15894	-1.47074	0.54450
F	3.69400	0.11886	-0.97311
H	3.03206	2.72009	0.04068
H	4.02882	4.49058	-1.36175
H	3.23212	4.83651	-3.69011
H	1.41156	3.40114	-4.58514
H	0.40075	1.64725	-3.15593
C	-5.71887	-1.23202	-0.00915
C	-6.84871	-2.03991	-0.08314
C	-6.72555	-3.37811	-0.45200
C	-5.46709	-3.89471	-0.74779
C	-4.33639	-3.08427	-0.67281
C	-4.45303	-1.74582	-0.29959
C	-3.22926	-0.86285	-0.16359
C	-2.88154	-0.66694	1.31544
O	-2.16104	-1.46244	-0.85488
H	-5.81441	-0.18393	0.26746
H	-7.82689	-1.62418	0.14069
H	-7.60590	-4.01095	-0.51367
H	-5.36448	-4.93531	-1.04233
H	-3.35121	-3.46892	-0.91173
H	-3.47570	0.11361	-0.60628
H	-1.97308	-0.06791	1.41660
H	-3.69606	-0.16836	1.85097
H	-2.70460	-1.64338	1.77650
H	-1.41602	-0.83204	-0.95127

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$B(C_6F_5)_3$-$(PhEtOH)_2$

C	-3.40019	-3.76890	1.05007
C	-2.41629	-4.75361	1.04113
C	-1.13040	-4.45230	1.48712
C	-0.83239	-3.16965	1.93303
C	-1.80593	-2.16796	1.91210
C	-3.09342	-2.47940	1.47943
C	-1.46099	-0.76308	2.35626
C	-1.00472	-0.70665	3.80592
O	-0.39659	-0.19250	1.53956
H	-4.40250	-3.99673	0.70134
H	-2.64865	-5.75194	0.68589
H	-0.36104	-5.21771	1.48687
H	0.16756	-2.93919	2.29180
H	-3.85398	-1.70272	1.45580
H	-2.31384	-0.09816	2.19390
H	-0.76868	0.31777	4.09113
H	-1.80103	-1.08948	4.44767
H	-0.11954	-1.33241	3.95043
H	0.51497	-0.61586	1.71377
B	-0.61994	0.50298	0.15660
C	0.87935	0.83494	-0.40723
C	-1.34220	1.94753	0.36828
C	-1.44965	-0.57152	-0.74104
C	-1.64668	2.67601	-0.78123
C	-2.15674	3.96298	-0.76939
C	-2.37090	4.59177	0.45178
C	-2.07168	3.91748	1.62312
C	-1.55855	2.62446	1.55952
C	1.83956	1.41743	0.41418
C	3.08681	1.84216	-0.01868
C	3.40699	1.71808	-1.36080
C	2.48765	1.14539	-2.22547
C	1.25556	0.71870	-1.74436
C	-0.84707	-1.79549	-1.01557
C	-1.47372	-2.85263	-1.64809
C	-2.78935	-2.69282	-2.06508
C	-3.43535	-1.49098	-1.83146
C	-2.76508	-0.46324	-1.17167
F	-1.43834	2.11050	-1.97903
F	-2.43330	4.60359	-1.90328
F	-2.85826	5.82819	0.49265
F	-2.26838	4.50783	2.80187
F	-1.29256	2.04938	2.74619
F	1.59081	1.57863	1.73522
F	3.97105	2.34937	0.84082
F	4.59645	2.10864	-1.80859
F	2.81163	0.97429	-3.50636
F	0.43501	0.17453	-2.64827
F	0.42310	-2.00524	-0.60477
F	-0.84823	-4.01443	-1.83553
F	-3.42942	-3.69827	-2.65450
F	-4.70544	-1.33822	-2.20485
F	-3.49017	0.63647	-0.92856
C	3.65196	-1.72880	-0.74409
C	4.65587	-1.21763	-1.56427
C	5.70097	-0.48173	-1.01314
C	5.73926	-0.25183	0.36100
C	4.74976	-0.78259	1.18191
C	3.69954	-1.52788	0.63530
C	2.64261	-2.13342	1.52935
C	3.21393	-3.06870	2.58491
O	1.86111	-1.11057	2.19513
H	2.82083	-2.28068	-1.17408
H	4.60620	-1.37336	-2.63735
H	6.47269	-0.06931	-1.65391
H	6.54194	0.33629	0.79293
H	4.80462	-0.61667	2.25635
H	1.92229	-2.67048	0.90818
H	2.40918	-3.48885	3.19425
H	3.76059	-3.88477	2.10688

H	3.90275	-2.53625	3.24654
H	2.40232	-0.32373	2.35726

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[$B(C_6F_5)_3$-(PhEtOH-PhEtO)]-

C	-3.64431	-3.39329	1.63774
C	-2.74076	-4.44351	1.50760
C	-1.37610	-4.20177	1.66770
C	-0.91727	-2.91849	1.94397
C	-1.81844	-1.85394	2.04725
C	-3.18166	-2.10560	1.90641
C	-1.29074	-0.45044	2.31607
C	-0.82273	-0.35332	3.76749
O	-0.21011	-0.13100	1.46229
H	-4.70816	-3.56883	1.50458
H	-3.09539	-5.44316	1.27551
H	-0.66589	-5.01706	1.56629
H	0.14494	-2.72127	2.07010
H	-3.88522	-1.27817	1.97432
H	-2.11452	0.26603	2.15582
H	-0.44444	0.64789	3.97341
H	-1.65347	-0.57578	4.44430
H	-0.02115	-1.07473	3.94550
B	-0.50643	0.48718	0.15507
C	0.93081	0.58328	-0.64687
C	-0.97824	2.07680	0.24787
C	-1.63400	-0.44041	-0.62589
C	-1.29955	2.74618	-0.93145
C	-1.59531	4.09748	-1.00497
C	-1.56227	4.85834	0.15629
C	-1.23637	4.24678	1.35343
C	-0.94528	2.88365	1.37556
C	2.02193	1.11532	0.03308
C	3.29642	1.22921	-0.50485
C	3.51222	0.82751	-1.81210
C	2.44768	0.33775	-2.55006
C	1.19016	0.23333	-1.96745
C	-1.30048	-1.74272	-0.99079
C	-2.20540	-2.68037	-1.45965
C	-3.53688	-2.31777	-1.60291
C	-3.92443	-1.03298	-1.26988
C	-2.97848	-0.13331	-0.78535
F	-1.33459	2.06080	-2.08644
F	-1.90347	4.67991	-2.16988
F	-1.84194	6.16542	0.11515
F	-1.19853	4.97128	2.47871
F	-0.63655	2.38682	2.58274
F	1.87792	1.54794	1.30106
F	4.31353	1.70272	0.22544
F	4.73353	0.88801	-2.34872
F	2.65739	-0.07985	-3.80442
F	0.22902	-0.26206	-2.76102
F	-0.03160	-2.16840	-0.86418
F	-1.82020	-3.92461	-1.76005
F	-4.43557	-3.20543	-2.03903
F	-5.21064	-0.67659	-1.38362
F	-3.47243	1.06505	-0.42361
C	5.07476	-1.46733	0.63009
C	5.41295	-1.75906	-0.68881
C	4.44845	-2.24339	-1.56941
C	3.14317	-2.42483	-1.12033
C	2.80640	-2.13248	0.19899
C	3.76720	-1.65203	1.09036
C	3.38244	-1.35993	2.53698
C	3.98824	-0.06177	3.07314
O	1.98863	-1.39118	2.73746
H	5.83794	-1.08296	1.30056
H	6.42927	-1.59279	-1.03340
H	4.70511	-2.44785	-2.60451
H	2.36784	-2.76742	-1.79972
H	1.78119	-2.24655	0.53210
H	3.76510	-2.18943	3.14862
H	3.61716	0.10296	4.08749
H	5.08008	-0.10820	3.10828
H	3.69994	0.78586	2.44971
H	1.52611	-0.70747	2.21311

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[$SiEt_3$-$(PhEtOH)_2$]$^+$

Si	-1.62530	1.50382	0.09880
O	-0.55914	0.15032	0.61647
C	-2.89252	1.65401	1.46166
C	-0.36581	2.89119	0.03579
C	-2.35331	1.10218	-1.57836
C	-0.86662	4.15808	-0.67914
C	-3.79499	0.57219	-1.56327
C	-3.65926	2.98749	1.38299
C	-1.02793	-1.04609	1.34557
C	0.18433	-1.89109	1.69472
C	-2.03303	-1.77467	0.49403
C	-1.70488	-2.16141	-0.80845
C	-2.62159	-2.86780	-1.57777
C	-3.86521	-3.20748	-1.04337
C	-4.19170	-2.83470	0.25703
C	-3.27787	-2.11295	1.02338
H	0.47821	0.32888	0.67185
H	-2.40187	1.57053	2.43905
H	-3.59201	0.81237	1.38370
H	-0.05933	3.13160	1.06191
H	0.53524	2.52421	-0.47315
H	-1.69074	0.38726	-2.08182
H	-2.30443	2.02168	-2.17509
H	-1.07112	3.96426	-1.73489
H	-1.78326	4.54875	-0.23038
H	-0.11718	4.95084	-0.63162
H	-4.48010	1.30167	-1.12164
H	-3.88147	-0.35491	-0.99180
H	-4.14174	0.36989	-2.57904
H	-4.08462	3.15889	0.38861
H	-3.00557	3.83196	1.61639
H	-4.48480	3.00448	2.09708
H	-1.50887	-0.67617	2.25640

H	-0.15804	-2.77634	2.23372
H	0.88909	-1.34830	2.32898
H	0.69584	-2.22284	0.78690
H	-0.73309	-1.89916	-1.22130
H	-2.36742	-3.16064	-2.59081
H	-4.57792	-3.76337	-1.64293
H	-5.15720	-3.09889	0.67433
H	-3.53283	-1.81704	2.03816
C	5.17297	0.77991	-0.71220
C	6.45712	0.29523	-0.47718
C	6.63493	-0.88340	0.24120
C	5.52834	-1.58121	0.72272
C	4.24574	-1.10276	0.48076
C	4.06354	0.08122	-0.23906
C	2.67215	0.58324	-0.53054
C	1.93286	-0.24843	-1.56428
O	1.87090	0.53097	0.68235
H	5.03453	1.70452	-1.26668
H	7.31691	0.84209	-0.84858
H	7.63523	-1.25833	0.42909
H	5.66684	-2.49871	1.28455
H	3.38084	-1.64487	0.85563
H	2.71946	1.62892	-0.85902
H	0.92410	0.14099	-1.74160
H	2.48127	-0.22531	-2.50743
H	1.86867	-1.28954	-1.23372
H	2.34381	0.95030	1.41403

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$SiEt_3$-(PhEtOH-PhEtO)

Si	-0.26623	1.04499	-0.43138
O	-0.37138	-0.64281	-0.50834
C	-0.12290	1.52156	1.38567
C	1.35176	1.41316	-1.31831
C	-1.73520	1.92279	-1.24339
C	1.51567	2.83226	-1.87643
C	-2.77261	2.49157	-0.26605
C	0.58107	2.86681	1.60657
C	-1.46156	-1.51593	-0.78670
C	-1.58838	-1.72673	-2.28816
C	-2.72594	-1.06028	-0.07731
C	-3.93260	-0.82960	-0.73650
C	-5.06054	-0.41869	-0.02646
C	-4.99380	-0.23523	1.35064
C	-3.79142	-0.46343	2.01935
C	-2.66948	-0.87345	1.30820
H	0.44572	0.72359	1.88021
H	-1.11824	1.52676	1.84595
H	2.15777	1.20212	-0.60470
H	1.47582	0.67697	-2.12285
H	-2.22525	1.23832	-1.94558
H	-1.33047	2.73628	-1.85854
H	0.82028	3.02388	-2.69895
H	1.33488	3.59567	-1.11264
H	2.52794	2.99060	-2.26029
H	-2.32097	3.23585	0.39788
H	-3.20477	1.70937	0.36408
H	-3.59469	2.98054	-0.79719
H	0.06051	3.68581	1.09684
H	1.60575	2.83697	1.22057
H	0.63519	3.12781	2.66772
H	-1.16738	-2.47721	-0.34206
H	-2.35497	-2.47248	-2.51529
H	-0.63261	-2.09074	-2.67193
H	-1.83993	-0.79505	-2.80382
H	-4.00037	-0.96646	-1.81121
H	-5.99190	-0.23987	-0.55414
H	-5.87217	0.08477	1.90157
H	-3.73029	-0.32425	3.09407
H	-1.72877	-1.05119	1.82455
C	3.98707	-0.86738	-0.63345
C	4.72883	0.29497	-0.46605
C	4.58783	1.05246	0.69802
C	3.71037	0.62830	1.69006
C	2.97826	-0.54933	1.52338
C	3.10384	-1.30716	0.35964
C	2.29969	-2.57281	0.08665
C	1.31739	-2.94087	1.19274
O	1.63908	-2.46324	-1.16261
H	4.06478	-1.44450	-1.55048
H	5.41019	0.61995	-1.24621
H	5.15925	1.96599	0.82823
H	3.59182	1.21075	2.59893
H	2.30522	-0.87032	2.31232
H	3.01034	-3.39995	-0.03750
H	0.77441	-3.84116	0.89631
H	1.82569	-3.13867	2.14082
H	0.59445	-2.13049	1.34035
H	1.05436	-1.68901	-1.08270

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$[SiPhH_2$-$(PhEtOH)_2]^+$

Si	0.709160	1.010040	-2.367516
O	0.196085	-0.639283	-2.043483
C	0.485739	2.089508	-0.890478
C	1.139770	-1.754086	-1.738620
C	0.306513	-3.010337	-1.588355
C	1.974327	-1.386275	-0.540861
C	1.413710	-1.361981	0.739286
C	2.195654	-1.009626	1.833311
C	3.540037	-0.680464	1.658832
C	4.102861	-0.700454	0.385003
C	3.319745	-1.051949	-0.712777
C	1.321773	1.997595	0.233681
C	1.108756	2.816944	1.336951
C	0.071319	3.749485	1.325571
C	-0.753015	3.869608	0.207986
C	-0.546956	3.042089	-0.892882
H	-0.232509	1.406377	-3.432475
H	2.088522	0.811416	-2.837033
H	-0.854101	-0.831781	-1.904323
H	1.773244	-1.818420	-2.627732

H	0.975972	-3.853454	-1.408706
H	-0.267124	-3.208968	-2.496802
H	-0.379196	-2.929079	-0.740789
H	0.366987	-1.610501	0.887428
H	1.751971	-0.995199	2.823456
H	4.149693	-0.413631	2.515733
H	5.148724	-0.449866	0.245192
H	3.760371	-1.075583	-1.706358
H	2.145783	1.289289	0.248768
H	1.759652	2.735668	2.201476
H	-0.086975	4.393704	2.184436
H	-1.547270	4.608225	0.192706
H	-1.189322	3.149570	-1.764509
O	-2.205445	-0.947324	-1.757552
C	-2.775926	-0.090363	-0.715736
C	-4.290010	-0.187711	-0.779228
C	-2.199772	-0.548351	0.599198
C	-2.327660	-1.884308	0.995863
C	-1.848101	-2.292819	2.236142
C	-1.247170	-1.366779	3.091304
C	-1.115337	-0.038667	2.696223
C	-1.585935	0.369914	1.449090
H	-2.730469	-0.879734	-2.568240
H	-2.450882	0.938988	-0.913457
H	-4.672230	0.157616	-1.745467
H	-4.726080	0.441427	-0.001151
H	-4.614657	-1.217274	-0.610288
H	-2.803817	-2.601753	0.332238
H	-1.951572	-3.328359	2.542281
H	-0.886407	-1.684625	4.064217
H	-0.644153	0.685125	3.353639
H	-1.479446	1.407275	1.142233

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$SiPhH_2$-(PhEtOH-PhEtO)

Si	0.244286	-0.657626	-2.069244
O	-0.157067	-1.699373	-0.815090
C	1.102703	0.887300	-1.490356
C	0.811344	-2.529756	-0.165638
C	0.065561	-3.377043	0.854676
C	1.902781	-1.691280	0.467989
C	1.559113	-0.599042	1.270320
C	2.547324	0.201240	1.826566
C	3.892897	-0.090676	1.599177
C	4.241952	-1.180315	0.809337
C	3.246677	-1.975420	0.240866
C	2.489855	1.047983	-1.599223
C	3.122614	2.159074	-1.050044
C	2.373241	3.124914	-0.381419
C	0.991901	2.982123	-0.268624
C	0.361842	1.872748	-0.823912
H	-1.066324	-0.333080	-2.674751
H	1.126633	-1.390778	-3.014396
H	1.268516	-3.185869	-0.921231
H	0.756717	-4.062007	1.351342
H	-0.727034	-3.951770	0.369140
H	-0.388933	-2.732335	1.612317
H	0.509565	-0.350103	1.407187
H	2.269796	1.066314	2.420752
H	4.665496	0.538977	2.029079
H	5.287035	-1.407753	0.624461
H	3.517618	-2.817174	-0.392114
H	3.086819	0.286256	-2.095662
H	4.199708	2.266508	-1.132796
H	2.867217	3.989302	0.052195
H	0.401950	3.731207	0.251159
H	-0.716435	1.768915	-0.724033
O	-2.838753	-2.136388	-0.109234
C	-3.566371	-0.989864	-0.476896
C	-5.010126	-1.231062	-0.048715
C	-3.027307	0.277616	0.170064
C	-2.212563	0.208645	1.300575
C	-1.785628	1.372153	1.938242
C	-2.177248	2.619166	1.457619
C	-2.984295	2.697398	0.323200
C	-3.399427	1.533203	-0.318098
H	-1.922196	-2.023774	-0.414440
H	-3.542500	-0.846951	-1.570614
H	-5.387718	-2.139166	-0.523824
H	-5.648482	-0.387516	-0.322502
H	-5.045412	-1.361274	1.036247
H	-1.930601	-0.770900	1.674475
H	-1.150742	1.303933	2.817173
H	-1.853492	3.525126	1.960526
H	-3.286149	3.665501	-0.064281
H	-4.025526	1.596626	-1.205639

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Phenol-BEt_3

C	-1.366016	-2.012429	0.475845
C	-1.945669	-2.996057	-0.315405
C	-1.178936	-3.713835	-1.232910
C	0.181325	-3.445120	-1.346780
C	0.774870	-2.458649	-0.562932
C	-0.006169	-1.738414	0.338535
O	0.505428	-0.724308	1.099177
B	0.348181	1.421839	-0.274350
C	0.582865	2.258719	1.048930
C	-0.598354	2.337749	2.017930
C	1.577706	1.007307	-1.186224
C	2.979947	1.058601	-0.575710
C	-1.123710	1.216874	-0.819016
C	-1.304523	0.440276	-2.125769
H	-1.944062	-1.442371	1.195267
H	-3.006028	-3.203423	-0.214471
H	-1.637899	-4.478601	-1.849401
H	0.790182	-4.000849	-2.052466
H	1.835980	-2.239127	-0.656354
H	1.462955	-0.676359	0.978657
H	1.475847	1.897973	1.577275
H	0.859254	3.273553	0.714428
H	-0.373289	2.950056	2.895967

H	-1.482489	2.764774	1.534683
H	-0.867074	1.336024	2.367930
H	1.536677	1.700303	-2.043052
H	1.385929	0.026517	-1.643369
H	3.758169	0.799302	-1.299095
H	3.093758	0.365069	0.269405
H	3.207018	2.053994	-0.183027
H	-1.558091	2.224950	-0.922022
H	-1.721959	0.757480	-0.019227
H	-2.354612	0.391371	-2.428847
H	-0.943580	-0.589544	-2.032452
H	-0.747839	0.907202	-2.945151

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[Phenoxide-BEt_3]-

C	-1.479864	-1.860349	0.380921
C	-1.980040	-3.034858	-0.168143
C	-1.182516	-3.836502	-0.984415
C	0.131741	-3.442137	-1.234017
C	0.640741	-2.269008	-0.688957
C	-0.158535	-1.441912	0.126706
O	0.314862	-0.335698	0.678508
B	0.382657	1.014992	-0.107851
C	0.645479	2.110867	1.079366
C	-0.532180	2.255051	2.046955
C	1.632956	0.947813	-1.168908
C	2.995275	0.724435	-0.506878
C	-1.048232	1.303627	-0.871135
C	-1.255840	0.641966	-2.239718
H	-2.092071	-1.225254	1.014231
H	-3.006748	-3.327957	0.040031
H	-1.576215	-4.752732	-1.414575
H	0.769768	-4.058374	-1.863713
H	1.663329	-1.957999	-0.879389
H	1.534851	1.816500	1.657443
H	0.882293	3.094675	0.641316
H	-0.325925	2.911673	2.904258
H	-1.415698	2.655758	1.535435
H	-0.808448	1.268822	2.437530
H	1.665089	1.877758	-1.761056
H	1.461085	0.147356	-1.905931
H	3.813270	0.545133	-1.219172
H	2.945476	-0.135375	0.172874
H	3.280609	1.588113	0.105095
H	-1.153712	2.394253	-1.001132
H	-1.882897	1.015343	-0.211675
H	-2.236680	0.867981	-2.681989
H	-1.171890	-0.449110	-2.176573
H	-0.493762	0.976596	-2.953577

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Phenol-BPh_3

C	-1.963698	-1.503931	-1.478419
C	-2.115399	-2.777749	-2.019272
C	-1.188223	-3.276157	-2.930789
C	-0.095363	-2.498191	-3.304151
C	0.076037	-1.226324	-2.768093
C	-0.866021	-0.750330	-1.866691
O	-0.706015	0.506412	-1.275010
B	0.099416	0.593737	0.401857
C	0.528392	2.138435	0.379034
C	1.643991	2.551430	1.124845
C	1.250437	-0.499659	0.195968
C	1.013415	-1.862984	0.437372
C	-1.112041	0.269012	1.388798
C	-2.419804	0.720554	1.153339
C	2.017406	3.889455	1.204696
C	1.284484	4.860902	0.526611
C	0.170104	4.481659	-0.214513
C	-0.204321	3.140538	-0.275450
C	1.943218	-2.841445	0.097273
C	3.147356	-2.479768	-0.501590
C	-3.445294	0.503688	2.068363
C	-3.181348	-0.155119	3.267891
C	-1.887951	-0.589154	3.538696
C	-0.871992	-0.380607	2.607247
C	3.411001	-1.136660	-0.756411
C	2.471990	-0.166563	-0.411747
H	-2.663890	-1.099544	-0.756698
H	-2.966724	-3.381493	-1.723459
H	-1.314049	-4.270149	-3.345924
H	0.638786	-2.884485	-4.002885
H	0.951549	-0.630688	-3.010534
H	2.231420	1.803914	1.653386
H	0.067200	-2.165163	0.878779
H	-2.641058	1.249119	0.228369
H	2.884133	4.175104	1.793203
H	1.576889	5.904829	0.580626
H	-0.415557	5.231073	-0.738617
H	-1.099617	2.877804	-0.836040
H	1.725157	-3.887258	0.291561
H	3.874877	-3.239932	-0.769879
H	-4.449363	0.856529	1.851801
H	-3.977435	-0.322255	3.986762
H	-1.668540	-1.094956	4.474217
H	0.133115	-0.728959	2.833565
H	4.347176	-0.844928	-1.223343
H	2.691724	0.877152	-0.625222
H	-0.108684	1.056943	-1.806214

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[Phenoxide-BPh_3]-

C	-1.008514	-1.945164	-1.446285
C	-1.418632	-2.999994	-2.254831
C	-1.672164	-2.819920	-3.612680
C	-1.507674	-1.546942	-4.158540
C	-1.097173	-0.484975	-3.365824
C	-0.836646	-0.659056	-1.992677
O	-0.464580	0.414863	-1.304129
B	0.047324	0.419017	0.119573
C	0.638650	1.930005	0.337710
C	1.684045	2.215749	1.226868

C	1.267783	-0.666294	0.278216
C	1.394745	-1.615899	1.299760
C	-1.179984	0.209634	1.181475
C	-2.506644	0.016317	0.771511
C	2.135236	3.516923	1.446501
C	1.552065	4.582171	0.765835
C	0.516485	4.326828	-0.131826
C	0.072040	3.022860	-0.335157
C	2.486288	-2.484011	1.374499
C	3.489668	-2.430372	0.413271
C	-3.553994	-0.114883	1.683572
C	-3.305444	-0.050956	3.051391
C	-1.999494	0.158342	3.491454
C	-0.966138	0.291014	2.568038
C	3.387423	-1.500923	-0.621896
C	2.297468	-0.638988	-0.677885
H	-0.821823	-2.101917	-0.390766
H	-1.542928	-3.983339	-1.808276
H	-1.991097	-3.652317	-4.232303
H	-1.699739	-1.379439	-5.215712
H	-0.962551	0.510495	-3.777466
H	2.169285	1.391903	1.748652
H	0.612889	-1.690356	2.052754
H	-2.724723	-0.028958	-0.292545
H	2.950368	3.699019	2.143410
H	1.902761	5.598278	0.928251
H	0.055429	5.149620	-0.674160
H	-0.732398	2.829574	-1.040510
H	2.548041	-3.208115	2.183853
H	4.340073	-3.105402	0.465384
H	-4.569108	-0.266278	1.323518
H	-4.118028	-0.154293	3.765897
H	-1.789214	0.226126	4.556423
H	0.043477	0.479148	2.931385
H	4.161423	-1.451129	-1.384255
H	2.226299	0.084363	-1.488312

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Phenol-B(C_6F_5)Ph_2

C	-2.345866	-1.267257	-1.592703
C	-2.684167	-2.478014	-2.193246
C	-1.748082	-3.170659	-2.954960
C	-0.467510	-2.649068	-3.129248
C	-0.115537	-1.435757	-2.548372
C	-1.064915	-0.770127	-1.786226
O	-0.681245	0.448129	-1.201145
B	0.195677	0.559816	0.318554
C	0.515123	2.128705	0.330839
C	0.446787	2.870069	1.517956
C	1.397485	-0.463117	0.077703
C	1.217538	-1.847880	0.223881
C	-0.907471	0.133675	1.438344
C	-2.246495	0.503362	1.367349
C	0.766789	4.224963	1.553600
C	1.152484	4.880310	0.387904
C	1.222613	4.169623	-0.807639
C	0.911605	2.812792	-0.829625
C	2.222225	-2.755294	-0.091723
C	3.449402	-2.293715	-0.564261
C	-3.199000	0.209326	2.330265
C	-2.802643	-0.463629	3.477355
C	-1.471246	-0.821245	3.626434
C	-0.556752	-0.512632	2.623485
C	3.660600	-0.925585	-0.706476
C	2.645204	-0.025672	-0.385027
F	-2.708069	1.197416	0.290629
F	-4.469719	0.573898	2.170289
F	-3.688566	-0.753848	4.423811
F	-1.076203	-1.445449	4.732937
F	0.711500	-0.851983	2.864629
H	-3.065427	-0.715134	-0.997785
H	-3.683238	-2.877947	-2.057918
H	-2.016052	-4.115962	-3.414134
H	0.265467	-3.187445	-3.720124
H	0.877830	-1.013176	-2.653601
H	0.137888	2.377823	2.437330
H	0.259351	-2.226567	0.575842
H	0.708408	4.770711	2.490356
H	1.395482	5.938025	0.410027
H	1.521278	4.672331	-1.722581
H	0.978044	2.269583	-1.769797
H	2.049813	-3.820523	0.027986
H	4.238503	-2.997165	-0.812093
H	4.618347	-0.557305	-1.061564
H	2.828831	1.039770	-0.491679
H	-1.449473	1.035977	-1.103009

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[Phenoxide-B(C_6F_5)Ph_2]-

C	-1.154807	-1.931738	-1.343691
C	-1.604385	-3.005469	-2.107216
C	-1.784773	-2.893678	-3.483022
C	-1.506995	-1.672141	-4.096942
C	-1.055534	-0.593297	-3.351233
C	-0.867940	-0.701071	-1.960923
O	-0.441354	0.387493	-1.321099
B	0.055229	0.416354	0.090068
C	0.641507	1.919610	0.333882
C	1.580427	2.216115	1.330902
C	1.302385	-0.681558	0.230958
C	1.313170	-1.866670	0.958974
C	-1.158727	0.222895	1.165525
C	-2.496552	0.272326	0.755381
C	2.015006	3.517088	1.575035
C	1.515157	4.572882	0.816964
C	0.581965	4.305886	-0.182382
C	0.156190	3.000037	-0.414264
C	2.399893	-2.735641	1.016198
C	3.548970	-2.436146	0.306103
C	-3.552033	0.225589	1.666734
C	-3.294566	0.135765	3.030528
C	-1.971106	0.097884	3.469130

C	-0.931019	0.144354	2.547783
C	3.587095	-1.278723	-0.456640
C	2.478334	-0.442037	-0.483224
F	0.231738	-2.272728	1.646987
F	2.342883	-3.861273	1.741213
F	4.605612	-3.256470	0.345841
F	4.690821	-0.988104	-1.157936
F	2.591461	0.641755	-1.259578
H	-1.043350	-2.035530	-0.270992
H	-1.820640	-3.946680	-1.608487
H	-2.135536	-3.739555	-4.065905
H	-1.639947	-1.559792	-5.170076
H	-0.827395	0.361393	-3.814357
H	1.995223	1.403489	1.926688
H	-2.714310	0.350255	-0.307247
H	2.748791	3.707650	2.354731
H	1.851404	5.590012	1.000315
H	0.186424	5.120625	-0.784777
H	-0.565948	2.797438	-1.200716
H	-4.578318	0.260519	1.308843
H	-4.112361	0.098431	3.745381
H	-1.753048	0.032541	4.532387
H	0.094997	0.116051	2.912691

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Phenol-B(C_6F_5)$_2$Ph

C	-2.259386	-1.301699	-1.722475
C	-2.625569	-2.533336	-2.260871
C	-1.677296	-3.335596	-2.888070
C	-0.356005	-2.905089	-2.991175
C	0.026875	-1.672872	-2.471849
C	-0.937491	-0.899950	-1.842408
O	-0.533354	0.350301	-1.323218
B	0.159017	0.512306	0.191636
C	0.517740	2.096347	0.276612
C	1.378595	2.503108	1.295997
C	1.404031	-0.481301	0.091420
C	1.286536	-1.846726	0.383423
C	-1.006584	0.181014	1.276020
C	-2.317139	0.610821	1.092309
C	1.733939	3.826756	1.515671
C	1.200434	4.818326	0.702488
C	0.318724	4.468077	-0.308232
C	-0.004738	3.129306	-0.490258
C	2.324264	-2.739059	0.132546
C	3.515001	-2.280792	-0.425685
C	-3.341420	0.425014	2.006383
C	-3.050663	-0.191352	3.215937
C	-1.751060	-0.599370	3.474753
C	-0.758188	-0.399090	2.519477
C	3.658845	-0.928280	-0.724935
C	2.613098	-0.045415	-0.466381
F	1.890510	1.590156	2.126982
F	-2.656104	1.265856	-0.048660
F	2.568313	4.154834	2.498053
F	1.524890	6.091661	0.897277
F	-0.213058	5.407269	-1.087044
F	-0.895416	2.877762	-1.481537
F	-4.578485	0.841120	1.744127
F	-4.007040	-0.379110	4.117998
F	-1.459843	-1.171147	4.639751
F	0.470351	-0.786234	2.864753
H	-2.986644	-0.662785	-1.234548
H	-3.656063	-2.862265	-2.183283
H	-1.967991	-4.296052	-3.299534
H	0.385039	-3.528205	-3.479657
H	1.049465	-1.316407	-2.529753
H	0.355531	-2.227446	0.797238
H	2.203173	-3.791679	0.368716
H	4.327567	-2.973009	-0.623543
H	4.585137	-0.561623	-1.156476
H	2.737551	1.006325	-0.714645
H	-1.217284	1.030596	-1.456909

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[Phenoxide-B(C_6F_5)$_2$Ph]-

C	-1.141981	-1.925560	-1.372529
C	-1.633004	-2.988341	-2.126541
C	-1.807114	-2.880657	-3.502712
C	-1.481260	-1.675920	-4.126647
C	-0.990062	-0.609095	-3.389645
C	-0.808970	-0.714108	-1.999763
O	-0.336532	0.363031	-1.370197
B	0.110170	0.404464	0.040118
C	0.637848	1.921656	0.311897
C	1.593064	2.247194	1.283102
C	1.339803	-0.694262	0.232276
C	1.317550	-1.887359	0.945556
C	-1.140964	0.203079	1.112649
C	-2.485139	0.333086	0.777168
C	1.972711	3.565856	1.524975
C	1.397220	4.604016	0.797032
C	0.442324	4.305670	-0.172390
C	0.072058	2.983561	-0.406085
C	2.393409	-2.764741	1.028292
C	3.568973	-2.462820	0.362241
C	-3.516541	0.296724	1.712789
C	-3.220456	0.143573	3.055966
C	-1.893689	0.029455	3.444775
C	-0.900715	0.072294	2.478054
C	3.642096	-1.295414	-0.381316
C	2.539740	-0.450743	-0.436843
F	0.207696	-2.290472	1.592427
F	-2.874922	0.511288	-0.493248
F	2.303435	-3.899056	1.734297
F	4.616712	-3.291567	0.427000
F	-4.793646	0.417934	1.327941
F	-4.198833	0.109748	3.968500
F	-1.592739	-0.110652	4.742273
F	0.362552	-0.027262	2.929203
F	4.770962	-1.000853	-1.038236
F	2.685385	0.644248	-1.191418

H	-1.025489	-2.031944	-0.300684
H	-1.884402	-3.916688	-1.620457
H	-2.190036	-3.716879	-4.079014
H	-1.610124	-1.567343	-5.200494
H	-0.728489	0.333657	-3.859021
H	2.053350	1.449097	1.861306
H	2.721989	3.783821	2.282053
H	1.690987	5.633898	0.981689
H	-0.013154	5.107074	-0.749252
H	-0.667738	2.753449	-1.168551

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Phenol-B(C_6F_5)$_3$

C	-1.795111	-1.689117	-1.664827
C	-1.830073	-2.877715	-2.391281
C	-0.895235	-3.119163	-3.394182
C	0.083654	-2.170708	-3.684673
C	0.129388	-0.974212	-2.976215
C	-0.814632	-0.764432	-1.984504
O	-0.708117	0.450958	-1.259459
B	-0.018232	0.491597	0.237730
C	0.525478	2.013395	0.364938
C	1.746835	2.380589	0.920073
C	1.092493	-0.670514	0.151412
C	0.970371	-1.929438	0.731111
C	-1.205340	0.306012	1.331762
C	-2.569696	0.442919	1.127765
C	2.132747	3.706906	1.080919
C	1.276429	4.725659	0.688139
C	0.040059	4.407809	0.141925
C	-0.300503	3.071729	0.006215
C	1.919186	-2.934223	0.573478
C	3.038287	-2.700006	-0.209452
C	-3.514834	0.389018	2.145735
C	-3.087656	0.212943	3.451768
C	-1.727874	0.089503	3.715337
C	-0.827739	0.148638	2.663960
C	3.194134	-1.466234	-0.827920
C	2.227537	-0.492580	-0.637221
F	2.618306	1.454464	1.328191
F	-0.101446	-2.250057	1.464945
F	-3.071686	0.624416	-0.123357
F	3.315518	4.006910	1.609626
F	1.634801	5.995726	0.835203
F	-0.796827	5.372195	-0.232147
F	-1.529054	2.807295	-0.502009
F	1.751607	-4.119917	1.154336
F	3.948567	-3.651397	-0.378963
F	-4.811470	0.512044	1.873831
F	-3.968503	0.161195	4.443803
F	-1.309523	-0.073882	4.966209
F	0.473484	0.041541	2.957197
F	4.251575	-1.238964	-1.604295
F	2.398750	0.660711	-1.302375
H	-2.509518	-1.487053	-0.876108
H	-2.588872	-3.617942	-2.162947
H	-0.927049	-4.050402	-3.949018
H	0.815424	-2.360506	-4.462140
H	0.885209	-0.218146	-3.160053
H	-1.550115	0.944049	-1.248938

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[Phenoxide-B(C_6F_5)$_3$]-

C	-1.125891	-1.901932	-1.405575
C	-1.565203	-2.966588	-2.187484
C	-1.610874	-2.873311	-3.575115
C	-1.208700	-1.683051	-4.181168
C	-0.766146	-0.614663	-3.415235
C	-0.714472	-0.706266	-2.015177
O	-0.281128	0.372790	-1.354795
B	0.106555	0.383597	0.066326
C	0.649278	1.917103	0.354133
C	1.810896	2.285023	1.022726
C	1.283731	-0.758325	0.274714
C	1.193130	-1.939517	0.997892
C	-1.161347	0.234491	1.113962
C	-2.505153	0.298053	0.765509
C	2.178841	3.607719	1.249096
C	1.355935	4.631597	0.811360
C	0.172983	4.316516	0.160702
C	-0.157556	2.982705	-0.042665
C	2.202461	-2.896269	1.047926
C	3.374112	-2.685906	0.342538
C	-3.532627	0.295959	1.707258
C	-3.228211	0.249691	3.056782
C	-1.898376	0.205188	3.453356
C	-0.909761	0.209302	2.482574
C	3.514604	-1.525116	-0.404012
C	2.478356	-0.603534	-0.425111
F	2.664778	1.365573	1.496534
F	0.078254	-2.250546	1.684798
F	-2.892541	0.360476	-0.512659
F	3.317625	3.901725	1.888317
F	1.693109	5.908497	1.021404
F	-0.639985	5.298805	-0.247007
F	-1.339860	2.754537	-0.628816
F	2.047843	-4.018588	1.760816
F	4.357629	-3.590605	0.376777
F	-4.813247	0.347532	1.321718
F	-4.203874	0.250688	3.971457
F	-1.595215	0.169487	4.756613
F	0.362584	0.186748	2.914080
F	4.645129	-1.310583	-1.087048
F	2.687262	0.502286	-1.152667
H	-1.110367	-1.994982	-0.325495
H	-1.879019	-3.883343	-1.695687
H	-1.954750	-3.710458	-4.174101
H	-1.237806	-1.586834	-5.263327
H	-0.447093	0.317590	-3.869281

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[Phenol-SiEt$_3$]$^+$

C	-1.489545	-1.944571	0.413262
C	-2.016015	-3.064664	-0.226347
C	-1.220988	-3.817831	-1.088673
C	0.107898	-3.466039	-1.318046
C	0.653363	-2.345521	-0.694403
C	-0.170565	-1.623138	0.150900
O	0.343860	-0.426701	0.763860
Si	0.417952	1.196128	-0.170859
C	0.673161	2.333870	1.277840
C	-0.552053	2.428696	2.202285
C	1.874010	0.967922	-1.305319
C	3.200490	0.693883	-0.579895
C	-1.255568	1.263704	-0.978368
C	-1.388726	0.509895	-2.311794
H	-2.079142	-1.340640	1.094547
H	-3.046826	-3.347707	-0.046210
H	-1.638658	-4.688219	-1.582066
H	0.723772	-4.059495	-1.984065
H	1.684429	-2.048613	-0.859623
H	1.000854	-0.603793	1.457806
H	1.563808	2.022199	1.839387
H	0.924754	3.323953	0.876416
H	-0.350387	3.088699	3.047528
H	-1.419621	2.828493	1.671125
H	-0.831308	1.450999	2.607002
H	1.957010	1.883328	-1.906123
H	1.642670	0.171383	-2.022813
H	4.015833	0.559503	-1.292749
H	3.155110	-0.217219	0.028329
H	3.475823	1.519926	0.080997
H	-1.464372	2.331759	-1.132143
H	-2.010332	0.927705	-0.256779
H	-2.386364	0.652849	-2.730856
H	-1.230500	-0.565396	-2.190198
H	-0.668036	0.875501	-3.047955

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Phenoxide-$SiEt_3$

C	-1.509693	-1.941845	0.398850
C	-2.036309	-3.071832	-0.218424
C	-1.244272	-3.850675	-1.059786
C	0.086005	-3.497286	-1.272438
C	0.622944	-2.368747	-0.659470
C	-0.180316	-1.584290	0.169686
O	0.328976	-0.464949	0.767153
Si	0.398811	1.007200	-0.068093
C	0.662972	2.270681	1.288546
C	-0.552466	2.396336	2.216958
C	1.839258	0.956534	-1.273434
C	3.192618	0.762639	-0.577360
C	-1.225431	1.293486	-0.975076
C	-1.362581	0.557722	-2.316183
H	-2.109343	-1.323390	1.059218
H	-3.071901	-3.344498	-0.041183
H	-1.659191	-4.729784	-1.540865
H	0.712810	-4.103601	-1.918700
H	1.660376	-2.084668	-0.807733
H	1.546461	1.972684	1.865758
H	0.904193	3.241291	0.836847
H	-0.370069	3.101196	3.032799
H	-1.433991	2.746032	1.670283
H	-0.801326	1.428102	2.661365
H	1.838908	1.884437	-1.860510
H	1.662454	0.147938	-1.994097
H	4.012751	0.674089	-1.295239
H	3.190031	-0.140533	0.041510
H	3.421706	1.605284	0.082178
H	-1.328378	2.376074	-1.131399
H	-2.047735	1.011084	-0.305222
H	-2.322255	0.773842	-2.794317
H	-1.293878	-0.526777	-2.186646
H	-0.573911	0.857670	-3.013111

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$[Phenol\text{-}SiPhH_2]^+$

C	-0.188521	-3.960562	0.632186
C	0.455792	-5.188930	0.501409
C	1.829716	-5.287562	0.714550
C	2.578094	-4.164807	1.062704
C	1.956504	-2.926256	1.208027
C	0.592640	-2.875765	0.990269
O	-0.039034	-1.579748	1.121199
Si	-0.331350	-0.548087	-0.382305
C	-1.467575	-1.465530	-1.475375
C	-2.854264	-1.246506	-1.400058
C	-3.722356	-1.968381	-2.210959
C	-3.213723	-2.910424	-3.103490
C	-1.839980	-3.134481	-3.192973
C	-0.968411	-2.415545	-2.384738
H	-1.254092	-3.852815	0.456452
H	-0.120043	-6.066076	0.229406
H	2.321117	-6.248260	0.608990
H	3.645937	-4.248617	1.228875
H	2.506250	-2.034912	1.489667
H	1.062452	-0.438541	-0.826721
H	-0.902747	0.628298	0.288177
H	-3.258962	-0.501790	-0.718824
H	-4.790812	-1.792154	-2.154713
H	-3.892142	-3.468632	-3.740192
H	-1.451932	-3.861800	-3.897515
H	0.101800	-2.591062	-2.464242
H	-0.655806	-1.532884	1.871295

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Phenoxide-$SiPhH_2$

C	-0.219614	-4.015751	0.964826
C	0.412582	-5.232878	0.732682
C	1.795141	-5.290798	0.568612
C	2.547197	-4.121158	0.642462
C	1.925903	-2.897503	0.877185
C	0.541536	-2.849784	1.037071
O	-0.083821	-1.648907	1.270592

Si	-0.414505	-0.645624	-0.031165
C	-1.462993	-1.518776	-1.301130
C	-2.810050	-1.174704	-1.474703
C	-3.604154	-1.833284	-2.410330
C	-3.059660	-2.853645	-3.184614
C	-1.722586	-3.213078	-3.025161
C	-0.931673	-2.548778	-2.093602
H	-1.295497	-3.945792	1.084602
H	-0.180164	-6.140270	0.676314
H	2.283358	-6.242231	0.386903
H	3.624950	-4.158391	0.520069
H	2.497098	-1.977329	0.946915
H	0.871221	-0.221891	-0.637939
H	-1.149395	0.506921	0.527334
H	-3.246126	-0.381158	-0.872426
H	-4.645090	-1.551884	-2.534060
H	-3.676498	-3.369515	-3.913913
H	-1.297777	-4.009165	-3.628251
H	0.110358	-2.840412	-1.977446

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BEt_3-$(Phenol)_2$

C	-0.05207	1.75310	-0.58261
C	-0.32804	2.96874	-1.19751
C	-1.34494	3.79475	-0.72116
C	-2.08525	3.40176	0.38932
C	-1.81948	2.18874	1.01974
C	-0.81180	1.36959	0.51970
O	-0.53199	0.14772	1.08772
H	0.72484	1.09179	-0.95208
H	0.25611	3.26852	-2.06115
H	-1.55633	4.73863	-1.21102
H	-2.87611	4.03804	0.77252
H	-2.39542	1.87478	1.88720
H	-1.17659	-0.05681	1.77830
B	-2.22979	-1.67503	-0.21543
C	-1.47897	-2.95746	0.33174
C	-0.60879	-3.74354	-0.65247
C	-3.38390	-1.01907	0.64947
C	-3.47455	-1.36778	2.13809
C	-1.90055	-1.11126	-1.65144
C	-2.73313	0.05985	-2.17871
H	-0.86552	-2.62675	1.18777
H	-2.22125	-3.62457	0.79481
H	-0.12251	-4.59641	-0.17042
H	-1.21072	-4.13430	-1.47916
H	0.17507	-3.11249	-1.07807
H	-4.30665	-1.36442	0.15158
H	-3.40869	0.06804	0.49805
H	-4.33045	-0.89069	2.62362
H	-2.58280	-1.06130	2.70435
H	-3.56403	-2.44654	2.29179
H	-1.94131	-1.95349	-2.35860
H	-0.82917	-0.84882	-1.63993
H	-2.41989	0.36100	-3.18257
H	-2.64728	0.94116	-1.53464
H	-3.79521	-0.20264	-2.23114
C	3.80098	-1.04583	-0.79963
C	5.04757	-0.50190	-0.51765
C	5.20197	0.42979	0.50810
C	4.09036	0.81279	1.25212
C	2.83434	0.27693	0.98103
C	2.69167	-0.65715	-0.04699
O	1.48929	-1.20771	-0.36884
H	3.66163	-1.77286	-1.59225
H	5.90721	-0.80988	-1.10465
H	6.17771	0.85092	0.72389
H	4.19525	1.53809	2.05299
H	1.96385	0.57421	1.55921
H	0.80628	-0.90038	0.24887

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[BEt_3-(Phenol-Phenoxide)]-

C	-1.65946	1.63157	-1.13830
C	-2.45343	2.77080	-1.06995
C	-2.94280	3.22157	0.15474
C	-2.61341	2.52334	1.31530
C	-1.81643	1.38522	1.25726
C	-1.34144	0.91516	0.02410
O	-0.56631	-0.18065	-0.05372
H	-1.27181	1.26592	-2.08437
H	-2.69525	3.30999	-1.98212
H	-3.56664	4.10885	0.20501
H	-2.97953	2.87028	2.27815
H	-1.55101	0.83600	2.15441
B	-1.21331	-1.64100	0.01149
C	0.00077	-2.59757	-0.52235
C	0.22434	-2.59427	-2.03914
C	-1.60061	-1.95912	1.56871
C	-0.42771	-1.88558	2.54945
C	-2.51800	-1.71002	-0.98039
C	-3.85859	-1.19414	-0.44113
H	0.94516	-2.31145	-0.03176
H	-0.19192	-3.63290	-0.19652
H	1.07543	-3.21566	-2.34707
H	-0.66083	-2.96580	-2.56822
H	0.41917	-1.58067	-2.40586
H	-2.03733	-2.97063	1.60825
H	-2.40159	-1.29231	1.92356
H	-0.70179	-2.13488	3.58353
H	0.00110	-0.87526	2.56312
H	0.37993	-2.56402	2.25093
H	-2.65584	-2.76554	-1.26817
H	-2.29061	-1.19003	-1.92493
H	-4.67422	-1.29397	-1.17031
H	-3.80550	-0.13721	-0.15714
H	-4.15728	-1.74888	0.45602
C	3.83509	0.87842	-1.18437
C	4.97597	0.91996	-0.39282
C	4.92425	0.55863	0.95259
C	3.70462	0.15401	1.49316
C	2.55351	0.10835	0.71599

C	2.60907	0.47102	-0.63920
O	1.53449	0.44744	-1.43715
H	3.86132	1.15503	-2.23338
H	5.91769	1.23773	-0.83332
H	5.81804	0.59064	1.56765
H	3.64344	-0.13354	2.53945
H	1.59982	-0.20615	1.12924
H	0.72679	0.13118	-0.92851

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BPh_3-$(Phenol)_2$

C	-1.81052	0.94286	2.22678
C	-3.02223	1.42902	2.70568
C	-3.64298	2.51515	2.09189
C	-3.03907	3.12193	0.99417
C	-1.82109	2.65479	0.51052
C	-1.22239	1.56330	1.12900
O	-0.02785	1.04069	0.68073
H	-1.32690	0.07725	2.66830
H	-3.48787	0.94673	3.55893
H	-4.59180	2.88438	2.46554
H	-3.51765	3.96260	0.50222
H	-1.35359	3.11420	-0.35585
H	0.15847	1.33125	-0.22448
B	-0.78224	-1.09082	-0.96209
C	0.59236	-0.97468	-1.72277
C	0.64462	-1.08354	-3.12368
C	-1.99967	-0.19733	-1.40388
C	-3.22543	-0.25376	-0.71308
C	-0.97122	-2.15614	0.18013
C	-0.18572	-2.20849	1.34307
C	1.85153	-1.00443	-3.81248
C	3.03790	-0.77877	-3.11763
C	3.01445	-0.66286	-1.73027
C	1.80795	-0.78670	-1.04619
C	-4.27722	0.60162	-1.02077
C	-4.12970	1.54794	-2.03271
C	-0.38297	-3.19728	2.30278
C	-1.35147	-4.17996	2.11126
C	-2.13175	-4.15873	0.95932
C	-1.95017	-3.15051	0.01604
C	-2.92387	1.64227	-2.72296
C	-1.87453	0.78459	-2.40489
H	-0.27464	-1.24380	-3.68229
H	-3.34373	-0.96715	0.09671
H	0.58172	-1.46131	1.52203
H	1.86504	-1.10761	-4.89323
H	3.97699	-0.69666	-3.65606
H	3.92962	-0.48121	-1.17236
H	1.81709	-0.72273	0.03654
H	-5.20576	0.54237	-0.46185
H	-4.94843	2.21969	-2.27349
H	0.23000	-3.20416	3.19887
H	-1.49636	-4.95709	2.85521
H	-2.88803	-4.92080	0.79819
H	-2.57926	-3.13834	-0.87148
H	-2.80030	2.38616	-3.50418
H	-0.93417	0.88346	-2.94015
C	4.49904	-0.01033	1.71358
C	5.64720	0.40436	1.04900
C	5.62742	1.53301	0.22959
C	4.44302	2.25062	0.08847
C	3.28792	1.84926	0.75285
C	3.31474	0.71443	1.56629
O	2.21284	0.26498	2.22229
H	4.49271	-0.89123	2.34604
H	6.56473	-0.16337	1.16829
H	6.52539	1.84975	-0.28925
H	4.41293	3.13195	-0.54441
H	2.36347	2.41103	0.65068
H	1.42473	0.71351	1.87297

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[BPh_3-(Phenol-Phenoxide)]-

C	-0.44397	-2.22173	1.47657
C	-0.52166	-3.60076	1.65111
C	-0.43583	-4.45989	0.55879
C	-0.27437	-3.92601	-0.71878
C	-0.19817	-2.55067	-0.90406
C	-0.27842	-1.68693	0.19527
O	-0.25845	-0.34375	0.00804
H	-0.50983	-1.54082	2.31823
H	-0.65150	-4.00483	2.65118
H	-0.49604	-5.53474	0.70032
H	-0.20402	-4.58557	-1.57911
H	-0.05188	-2.11651	-1.88833
B	1.07806	0.44282	-0.07495
C	0.65981	1.92213	-0.60956
C	1.55949	2.99549	-0.51373
C	2.06863	-0.31799	-1.13242
C	2.77125	-1.48163	-0.77352
C	1.71748	0.56906	1.42552
C	0.88475	0.81240	2.53163
C	1.25741	4.26128	-1.00654
C	0.02370	4.49891	-1.61134
C	-0.89027	3.45539	-1.71741
C	-0.56936	2.18921	-1.22663
C	3.55136	-2.19074	-1.68328
C	3.65683	-1.75113	-3.00149
C	1.39004	1.00083	3.81481
C	2.76608	0.96774	4.03741
C	3.61896	0.75052	2.96053
C	3.09621	0.55432	1.68119
C	2.97530	-0.60131	-3.38967
C	2.19850	0.09783	-2.46522
H	2.52113	2.82882	-0.03076
H	2.69064	-1.84630	0.24937
H	-0.19210	0.86737	2.38117
H	1.98093	5.06789	-0.91380
H	-0.22146	5.48710	-1.99180
H	-1.85845	3.62472	-2.18218
H	-1.29480	1.38578	-1.32866

H	4.07326	-3.09027	-1.36625
H	4.26403	-2.29944	-3.71727
H	0.71008	1.18242	4.64365
H	3.16615	1.11550	5.03714
H	4.69527	0.72937	3.11512
H	3.78178	0.38072	0.85433
H	3.04960	-0.24625	-4.41487
H	1.67255	0.99412	-2.78647
C	-4.71298	0.74554	1.04359
C	-5.88713	0.45367	0.36242
C	-5.85758	-0.25395	-0.83872
C	-4.62766	-0.66659	-1.34575
C	-3.44245	-0.38373	-0.67543
C	-3.47591	0.32993	0.53211
O	-2.37139	0.63437	1.22888
H	-4.71918	1.29806	1.97727
H	-6.83706	0.78458	0.77392
H	-6.77710	-0.48016	-1.36884
H	-4.58419	-1.22148	-2.27881
H	-2.48490	-0.71312	-1.06798
H	-1.55459	0.32698	0.74838

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$B(C_6F_5)Ph_2$-$(Phenol)_2$

C	1.46982	1.55791	-2.38155
C	2.24191	2.69590	-2.60456
C	1.88349	3.91703	-2.04358
C	0.73605	3.99851	-1.25571
C	-0.04545	2.87382	-1.02002
C	0.33323	1.65460	-1.58143
O	-0.46123	0.56836	-1.30309
H	1.74886	0.60867	-2.82843
H	3.12888	2.61815	-3.22510
H	2.48888	4.79886	-2.22137
H	0.44285	4.94778	-0.81909
H	-0.94016	2.91885	-0.40613
H	-0.09902	-0.23922	-1.69465
B	0.32631	-1.09481	0.99664
C	-0.48657	-2.26758	0.36889
C	0.12145	-3.47472	-0.01878
C	-0.33095	-0.05484	1.94499
C	0.11295	1.27910	1.95423
C	1.85284	-0.91639	0.60189
C	2.31071	-1.06462	-0.70516
C	-0.61363	-4.49737	-0.60491
C	-1.97489	-4.31927	-0.85387
C	-2.59885	-3.12565	-0.50034
C	-1.86295	-2.12080	0.12066
C	-0.53252	2.24905	2.71075
C	-1.61708	1.89420	3.51024
C	3.61240	-0.79850	-1.09976
C	4.53883	-0.40630	-0.14407
C	4.14471	-0.27804	1.18170
C	2.82199	-0.52282	1.52818
C	-2.05539	0.57296	3.54607
C	-1.42604	-0.38575	2.76092
F	1.46551	-1.43234	-1.69214
F	3.96485	-0.89316	-2.38027
F	5.79268	-0.15522	-0.49477
F	5.03356	0.08363	2.10141
F	2.50315	-0.38292	2.81410
H	1.18704	-3.61271	0.15066
H	0.95879	1.56584	1.33314
H	-0.12824	-5.42787	-0.88146
H	-2.54601	-5.11139	-1.32834
H	-3.65378	-2.96969	-0.70456
H	-2.35894	-1.19696	0.40420
H	-0.18944	3.27860	2.68055
H	-2.11941	2.64861	4.10804
H	-2.89440	0.29471	4.17571
H	-1.78533	-1.41108	2.77905
C	-3.93933	0.15977	-1.45867
C	-5.17202	-0.22236	-1.98149
C	-6.35551	0.12420	-1.33621
C	-6.29588	0.86269	-0.15477
C	-5.07342	1.24718	0.38076
C	-3.88985	0.89673	-0.27231
O	-2.72085	1.28210	0.29858
H	-3.01295	-0.10291	-1.96213
H	-5.20212	-0.79327	-2.90463
H	-7.31289	-0.17475	-1.74855
H	-7.21197	1.13944	0.35789
H	-5.00516	1.81430	1.30290
H	-1.96839	0.92465	-0.20219

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$[B(C_6F_5)Ph_2$-(Phenol-Phenoxide)]-

C	-1.23032	-0.14096	-2.52718
C	-1.65843	-0.82572	-3.66086
C	-0.85706	-1.79048	-4.26487
C	0.39209	-2.07052	-3.71404
C	0.83150	-1.40152	-2.57908
C	0.02686	-0.42549	-1.97447
O	0.52317	0.20355	-0.88549
H	-1.85952	0.61599	-2.07236
H	-2.63539	-0.59423	-4.07596
H	-1.20074	-2.31764	-5.14925
H	1.03111	-2.82353	-4.16662
H	1.79678	-1.62563	-2.13523
B	-0.35665	0.84363	0.18177
C	0.58833	1.08062	1.49151
C	0.20910	0.76006	2.80093
C	-1.54423	-0.26123	0.52597
C	-2.91565	-0.11715	0.34992
C	-0.86332	2.31618	-0.29115
C	-0.40999	2.90442	-1.47716
C	1.03039	1.02601	3.89630
C	2.27421	1.61946	3.70813
C	2.67467	1.95927	2.41743
C	1.83529	1.70624	1.33693
C	-3.84250	-1.11216	0.64920
C	-3.40250	-2.33066	1.13639

C	-0.75194	4.21129	-1.83015
C	-1.56052	4.97118	-0.99297
C	-2.01430	4.41451	0.20364
C	-1.66132	3.11437	0.54322
C	-2.04195	-2.53883	1.30688
C	-1.15565	-1.51658	0.99480
F	-3.43550	1.00637	-0.16966
F	-5.15249	-0.90948	0.45903
F	-4.27672	-3.29891	1.43005
F	-1.60632	-3.71843	1.76458
F	0.14380	-1.80078	1.16693
H	-0.75473	0.28504	2.97540
H	0.22928	2.32588	-2.14112
H	0.70042	0.75961	4.89748
H	2.92424	1.81694	4.55615
H	3.64305	2.42363	2.25149
H	2.16249	2.00301	0.34258
H	-0.38244	4.63445	-2.76087
H	-1.83078	5.98859	-1.26262
H	-2.63894	5.00119	0.87261
H	-2.00895	2.70040	1.48912
C	5.27228	-0.26710	-1.10824
C	6.11077	-1.14810	-0.43666
C	5.60462	-2.00761	0.53687
C	4.24289	-1.97060	0.82941
C	3.38851	-1.09529	0.16741
C	3.90523	-0.23463	-0.81078
O	3.13360	0.63417	-1.49546
H	5.64817	0.40826	-1.86979
H	7.17049	-1.16288	-0.67710
H	6.26214	-2.69410	1.06058
H	3.83118	-2.62905	1.58862
H	2.32878	-1.05928	0.40413
H	2.19534	0.54047	-1.21077

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$B(C_6F_5)_2Ph$-(Phenol)$_2$

C	2.66876	2.11166	-1.86761
C	3.45987	3.25491	-1.96092
C	2.97429	4.48381	-1.52545
C	1.68389	4.58147	-1.00855
C	0.87187	3.45580	-0.92241
C	1.39125	2.24307	-1.34737
O	0.56103	1.10201	-1.20317
H	3.03596	1.14654	-2.19602
H	4.46171	3.17601	-2.36884
H	3.60076	5.36677	-1.58964
H	1.30314	5.53765	-0.66683
H	-0.13029	3.49931	-0.50972
H	0.68629	0.48918	-1.95155
B	0.63974	0.17153	0.25301
C	-0.78922	-0.58814	0.28229
C	-1.45097	-0.90049	1.46998
C	0.92320	1.29314	1.34490
C	2.23103	1.65398	1.69313
C	1.82636	-0.91757	0.00736
C	2.33670	-1.36498	-1.20375
C	-2.65493	-1.59606	1.50401
C	-3.23239	-2.03801	0.32302
C	-2.58669	-1.79278	-0.87889
C	-1.39701	-1.08284	-0.86521
C	2.49192	2.74367	2.51881
C	1.43701	3.50044	3.02123
C	3.29945	-2.35761	-1.32934
C	3.77552	-2.97938	-0.18564
C	3.27889	-2.59548	1.05308
C	2.31965	-1.59383	1.12470
C	0.12672	3.15789	2.69547
C	-0.12152	2.06783	1.86701
F	-0.94222	-0.54420	2.65158
F	1.91113	-0.82556	-2.38070
F	-3.26271	-1.83677	2.66324
F	-4.38923	-2.69006	0.34320
F	-3.12334	-2.20054	-2.02673
F	-0.83018	-0.85518	-2.07822
F	3.75436	-2.71583	-2.52767
F	4.69288	-3.93538	-0.27458
F	3.71728	-3.19685	2.15448
F	1.85168	-1.29425	2.33842
H	3.06805	1.08364	1.29551
H	3.51608	3.00244	2.76902
H	1.63450	4.35144	3.66593
H	-0.70118	3.74196	3.08582
H	-1.14611	1.82837	1.59484
C	-3.80202	0.87007	-1.92296
C	-4.99686	0.15668	-1.89338
C	-5.72932	0.05554	-0.71371
C	-5.26355	0.68680	0.43883
C	-4.06825	1.39739	0.42322
C	-3.33238	1.47685	-0.75838
O	-2.14717	2.15629	-0.72254
H	-3.21814	0.93368	-2.83789
H	-5.34507	-0.33412	-2.79608
H	-6.65261	-0.51223	-0.69062
H	-5.82614	0.61209	1.36398
H	-3.68352	1.88172	1.31481
H	-1.55756	1.82022	-1.40996

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[$B(C_6F_5)_2Ph$-(Phenol-Phenoxide)]-

C	0.28732	-2.95359	-1.28298
C	0.47775	-4.33270	-1.27547
C	1.25625	-4.93384	-0.29022
C	1.85374	-4.14011	0.68735
C	1.66721	-2.76262	0.69299
C	0.87203	-2.16232	-0.29036
O	0.72404	-0.81009	-0.32035
H	-0.28511	-2.46704	-2.06384
H	0.01953	-4.93869	-2.05203
H	1.40342	-6.00949	-0.28832
H	2.46955	-4.59629	1.45684
H	2.11784	-2.13214	1.45375

B	-0.40980	-0.13404	0.42638
C	-0.20481	1.48794	0.21995
C	-1.04668	2.35243	0.91828
C	-0.29300	-0.57899	1.98477
C	-0.79127	-1.80967	2.43774
C	-1.86245	-0.47474	-0.29910
C	-1.95526	-0.47682	-1.69116
C	-1.00005	3.73502	0.81454
C	-0.07614	4.31585	-0.04192
C	0.77306	3.50252	-0.77195
C	0.69276	2.11785	-0.63759
C	-0.54320	-2.28008	3.72318
C	0.22774	-1.52456	4.60440
C	-3.13217	-0.69372	-2.39541
C	-4.31447	-0.88107	-1.69639
C	-4.28908	-0.84668	-0.31303
C	-3.08422	-0.63379	0.35282
C	0.74680	-0.30555	4.18012
C	0.48825	0.15196	2.88845
F	-1.97859	1.84843	1.74078
F	-0.86513	-0.26138	-2.44561
F	-1.83455	4.51124	1.51630
F	-0.01189	5.64580	-0.16370
F	1.65737	4.05655	-1.60826
F	1.54484	1.42505	-1.40329
F	-3.14334	-0.70477	-3.73386
F	-5.46267	-1.08490	-2.34966
F	-5.42762	-1.00865	0.37152
F	-3.18071	-0.58722	1.68626
H	-1.37882	-2.42497	1.75828
H	-0.94552	-3.23974	4.03657
H	0.42612	-1.88670	5.60959
H	1.35885	0.28963	4.85258
H	0.92681	1.09516	2.56909
C	3.83788	-0.53112	-1.39323
C	4.94154	-0.75521	-2.20803
C	6.22737	-0.42506	-1.78442
C	6.39794	0.13990	-0.52191
C	5.30580	0.36793	0.30602
C	4.01666	0.03287	-0.12297
O	2.99103	0.26364	0.71893
H	2.83279	-0.77127	-1.72621
H	4.79013	-1.19331	-3.19049
H	7.08239	-0.60311	-2.42861
H	7.39311	0.40548	-0.17557
H	5.42078	0.80422	1.29270
H	2.15338	-0.06333	0.31402

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$B(C_6F_5)_3$-$(Phenol)_2$

C	-2.45050	-0.13911	-2.22743
C	-3.41424	-0.54818	-3.14464
C	-3.10563	-1.47983	-4.13261
C	-1.82406	-2.01779	-4.20228
C	-0.85103	-1.63470	-3.28349
C	-1.18261	-0.69628	-2.31667
O	-0.17991	-0.32834	-1.40487
H	-2.68568	0.58430	-1.45461
H	-4.41211	-0.12757	-3.08478
H	-3.86364	-1.78731	-4.84450
H	-1.57723	-2.74746	-4.96580
H	0.15077	-2.04952	-3.31542
H	0.69450	-0.15746	-1.87974
B	-0.41957	0.13978	0.11110
C	1.06165	0.07399	0.79028
C	1.42543	-0.67462	1.90764
C	-1.49128	-0.96157	0.62938
C	-2.80662	-0.71890	1.00821
C	-0.88906	1.69396	0.12655
C	-0.84319	2.57801	-0.94335
C	2.71455	-0.68026	2.43103
C	3.69822	0.10931	1.85517
C	3.37465	0.91066	0.77119
C	2.08201	0.86917	0.27436
C	-3.69448	-1.72628	1.37273
C	-3.27747	-3.04707	1.34830
C	-1.16158	3.92692	-0.82793
C	-1.52410	4.43773	0.40842
C	-1.56101	3.59583	1.51367
C	-1.23538	2.25898	1.35038
C	-1.98042	-3.34489	0.95073
C	-1.13320	-2.30793	0.59822
F	0.54038	-1.44216	2.54864
F	-3.31606	0.52104	0.98912
F	-0.46997	2.16294	-2.16912
F	3.01070	-1.43774	3.48485
F	4.93741	0.09699	2.33281
F	4.30045	1.68556	0.20712
F	1.84432	1.62822	-0.82006
F	-4.94461	-1.43076	1.72283
F	-4.11324	-4.02202	1.68819
F	-1.10693	4.72945	-1.89058
F	-1.82853	5.72519	0.53826
F	-1.89696	4.08115	2.70649
F	-1.26148	1.47720	2.43816
F	-1.57020	-4.61103	0.90819
F	0.10629	-2.65383	0.20671
C	4.30764	-0.12438	-2.18952
C	5.35157	-0.66796	-1.44263
C	5.14108	-1.79228	-0.65180
C	3.87830	-2.38548	-0.61373
C	2.82743	-1.85722	-1.35350
C	3.05838	-0.72254	-2.12500
O	1.96719	-0.18677	-2.79962
H	4.45961	0.77005	-2.78712
H	6.32675	-0.19423	-1.47114
H	5.95288	-2.20140	-0.06087
H	3.70248	-3.25755	0.00735
H	1.83112	-2.28396	-1.29991
H	2.16584	0.71836	-3.07781

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[$B(C_6F_5)_3$-(Phenol-Phenoxide)]-

C	1.82159	-0.07803	2.62939
C	2.44511	-0.35204	3.84288
C	1.80967	-1.10745	4.82417
C	0.52867	-1.59656	4.57554
C	-0.10554	-1.33538	3.36821
C	0.53328	-0.56994	2.38406
O	-0.15250	-0.34029	1.24329
H	2.33056	0.51489	1.87716
H	3.44434	0.03574	4.01908
H	2.30563	-1.31437	5.76690
H	0.01723	-2.19307	5.32544
H	-1.09628	-1.72743	3.15733
B	0.48022	0.08288	-0.04827
C	-0.77784	0.00423	-1.11109
C	-0.88938	-0.77754	-2.25432
C	1.68994	-0.99436	-0.35467
C	3.05163	-0.73465	-0.43677
C	0.95920	1.65569	-0.06562
C	0.68593	2.59588	0.92003
C	-2.05915	-0.87005	-3.00078
C	-3.17713	-0.14492	-2.62166
C	-3.10581	0.68192	-1.51107
C	-1.91218	0.75640	-0.80705
C	4.01674	-1.72236	-0.60884
C	3.62833	-3.04797	-0.68996
C	1.01861	3.94259	0.79648
C	1.63077	4.39453	-0.36038
C	1.90312	3.49555	-1.38248
C	1.55478	2.16456	-1.21531
C	2.28158	-3.36626	-0.58947
C	1.35806	-2.34661	-0.41598
F	0.14126	-1.50770	-2.70499
F	3.53389	0.51382	-0.30399
F	0.07223	2.25065	2.05826
F	-2.11551	-1.65001	-4.08635
F	-4.30602	-0.22975	-3.33020
F	-4.16793	1.40017	-1.14292
F	-1.89486	1.60534	0.23256
F	5.31470	-1.40466	-0.67752
F	4.53941	-4.01117	-0.85292
F	0.74239	4.80785	1.77878
F	1.95362	5.68461	-0.49491
F	2.48576	3.92536	-2.50749
F	1.82310	1.33433	-2.23597
F	1.89686	-4.64435	-0.65653
F	0.07512	-2.72013	-0.31509
C	-3.38999	-0.16326	1.91817
C	-4.56594	0.48653	2.27916
C	-5.80993	-0.03479	1.93382
C	-5.86761	-1.22371	1.20845
C	-4.70311	-1.88122	0.83308
C	-3.45567	-1.35336	1.18385
O	-2.35792	-2.03464	0.79183
H	-2.42038	0.25677	2.16849
H	-4.50190	1.41666	2.83609
H	-6.72119	0.48110	2.21818
H	-6.82963	-1.64108	0.92456
H	-4.72718	-2.80031	0.25716
H	-1.55163	-1.49759	0.93245

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[$SiEt_3$-$(Phenol)_2$]$^+$

C	-0.71119	1.50929	0.52314
C	-1.11031	2.81251	0.81244
C	-0.48598	3.89348	0.19397
C	0.54129	3.68263	-0.72338
C	0.95029	2.38708	-1.03032
C	0.31249	1.33318	-0.39615
O	0.74313	0.00965	-0.71509
Si	1.96979	-0.85894	0.31638
C	2.25848	-2.42277	-0.65504
C	1.11711	-3.45025	-0.64564
C	3.41961	0.30768	0.31573
C	4.16144	0.36879	-1.02786
C	1.16623	-1.11434	1.98339
C	1.38294	0.02737	2.99021
H	-1.18961	0.65429	0.99237
H	-1.91110	2.97729	1.52470
H	-0.80094	4.90435	0.42768
H	1.02610	4.52474	-1.20427
H	1.74429	2.19389	-1.74364
H	0.01704	-0.50211	-1.26071
H	2.53739	-2.16163	-1.68293
H	3.16217	-2.86901	-0.21655
H	1.43105	-4.38476	-1.11487
H	0.79965	-3.68861	0.37473
H	0.24704	-3.08661	-1.19911
H	4.10286	-0.02537	1.10788
H	3.07959	1.30323	0.62641
H	4.95762	1.11527	-1.00325
H	3.49070	0.62743	-1.85370
H	4.61903	-0.59370	-1.27100
H	1.58128	-2.04812	2.38659
H	0.09551	-1.31283	1.84139
H	0.90495	-0.20141	3.94490
H	0.97030	0.97314	2.62848
H	2.44699	0.18482	3.18520
C	-2.23710	-1.78544	0.11311
C	-3.24197	-1.61487	1.06370
C	-4.23106	-0.65170	0.87604
C	-4.22200	0.14272	-0.26858
C	-3.21530	-0.00318	-1.21975
C	-2.23945	-0.96523	-1.00593
O	-1.15141	-1.09473	-1.88431
H	-1.47193	-2.54683	0.22439
H	-3.25806	-2.24901	1.94346
H	-5.01537	-0.52885	1.61424
H	-4.99565	0.88679	-0.42253
H	-3.18280	0.63407	-2.09899
H	-1.39209	-0.81635	-2.77949

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$SiEt_3$-(Phenol-Phenoxide)

C	-0.24337	1.44722	1.06126
C	-0.45093	2.78637	1.37569
C	0.02933	3.79195	0.53880
C	0.70642	3.45323	-0.62993
C	0.91754	2.11667	-0.95862
C	0.45413	1.12122	-0.10095
O	0.66959	-0.20671	-0.40610
Si	2.18766	-0.91936	-0.05506
C	1.84868	-2.76038	-0.12769
C	1.21591	-3.33620	1.14832
C	3.39774	-0.38752	-1.38759
C	2.94882	-0.80920	-2.79313
C	2.74262	-0.36985	1.65353
C	3.37383	1.02783	1.73391
H	-0.62091	0.64614	1.68970
H	-0.99356	3.04397	2.27932
H	-0.13310	4.83419	0.79118
H	1.07052	4.23119	-1.29319
H	1.43247	1.83240	-1.87111
H	1.19944	-2.95302	-0.99123
H	2.79549	-3.27224	-0.34480
H	1.04837	-4.41254	1.05503
H	1.86363	-3.17847	2.01618
H	0.24883	-2.87287	1.36205
H	4.37905	-0.82082	-1.15313
H	3.53296	0.69991	-1.33810
H	3.64441	-0.46596	-3.56360
H	1.96006	-0.40249	-3.02884
H	2.87723	-1.89820	-2.87473
H	3.45851	-1.12176	2.01327
H	1.88024	-0.43769	2.32946
H	3.69976	1.25714	2.75223
H	2.66810	1.80600	1.42867
H	4.25109	1.10292	1.08394
C	-3.91994	-1.36978	0.78223
C	-5.13485	-0.85630	0.34611
C	-5.18640	0.04352	-0.71742
C	-4.00317	0.42391	-1.34374
C	-2.77892	-0.08297	-0.91845
C	-2.73728	-0.98254	0.14923
O	-1.57172	-1.50454	0.61129
H	-3.86103	-2.07097	1.60761
H	-6.05057	-1.16246	0.84253
H	-6.13748	0.44162	-1.05369
H	-4.02728	1.12362	-2.17341
H	-1.85458	0.21184	-1.40821
H	-0.82284	-1.14343	0.10291

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$[SiPhH_2$-$(Phenol)_2]^+$

C	0.111092	-2.498330	3.036192
C	-0.575400	-3.553948	3.632401
C	-0.435726	-4.849347	3.138549
C	0.384171	-5.103375	2.040611
C	1.074365	-4.061450	1.425724
C	0.920090	-2.786918	1.950824
O	1.630210	-1.706819	1.344675
Si	0.959635	-0.949822	-0.135141
C	0.735816	-2.273061	-1.385494
C	-0.491046	-2.947502	-1.497364
C	-0.630158	-4.012130	-2.380688
C	0.455456	-4.416608	-3.156094
C	1.678681	-3.756094	-3.055950
C	1.818874	-2.686630	-2.178188
C	4.963464	-1.390997	-0.578205
C	5.426731	-1.683648	-1.859655
C	5.465945	-3.003057	-2.308680
C	5.041461	-4.038468	-1.478038
C	4.567097	-3.762100	-0.197524
C	4.541405	-2.440352	0.225211
O	4.038929	-2.106038	1.498547
H	0.031496	-1.480651	3.402631
H	-1.215945	-3.360957	4.485497
H	-0.972160	-5.665365	3.609712
H	0.481225	-6.111528	1.653646
H	1.693590	-4.221041	0.547179
H	2.681352	-1.838623	1.448385
H	2.034729	0.013175	-0.421032
H	-0.292514	-0.367232	0.368212
H	-1.341508	-2.641500	-0.892912
H	-1.582169	-4.524259	-2.467879
H	0.344659	-5.246318	-3.846621
H	2.520282	-4.066634	-3.666597
H	2.775007	-2.171286	-2.118104
H	4.947005	-0.377154	-0.192789
H	5.770234	-0.878973	-2.500336
H	5.838870	-3.225167	-3.302389
H	5.078943	-5.065958	-1.822964
H	4.233254	-4.559472	0.460576
H	4.346161	-2.728904	2.173188

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$SiPhH_2$-(Phenol-Phenoxide)

C	0.026495	-1.985354	3.080629
C	-0.846998	-2.736976	3.859934
C	-0.950216	-4.113748	3.672410
C	-0.173372	-4.739078	2.700825
C	0.705120	-3.999649	1.912541
C	0.798566	-2.623234	2.112650
O	1.683656	-1.876205	1.352849
Si	1.121483	-1.273303	-0.128546
C	0.960520	-2.606059	-1.415138
C	-0.163763	-3.447199	-1.435337
C	-0.284397	-4.454378	-2.386734
C	0.718086	-4.632478	-3.338830
C	1.836617	-3.804377	-3.337642
C	1.956187	-2.797579	-2.383250
H	0.127083	-0.912992	3.211652
H	-1.448111	-2.243832	4.616963

H	-1.631461	-4.696352	4.283222
H	-0.246812	-5.811504	2.552333
H	1.326470	-4.468965	1.156026
H	2.103855	-0.252386	-0.538978
H	-0.206180	-0.675712	0.150124
H	-0.952269	-3.315720	-0.697231
H	-1.158279	-5.098034	-2.389222
H	0.624610	-5.417930	-4.082522
H	2.622393	-3.942533	-4.073743
H	2.840993	-2.164395	-2.389923
C	4.607679	-1.853785	-0.210638
C	5.254208	-1.313454	-1.320133
C	5.693372	-2.136169	-2.353677
C	5.486851	-3.513841	-2.262834
C	4.837130	-4.064050	-1.165724
C	4.384770	-3.231031	-0.139901
O	3.734592	-3.801956	0.904006
H	4.271539	-1.216174	0.602842
H	5.415553	-0.241027	-1.370525
H	6.197759	-1.712627	-3.215195
H	5.830471	-4.166549	-3.059625
H	4.648226	-5.129121	-1.089568
H	3.247232	-3.108485	1.376629

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Thiophenol-BEt_3

C	-1.660716	-2.599408	-0.000052
C	-1.781952	-3.623765	-0.932761
C	-0.650343	-4.161552	-1.540383
C	0.606854	-3.662273	-1.213478
C	0.738597	-2.628613	-0.290735
C	-0.397650	-2.097326	0.322266
S	-0.315255	-0.752940	1.483603
B	0.342654	1.632281	-0.246456
C	0.919646	2.435535	0.992049
C	-0.093290	3.040226	1.965755
C	1.321942	0.798240	-1.171278
C	2.731608	0.525407	-0.645203
C	-1.150849	1.871852	-0.712815
C	-1.696554	0.932308	-1.789894
H	-2.543875	-2.189639	0.480893
H	-2.766973	-4.006577	-1.178971
H	-0.747847	-4.963935	-2.263541
H	1.495448	-4.072349	-1.682337
H	1.722409	-2.233190	-0.054324
H	1.001197	-0.836612	1.728178
H	1.655088	1.825908	1.535092
H	1.528931	3.241693	0.547317
H	0.390051	3.600524	2.771274
H	-0.777420	3.722409	1.452026
H	-0.707239	2.259177	2.427604
H	1.388339	1.359886	-2.118254
H	0.832689	-0.142203	-1.462026
H	3.332770	-0.057719	-1.349488
H	2.705603	-0.031065	0.300122
H	3.270017	1.456148	-0.440961
H	-1.184920	2.913662	-1.075969
H	-1.813510	1.872793	0.162297
H	-2.727412	1.173669	-2.065419
H	-1.679707	-0.108251	-1.446522
H	-1.092543	0.976545	-2.701610

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[Thiophenoxide-BEt_3]-

C	-1.577533	-2.206017	0.346815
C	-2.094361	-3.210504	-0.465936
C	-1.272512	-3.877209	-1.372569
C	0.075699	-3.531734	-1.446146
C	0.592619	-2.530805	-0.629046
C	-0.225375	-1.836358	0.276705
S	0.417785	-0.531860	1.283726
B	0.423824	1.100514	0.009557
C	0.722892	2.324459	1.052707
C	-0.437565	2.703200	1.977407
C	1.624827	0.900743	-1.074640
C	3.043492	0.882396	-0.502794
C	-1.042643	1.248320	-0.703794
C	-1.258033	0.490421	-2.020150
H	-2.219567	-1.673199	1.041665
H	-3.148327	-3.468734	-0.397553
H	-1.676951	-4.656544	-2.012313
H	0.729768	-4.044678	-2.146975
H	1.642371	-2.258353	-0.686281
H	1.609734	2.107202	1.667259
H	0.998115	3.207130	0.448821
H	-0.191468	3.522749	2.666634
H	-1.314140	3.015246	1.397869
H	-0.744017	1.839457	2.577296
H	1.550255	1.721632	-1.810495
H	1.459716	-0.017687	-1.658941
H	3.816000	0.702143	-1.263180
H	3.131440	0.101721	0.261530
H	3.283053	1.835032	-0.015448
H	-1.198790	2.322793	-0.909458
H	-1.840511	0.975142	0.003016
H	-2.263512	0.644834	-2.435695
H	-1.118475	-0.588427	-1.897176
H	-0.539584	0.818418	-2.780553

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Thiophenol-BPh_3

C	-1.954431	-1.674203	-1.619760
C	-1.957723	-3.046259	-1.850524
C	-0.944914	-3.636499	-2.601501
C	0.076726	-2.849757	-3.126487
C	0.091952	-1.477167	-2.904947
C	-0.925965	-0.896481	-2.151544
S	-0.910812	0.832243	-1.732503
B	0.084412	0.759262	0.411169
C	0.572588	2.277573	0.517035
C	1.841471	2.585559	1.030463

C	1.151411	-0.382139	0.079625
C	0.897725	-1.733336	0.365896
C	-1.164396	0.388768	1.338355
C	-2.505499	0.710496	1.084041
C	2.256243	3.903461	1.214921
C	1.410094	4.954857	0.878101
C	0.139628	4.677886	0.377330
C	-0.270641	3.358977	0.215071
C	1.766867	-2.745420	-0.034553
C	2.922195	-2.432533	-0.744781
C	-3.517432	0.426756	1.999063
C	-3.211180	-0.177184	3.214532
C	-1.885806	-0.489782	3.503981
C	-0.884697	-0.212074	2.577488
C	3.196624	-1.102179	-1.054952
C	2.320712	-0.099166	-0.648162
H	-2.728261	-1.216146	-1.010982
H	-2.753468	-3.654439	-1.433429
H	-0.948848	-4.707654	-2.772942
H	0.877483	-3.304374	-3.700332
H	0.909382	-0.873090	-3.285897
H	2.515354	1.776804	1.300872
H	-0.012250	-2.001002	0.895494
H	-2.780522	1.200885	0.152358
H	3.242877	4.107634	1.619915
H	1.732970	5.982561	1.012291
H	-0.534445	5.490579	0.124100
H	-1.280040	3.166543	-0.144524
H	1.534017	-3.780366	0.197555
H	3.601560	-3.218751	-1.060262
H	-4.545640	0.684635	1.763191
H	-3.996495	-0.398059	3.930509
H	-1.630506	-0.954061	4.451809
H	0.144429	-0.466812	2.821305
H	4.092870	-0.846900	-1.612894
H	2.545948	0.933130	-0.909094
H	0.235319	1.151064	-2.353096

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[Thiophenoxide-BPh_3]-

C	-2.057235	-1.640325	-1.707061
C	-2.147123	-3.005710	-1.967734
C	-1.157932	-3.648525	-2.707675
C	-0.074143	-2.913002	-3.182075
C	0.017622	-1.550054	-2.919422
C	-0.972146	-0.892019	-2.178629
S	-0.804195	0.840146	-1.811305
B	-0.010193	0.742440	0.044000
C	0.524531	2.247110	0.369446
C	1.627830	2.454089	1.212660
C	1.171361	-0.366397	-0.073618
C	0.975575	-1.714950	0.261443
C	-1.148226	0.381992	1.157624
C	-2.517020	0.637631	0.990668
C	2.054359	3.728927	1.580222
C	1.381953	4.853853	1.110332
C	0.279275	4.681321	0.276944
C	-0.137376	3.400736	-0.078787
C	1.943721	-2.689460	0.021416
C	3.156202	-2.341422	-0.565455
C	-3.446121	0.406494	2.004334
C	-3.031343	-0.088636	3.237557
C	-1.676208	-0.339789	3.441096
C	-0.760612	-0.103636	2.418402
C	3.381860	-1.010073	-0.912940
C	2.403419	-0.049589	-0.670889
H	-2.818487	-1.144084	-1.113609
H	-2.993074	-3.570215	-1.584467
H	-1.226695	-4.714540	-2.905594
H	0.714459	-3.405566	-3.744406
H	0.879769	-0.980520	-3.252528
H	2.171470	1.587595	1.584326
H	0.025144	-2.014397	0.697474
H	-2.854117	1.027444	0.032707
H	2.915816	3.844506	2.234038
H	1.711570	5.851001	1.390355
H	-0.259306	5.548952	-0.097026
H	-1.007328	3.290735	-0.723538
H	1.742687	-3.725930	0.281518
H	3.914064	-3.096880	-0.757055
H	-4.499400	0.615149	1.830268
H	-3.752147	-0.273840	4.029769
H	-1.332174	-0.721065	4.399840
H	0.293930	-0.306252	2.598284
H	4.321354	-0.722301	-1.379489
H	2.585208	0.981384	-0.968257

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Thiophenol-B(C_6F_5)Ph_2

C	-2.237879	-1.353080	-1.984922
C	-2.579768	-2.676968	-2.243367
C	-1.608349	-3.588328	-2.649770
C	-0.287701	-3.175917	-2.802819
C	0.066917	-1.852244	-2.563503
C	-0.914564	-0.948635	-2.157748
S	-0.388799	0.725449	-1.818091
B	0.216680	0.731161	0.265089
C	0.614944	2.265634	0.492940
C	1.843726	2.616907	1.067628
C	1.377404	-0.356186	0.046616
C	1.224669	-1.705553	0.394732
C	-1.026643	0.293112	1.212710
C	-2.386561	0.489159	0.999307
C	2.165032	3.945270	1.340557
C	1.262165	4.959322	1.037471
C	0.027432	4.635034	0.479055
C	-0.289296	3.305124	0.223873
C	2.188288	-2.659493	0.077850
C	3.336335	-2.288124	-0.616321
C	-3.376574	0.143742	1.910548
C	-3.015386	-0.392893	3.135851
C	-1.669558	-0.565746	3.424882

C	-0.717101	-0.211588	2.478221
C	3.510596	-0.956903	-0.989006
C	2.542440	-0.011102	-0.660491
F	-2.842564	1.062026	-0.140371
F	-4.661881	0.341572	1.619553
F	-3.944825	-0.723991	4.026459
F	-1.303445	-1.053969	4.607598
F	0.562014	-0.361385	2.841489
H	-2.989292	-0.646827	-1.649128
H	-3.609088	-2.995596	-2.117536
H	-1.881030	-4.620348	-2.843431
H	0.475668	-3.883464	-3.108501
H	1.099068	-1.529024	-2.669141
H	2.556576	1.835136	1.315456
H	0.321091	-2.027712	0.905930
H	3.123244	4.187420	1.790042
H	1.513305	5.995182	1.242612
H	-0.690138	5.417546	0.252214
H	-1.274208	3.069274	-0.177914
H	2.036684	-3.695679	0.364490
H	4.088889	-3.029428	-0.866893
H	4.399720	-0.655155	-1.534245
H	2.687504	1.021868	-0.969502
H	-1.599143	1.299554	-1.887906

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[Thiophenoxide-B(C_6F_5)Ph_2]-

C	-1.768004	-1.777892	-1.590009
C	-1.696337	-3.139928	-1.870491
C	-0.756510	-3.626446	-2.775770
C	0.112689	-2.736025	-3.402928
C	0.048240	-1.375499	-3.116521
C	-0.887633	-0.877374	-2.200661
S	-0.860955	0.849490	-1.768228
B	-0.095839	0.746879	0.086812
C	0.504980	2.217943	0.423820
C	1.672021	2.394438	1.180067
C	1.044414	-0.425818	-0.047107
C	0.839468	-1.761817	0.300066
C	-1.229931	0.458991	1.220118
C	-2.605980	0.606284	1.014170
C	2.124181	3.655916	1.560634
C	1.413775	4.794466	1.189967
C	0.247148	4.649649	0.443000
C	-0.196031	3.381776	0.076177
C	1.715123	-2.792199	-0.029496
C	2.871298	-2.508805	-0.734407
C	-3.529625	0.454761	2.050584
C	-3.097469	0.155938	3.337415
C	-1.729769	0.016718	3.575619
C	-0.823088	0.171849	2.534280
C	3.125685	-1.198381	-1.106760
C	2.219515	-0.201023	-0.768840
F	-0.261874	-2.152698	0.956665
F	1.448791	-4.055367	0.325865
F	3.730126	-3.484138	-1.055875
F	4.235309	-0.912829	-1.802829
F	2.514212	1.021015	-1.229295
H	-2.476712	-1.405791	-0.856762
H	-2.370625	-3.825907	-1.365772
H	-0.695316	-4.690483	-2.983801
H	0.857853	-3.103754	-4.103119
H	0.745226	-0.680376	-3.575586
H	2.247987	1.518296	1.474262
H	-2.957144	0.845304	0.012948
H	3.036908	3.750762	2.144020
H	1.763953	5.781403	1.480226
H	-0.321352	5.528211	0.147844
H	-1.118385	3.289230	-0.494737
H	-4.591642	0.573040	1.848282
H	-3.812675	0.035154	4.146705
H	-1.373335	-0.212778	4.576922
H	0.241367	0.063954	2.741062

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Thiophenol-B(C_6F_5)$_2$Ph

C	-2.056118	-1.564825	-1.851714
C	-2.222268	-2.919070	-2.125618
C	-1.204778	-3.641822	-2.743687
C	-0.017785	-3.009263	-3.102557
C	0.155991	-1.652467	-2.850800
C	-0.864983	-0.943332	-2.222723
S	-0.547970	0.770432	-1.827932
B	0.087869	0.733140	0.202174
C	0.598838	2.245277	0.467197
C	1.752382	2.534443	1.195243
C	1.203053	-0.397171	-0.003746
C	0.974251	-1.733512	0.346009
C	-1.128847	0.374710	1.213426
C	-2.503435	0.480247	1.036907
C	2.140668	3.834706	1.505153
C	1.356385	4.903575	1.098581
C	0.186692	4.663069	0.389675
C	-0.163812	3.352470	0.107236
C	1.888177	-2.736093	0.032275
C	3.058634	-2.422901	-0.652836
C	-3.434773	0.187128	2.027109
C	-2.997312	-0.198602	3.283461
C	-1.633352	-0.285059	3.527455
C	-0.741259	0.010289	2.506536
C	3.310157	-1.100939	-1.014554
C	2.390904	-0.106924	-0.692043
F	2.543945	1.560422	1.645312
F	-3.036992	0.872998	-0.140634
F	3.255598	4.060019	2.195862
F	1.717779	6.148670	1.387807
F	-0.581612	5.678587	0.001735
F	-1.319915	3.165675	-0.562918
F	-4.738687	0.288598	1.775922
F	-3.871565	-0.476343	4.244095
F	-1.196396	-0.634976	4.733913
F	0.559281	-0.049645	2.810336

H	-2.839441	-1.000306	-1.358574
H	-3.148442	-3.409884	-1.846122
H	-1.337795	-4.699598	-2.944565
H	0.780131	-3.570067	-3.577197
H	1.086224	-1.156962	-3.109494
H	0.052796	-2.003114	0.856855
H	1.681922	-3.763458	0.316219
H	3.773137	-3.201927	-0.900074
H	4.223699	-0.844571	-1.542328
H	2.600041	0.921084	-0.983623
H	-1.813206	1.208358	-1.834334

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[Thiophenoxide-B(C_6F_5)$_2$Ph]-

C	-1.877972	-1.645657	-1.703438
C	-1.923588	-3.019369	-1.926165
C	-0.955086	-3.639036	-2.711912
C	0.057529	-2.871321	-3.283480
C	0.109738	-1.499607	-3.053927
C	-0.850717	-0.870496	-2.252022
S	-0.693919	0.863498	-1.878770
B	-0.045183	0.753072	-0.005799
C	0.496960	2.231276	0.388521
C	1.649761	2.427375	1.160536
C	1.109130	-0.404783	-0.093421
C	0.923111	-1.738006	0.267596
C	-1.204531	0.429442	1.126386
C	-2.581032	0.600914	1.016361
C	2.054649	3.696712	1.566203
C	1.308679	4.817125	1.209912
C	0.152850	4.649384	0.451409
C	-0.244118	3.374582	0.055636
C	1.834629	-2.751544	-0.005929
C	3.009563	-2.450892	-0.672839
C	-3.469055	0.422910	2.076782
C	-2.991550	0.081132	3.327960
C	-1.625134	-0.087342	3.498511
C	-0.781247	0.096273	2.415254
C	3.246198	-1.140712	-1.057485
C	2.305021	-0.159396	-0.770321
F	-0.194096	-2.137553	0.896427
F	-3.166931	0.938891	-0.143294
F	1.586925	-4.013343	0.364900
F	3.903860	-3.409182	-0.942975
F	-4.785313	0.592624	1.894451
F	-3.830571	-0.086840	4.356506
F	-1.143090	-0.416474	4.703566
F	0.527768	-0.080556	2.661634
F	4.375907	-0.837390	-1.711283
F	2.592130	1.066285	-1.224907
H	-2.631153	-1.157331	-1.094027
H	-2.716900	-3.609315	-1.476056
H	-0.986939	-4.712052	-2.875205
H	0.821006	-3.344440	-3.894818
H	0.913592	-0.899499	-3.470291
H	2.242672	1.563628	1.452307
H	2.957312	3.811857	2.160939
H	1.623094	5.809365	1.521866
H	-0.442546	5.513879	0.168897
H	-1.157377	3.258049	-0.525661

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Thiophenol-B(C_6F_5)$_3$

C	-1.807076	-1.689113	-1.715877
C	-1.798805	-3.057602	-1.966911
C	-0.796439	-3.622942	-2.752118
C	0.192648	-2.818410	-3.312913
C	0.189863	-1.446093	-3.081118
C	-0.805928	-0.897795	-2.275111
S	-0.630647	0.826348	-1.839022
B	0.000236	0.720593	0.172177
C	0.566437	2.201713	0.473149
C	1.768638	2.466039	1.122554
C	1.074725	-0.466276	-0.019075
C	0.832635	-1.793869	0.329093
C	-1.219560	0.436287	1.202747
C	-2.593679	0.538961	1.042244
C	2.170002	3.753045	1.462850
C	1.349982	4.831557	1.162999
C	0.134531	4.614034	0.527395
C	-0.226811	3.313764	0.213218
C	1.698922	-2.833994	0.013639
C	2.868981	-2.563489	-0.679180
C	-3.506478	0.359945	2.077547
C	-3.046760	0.089375	3.354818
C	-1.678080	-0.007406	3.575650
C	-0.809896	0.172469	2.512131
C	3.151734	-1.257960	-1.056543
C	2.255222	-0.251366	-0.729025
F	2.598739	1.475318	1.455666
F	-0.291505	-2.147626	0.963629
F	-3.151019	0.792575	-0.163852
F	3.331180	3.958745	2.078030
F	1.724145	6.065199	1.481396
F	-0.663889	5.638527	0.238282
F	-1.421826	3.134941	-0.389477
F	1.405053	-4.085827	0.356835
F	3.703979	-3.546907	-0.994928
F	-4.813345	0.456224	1.843155
F	-3.901975	-0.078422	4.356540
F	-1.219029	-0.262936	4.796835
F	0.500874	0.082671	2.772601
F	4.257599	-0.988959	-1.746985
F	2.537599	0.975178	-1.191673
H	-2.570666	-1.244405	-1.087300
H	-2.569761	-3.684434	-1.532369
H	-0.786873	-4.693183	-2.927872
H	0.970861	-3.256902	-3.928364
H	0.960028	-0.809648	-3.506302
H	-1.923829	1.163668	-1.755646

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[Thiophenoxide-B(C_6F_5)$_3$]-

C	-1.764517	-1.736684	-1.743577
C	-1.720376	-3.102609	-2.010403
C	-0.723165	-3.628740	-2.827924
C	0.226730	-2.775993	-3.386672
C	0.190569	-1.411914	-3.111774
C	-0.796941	-0.877800	-2.275940
S	-0.765946	0.850019	-1.843016
B	-0.099934	0.731350	0.022986
C	0.503402	2.210849	0.400575
C	1.724814	2.456954	1.023472
C	1.009737	-0.462196	-0.055519
C	0.763957	-1.778119	0.324284
C	-1.247621	0.471558	1.175052
C	-2.632645	0.512492	1.055155
C	2.158608	3.729737	1.380424
C	1.346203	4.825697	1.143230
C	0.105557	4.630623	0.556979
C	-0.288806	3.343418	0.217105
C	1.619320	-2.838143	0.039614
C	2.794931	-2.600582	-0.649231
C	-3.497728	0.354039	2.137951
C	-2.989548	0.163606	3.409598
C	-1.613545	0.125555	3.585016
C	-0.791495	0.284064	2.481397
C	3.089194	-1.305823	-1.050562
C	2.201034	-0.281779	-0.758039
F	2.565914	1.462575	1.332776
F	-0.362757	-2.116303	0.973332
F	-3.244416	0.681899	-0.123827
F	3.349593	3.905421	1.964779
F	1.748801	6.054247	1.483233
F	-0.700260	5.677142	0.343202
F	-1.518962	3.221944	-0.302082
F	1.312537	-4.082552	0.422860
F	3.634432	-3.603250	-0.929887
F	-4.823269	0.391907	1.955805
F	-3.809913	0.015555	4.454848
F	-1.104198	-0.056369	4.808884
F	0.530242	0.244748	2.716535
F	4.216635	-1.064139	-1.731644
F	2.527690	0.928713	-1.231498
H	-2.537988	-1.320616	-1.106586
H	-2.465033	-3.759413	-1.570218
H	-0.683936	-4.695607	-3.025746
H	1.011520	-3.176433	-4.022345
H	0.947470	-0.745785	-3.515659

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[Thiophenol-$SiEt_3$]$^+$

C	-1.607661	-2.262882	0.356658
C	-2.078648	-3.209985	-0.549484
C	-1.211207	-3.788726	-1.472283
C	0.136341	-3.431070	-1.494897
C	0.622348	-2.475429	-0.608222
C	-0.263509	-1.904184	0.303174
S	0.257220	-0.595943	1.416138
Si	0.402447	1.231601	-0.034984
C	0.730376	2.603399	1.186643
C	-0.454285	2.902562	2.118259
C	1.798195	0.831673	-1.207798
C	3.180136	0.659933	-0.564608
C	-1.306568	1.215733	-0.795472
C	-1.419876	0.428058	-2.110715
H	-2.273597	-1.821432	1.091538
H	-3.122824	-3.500739	-0.523480
H	-1.583089	-4.530030	-2.170802
H	0.812953	-3.895023	-2.203910
H	1.670850	-2.191815	-0.625657
H	1.557540	-0.915540	1.550909
H	1.636894	2.383475	1.763149
H	0.975135	3.491303	0.587374
H	-0.220362	3.736229	2.782550
H	-1.349718	3.173204	1.552499
H	-0.703454	2.043451	2.748278
H	1.819888	1.675165	-1.913302
H	1.523729	-0.040440	-1.812156
H	3.947770	0.512299	-1.326401
H	3.220819	-0.211958	0.098370
H	3.465154	1.535991	0.023831
H	-1.566097	2.269607	-0.965836
H	-2.038500	0.860086	-0.059150
H	-2.435296	0.493980	-2.506161
H	-1.182539	-0.631330	-1.977032
H	-0.744771	0.829623	-2.871023

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Thiophenoxide-$SiEt_3$

C	-1.582033	-2.191699	0.380781
C	-2.124052	-3.105847	-0.518326
C	-1.309348	-3.733032	-1.458262
C	0.055027	-3.454715	-1.486056
C	0.602657	-2.544646	-0.585474
C	-0.216827	-1.897451	0.343135
S	0.467260	-0.679494	1.465472
Si	0.428659	1.012011	0.094389
C	0.711873	2.509741	1.201503
C	-0.473818	2.820226	2.123645
C	1.809821	0.842449	-1.175596
C	3.213357	0.810171	-0.562184
C	-1.245900	1.114389	-0.774078
C	-1.332537	0.364205	-2.110572
H	-2.211658	-1.694191	1.111530
H	-3.186665	-3.324588	-0.486846
H	-1.735161	-4.440609	-2.162047
H	0.697085	-3.947678	-2.209064
H	1.666536	-2.327142	-0.596784
H	1.621249	2.349778	1.793155
H	0.922408	3.367990	0.549199
H	-0.280784	3.698026	2.746523
H	-1.382792	3.018099	1.546904

H	-0.685152	1.977843	2.788449
H	1.716353	1.684533	-1.875609
H	1.627781	-0.061210	-1.770421
H	3.987107	0.694450	-1.326295
H	3.311202	-0.019709	0.144647
H	3.427688	1.732802	-0.013732
H	-1.454915	2.181326	-0.934558
H	-2.020655	0.757349	-0.085090
H	-2.324084	0.471101	-2.560002
H	-1.138086	-0.705623	-1.988242
H	-0.603370	0.752588	-2.828228

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[Thiophenol-$SiPhH_2$]$^+$

C	-0.259503	-3.751052	0.551795
C	0.214302	-5.008760	0.193468
C	1.571107	-5.308102	0.304468
C	2.467841	-4.356579	0.783317
C	2.013749	-3.096287	1.162174
C	0.655178	-2.816837	1.035033
S	0.137116	-1.163902	1.515633
Si	-0.388151	-0.165473	-0.500692
C	-1.415204	-1.350331	-1.443270
C	-2.804056	-1.406398	-1.233810
C	-3.570028	-2.366298	-1.884588
C	-2.957171	-3.271410	-2.751795
C	-1.582311	-3.219888	-2.974245
C	-0.810606	-2.265570	-2.320616
H	-1.313942	-3.511141	0.450744
H	-0.482422	-5.753496	-0.174858
H	1.929882	-6.291659	0.021775
H	3.521363	-4.594463	0.876918
H	2.701438	-2.357001	1.560192
H	0.986793	0.039300	-0.980889
H	-1.067724	1.034376	0.015038
H	-3.292406	-0.693627	-0.572883
H	-4.642307	-2.403812	-1.726907
H	-3.558230	-4.015626	-3.263774
H	-1.114139	-3.919425	-3.658053
H	0.262209	-2.235531	-2.493824
H	-1.104228	-1.432837	1.960751

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Thiophenoxide-$SiPhH_2$

C	-0.653475	-3.037277	0.821897
C	-0.680535	-4.346930	0.350543
C	0.424530	-4.876644	-0.310217
C	1.559655	-4.092651	-0.500643
C	1.592458	-2.782440	-0.032572
C	0.485111	-2.251215	0.632164
S	0.535187	-0.570780	1.266024
Si	-0.267920	0.376628	-0.491728
C	-0.201597	2.222459	-0.221117
C	-1.378417	2.981318	-0.183751
C	-1.334207	4.358511	0.018559
C	-0.108659	4.995632	0.189020
C	1.072100	4.256020	0.157791
C	1.024259	2.881142	-0.045934
H	-1.508526	-2.618298	1.342726
H	-1.567441	-4.953670	0.502303
H	0.401718	-5.898238	-0.675161
H	2.424013	-4.500882	-1.014458
H	2.474074	-2.165646	-0.174514
H	-1.675493	-0.037107	-0.707795
H	0.552349	-0.048058	-1.651392
H	-2.340590	2.492106	-0.312852
H	-2.254751	4.932846	0.044787
H	-0.072260	6.068783	0.347925
H	2.028073	4.751818	0.292701
H	1.951502	2.312829	-0.063836

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BEt_3-(Thiophenol)$_2$

C	-0.65029	1.45532	-1.04333
C	-0.67357	2.84613	-1.05245
C	-0.80131	3.55660	0.13836
C	-0.89914	2.86726	1.34361
C	-0.87628	1.47582	1.36512
C	-0.75892	0.76746	0.16818
S	-0.72938	-1.00878	0.10641
H	-0.54539	0.90452	-1.97403
H	-0.58921	3.37347	-1.99677
H	-0.81881	4.64078	0.12743
H	-0.99159	3.41158	2.27764
H	-0.95014	0.94555	2.31014
H	-0.81008	-1.21260	1.43025
B	-3.88932	-0.98749	-0.09719
C	-3.87486	-2.48955	-0.59332
C	-3.46447	-2.73976	-2.04546
C	-4.01013	-0.65514	1.44529
C	-3.80886	-1.79886	2.43967
C	-3.97049	0.18295	-1.16001
C	-4.13640	1.61375	-0.64397
H	-3.27177	-3.10858	0.08364
H	-4.90727	-2.84887	-0.43464
H	-3.52625	-3.79783	-2.31560
H	-4.09853	-2.18343	-2.74240
H	-2.43270	-2.41490	-2.21726
H	-5.01713	-0.22493	1.57662
H	-3.34452	0.18922	1.67846
H	-3.93427	-1.47551	3.47712
H	-2.80680	-2.23445	2.35003
H	-4.51889	-2.61161	2.25834
H	-4.79387	-0.06382	-1.84916
H	-3.07518	0.11029	-1.79760
H	-4.17254	2.34114	-1.46064
H	-3.31034	1.90292	0.01328
H	-5.06188	1.71997	-0.06830
C	5.39013	0.53062	-0.12988
C	6.50026	-0.28604	0.05371
C	6.34614	-1.65857	0.23137
C	5.06769	-2.20885	0.22282

C	3.95102	-1.39979	0.03838
C	4.10746	-0.02324	-0.13843
S	2.72340	1.06450	-0.37966
H	5.51670	1.60053	-0.26584
H	7.49174	0.15560	0.05846
H	7.21410	-2.29295	0.37503
H	4.93353	-3.27732	0.35927
H	2.95683	-1.83802	0.03047
H	1.77862	0.11839	-0.26386

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[BEt_3-(Thiophenol-Thiophenoxide)]-

C	-1.96740	1.81532	-0.53729
C	-2.98560	2.73986	-0.75329
C	-4.06464	2.81903	0.12360
C	-4.11101	1.96680	1.22546
C	-3.09402	1.04290	1.44270
C	-2.00867	0.94274	0.56027
S	-0.73741	-0.26041	0.82796
H	-1.13426	1.74636	-1.23146
H	-2.93632	3.39906	-1.61569
H	-4.86061	3.53759	-0.04875
H	-4.94745	2.01868	1.91756
H	-3.13008	0.36986	2.29386
B	-1.20278	-1.89449	-0.40745
C	0.28690	-2.47742	-0.73006
C	1.07807	-1.69316	-1.78053
C	-2.10406	-2.89033	0.51166
C	-1.38411	-3.52953	1.70045
C	-1.97771	-1.38744	-1.74702
C	-3.49196	-1.17345	-1.64096
H	0.88631	-2.55907	0.19177
H	0.16977	-3.51836	-1.07865
H	2.11083	-2.04537	-1.89776
H	0.59191	-1.75734	-2.76055
H	1.12340	-0.62772	-1.52164
H	-2.48634	-3.69312	-0.14373
H	-2.99896	-2.36218	0.87411
H	-2.03725	-4.17174	2.30605
H	-0.97539	-2.75443	2.35859
H	-0.54147	-4.14535	1.36478
H	-1.80033	-2.16004	-2.51610
H	-1.51054	-0.47840	-2.15302
H	-3.93741	-0.85072	-2.59123
H	-3.74466	-0.41780	-0.89037
H	-3.99551	-2.10030	-1.34290
C	4.46362	1.61885	-0.22953
C	5.59293	0.82720	-0.04999
C	5.47119	-0.48116	0.41142
C	4.20445	-0.98632	0.69589
C	3.06992	-0.20012	0.52668
C	3.19130	1.11194	0.05552
S	1.77844	2.15256	-0.19146
H	4.56263	2.63668	-0.59638
H	6.57358	1.23625	-0.27687
H	6.35287	-1.10004	0.54591
H	4.08879	-2.00603	1.05152
H	2.08555	-0.60190	0.74894
H	0.83301	1.20928	0.15551

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BPh_3-(Thiophenol)$_2$

C	1.71484	-2.30220	-0.24315
C	2.90826	-2.94890	0.06553
C	4.05943	-2.69952	-0.67620
C	4.01191	-1.79970	-1.73785
C	2.82312	-1.15628	-2.06392
C	1.67427	-1.40616	-1.31356
S	0.12485	-0.60357	-1.66924
H	0.82475	-2.47487	0.35518
H	2.93596	-3.64206	0.90014
H	4.98925	-3.19982	-0.42647
H	4.90644	-1.58853	-2.31545
H	2.79459	-0.45046	-2.88838
H	0.64367	0.44385	-2.32987
B	0.58499	1.33736	0.76539
C	-0.49097	2.36881	0.26016
C	-0.16721	3.73483	0.20284
C	2.07935	1.43702	0.27888
C	3.10033	0.68704	0.88937
C	0.20729	0.33355	1.92152
C	-0.71262	-0.71673	1.78907
C	-1.10734	4.69410	-0.16619
C	-2.39521	4.30103	-0.51421
C	-2.74084	2.95137	-0.46803
C	-1.80794	2.00135	-0.06676
C	4.41557	0.74169	0.43860
C	4.74196	1.53346	-0.65917
C	-1.01037	-1.55926	2.85661
C	-0.42312	-1.34984	4.10166
C	0.47226	-0.29691	4.26617
C	0.78940	0.52299	3.18612
C	3.74627	2.26057	-1.30851
C	2.43671	2.21135	-0.84095
H	0.83830	4.05391	0.46557
H	2.85478	0.03712	1.72377
H	-1.18721	-0.90129	0.82999
H	-0.83163	5.74396	-0.18818
H	-3.12977	5.04199	-0.81477
H	-3.74449	2.63590	-0.73364
H	-2.11120	0.95662	-0.01819
H	5.18148	0.15007	0.93035
H	5.76631	1.57251	-1.01807
H	-1.69966	-2.38668	2.71087
H	-0.65948	-2.00259	4.93616
H	0.93374	-0.11986	5.23287
H	1.50494	1.32995	3.32975
H	3.99224	2.86742	-2.17475
H	1.66880	2.78097	-1.35832
C	-3.87925	-1.58252	0.36883
C	-4.78617	-0.52903	0.32316
C	-4.95795	0.20063	-0.85025

C	-4.20323	-0.12086	-1.97565
C	-3.29945	-1.17857	-1.94190
C	-3.13907	-1.91927	-0.76803
S	-2.03651	-3.30778	-0.65651
H	-3.74435	-2.14362	1.28879
H	-5.35653	-0.27752	1.21114
H	-5.67207	1.01692	-0.88567
H	-4.31944	0.45034	-2.89123
H	-2.72134	-1.42971	-2.82571
H	-1.35789	-3.05385	-1.78635

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$[BPh_3$-(Thiophenol-Thiophenoxide)]-

C	-0.85031	3.26707	-1.67758
C	-1.60563	4.43290	-1.68263
C	-2.80703	4.49841	-0.97891
C	-3.23436	3.37964	-0.26970
C	-2.48184	2.20813	-0.25823
C	-1.27410	2.13284	-0.96647
S	-0.24515	0.69183	-1.02618
H	0.08583	3.22032	-2.22691
H	-1.25179	5.29648	-2.23946
H	-3.39903	5.40863	-0.98252
H	-4.16720	3.41223	0.28633
H	-2.82924	1.34734	0.30243
B	-1.03205	-0.78739	0.07970
C	-0.01557	-1.99621	-0.34290
C	-0.38368	-3.08265	-1.14764
C	-2.56806	-1.06885	-0.38935
C	-3.58202	-1.40483	0.52038
C	-0.88656	-0.47879	1.67215
C	-0.69339	0.78690	2.24228
C	0.52956	-4.07236	-1.51306
C	1.85288	-3.99742	-1.08911
C	2.24839	-2.93129	-0.28281
C	1.32197	-1.96117	0.08895
C	-4.88622	-1.68419	0.10992
C	-5.22191	-1.63625	-1.23878
C	-0.58612	0.97240	3.62109
C	-0.67278	-0.11491	4.48398
C	-0.85947	-1.38851	3.94993
C	-0.95655	-1.55812	2.57181
C	-4.23740	-1.30299	-2.16764
C	-2.94157	-1.02334	-1.74440
H	-1.41047	-3.15733	-1.49678
H	-3.34892	-1.43866	1.58164
H	-0.61802	1.65591	1.59248
H	0.20545	-4.90299	-2.13568
H	2.56842	-4.76222	-1.37970
H	3.27824	-2.85140	0.05609
H	1.64246	-1.14608	0.73804
H	-5.64252	-1.93604	0.84958
H	-6.23695	-1.84926	-1.56341
H	-0.42818	1.97172	4.01858
H	-0.58650	0.02508	5.55814
H	-0.91685	-2.25178	4.60852
H	-1.07908	-2.56265	2.16931
H	-4.48369	-1.25273	-3.22546
H	-2.18725	-0.75092	-2.47940
C	5.26086	1.20241	0.48111
C	6.26961	0.64773	-0.29822
C	5.95570	-0.08742	-1.43902
C	4.61953	-0.25524	-1.79316
C	3.60216	0.30212	-1.02447
C	3.91802	1.03230	0.12601
S	2.67545	1.73710	1.17572
H	5.51010	1.76802	1.37455
H	7.30696	0.78786	-0.00775
H	6.74370	-0.52600	-2.04312
H	4.35469	-0.83243	-2.67392
H	2.56380	0.16258	-1.30990
H	1.59697	1.32845	0.45593

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$B(C_6F_5)Ph$-$(Thiophenol)_2$

C	1.04392	-2.06794	2.00119
C	1.64547	-3.29692	1.75296
C	1.01272	-4.24414	0.94998
C	-0.23672	-3.95409	0.40908
C	-0.84022	-2.72120	0.63922
C	-0.19875	-1.76763	1.43321
S	-0.88714	-0.15457	1.70716
H	1.53213	-1.34655	2.64915
H	2.61507	-3.51365	2.19043
H	1.48752	-5.19898	0.75228
H	-0.74055	-4.68241	-0.21790
H	-1.80236	-2.49087	0.19213
H	-1.99795	-0.34265	0.97588
B	1.20875	1.65442	-0.32497
C	0.18093	2.37612	-1.25931
C	0.17152	2.15055	-2.64615
C	1.73730	0.21660	-0.72130
C	3.05853	-0.19120	-0.51044
C	1.78182	2.38447	0.93173
C	2.23557	1.66447	2.04961
C	-0.70292	2.83021	-3.48752
C	-1.61145	3.74285	-2.95281
C	-1.63519	3.97380	-1.57894
C	-0.74452	3.30104	-0.74653
C	3.51869	-1.46394	-0.82099
C	2.64691	-2.38607	-1.38279
C	2.72466	2.30444	3.17969
C	2.80135	3.69691	3.20672
C	2.38319	4.43659	2.10490
C	1.87000	3.78527	0.98623
C	1.33525	-2.01924	-1.64387
C	0.90595	-0.74613	-1.30113
F	3.96073	0.65695	-0.01165
F	4.78512	-1.80567	-0.59043
F	3.06616	-3.61093	-1.67327
F	0.49651	-2.89463	-2.19439
F	-0.38940	-0.48849	-1.51271

H	0.87214	1.43687	-3.07288
H	2.19456	0.57890	2.02230
H	-0.68146	2.64798	-4.55722
H	-2.30001	4.27058	-3.60536
H	-2.34506	4.68044	-1.15922
H	-0.76869	3.48446	0.32470
H	3.05459	1.72467	4.03578
H	3.19237	4.20211	4.08453
H	2.45389	5.51957	2.11777
H	1.54609	4.37280	0.13184
C	-4.17657	-1.27367	-0.43891
C	-3.37343	-0.59709	-1.35362
C	-3.12344	0.76538	-1.20382
C	-3.69709	1.44732	-0.13331
C	-4.50564	0.78089	0.78445
C	-4.74393	-0.58765	0.63938
S	-5.76793	-1.50727	1.76384
H	-4.35487	-2.33939	-0.55214
H	-2.91762	-1.14465	-2.17229
H	-2.47521	1.28589	-1.90149
H	-3.50620	2.50802	-0.00658
H	-4.94831	1.32563	1.61282
H	-5.72800	-0.61656	2.76492

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[B(C_6F_5)Ph_2-(Thiophenol-Thiophenoxide)]-

C	-0.40990	-2.72453	-1.10932
C	-0.44497	-4.04754	-0.67852
C	0.49238	-4.51269	0.24127
C	1.46739	-3.64355	0.72359
C	1.49944	-2.31718	0.30116
C	0.55672	-1.83693	-0.61734
S	0.59535	-0.14916	-1.18307
H	-1.12230	-2.36429	-1.84393
H	-1.20607	-4.71824	-1.06736
H	0.46475	-5.54542	0.57638
H	2.20477	-3.99343	1.44024
H	2.24669	-1.63894	0.70286
B	-0.74242	0.84440	-0.01973
C	-0.77316	2.32632	-0.68224
C	-1.97011	3.02630	-0.88780
C	-0.10636	0.78980	1.47234
C	-0.12622	-0.40059	2.22126
C	-2.22754	0.13684	-0.10317
C	-2.78243	-0.38661	-1.27342
C	-1.99642	4.31534	-1.41840
C	-0.80985	4.95163	-1.76776
C	0.39761	4.28376	-1.57581
C	0.40875	2.99775	-1.04320
C	0.49634	-0.50880	3.45982
C	1.15893	0.58797	4.00815
C	-4.03926	-0.97670	-1.34604
C	-4.84497	-1.01536	-0.22066
C	-4.37211	-0.45957	0.95510
C	-3.10308	0.11172	0.98632
C	1.17613	1.78673	3.30344
C	0.55120	1.88075	2.05859
F	-2.11311	-0.36155	-2.43377
F	-4.48730	-1.48841	-2.49963
F	-6.06214	-1.56646	-0.27330
F	-5.15072	-0.45499	2.04437
F	-2.77530	0.67619	2.15573
H	-2.91304	2.55170	-0.62615
H	-0.64523	-1.26834	1.81807
H	-2.94781	4.82157	-1.56102
H	-0.82413	5.95496	-2.18462
H	1.33484	4.76485	-1.84267
H	1.36574	2.49960	-0.89808
H	0.46578	-1.45286	3.99794
H	1.65254	0.50813	4.97265
H	1.68218	2.65482	3.71833
H	0.57892	2.83027	1.53063
C	4.35026	-0.54438	-1.23806
C	5.29559	-1.17056	-2.04469
C	6.65132	-1.11428	-1.73204
C	7.05805	-0.42011	-0.59503
C	6.12163	0.20665	0.21900
C	4.75889	0.15028	-0.09446
S	3.61642	0.96125	0.99437
H	3.29511	-0.58618	-1.49380
H	4.96192	-1.70724	-2.92774
H	7.38251	-1.60510	-2.36653
H	8.11185	-0.36612	-0.33680
H	6.44336	0.74389	1.10689
H	2.48297	0.62337	0.32933

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B(C_6F_5)$_2$Ph-(Thiophenol)$_2$

C	2.62210	-2.49030	-1.77175
C	3.99425	-2.54555	-1.99325
C	4.69395	-1.40669	-2.38318
C	4.00534	-0.21083	-2.57148
C	2.63272	-0.14249	-2.35493
C	1.93955	-1.28410	-1.94406
S	0.20064	-1.12777	-1.59773
H	2.08969	-3.37837	-1.44652
H	4.51938	-3.48238	-1.83985
H	5.76618	-1.45126	-2.54000
H	4.53890	0.68227	-2.88103
H	2.10562	0.79322	-2.49602
H	0.03440	-2.33111	-1.02839
B	0.18889	0.26952	1.22931
C	-0.57798	-0.91361	1.89392
C	-0.06684	-1.62725	2.98784
C	-0.65976	1.49900	0.71110
C	-0.35520	2.20233	-0.45449
C	1.76264	0.27452	1.13416
C	2.50556	-0.91027	1.05577
C	-0.77833	-2.67865	3.55506
C	-2.00326	-3.06182	3.01184
C	-2.52875	-2.37443	1.91894
C	-1.83023	-1.29745	1.38698

C	-1.13127	3.23552	-0.95249
C	-2.26475	3.62698	-0.25058
C	3.88523	-0.93802	0.91086
C	4.58151	0.25647	0.80880
C	3.89443	1.46103	0.88202
C	2.51741	1.44961	1.04714
C	-2.60101	2.97694	0.92653
C	-1.80421	1.93407	1.38446
F	0.73366	1.88030	-1.16586
F	1.90080	-2.10148	1.05909
F	-0.79790	3.85962	-2.08024
F	-3.01488	4.62279	-0.70191
F	4.53899	-2.09529	0.84943
F	5.89694	0.24848	0.64375
F	4.56133	2.60980	0.79883
F	1.92448	2.64274	1.13198
F	-3.67547	3.35984	1.61166
F	-2.16985	1.37784	2.53940
H	0.89941	-1.35144	3.40341
H	-0.37368	-3.20869	4.41135
H	-2.54941	-3.89517	3.44328
H	-3.48082	-2.66548	1.48507
H	-2.25718	-0.74565	0.55210
C	-3.31650	-2.30990	-1.90630
C	-3.84810	-3.54721	-1.55419
C	-4.99475	-3.62815	-0.76884
C	-5.60509	-2.45624	-0.32699
C	-5.07566	-1.21461	-0.66383
C	-3.93238	-1.13662	-1.46396
S	-3.31233	0.48025	-1.86408
H	-2.43018	-2.25701	-2.53258
H	-3.36290	-4.45269	-1.90434
H	-5.40903	-4.59475	-0.50356
H	-6.49850	-2.50463	0.28732
H	-5.55277	-0.30481	-0.31200
H	-2.24305	0.06539	-2.56146

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[$B(C_6F_5)_2$Ph-(Thiophenol-Thiophenoxide)]-

C	-2.05389	-2.16437	-2.09243
C	-2.99973	-3.17354	-1.94037
C	-2.86026	-4.11744	-0.92441
C	-1.76278	-4.04994	-0.07056
C	-0.81134	-3.04399	-0.22423
C	-0.95395	-2.08223	-1.23063
S	0.19638	-0.72980	-1.38960
H	-2.16984	-1.40848	-2.86347
H	-3.85705	-3.21254	-2.60635
H	-3.60637	-4.89553	-0.79523
H	-1.64988	-4.77398	0.73065
H	0.02336	-2.96958	0.46745
B	-0.31137	0.40198	0.19870
C	0.49261	0.01332	1.55268
C	0.13577	0.65222	2.75237
C	-1.92963	0.19509	0.28234
C	-2.79358	0.79510	-0.63341
C	0.14611	1.94646	-0.14080
C	1.38356	2.24730	-0.70140
C	0.83399	0.43690	3.93466
C	1.93201	-0.42452	3.95169
C	2.31162	-1.06188	2.77615
C	1.59615	-0.84181	1.59853
C	-4.14178	0.48872	-0.74406
C	-4.69076	-0.47827	0.08498
C	1.86318	3.53591	-0.89694
C	1.09034	4.61505	-0.50168
C	-0.14199	4.37554	0.08518
C	-0.57701	3.06750	0.26112
C	-3.87826	-1.10983	1.00924
C	-2.53327	-0.76120	1.09654
F	-2.32958	1.70588	-1.50239
F	2.21416	1.26255	-1.08643
F	-4.91603	1.10323	-1.64791
F	-5.98649	-0.79495	-0.01179
F	3.06697	3.73985	-1.44576
F	1.52824	5.86624	-0.67550
F	-0.89424	5.40706	0.48661
F	-1.76451	2.93633	0.87647
F	-4.38960	-2.05457	1.80644
F	-1.82824	-1.44995	2.00350
H	-0.71425	1.33431	2.75225
H	0.52634	0.94272	4.84642
H	2.48395	-0.59139	4.87260
H	3.16922	-1.72989	2.76207
H	1.90664	-1.34906	0.69069
C	3.98498	-1.14352	-0.96464
C	5.01384	-0.24703	-0.69794
C	6.22678	-0.69868	-0.18373
C	6.39846	-2.05706	0.07311
C	5.36710	-2.95852	-0.17190
C	4.15348	-2.50288	-0.69281
S	2.84638	-3.67057	-0.98690
H	3.03965	-0.78773	-1.36011
H	4.84781	0.80831	-0.89158
H	7.02962	0.00185	0.02276
H	7.33844	-2.41989	0.47876
H	5.49841	-4.01410	0.04836
H	1.89011	-2.74847	-1.23356

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$B(C_6F_5)_3$-$(Thiophenol)_2$

C	3.39248	-0.35198	2.11293
C	4.64708	-0.94184	1.99389
C	4.76785	-2.32626	1.89804
C	3.63391	-3.13378	1.94680
C	2.37378	-2.55827	2.07843
C	2.26553	-1.17017	2.14793
S	0.60917	-0.49819	2.10174
H	3.28923	0.72583	2.16849
H	5.53072	-0.31396	1.95976
H	5.74822	-2.77679	1.78688
H	3.72700	-4.21240	1.87888

H	1.48136	-3.17615	2.11155
H	0.78751	0.58657	2.86596
B	0.51142	0.27677	0.15201
C	-1.04934	0.59782	-0.10598
C	-1.71502	0.30615	-1.29253
C	1.13730	-1.00906	-0.59612
C	2.45565	-1.09383	-1.03880
C	1.32082	1.67603	-0.00944
C	1.73985	2.59588	0.94159
C	-2.99557	0.77236	-1.57156
C	-3.66015	1.55079	-0.63804
C	-3.04644	1.84098	0.57386
C	-1.76138	1.37833	0.79895
C	3.01802	-2.26460	-1.53391
C	2.25109	-3.41775	-1.60168
C	2.31977	3.82165	0.62769
C	2.47405	4.18498	-0.69888
C	2.05341	3.31012	-1.69305
C	1.48802	2.09919	-1.33068
C	0.93320	-3.38663	-1.16663
C	0.41563	-2.19800	-0.67441
F	-1.13361	-0.43778	-2.23882
F	3.27571	-0.03836	-0.97262
F	1.64361	2.34199	2.26659
F	-3.59166	0.46205	-2.72077
F	-4.88156	2.00863	-0.89090
F	-3.69485	2.55170	1.49540
F	-1.17742	1.71568	1.96789
F	4.28916	-2.28987	-1.92743
F	2.77593	-4.54604	-2.06681
F	2.71616	4.64385	1.59702
F	3.01944	5.35297	-1.01842
F	2.19008	3.64455	-2.97274
F	1.08303	1.29703	-2.32364
F	0.18973	-4.49041	-1.20780
F	-0.84161	-2.24161	-0.20200
C	-5.16056	-0.54129	1.40672
C	-6.10919	-0.32987	0.41247
C	-5.97641	-0.94506	-0.83089
C	-4.89914	-1.79339	-1.06656
C	-3.95636	-2.03140	-0.06919
C	-4.08200	-1.39754	1.16755
S	-2.80649	-1.66330	2.38257
H	-5.24675	-0.02646	2.35921
H	-6.94050	0.34116	0.60224
H	-6.70564	-0.75839	-1.61164
H	-4.78556	-2.27398	-2.03274
H	-3.12317	-2.70112	-0.25206
H	-3.57692	-1.44483	3.45877

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[B(C_6F_5)$_3$-(Thiophenol-Thiophenoxide)]-

C	-2.69466	-0.25613	-2.66634
C	-3.98722	-0.70726	-2.91949
C	-4.29578	-2.06044	-2.80295
C	-3.29945	-2.96385	-2.43897
C	-2.00861	-2.51410	-2.17515
C	-1.69643	-1.15430	-2.27443
S	-0.07698	-0.56168	-1.82982
H	-2.44654	0.79675	-2.74993
H	-4.75788	0.00414	-3.20113
H	-5.30677	-2.40892	-2.99039
H	-3.53126	-4.02049	-2.34053
H	-1.23499	-3.20798	-1.85848
B	-0.44334	0.24975	-0.04305
C	1.00039	0.26649	0.73047
C	1.23893	-0.17857	2.02859
C	-1.56564	-0.75078	0.58923
C	-2.93152	-0.48209	0.57654
C	-0.92175	1.82081	-0.07010
C	-0.98021	2.70651	-1.14013
C	2.49589	-0.15534	2.62159
C	3.57701	0.36056	1.92505
C	3.37896	0.87682	0.65492
C	2.10827	0.82942	0.09913
C	-3.90763	-1.41792	0.90421
C	-3.53179	-2.69533	1.27882
C	-1.33544	4.04793	-1.00129
C	-1.63718	4.55926	0.24753
C	-1.58731	3.71744	1.34964
C	-1.23173	2.39127	1.16592
C	-2.18344	-3.01872	1.30354
C	-1.24666	-2.05870	0.95224
F	0.25051	-0.66342	2.79153
F	-3.40124	0.71717	0.19576
F	-0.72218	2.32590	-2.39867
F	2.67211	-0.61960	3.86344
F	4.79334	0.37409	2.47747
F	4.40529	1.39490	-0.02211
F	1.98028	1.35601	-1.13014
F	-5.20398	-1.09390	0.85511
F	-4.45300	-3.60835	1.60149
F	-1.38182	4.84950	-2.07186
F	-1.97491	5.84427	0.39251
F	-1.87706	4.19559	2.56473
F	-1.19772	1.62579	2.26853
F	-1.80506	-4.25734	1.63904
F	0.02968	-2.47526	0.92632
C	3.70268	-0.89919	-2.20009
C	4.65994	-0.09917	-2.81562
C	5.97369	-0.08002	-2.35586
C	6.32182	-0.85629	-1.25394
C	5.36883	-1.64544	-0.61943
C	4.05477	-1.68123	-1.09632
S	2.88506	-2.71688	-0.25580
H	2.67911	-0.90512	-2.56387
H	4.36765	0.51644	-3.66068
H	6.71516	0.54671	-2.84080
H	7.33810	-0.83676	-0.87169
H	5.63615	-2.22750	0.25795
H	1.76849	-2.14700	-0.75741

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[$SiEt_3$-(Thiophenol)$_2$]$^+$

C	-0.86152	1.24351	0.72361
C	-1.78504	2.21298	1.09933
C	-2.10920	3.25209	0.22857
C	-1.51669	3.32489	-1.02862
C	-0.59303	2.35976	-1.42298
C	-0.27522	1.33233	-0.53686
S	0.92517	0.13219	-1.12559
Si	2.63062	-0.07081	0.44490
C	2.25674	-1.68389	1.31405
C	1.02312	-1.68308	2.22334
C	4.10305	-0.15409	-0.70052
C	4.13892	-1.41660	-1.57391
C	2.51590	1.48098	1.47435
C	2.77607	2.77420	0.68745
H	-0.62312	0.42585	1.39575
H	-2.25696	2.14844	2.07375
H	-2.82789	4.00579	0.53151
H	-1.77059	4.13082	-1.70819
H	-0.13046	2.40418	-2.40360
H	0.27882	-1.06780	-0.90791
H	2.18217	-2.48334	0.56675
H	3.15712	-1.91485	1.90059
H	0.92359	-2.63743	2.74508
H	1.07587	-0.89458	2.98004
H	0.10251	-1.53591	1.64751
H	5.00282	-0.10087	-0.07334
H	4.11940	0.74804	-1.32288
H	5.00122	-1.40129	-2.24298
H	3.24526	-1.50162	-2.20231
H	4.20875	-2.32262	-0.96647
H	3.26726	1.36334	2.26785
H	1.54831	1.52565	1.98478
H	2.73155	3.64204	1.34817
H	2.02826	2.92451	-0.09778
H	3.76333	2.76696	0.21842
C	-2.69407	-1.84236	0.98969
C	-3.69841	-0.92029	1.27766
C	-4.15735	-0.05116	0.29183
C	-3.60609	-0.09594	-0.98713
C	-2.59076	-1.00065	-1.28046
C	-2.14123	-1.87745	-0.29048
S	-0.79183	-3.01733	-0.59581
H	-2.35942	-2.54710	1.74485
H	-4.13675	-0.90079	2.26995
H	-4.94882	0.65592	0.51621
H	-3.96256	0.57743	-1.75952
H	-2.15934	-1.02940	-2.27795
H	-1.13341	-3.35913	-1.84803

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$SiEt_3$-(Thiophenol-Thiophenoxide)

C	0.83114	-0.77001	0.94870
C	1.48512	-1.89765	1.43412
C	1.36719	-3.11806	0.77150
C	0.60314	-3.20508	-0.38903
C	-0.04582	-2.07683	-0.88609
C	0.06014	-0.85858	-0.21247
S	-0.77289	0.59685	-0.84429
Si	-2.71187	0.26419	0.09855
C	-3.58253	1.92735	-0.05303
C	-2.97569	3.01413	0.84339
C	-3.63506	-1.08232	-0.83920
C	-3.92428	-0.73141	-2.30227
C	-2.48774	-0.22871	1.90694
C	-2.38127	-1.73907	2.16010
H	0.92740	0.18644	1.45430
H	2.09322	-1.81891	2.32970
H	1.87548	-3.99669	1.15521
H	0.51332	-4.15127	-0.91328
H	-0.63412	-2.13207	-1.79731
H	-3.56501	2.24570	-1.10232
H	-4.64045	1.77312	0.19844
H	-3.49944	3.96747	0.73273
H	-3.02501	2.73016	1.89914
H	-1.92202	3.18206	0.60060
H	-4.57182	-1.27826	-0.29913
H	-3.05217	-2.00959	-0.77294
H	-4.44313	-1.54409	-2.81817
H	-2.99638	-0.52676	-2.84530
H	-4.55255	0.16148	-2.37941
H	-3.35067	0.17801	2.45274
H	-1.60844	0.28942	2.30768
H	-2.26425	-1.95263	3.22640
H	-1.52511	-2.17726	1.63866
H	-3.28035	-2.26037	1.81742
C	3.84648	0.94817	0.74049
C	4.44802	-0.27686	0.46697
C	4.13319	-0.96917	-0.69942
C	3.23808	-0.41348	-1.60955
C	2.65967	0.82720	-1.35927
C	2.94258	1.49980	-0.16910
S	2.16724	3.05870	0.22271
H	4.05917	1.47085	1.66789
H	5.14803	-0.70085	1.18029
H	4.58136	-1.93719	-0.89757
H	2.98648	-0.94552	-2.52147
H	1.97066	1.26476	-2.07538
H	0.93812	2.69806	-0.19003

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[$SiPhH_2$-(Thiophenol)$_2$]$^+$

C	-0.019146	-3.286179	2.402457
C	-0.385775	-4.623342	2.268396
C	0.306988	-5.453365	1.391436
C	1.373840	-4.955996	0.643908
C	1.749441	-3.622538	0.756458
C	1.043109	-2.808294	1.639441
S	1.392832	-1.052451	1.776919
Si	0.777976	-0.216096	-0.284069
C	0.395173	-1.671510	-1.332093

C	-0.791682	-2.392009	-1.117388
C	-1.025332	-3.577145	-1.803130
C	-0.079603	-4.050006	-2.712934
C	1.094293	-3.336948	-2.946302
C	1.333125	-2.152279	-2.257648
C	4.741223	-2.084268	-0.922291
C	4.677494	-3.273640	-1.645246
C	4.852124	-4.497379	-1.003158
C	5.099198	-4.528295	0.368131
C	5.152791	-3.347367	1.103159
C	4.971367	-2.125594	0.454312
S	4.942502	-0.570156	1.328884
H	-0.546437	-2.634055	3.091367
H	-1.208989	-5.013029	2.856645
H	0.017642	-6.494084	1.293411
H	1.918066	-5.599827	-0.038928
H	2.562956	-3.230989	0.154036
H	2.767331	-0.998377	1.638667
H	1.986841	0.544998	-0.649026
H	-0.367450	0.612146	0.122173
H	-1.534028	-2.032696	-0.408303
H	-1.942678	-4.130246	-1.633649
H	-0.264818	-4.974192	-3.250575
H	1.817831	-3.701178	-3.668041
H	2.253005	-1.603231	-2.440649
H	4.641516	-1.127796	-1.429047
H	4.513183	-3.238711	-2.717690
H	4.817318	-5.420674	-1.571100
H	5.250583	-5.476098	0.873809
H	5.335227	-3.383546	2.172818
H	5.434563	-1.018106	2.493955

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$SiPhH_2$-(Thiophenol-Thiophenoxide)

C	-0.271522	-3.244693	2.457048
C	-0.769575	-4.540361	2.344170
C	0.031234	-5.556972	1.826621
C	1.336569	-5.275879	1.430578
C	1.838123	-3.981149	1.531214
C	1.030051	-2.962247	2.035088
S	1.663330	-1.282494	2.083810
Si	0.476593	-0.541805	0.438143
C	0.645857	-1.518422	-1.147194
C	0.244462	-2.859644	-1.251273
C	0.358018	-3.543580	-2.458690
C	0.853033	-2.893465	-3.587866
C	1.239847	-1.557555	-3.506522
C	1.144430	-0.880880	-2.292663
H	-0.889548	-2.449020	2.861479
H	-1.784243	-4.754663	2.664105
H	-0.361009	-6.564946	1.738196
H	1.971415	-6.058718	1.026847
H	2.846332	-3.753420	1.205097
H	0.947398	0.844656	0.212782
H	-0.939645	-0.541612	0.877864
H	-0.161425	-3.380087	-0.387043
H	0.051259	-4.583228	-2.519155
H	0.933210	-3.425784	-4.530693
H	1.624693	-1.046337	-4.383152
H	1.473541	0.152986	-2.233967
C	3.775450	-3.130586	-1.333288
C	3.856407	-4.520965	-1.274195
C	4.649722	-5.138764	-0.311790
C	5.367871	-4.360145	0.595890
C	5.302381	-2.971333	0.533057
C	4.500050	-2.353074	-0.430268
S	4.436312	-0.569151	-0.560233
H	3.142819	-2.649935	-2.071517
H	3.281638	-5.115306	-1.977872
H	4.710698	-6.221632	-0.266011
H	5.987428	-4.834266	1.350308
H	5.873867	-2.362564	1.226305
H	3.981695	-0.356068	0.686747

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Aniline-BEt_3

C	-1.543827	-1.919901	0.302358
C	-2.035926	-3.024942	-0.384389
C	-1.190573	-3.785212	-1.188009
C	0.154230	-3.440629	-1.298121
C	0.654735	-2.335280	-0.617764
C	-0.201809	-1.577259	0.174508
N	0.293566	-0.385534	0.818211
B	0.359683	1.073140	-0.107822
C	0.659695	2.170025	1.059368
C	-0.511417	2.484158	1.998261
C	1.586182	0.876593	-1.149106
C	2.982341	0.709346	-0.538751
C	-1.094259	1.259773	-0.808328
C	-1.315377	0.574130	-2.162851
H	-2.201343	-1.314452	0.919720
H	-3.083881	-3.289087	-0.291330
H	-1.577509	-4.644683	-1.724442
H	0.819041	-4.030890	-1.919656
H	1.698882	-2.050881	-0.710009
H	1.244742	-0.528833	1.159437
H	1.535249	1.885475	1.666265
H	0.960501	3.101839	0.559779
H	-0.252806	3.219551	2.766624
H	-1.368211	2.873551	1.440520
H	-0.872587	1.595251	2.538361
H	1.597037	1.771362	-1.788675
H	1.389088	0.046395	-1.842855
H	3.762780	0.581387	-1.295753
H	3.053399	-0.170542	0.120283
H	3.256048	1.575412	0.071708
H	-1.237118	2.341926	-0.950559
H	-1.906689	0.973083	-0.119654
H	-2.318973	0.759397	-2.560662
H	-1.181877	-0.511821	-2.106823
H	-0.598222	0.943562	-2.902891
H	-0.282839	-0.158828	1.628806

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[Anilide-BEt_3]-

C	-1.451415	-1.496905	0.007309
C	-2.216635	-2.644302	0.142619
C	-1.663986	-3.921559	0.024898
C	-0.296580	-4.011686	-0.238942
C	0.485044	-2.877180	-0.380582
C	-0.057033	-1.566054	-0.263755
N	0.721007	-0.473432	-0.414311
H	-1.908339	-0.521034	0.113698
H	-3.279745	-2.536370	0.349207
H	-2.275117	-4.811451	0.135359
H	0.173294	-4.988662	-0.337697
H	1.549059	-2.976420	-0.588565
H	1.680969	-0.726522	-0.613124
B	0.469645	1.092570	-0.387784
C	0.447836	1.659784	1.160843
C	-0.676847	1.134814	2.057879
C	1.772299	1.733056	-1.185189
C	3.131149	1.591684	-0.487521
C	-0.894399	1.531589	-1.206525
C	-1.069498	0.857128	-2.570625
H	1.403043	1.416716	1.652773
H	0.401427	2.762663	1.140547
H	-0.648881	1.546179	3.077327
H	-1.664755	1.373067	1.644013
H	-0.623900	0.043619	2.143243
H	1.591942	2.805197	-1.359653
H	1.850185	1.282512	-2.188030
H	3.974987	1.936924	-1.100980
H	3.346051	0.549521	-0.212970
H	3.152923	2.163043	0.446739
H	-0.843863	2.622920	-1.354652
H	-1.817213	1.379685	-0.625658
H	-1.944222	1.220768	-3.128051
H	-1.179201	-0.226885	-2.454047
H	-0.189409	1.021125	-3.203565

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Aniline-BPh_3

C	-2.261074	-1.485482	-1.221094
C	-2.604782	-2.779341	-1.602548
C	-1.820282	-3.479601	-2.515254
C	-0.683254	-2.883286	-3.053458
C	-0.330076	-1.590939	-2.680754
C	-1.123254	-0.902554	-1.769844
N	-0.715375	0.423951	-1.344532
B	0.109674	0.575927	0.135944
C	0.464317	2.156008	0.238157
C	1.004481	2.611058	1.454469
C	1.411071	-0.375172	-0.012721
C	1.319403	-1.779737	-0.009236
C	-0.992439	0.182348	1.259624
C	-2.182319	0.928606	1.335243
C	1.362296	3.937728	1.654322
C	1.178839	4.873492	0.635296
C	0.639593	4.459775	-0.574828
C	0.293162	3.119245	-0.763084
C	2.432232	-2.594526	-0.198263
C	3.687322	-2.024683	-0.398645
C	-3.190676	0.632359	2.246053
C	-3.022133	-0.420807	3.144625
C	-1.837470	-1.147938	3.125628
C	-0.841078	-0.847281	2.195302
C	3.811956	-0.639226	-0.410541
C	2.689042	0.165503	-0.221492
H	-2.854392	-0.943506	-0.491421
H	-3.489364	-3.240805	-1.177049
H	-2.093291	-4.488671	-2.804719
H	-0.062222	-3.424819	-3.758679
H	0.575196	-1.131501	-3.067974
H	-0.092683	0.825199	-2.046604
H	1.143060	1.894582	2.261757
H	0.349499	-2.251911	0.133233
H	-2.314419	1.789336	0.676775
H	1.780010	4.248612	2.607349
H	1.451990	5.912827	0.787934
H	0.486959	5.175389	-1.377415
H	-0.123402	2.854331	-1.735590
H	2.319283	-3.674795	-0.189378
H	4.559049	-2.655803	-0.543405
H	-4.097775	1.229317	2.269741
H	-3.800900	-0.657428	3.863047
H	-1.685143	-1.954532	3.836859
H	0.078417	-1.424743	2.206058
H	4.784945	-0.181970	-0.565178
H	2.810132	1.245717	-0.230553
H	-1.528717	1.039475	-1.282490

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[Anilide-BPh_3]-

C	-0.959623	-1.959119	-1.592346
C	-1.341748	-3.008872	-2.413956
C	-1.584109	-2.825337	-3.776188
C	-1.430823	-1.542951	-4.301561
C	-1.047698	-0.481274	-3.496153
C	-0.800396	-0.650682	-2.111992
N	-0.440801	0.401140	-1.326864
H	-0.778036	-2.127536	-0.536575
H	-1.452440	-3.998091	-1.975973
H	-1.882349	-3.655864	-4.407789
H	-1.610430	-1.364078	-5.359547
H	-0.931254	0.511928	-3.925522
H	-0.339925	1.266918	-1.838379
B	0.038332	0.415480	0.157918
C	0.637684	1.929054	0.398374
C	1.934782	2.209969	0.846919
C	1.224250	-0.702331	0.378623
C	1.356590	-1.527113	1.504010
C	-1.213033	0.220621	1.202351
C	-2.504750	-0.134427	0.789014
C	2.386650	3.517488	1.035656

C	1.546996	4.595180	0.773085
C	0.247688	4.349018	0.330266
C	-0.190643	3.039574	0.157001
C	2.417457	-2.423249	1.649575
C	3.389952	-2.525121	0.660506
C	-3.561563	-0.271565	1.690204
C	-3.358921	-0.049094	3.048868
C	-2.089859	0.322495	3.490970
C	-1.047376	0.458118	2.578295
C	3.283019	-1.724408	-0.476208
C	2.218503	-0.838065	-0.605845
H	2.610656	1.382275	1.049695
H	0.602444	-1.478567	2.285956
H	-2.685647	-0.303221	-0.269802
H	3.401092	3.694199	1.386201
H	1.896340	5.614589	0.915684
H	-0.424555	5.180335	0.129957
H	-1.216218	2.859340	-0.164697
H	2.480113	-3.047392	2.538313
H	4.216705	-3.222618	0.768187
H	-4.548480	-0.551451	1.328323
H	-4.179304	-0.154485	3.754271
H	-1.917603	0.516340	4.547366
H	-0.068047	0.774536	2.936779
H	4.028968	-1.798217	-1.264287
H	2.138720	-0.225970	-1.502556

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Aniline-B(C_6F_5)Ph_2

C	-2.263602	-1.350098	-1.699561
C	-2.577074	-2.626288	-2.160039
C	-1.617839	-3.394103	-2.812500
C	-0.336996	-2.883363	-3.007729
C	-0.010877	-1.611290	-2.551630
C	-0.980517	-0.854164	-1.901254
N	-0.632686	0.468277	-1.397713
B	0.065647	0.588819	0.128452
C	0.475516	2.144031	0.303434
C	1.335065	2.475889	1.364915
C	1.320129	-0.421642	0.030196
C	1.207771	-1.791976	0.307292
C	-1.073726	0.217339	1.241974
C	-2.418526	0.549267	1.120124
C	1.715104	3.788182	1.617017
C	1.244711	4.821365	0.806312
C	0.390934	4.524114	-0.248027
C	0.013474	3.201682	-0.488042
C	2.243975	-2.681999	0.044554
C	3.433121	-2.220632	-0.516948
C	-3.381047	0.321640	2.092521
C	-2.992758	-0.234698	3.301811
C	-1.655594	-0.542236	3.503287
C	-0.732623	-0.301291	2.491355
C	3.575548	-0.865691	-0.800719
C	2.531007	0.016643	-0.524341
F	-2.875704	1.144542	-0.014472
F	-4.656096	0.645972	1.880816
F	-3.888800	-0.458316	4.258341
F	-1.264383	-1.052512	4.669102
F	0.542573	-0.577550	2.790710
H	-3.011659	-0.743161	-1.202376
H	-3.577940	-3.015536	-2.007670
H	-1.866897	-4.388023	-3.168264
H	0.419030	-3.478070	-3.508740
H	0.997307	-1.222643	-2.667756
H	0.062466	0.894056	-2.013843
H	-1.459559	1.065888	-1.414892
H	0.276373	-2.176523	0.719029
H	2.123054	-3.737110	0.271007
H	4.243840	-2.911894	-0.725992
H	4.501218	-0.493637	-1.229916
H	2.662435	1.075025	-0.741317
H	1.713355	1.677552	2.000121
H	2.382067	4.008868	2.444992
H	1.541597	5.847549	0.998174
H	0.013808	5.318200	-0.885455
H	-0.667306	3.023433	-1.320410

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[Anilide-B(C_6F_5)Ph_2]-

C	-1.160383	-1.930306	-1.402635
C	-1.592558	-3.030916	-2.130316
C	-1.687356	-2.998531	-3.521020
C	-1.332942	-1.820436	-4.177432
C	-0.900272	-0.711274	-3.466969
C	-0.803301	-0.728187	-2.056607
N	-0.398350	0.381841	-1.367133
H	-1.102229	-1.984703	-0.321161
H	-1.858842	-3.937634	-1.592719
H	-2.024266	-3.867010	-4.077618
H	-1.391220	-1.763369	-5.261941
H	-0.625017	0.199375	-3.994875
H	-0.017859	1.100242	-1.969559
B	0.078882	0.445423	0.102777
C	0.636616	1.959860	0.376055
C	1.746771	2.253508	1.179379
C	1.316776	-0.662390	0.281924
C	1.292734	-1.855123	0.996781
C	-1.144511	0.247399	1.169305
C	-2.482772	0.217058	0.760823
C	2.144108	3.562213	1.446084
C	1.435145	4.632792	0.907815
C	0.322045	4.373484	0.111547
C	-0.066643	3.059813	-0.138935
C	2.353505	-2.757588	1.038404
C	3.508871	-2.487326	0.327163
C	-3.534059	0.161150	1.677467
C	-3.271346	0.142439	3.042816
C	-1.946663	0.184855	3.479243
C	-0.911596	0.239934	2.553294
C	3.579679	-1.323922	-0.424968
C	2.494942	-0.457928	-0.438252

F	0.204564	-2.232658	1.688828
F	2.265756	-3.888753	1.751803
F	4.540429	-3.340115	0.354817
F	4.688321	-1.059678	-1.130115
F	2.630790	0.629617	-1.214255
H	2.323259	1.433339	1.604584
H	-2.700623	0.236876	-0.304634
H	3.014410	3.747253	2.071270
H	1.743682	5.655205	1.108740
H	-0.247979	5.198294	-0.309703
H	-0.952542	2.872313	-0.743556
H	-4.561441	0.132092	1.321865
H	-4.085869	0.099178	3.761193
H	-1.725265	0.178269	4.543877
H	0.116837	0.283642	2.911861

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Aniline-B(C_6F_5)$_2$Ph

C	-2.333652	-1.331494	-1.567040
C	-2.732425	-2.607555	-1.954588
C	-1.838232	-3.457393	-2.598896
C	-0.539974	-3.028624	-2.863339
C	-0.129212	-1.756463	-2.479972
C	-1.031945	-0.920575	-1.830972
N	-0.601577	0.406511	-1.411949
B	0.121376	0.548559	0.094172
C	0.490557	2.133697	0.281034
C	1.123539	2.499747	1.469492
C	1.423603	-0.389835	-0.035434
C	1.375602	-1.773731	0.190207
C	-0.994870	0.159652	1.222457
C	-2.306277	0.619108	1.128550
C	1.489576	3.802032	1.777003
C	1.219183	4.817666	0.868088
C	0.590323	4.508499	-0.326984
C	0.244865	3.187397	-0.588529
C	2.458357	-2.599963	-0.090395
C	3.629485	-2.060185	-0.618998
C	-3.294780	0.395978	2.073521
C	-2.966894	-0.297125	3.229780
C	-1.666416	-0.743818	3.401715
C	-0.710910	-0.502219	2.417869
C	3.705130	-0.691938	-0.858391
C	2.613672	0.125660	-0.566202
F	1.400389	1.561203	2.380310
F	-2.694697	1.334302	0.040478
F	2.092518	4.088615	2.927592
F	1.561402	6.071917	1.142549
F	0.324575	5.467364	-1.212054
F	-0.359959	2.969670	-1.782363
F	-4.534157	0.847206	1.887253
F	-3.887269	-0.523853	4.160581
F	-1.335600	-1.394122	4.514421
F	0.516757	-0.942523	2.694209
H	-3.030653	-0.656001	-1.083152
H	-3.747686	-2.932194	-1.754275
H	-2.153679	-4.450872	-2.898711
H	0.161801	-3.685686	-3.365283
H	0.889522	-1.424002	-2.659266
H	-1.387070	1.055543	-1.460243
H	0.463256	-2.219625	0.579386
H	2.388115	-3.666717	0.099120
H	4.476944	-2.701881	-0.839235
H	4.613906	-0.258832	-1.265144
H	2.695313	1.194719	-0.755106
H	0.090772	0.759108	-2.073991

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[Anilide-B(C_6F_5)$_2$Ph]-

C	-1.171734	-1.914781	-1.436689
C	-1.643052	-3.004305	-2.156425
C	-1.735258	-2.976401	-3.547046
C	-1.339271	-1.815537	-4.210417
C	-0.867418	-0.718195	-3.506846
C	-0.770623	-0.732438	-2.097756
N	-0.319237	0.361130	-1.414492
H	-1.108750	-1.970046	-0.355141
H	-1.942656	-3.897344	-1.613676
H	-2.103593	-3.835200	-4.098500
H	-1.397003	-1.762698	-5.295037
H	-0.562281	0.179877	-4.039518
H	0.062393	1.082880	-2.010403
B	0.109093	0.433025	0.054867
C	0.625342	1.955357	0.351090
C	1.716809	2.270957	1.170144
C	1.327439	-0.678512	0.281382
C	1.275660	-1.872544	0.990642
C	-1.145769	0.232206	1.122019
C	-2.498705	0.296755	0.802533
C	2.082836	3.589206	1.432015
C	1.357496	4.641759	0.879253
C	0.260057	4.357718	0.070514
C	-0.096654	3.034682	-0.180117
C	2.327097	-2.781475	1.061306
C	3.506580	-2.512697	0.388953
C	-3.513735	0.259922	1.757519
C	-3.193933	0.171523	3.100419
C	-1.858137	0.119353	3.472492
C	-0.882793	0.160598	2.488876
C	3.608154	-1.345014	-0.352066
C	2.528467	-0.473027	-0.397263
F	0.161806	-2.242719	1.649397
F	-2.920574	0.404223	-0.464634
F	2.209107	-3.915085	1.764412
F	4.531187	-3.371350	0.444365
F	-4.800379	0.318580	1.388343
F	-4.157490	0.138804	4.029012
F	-1.533590	0.040413	4.769836
F	0.390219	0.118948	2.919663
F	4.740274	-1.079620	-1.016877
F	2.694519	0.620312	-1.158675
H	2.294048	1.463230	1.614416

H	2.939456	3.796372	2.068516
H	1.641889	5.671105	1.079859
H	-0.321482	5.168408	-0.361545
H	-0.967220	2.823810	-0.799631

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Aniline-B(C_6F_5)$_3$

C	-1.824321	-1.651774	-1.662075
C	-1.904672	-2.904588	-2.263932
C	-0.981887	-3.284830	-3.233914
C	0.029569	-2.405729	-3.610874
C	0.119098	-1.150411	-3.018804
C	-0.809797	-0.785197	-2.050639
N	-0.662677	0.512706	-1.395076
B	-0.051615	0.508195	0.153473
C	0.514419	2.023544	0.396128
C	1.731938	2.340435	0.992971
C	1.092834	-0.639734	0.098784
C	1.050244	-1.878720	0.725383
C	-1.240188	0.307771	1.245334
C	-2.605061	0.463344	1.055300
C	2.125377	3.647843	1.258959
C	1.283824	4.701853	0.933421
C	0.053020	4.436303	0.349313
C	-0.296776	3.116850	0.107258
C	2.037539	-2.846426	0.558532
C	3.109706	-2.597497	-0.283053
C	-3.542283	0.412424	2.081336
C	-3.107558	0.229735	3.383587
C	-1.746390	0.099936	3.635832
C	-0.854826	0.155876	2.577279
C	3.180610	-1.384290	-0.956646
C	2.179202	-0.452742	-0.749750
F	2.594592	1.384067	1.346150
F	0.025743	-2.221426	1.513786
F	-3.114474	0.664139	-0.186147
F	3.303546	3.896236	1.823659
F	1.651223	5.953807	1.179917
F	-0.770972	5.433428	0.036600
F	-1.516968	2.907102	-0.440335
F	1.948871	-4.015585	1.188067
F	4.052504	-3.516461	-0.460427
F	-4.840309	0.550018	1.819922
F	-3.981182	0.182622	4.382822
F	-1.317430	-0.058680	4.884352
F	0.448804	0.066981	2.868054
F	4.183591	-1.141840	-1.798689
F	2.247582	0.684712	-1.480123
H	-2.544608	-1.353679	-0.911081
H	-2.694532	-3.585715	-1.966759
H	-1.049584	-4.264478	-3.694047
H	0.754985	-2.694720	-4.363454
H	0.919467	-0.466999	-3.290319
H	-1.550348	1.019325	-1.388582
H	0.000250	1.074206	-1.933925

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[Anilide-B(C_6F_5)$_3$]-

C	-1.089533	-1.955013	-1.452285
C	-1.558405	-3.042807	-2.176510
C	-1.690592	-2.994837	-3.562962
C	-1.341823	-1.814089	-4.217603
C	-0.867302	-0.720330	-3.510682
C	-0.722244	-0.758273	-2.106403
N	-0.252493	0.327041	-1.424406
H	-1.019986	-2.019861	-0.371991
H	-1.832004	-3.947275	-1.639212
H	-2.059176	-3.851317	-4.117625
H	-1.437521	-1.742946	-5.298336
H	-0.594423	0.191470	-4.037305
H	-0.097467	1.139167	-2.001567
B	0.130628	0.408093	0.050380
C	0.651875	1.950682	0.353709
C	1.790738	2.320392	1.064025
C	1.319511	-0.720188	0.298639
C	1.226606	-1.905570	1.013611
C	-1.138097	0.248724	1.102399
C	-2.486358	0.279124	0.762987
C	2.129376	3.642026	1.337714
C	1.302708	4.667517	0.909897
C	0.144006	4.353266	0.217711
C	-0.156187	3.020116	-0.031491
C	2.240482	-2.858302	1.070504
C	3.421629	-2.637378	0.385741
C	-3.507140	0.255293	1.712744
C	-3.195286	0.219284	3.060434
C	-1.862423	0.207310	3.448484
C	-0.881057	0.231991	2.470957
C	3.566317	-1.469927	-0.350936
C	2.524620	-0.556555	-0.381315
F	2.647136	1.406238	1.537510
F	0.105960	-2.226624	1.686935
F	-2.892655	0.331667	-0.509320
F	3.245289	3.934131	2.015190
F	1.615331	5.941675	1.164969
F	-0.672976	5.331473	-0.189725
F	-1.313869	2.793700	-0.674906
F	2.081052	-3.986165	1.773799
F	4.410302	-3.536815	0.428019
F	-4.791098	0.276060	1.334367
F	-4.165651	0.199621	3.980789
F	-1.549588	0.183282	4.750023
F	0.393631	0.237941	2.897987
F	4.706508	-1.243093	-1.014920
F	2.735904	0.556898	-1.102107

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[Aniline-$SiEt_3$]$^+$

C	-1.491445	-1.960941	0.407916
C	-2.037529	-3.006656	-0.331027
C	-1.246636	-3.715059	-1.232992
C	0.098377	-3.389591	-1.392072

C	0.657625	-2.344685	-0.661004
C	-0.151824	-1.645373	0.224837
N	0.408672	-0.485122	0.932508
Si	0.402432	1.145404	-0.113832
C	0.653972	2.416684	1.231494
C	-0.552967	2.569644	2.171775
C	1.845754	0.905966	-1.269837
C	3.197737	0.670976	-0.579424
C	-1.278751	1.201212	-0.921176
C	-1.401396	0.435807	-2.249146
H	-2.103755	-1.405077	1.113251
H	-3.081343	-3.267326	-0.197482
H	-1.677172	-4.528296	-1.806146
H	0.717893	-3.949257	-2.083664
H	1.707052	-2.087054	-0.777774
H	1.371583	-0.685527	1.222054
H	1.562541	2.184817	1.801510
H	0.860710	3.374534	0.737685
H	-0.363476	3.331686	2.929671
H	-1.452207	2.863990	1.624532
H	-0.784850	1.643519	2.711677
H	1.898261	1.815538	-1.882840
H	1.615300	0.097818	-1.973947
H	4.002811	0.598615	-1.312907
H	3.216980	-0.263665	-0.005190
H	3.451426	1.485035	0.104910
H	-1.495212	2.265911	-1.084287
H	-2.039823	0.863829	-0.205949
H	-2.400778	0.561073	-2.670152
H	-1.225752	-0.636151	-2.121733
H	-0.685849	0.808719	-2.986808
H	-0.115065	-0.324953	1.798459

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Anilide-$SiEt_3$

C	-0.930777	-2.580598	0.946961
C	-1.054651	-3.888375	0.497992
C	-0.678417	-4.235579	-0.797317
C	-0.174644	-3.244940	-1.635191
C	-0.047375	-1.932214	-1.196005
C	-0.424990	-1.574973	0.108046
N	-0.299658	-0.270004	0.577302
Si	0.288652	1.197863	-0.193633
C	0.552517	2.396486	1.238094
C	-0.700663	2.705939	2.067369
C	1.937424	0.897501	-1.059253
C	2.871104	-0.030937	-0.272829
C	-0.967795	1.929541	-1.393361
C	-1.387589	1.008124	-2.545711
H	-1.227707	-2.323392	1.960681
H	-1.450418	-4.643298	1.170579
H	-0.776197	-5.257398	-1.146200
H	0.125452	-3.491931	-2.648989
H	0.344005	-1.176205	-1.869385
H	-0.591043	-0.171643	1.541585
H	1.344285	1.999641	1.885688
H	0.951110	3.328126	0.816497
H	-0.487439	3.411331	2.875417
H	-1.488910	3.144013	1.448190
H	-1.118230	1.805774	2.530761
H	2.405649	1.882495	-1.190848
H	1.785316	0.510969	-2.073814
H	3.843442	-0.136201	-0.762224
H	2.433686	-1.028359	-0.171160
H	3.050581	0.351308	0.737177
H	-0.546043	2.862557	-1.791706
H	-1.854608	2.220962	-0.817043
H	-2.117550	1.490629	-3.202087
H	-1.836158	0.084650	-2.168156
H	-0.529814	0.726514	-3.165923

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[Aniline-$SiPhH_2$]$^+$

C	-0.287932	-3.960806	0.848200
C	0.342919	-5.179001	0.611967
C	1.730561	-5.242203	0.511366
C	2.498606	-4.087851	0.646679
C	1.883358	-2.861702	0.883547
C	0.499011	-2.825916	0.988191
N	-0.162056	-1.519736	1.180371
Si	-0.426400	-0.604748	-0.488214
C	-1.466201	-1.711862	-1.509465
C	-2.854161	-1.505651	-1.577506
C	-3.653996	-2.359449	-2.329707
C	-3.074242	-3.420386	-3.021905
C	-1.696886	-3.633492	-2.967566
C	-0.894198	-2.784085	-2.216790
H	-1.371082	-3.900644	0.910524
H	-0.254910	-6.077199	0.506995
H	2.215971	-6.194430	0.329585
H	3.578953	-4.137460	0.572518
H	2.476664	-1.957666	0.991980
H	0.392072	-0.942049	1.820924
H	-1.066488	-1.661558	1.641024
H	0.975052	-0.429971	-0.897298
H	-1.089493	0.629171	-0.032782
H	-3.313605	-0.669619	-1.055578
H	-4.724160	-2.192893	-2.383494
H	-3.698230	-4.081644	-3.614003
H	-1.251385	-4.455903	-3.516445
H	0.179259	-2.956493	-2.180540

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Anilide-$SiPhH_2$

C	0.229755	-3.638561	2.438945
C	0.786117	-4.897232	2.625218
C	1.356829	-5.586555	1.558223
C	1.358384	-4.993996	0.298656
C	0.802013	-3.735879	0.099420
C	0.230684	-3.037462	1.172789
N	-0.333139	-1.771569	0.993291
Si	-0.310361	-0.783617	-0.439903

C	-1.245954	-1.611952	-1.832386
C	-2.139985	-2.656868	-1.565882
C	-2.850844	-3.267987	-2.595468
C	-2.678178	-2.839775	-3.909150
C	-1.788871	-1.805826	-4.193135
C	-1.075766	-1.202518	-3.161368
H	-0.210251	-3.106779	3.278766
H	0.773486	-5.340707	3.616070
H	1.791602	-6.568750	1.705951
H	1.795212	-5.516302	-0.546801
H	0.800363	-3.301965	-0.896737
H	-0.704516	-1.364023	1.840064
H	1.067522	-0.500531	-0.915948
H	-0.946258	0.483840	-0.009472
H	-2.267293	-3.002239	-0.542424
H	-3.536250	-4.079990	-2.373997
H	-3.231524	-3.315466	-4.712858
H	-1.647475	-1.475732	-5.217485
H	-0.373320	-0.405797	-3.398482

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$(Aniline)_2$

C	3.50941	0.40172	0.48546
C	3.86153	-0.94137	0.43036
C	3.04411	-1.86531	-0.21672
C	1.86755	-1.42275	-0.81558
C	1.50957	-0.07946	-0.77588
C	2.32759	0.84774	-0.11816
N	1.93299	2.18833	-0.00799
H	4.14646	1.11450	1.00241
H	4.78378	-1.26761	0.90124
H	3.32113	-2.91302	-0.25439
H	1.21485	-2.12628	-1.32357
H	0.58826	0.26040	-1.24205
H	2.70337	2.83906	0.06538
H	1.26802	2.46935	-0.71819
C	-1.57258	-0.49319	0.62327
C	-2.46096	-1.56158	0.58295
C	-3.75773	-1.39439	0.10366
C	-4.15590	-0.13534	-0.33891
C	-3.27453	0.93841	-0.30871
C	-1.97024	0.77229	0.17314
N	-1.06430	1.83959	0.14538
H	-0.56265	-0.63178	0.99893
H	-2.13361	-2.53433	0.93717
H	-4.44779	-2.23049	0.07790
H	-5.16364	0.01574	-0.71367
H	-3.58993	1.91564	-0.66487
H	-1.50192	2.74582	0.24805
H	-0.27424	1.74688	0.77472

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[Aniline-Anilide]-

C	2.39624	0.78407	0.51567
C	3.62250	1.01454	1.10779
C	4.75750	0.25971	0.77962
C	4.60336	-0.74560	-0.17678
C	3.38211	-0.99319	-0.78407
C	2.20491	-0.23935	-0.47108
N	1.00058	-0.42466	-1.02184
H	1.52725	1.37865	0.78760
H	3.70379	1.80680	1.85163
H	5.71673	0.44810	1.25139
H	5.46180	-1.35521	-0.45901
H	3.29916	-1.78572	-1.52722
H	1.04277	-1.17819	-1.70665
C	-2.20204	-0.75028	0.30077
C	-3.33110	-1.40410	0.76289
C	-4.60297	-0.83087	0.65885
C	-4.71177	0.42596	0.06960
C	-3.59045	1.09785	-0.40234
C	-2.30182	0.53051	-0.29639
N	-1.17471	1.16700	-0.71317
H	-1.21149	-1.19217	0.36903
H	-3.22006	-2.38716	1.21516
H	-5.48142	-1.35206	1.02583
H	-5.68820	0.89602	-0.02811
H	-3.69542	2.07939	-0.86008
H	-1.31287	1.97435	-1.30187
H	-0.28198	0.57522	-0.85988

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BEt_3-$(Aniline)_2$

C	1.40698	1.51902	1.12638
C	1.94942	2.79924	1.05535
C	1.88753	3.52443	-0.13159
C	1.27270	2.96763	-1.25126
C	0.72599	1.69081	-1.18852
C	0.80462	0.96829	-0.00118
N	0.27645	-0.36819	0.06272
B	1.30751	-1.69898	-0.19201
C	0.22187	-2.91350	-0.30145
C	-0.60396	-2.95233	-1.59286
C	2.12122	-1.43548	-1.57506
C	3.40990	-0.60876	-1.47727
C	2.24814	-1.79183	1.12821
C	1.52885	-2.08636	2.45032
H	1.45601	0.93842	2.04320
H	2.42584	3.22805	1.93086
H	2.31501	4.51995	-0.18414
H	1.21787	3.52887	-2.17815
H	0.24173	1.24815	-2.05452
H	-0.14954	-0.50401	0.98591
H	-0.48612	-0.46269	-0.61171
H	0.76765	-3.86344	-0.20818
H	-0.46932	-2.90058	0.55922
H	0.04218	-3.07511	-2.46751
H	-1.33552	-3.76791	-1.60428
H	-1.17672	-2.02663	-1.75415
H	2.38168	-2.42179	-1.98872
H	1.46260	-0.98943	-2.33939

H	3.89467	-0.47703	-2.45099
H	3.23061	0.39043	-1.06462
H	4.13279	-1.09831	-0.81660
H	2.85912	-0.88375	1.24110
H	2.97828	-2.59436	0.94707
H	1.01937	-3.05475	2.41391
H	0.75594	-1.33734	2.68308
H	2.20950	-2.10661	3.30837
C	-2.40726	1.53242	0.39157
C	-2.98981	1.56310	-0.87130
C	-3.59862	0.42810	-1.40159
C	-3.62588	-0.74321	-0.64653
C	-3.04418	-0.78619	0.61586
C	-2.42719	0.35388	1.14476
N	-1.69932	0.26778	2.34360
H	-1.90122	2.41109	0.78322
H	-2.95560	2.48271	-1.44693
H	-4.04583	0.45455	-2.38883
H	-4.08922	-1.63917	-1.04699
H	-3.04120	-1.71138	1.18606
H	-1.55049	1.15759	2.80179
H	-2.04947	-0.42336	2.99468

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[BEt_3-(Aniline-Anilide)]-

C	1.86643	1.89847	0.14599
C	1.77101	3.28282	0.13861
C	0.65069	3.94201	-0.36897
C	-0.38319	3.16120	-0.88853
C	-0.30484	1.77728	-0.89306
C	0.81906	1.08720	-0.36140
N	0.83420	-0.27066	-0.30323
H	2.75394	1.41537	0.53563
H	2.59980	3.86224	0.53989
H	0.58910	5.02540	-0.36766
H	-1.27082	3.63672	-1.30095
H	-1.12788	1.19000	-1.29622
H	0.03593	-0.65975	-0.79440
B	1.95448	-1.35155	0.01961
C	1.12478	-2.76210	0.26607
C	0.34374	-3.32696	-0.92794
C	2.97655	-1.53503	-1.25943
C	3.78612	-0.29654	-1.65528
C	2.78356	-1.01209	1.40574
C	1.92555	-0.53871	2.58288
H	1.84167	-3.53264	0.58947
H	0.43187	-2.64759	1.11803
H	1.02267	-3.59986	-1.74281
H	-0.24180	-4.22269	-0.67706
H	-0.36731	-2.60131	-1.34685
H	3.67364	-2.36392	-1.04744
H	2.40524	-1.85529	-2.14554
H	4.45729	-0.47124	-2.50810
H	3.12109	0.53089	-1.92635
H	4.40891	0.05824	-0.82478
H	3.59740	-0.28572	1.25648
H	3.30030	-1.93942	1.70106
H	1.10383	-1.23800	2.78200
H	1.47310	0.43798	2.36845
H	2.48828	-0.43216	3.52023
C	-3.47512	0.83507	0.53806
C	-4.49092	0.43315	-0.32038
C	-4.50425	-0.85136	-0.86100
C	-3.47590	-1.73022	-0.52416
C	-2.45843	-1.34163	0.33788
C	-2.43935	-0.04742	0.88392
N	-1.43487	0.32414	1.76693
H	-3.46026	1.84565	0.93810
H	-5.27714	1.13808	-0.57742
H	-5.29516	-1.15788	-1.53769
H	-3.45538	-2.73310	-0.94209
H	-1.65555	-2.02896	0.59109
H	-1.25402	1.32181	1.74801
H	-0.55954	-0.16031	1.56910

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BPh_3-$(Aniline)_2$

C	2.42158	1.90618	-1.59290
C	2.83025	3.23665	-1.54498
C	1.91082	4.24522	-1.27338
C	0.57429	3.92280	-1.04768
C	0.15430	2.59908	-1.09895
C	1.08379	1.60083	-1.37315
N	0.64853	0.21881	-1.35578
H	3.13767	1.10924	-1.77030
H	3.87394	3.48060	-1.71293
H	2.23571	5.27929	-1.22914
H	-0.14383	4.70255	-0.81699
H	-0.87384	2.32674	-0.87472
H	-0.34763	0.16491	-1.64558
H	1.17403	-0.30012	-2.05890
B	0.80052	-0.60355	0.11173
C	-0.17473	-1.89718	-0.04195
C	-0.81461	-2.45968	1.07259
C	0.35915	0.48842	1.22519
C	1.29225	1.38751	1.76917
C	2.33603	-1.12585	0.22141
C	3.11407	-1.51449	-0.87883
C	-1.59333	-3.61117	0.97700
C	-1.75626	-4.24980	-0.25053
C	-1.11790	-3.72981	-1.37453
C	-0.34071	-2.57782	-1.25931
C	0.90945	2.44936	2.58341
C	-0.43645	2.64852	2.88338
C	4.39295	-2.05123	-0.74182
C	4.93523	-2.23457	0.52582
C	4.17986	-1.88476	1.64203
C	2.90738	-1.34262	1.48531
C	-1.38552	1.77443	2.36322
C	-0.98755	0.71371	1.54932
H	-0.70286	-1.97529	2.03951
H	2.34583	1.26613	1.52818

H	2.72696	-1.42427	-1.89582
H	-2.07368	-4.01331	1.86451
H	-2.36133	-5.14769	-0.32882
H	-1.21406	-4.22870	-2.33512
H	0.16501	-2.22029	-2.15772
H	1.66107	3.12672	2.97863
H	-0.74049	3.47675	3.51687
H	4.96059	-2.33239	-1.62415
H	5.93048	-2.65186	0.64249
H	4.58417	-2.03325	2.63914
H	2.33546	-1.07415	2.37030
H	-2.44053	1.91245	2.58382
H	-1.75368	0.05434	1.14977
C	-3.48996	1.40265	-0.97619
C	-4.30344	1.59020	0.13620
C	-4.69058	0.50526	0.91917
C	-4.26377	-0.77411	0.56972
C	-3.45349	-0.97329	-0.54250
C	-3.05407	0.11937	-1.31468
N	-2.14374	-0.06021	-2.38698
H	-3.18332	2.25217	-1.58166
H	-4.63049	2.59255	0.39382
H	-5.31914	0.65559	1.79019
H	-4.55172	-1.63084	1.17084
H	-3.10466	-1.97103	-0.79560
H	-2.12148	-1.02618	-2.69888
H	-2.33852	0.55406	-3.17033

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[BPh_3-(Aniline-Anilide)]-

C	0.42703	-2.68993	0.30040
C	0.09320	-4.03637	0.36363
C	-1.14153	-4.50453	-0.08457
C	-2.04360	-3.58227	-0.61465
C	-1.72543	-2.23381	-0.68850
C	-0.48401	-1.74337	-0.22000
N	-0.20909	-0.39889	-0.23956
H	1.39616	-2.34871	0.64805
H	0.81988	-4.73515	0.77056
H	-1.39101	-5.55927	-0.02893
H	-3.01270	-3.91435	-0.97974
H	-2.44225	-1.52819	-1.10390
H	-0.88402	0.11897	-0.79075
B	1.17588	0.31380	-0.04392
C	0.91443	1.84314	-0.59546
C	1.41038	2.35088	-1.80308
C	2.33815	-0.43429	-0.93421
C	3.67325	-0.58636	-0.53374
C	1.57770	0.41749	1.54315
C	0.92991	-0.29869	2.55967
C	1.09216	3.63362	-2.25380
C	0.25503	4.45403	-1.50439
C	-0.24915	3.98216	-0.29291
C	0.08752	2.70470	0.14768
C	4.63151	-1.19026	-1.34900
C	4.28058	-1.67040	-2.60663
C	1.27557	-0.16386	3.90547
C	2.29380	0.70510	4.28290
C	2.95211	1.44220	3.29923
C	2.58988	1.29981	1.96305
C	2.95938	-1.54390	-3.03224
C	2.01571	-0.94163	-2.20502
H	2.06275	1.72524	-2.40779
H	3.97321	-0.23466	0.45041
H	0.13337	-0.98990	2.29189
H	1.49964	3.99211	-3.19629
H	0.00258	5.45152	-1.85440
H	-0.89663	4.61333	0.31127
H	-0.28891	2.36077	1.11149
H	5.65565	-1.29036	-0.99657
H	5.02264	-2.14375	-3.24432
H	0.74378	-0.73804	4.66037
H	2.56631	0.81497	5.32922
H	3.74034	2.13773	3.57795
H	3.09438	1.90550	1.21105
H	2.66369	-1.92362	-4.00740
H	0.98480	-0.86354	-2.54645
C	-4.76372	-0.55192	0.60056
C	-5.71691	-0.17989	-0.33890
C	-5.51363	0.92427	-1.16440
C	-4.33169	1.65059	-1.03123
C	-3.37200	1.29097	-0.09308
C	-3.57318	0.17909	0.74188
H	-4.92404	-1.42360	1.22985
H	-6.62700	-0.76657	-0.43092
H	-6.25794	1.20820	-1.90097
H	-4.14473	2.50964	-1.66931
H	-2.45270	1.86412	-0.00227
N	-2.63088	-0.16085	1.70323
H	-1.68150	0.09352	1.43221
H	-2.65029	-1.14608	1.93865

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$B(C_6F_5)Ph_2$-$(Aniline)_2$

C	1.52900	2.03883	-2.24630
C	2.18654	3.23552	-2.51884
C	1.75447	4.42424	-1.93908
C	0.65785	4.41521	-1.08077
C	-0.00512	3.22557	-0.80092
C	0.43411	2.04065	-1.38742
N	-0.25510	0.80031	-1.08206
H	1.85575	1.11269	-2.70570
H	3.03906	3.23347	-3.18967
H	2.27074	5.35387	-2.15330
H	0.32016	5.33540	-0.61593
H	-0.83420	3.20558	-0.10005
H	-1.26862	1.00331	-0.94443
H	-0.16653	0.16894	-1.87715
B	0.17694	-0.05294	0.28401
C	-0.86503	-1.29005	0.37745
C	-0.97838	-1.98162	1.59505
C	0.04696	1.03293	1.47793

C	1.06720	1.95172	1.76474
C	1.68382	-0.66199	0.06517
C	2.16082	-1.13197	-1.15386
C	-1.81837	-3.08068	1.74040
C	-2.57280	-3.53194	0.65848
C	-2.47199	-2.87573	-0.56265
C	-1.62840	-1.77356	-0.69287
C	0.88882	2.99408	2.66959
C	-0.33267	3.15208	3.32103
C	3.40090	-1.72434	-1.34297
C	4.22719	-1.91481	-0.24602
C	3.78711	-1.51210	1.00576
C	2.53779	-0.91593	1.13873
C	-1.36026	2.24620	3.07239
C	-1.16109	1.20133	2.16899
F	1.39554	-1.03146	-2.27303
F	3.79085	-2.12178	-2.55444
F	5.41986	-2.48598	-0.39132
F	4.55947	-1.71230	2.07248
F	2.17369	-0.60740	2.38981
H	-0.39240	-1.64093	2.44665
H	2.02184	1.86247	1.24864
H	-1.88386	-3.58841	2.69834
H	-3.23307	-4.38689	0.76810
H	-3.06174	-3.20669	-1.41217
H	-1.59773	-1.28748	-1.66732
H	1.70143	3.68789	2.86337
H	-0.47709	3.96531	4.02567
H	-2.30905	2.34250	3.59363
H	-1.95847	0.48019	2.00218
C	-4.41634	0.11171	-1.87471
C	-5.28850	-0.96583	-1.98055
C	-5.72881	-1.63320	-0.84009
C	-5.29239	-1.20546	0.41043
C	-4.43249	-0.11918	0.52604
C	-3.98541	0.54270	-0.61804
N	-3.04373	1.60186	-0.52792
H	-4.05988	0.62106	-2.76644
H	-5.62095	-1.28771	-2.96246
H	-6.40290	-2.47844	-0.92598
H	-5.61977	-1.72019	1.30782
H	-4.10393	0.21490	1.50601
H	-3.27216	2.37382	-1.14634
H	-2.94149	1.94871	0.42216

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[$B(C_6F_5)Ph_2$-(Aniline-Anilide)]-

C	-0.43375	1.56298	-2.29216
C	-0.95634	2.08423	-3.46784
C	-2.32244	2.32278	-3.61203
C	-3.16363	2.02758	-2.54074
C	-2.65467	1.50675	-1.35891
C	-1.27520	1.25826	-1.20400
N	-0.79399	0.69406	-0.03964
H	0.63352	1.39313	-2.19762
H	-0.27893	2.31090	-4.28714
H	-2.72050	2.73108	-4.53550
H	-4.23364	2.20138	-2.62236
H	-3.32527	1.27230	-0.53427
H	-1.47152	0.75403	0.71219
B	0.68209	0.65020	0.45203
C	0.55734	0.25302	2.03972
C	0.96824	1.07417	3.09633
C	1.41738	2.09889	0.23428
C	2.71927	2.29408	-0.24422
C	1.55130	-0.58405	-0.26262
C	1.14961	-1.40944	-1.30820
C	0.77665	0.71011	4.42924
C	0.16158	-0.49738	4.74728
C	-0.24946	-1.34137	3.71752
C	-0.04465	-0.96684	2.39134
C	3.27737	3.56476	-0.38703
C	2.54166	4.69504	-0.04733
C	1.91014	-2.46911	-1.79911
C	3.14061	-2.74945	-1.23297
C	3.59051	-1.96376	-0.18207
C	2.79498	-0.92241	0.27503
C	1.24092	4.53672	0.42741
C	0.69802	3.26220	0.55634
F	-0.02894	-1.23576	-1.93317
F	1.46232	-3.22039	-2.81307
F	3.88732	-3.76055	-1.69185
F	4.77885	-2.22551	0.37742
F	3.29704	-0.21298	1.29806
H	1.45149	2.02091	2.86815
H	3.31984	1.43385	-0.52937
H	1.10983	1.37356	5.22363
H	0.00875	-0.78128	5.78497
H	-0.72426	-2.29221	3.94643
H	-0.35662	-1.64807	1.59859
H	4.29068	3.67012	-0.76694
H	2.97159	5.68696	-0.15724
H	0.64695	5.40919	0.68797
H	-0.32555	3.15620	0.91198
C	-3.65792	-1.04113	1.34559
C	-4.84310	-0.74374	2.00584
C	-6.07481	-0.87082	1.36544
C	-6.09699	-1.30167	0.04081
C	-4.91844	-1.59465	-0.63361
C	-3.67417	-1.46924	0.00560
N	-2.49211	-1.79142	-0.63958
H	-2.70506	-0.95587	1.86230
H	-4.79943	-0.40941	3.03859
H	-6.99695	-0.63656	1.88681
H	-7.04471	-1.40358	-0.48116
H	-4.94670	-1.91459	-1.67197
H	-1.69897	-1.21251	-0.36085
H	-2.56169	-1.79122	-1.64888

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$B(C_6F_5)_2Ph$-$(Aniline)_2$

C	0.97840	-2.70933	-1.46811

C	1.54165	-3.97981	-1.38740
C	2.60865	-4.22065	-0.52612
C	3.12095	-3.18543	0.25196
C	2.56497	-1.91268	0.18219
C	1.49298	-1.68944	-0.67572
N	0.90611	-0.35846	-0.73877
H	0.16234	-2.50663	-2.15313
H	1.14546	-4.77960	-2.00386
H	3.04404	-5.21255	-0.46636
H	3.95781	-3.36286	0.91916
H	2.95626	-1.09821	0.78833
H	0.63768	-0.15787	-1.70258
H	1.65276	0.31095	-0.52723
B	-0.31301	-0.00370	0.32578
C	-0.77897	1.54305	0.03161
C	-1.75871	2.08123	0.86766
C	0.40856	-0.16034	1.76047
C	0.51307	-1.39266	2.42200
C	-1.59035	-0.96835	-0.00587
C	-1.98508	-1.19856	-1.32156
C	-2.25724	3.36994	0.74132
C	-1.77389	4.19245	-0.26915
C	-0.80341	3.70653	-1.12922
C	-0.34017	2.40677	-0.96075
C	1.29691	-1.55006	3.56014
C	2.01539	-0.46977	4.06857
C	-3.09004	-1.94519	-1.69791
C	-3.90371	-2.47785	-0.70838
C	-3.58647	-2.24805	0.62073
C	-2.45955	-1.49802	0.94813
C	1.93774	0.76334	3.42978
C	1.14238	0.90798	2.29350
F	-2.26439	1.33219	1.85175
F	-1.25722	-0.68181	-2.34359
F	-3.19087	3.82578	1.57226
F	-2.23693	5.43070	-0.40695
F	-0.32224	4.47705	-2.10495
F	0.61226	2.01419	-1.84736
F	-3.37955	-2.13998	-2.98417
F	-4.97539	-3.19392	-1.03313
F	-4.36957	-2.73906	1.57877
F	-2.26031	-1.30770	2.25315
H	-0.01592	-2.25658	2.02720
H	1.35297	-2.51840	4.04807
H	2.62837	-0.58906	4.95662
H	2.48950	1.61453	3.81862
H	1.09673	1.88203	1.80776
C	4.84582	-0.21406	-1.50499
C	5.58577	-0.25925	-0.33096
C	5.30638	0.60832	0.72474
C	4.28171	1.53865	0.58017
C	3.53974	1.60171	-0.59711
C	3.80731	0.71503	-1.65115
N	2.98173	0.69198	-2.77992
H	5.05294	-0.91310	-2.31046
H	6.38424	-0.98871	-0.23685
H	5.88056	0.56150	1.64299
H	4.04798	2.22322	1.38936
H	2.74911	2.34007	-0.70996
H	2.55780	1.58231	-3.00665
H	3.40274	0.26261	-3.59257

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[B(C_6F_5)$_2$Ph-(Aniline-Anilide)]-

C	1.26339	2.71620	-0.25188
C	2.36350	3.54797	-0.41305
C	2.88704	3.83615	-1.67389
C	2.26964	3.27024	-2.78852
C	1.16703	2.43933	-2.64783
C	0.62871	2.13475	-1.37489
N	-0.45675	1.31433	-1.25507
H	0.88161	2.51548	0.74127
H	2.82489	3.97549	0.47350
H	3.75346	4.47924	-1.78445
H	2.65641	3.46867	-3.78459
H	0.70118	2.00260	-3.52922
H	-0.83927	1.01384	-2.13809
B	-0.99907	0.67702	0.03862
C	-2.31618	-0.26996	-0.33074
C	-2.70954	-1.33443	0.48017
C	-1.60025	1.76380	1.09823
C	-1.91724	3.06317	0.68534
C	0.21939	-0.28616	0.64025
C	0.54542	-1.45342	-0.04607
C	-3.84964	-2.09846	0.26903
C	-4.68058	-1.80536	-0.80068
C	-4.34886	-0.74932	-1.63118
C	-3.19725	-0.01122	-1.37730
C	-2.53168	3.97768	1.54072
C	-2.85587	3.60768	2.84212
C	1.55604	-2.32491	0.32021
C	2.34998	-2.02587	1.41676
C	2.09626	-0.86108	2.11903
C	1.04955	-0.02809	1.72547
C	-2.56098	2.31558	3.27515
C	-1.94524	1.41448	2.41273
F	-1.98033	-1.68756	1.55438
F	-0.13315	-1.79702	-1.16344
F	-4.15768	-3.11139	1.08721
F	-5.78412	-2.52705	-1.02317
F	-5.14139	-0.44432	-2.66595
F	-2.97927	1.00397	-2.23746
F	1.81109	-3.41449	-0.42100
F	3.34065	-2.84224	1.78112
F	2.85657	-0.54530	3.17334
F	0.88715	1.07211	2.48148
H	-1.67133	3.35800	-0.33239
H	-2.75691	4.98141	1.18897
H	-3.33397	4.31617	3.51322
H	-2.81105	2.01222	4.28868
H	-1.72548	0.40890	2.76597
C	3.78237	0.32904	-0.99282

C	4.81175	0.41452	-0.06453
C	5.57782	-0.70376	0.26067
C	5.30564	-1.91256	-0.37581
C	4.27961	-2.01032	-1.30843
C	3.48942	-0.89285	-1.61063
N	2.43567	-0.98790	-2.52573
H	3.18070	1.20072	-1.22610
H	5.00017	1.36962	0.41789
H	6.36862	-0.63652	1.00041
H	5.88621	-2.79777	-0.13225
H	4.05627	-2.96203	-1.78177
H	1.95585	-1.87941	-2.48022
H	1.76416	-0.23402	-2.41286

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$B(C_6F_5)_3$-(Aniline)$_2$

C	2.58226	0.07153	-2.66626
C	3.77082	0.65185	-3.10197
C	3.92406	2.03473	-3.10362
C	2.87749	2.84708	-2.67427
C	1.68562	2.27711	-2.24137
C	1.54565	0.89210	-2.23621
N	0.32184	0.31233	-1.70144
H	2.46150	-1.00479	-2.66613
H	4.58170	0.01384	-3.43627
H	4.85580	2.47885	-3.43635
H	2.98862	3.92613	-2.66957
H	0.87303	2.90105	-1.88207
H	0.02517	-0.47692	-2.27666
H	-0.44923	1.01676	-1.75796
B	0.39998	-0.20743	-0.13717
C	-1.14077	-0.33097	0.39482
C	-1.57890	0.02914	1.66661
C	1.30601	0.92464	0.60489
C	2.66408	0.79041	0.87681
C	0.98990	-1.73036	-0.06872
C	1.03245	-2.67075	-1.08819
C	-2.87309	-0.20623	2.11711
C	-3.78391	-0.84598	1.29122
C	-3.39107	-1.24394	0.02292
C	-2.09458	-0.97755	-0.38585
C	3.45039	1.82200	1.37984
C	2.88321	3.06414	1.61660
C	1.42542	-3.99337	-0.91145
C	1.77289	-4.43245	0.35459
C	1.72630	-3.53920	1.41846
C	1.33072	-2.23187	1.18777
C	1.53620	3.25573	1.34383
C	0.79592	2.19478	0.84825
F	-0.75854	0.63653	2.53104
F	3.30437	-0.35913	0.63329
F	0.70494	-2.33774	-2.36259
F	-3.25298	0.19707	3.32919
F	-5.03672	-1.03755	1.69383
F	-4.25504	-1.85432	-0.78578
F	-1.76391	-1.39253	-1.63010
F	4.74536	1.62960	1.62033
F	3.62165	4.06391	2.08738
F	1.45884	-4.83246	-1.94535
F	2.14686	-5.69235	0.55163
F	2.04943	-3.95018	2.64185
F	1.27992	-1.41699	2.24910
F	0.97552	4.45040	1.53582
F	-0.49204	2.46848	0.53856
C	-3.90203	1.15170	-2.38682
C	-5.15764	0.73740	-1.95624
C	-5.62076	1.08430	-0.68908
C	-4.81195	1.85097	0.14575
C	-3.55481	2.27316	-0.27603
C	-3.10088	1.93223	-1.55074
N	-1.80434	2.33136	-1.98442
H	-3.53559	0.86602	-3.36915
H	-5.77010	0.12596	-2.61047
H	-6.59359	0.74718	-0.34942
H	-5.15270	2.11181	1.14336
H	-2.92102	2.86017	0.38248
H	-1.45739	3.09795	-1.41619
H	-1.81179	2.61861	-2.95859

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[$B(C_6F_5)_3$-(Aniline-Anilide)]-

C	0.85054	1.91798	-2.23024
C	1.08010	2.92907	-3.15452
C	0.18708	3.98701	-3.31458
C	-0.95194	4.01831	-2.51142
C	-1.19317	3.01971	-1.57795
C	-0.30402	1.93409	-1.41956
N	-0.58327	0.92978	-0.52700
H	1.56569	1.10778	-2.13063
H	1.97931	2.88509	-3.76326
H	0.37697	4.76945	-4.04164
H	-1.66235	4.83627	-2.60350
H	-2.07987	3.06361	-0.94882
H	-1.37688	1.14457	0.06451
B	0.43992	-0.04817	0.06785
C	-0.37339	-0.91167	1.22027
C	-0.03027	-1.09124	2.55696
C	1.68060	0.85738	0.68665
C	2.98540	0.93398	0.22024
C	0.95824	-1.21318	-0.98223
C	0.43989	-1.47496	-2.24436
C	-0.80931	-1.81235	3.45729
C	-1.98495	-2.40897	3.03120
C	-2.35169	-2.29286	1.69979
C	-1.53648	-1.57555	0.83590
C	3.93402	1.82390	0.71747
C	3.58367	2.69869	1.72990
C	0.85223	-2.54909	-3.03063
C	1.81078	-3.42366	-2.54921
C	2.34718	-3.21463	-1.28578
C	1.90585	-2.13336	-0.54057
C	2.28666	2.67503	2.22410

C	1.37830	1.77510	1.69070
F	1.09240	-0.56979	3.06619
F	3.41276	0.15188	-0.78818
F	-0.50478	-0.69587	-2.79362
F	-0.43434	-1.93660	4.73444
F	-2.74483	-3.09715	3.88670
F	-3.47590	-2.86955	1.25919
F	-1.93054	-1.56666	-0.45365
F	5.17570	1.84805	0.21874
F	4.47882	3.55998	2.22330
F	0.32538	-2.74907	-4.24359
F	2.21486	-4.46030	-3.28987
F	3.26813	-4.05910	-0.80768
F	2.44566	-1.98188	0.68012
F	1.93481	3.51766	3.20181
F	0.13917	1.80634	2.21021
C	-4.49178	0.22390	-0.27257
C	-5.43022	0.69270	0.63782
C	-5.99444	1.95976	0.50293
C	-5.59928	2.75569	-0.57004
C	-4.66062	2.30027	-1.48726
C	-4.08588	1.02422	-1.35519
N	-3.18536	0.54966	-2.29525
H	-4.07292	-0.77069	-0.16317
H	-5.72075	0.05337	1.46690
H	-6.72375	2.32053	1.22037
H	-6.02225	3.74876	-0.69458
H	-4.35007	2.93105	-2.31670
H	-2.68929	1.28259	-2.78912
H	-2.51707	-0.12068	-1.93155

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$[SiEt_3\text{-}(Aniline)_2]^+$

C	0.57461	1.93467	-1.34634
C	0.56960	3.31394	-1.54137
C	0.25334	4.16939	-0.48938
C	-0.06388	3.64753	0.76269
C	-0.06319	2.27115	0.97000
C	0.25991	1.43045	-0.08858
N	0.27254	-0.01896	0.10529
Si	1.99032	-0.80785	0.28930
C	1.54977	-2.52234	0.89008
C	0.57627	-3.25893	-0.04339
C	2.70048	-0.80166	-1.44033
C	3.89138	-1.77142	-1.54826
C	2.89592	0.26142	1.51947
C	2.35930	0.15807	2.95487
H	0.81500	1.25938	-2.16265
H	0.81166	3.71715	-2.51845
H	0.25022	5.24221	-0.64552
H	-0.31706	4.31105	1.58205
H	-0.32699	1.85997	1.94050
H	-0.23110	-0.45292	-0.73107
H	-0.31526	-0.25541	0.91133
H	2.48302	-3.09063	0.98853
H	1.13483	-2.46393	1.90361
H	-0.39926	-2.75945	-0.07512
H	0.96163	-3.31371	-1.06709
H	0.40109	-4.28168	0.29637
H	1.92299	-1.08298	-2.16283
H	3.01774	0.21455	-1.70018
H	4.67957	-1.52357	-0.83073
H	3.58417	-2.80468	-1.36270
H	4.33659	-1.73341	-2.54419
H	2.86300	1.29888	1.16470
H	3.95424	-0.02649	1.49366
H	2.48761	-0.84980	3.35761
H	1.29272	0.40262	3.01224
H	2.88192	0.84833	3.61978
C	-4.46619	-0.60555	1.09865
C	-3.91867	0.55242	0.55068
C	-2.95907	0.47206	-0.45400
C	-2.55363	-0.77902	-0.92513
C	-3.09918	-1.94138	-0.38088
C	-4.05452	-1.84921	0.62842
N	-1.49349	-0.85128	-1.88515
H	-5.21545	-0.53836	1.87916
H	-4.24192	1.52679	0.90158
H	-2.53304	1.37654	-0.88233
H	-2.79298	-2.91395	-0.75782
H	-4.48384	-2.75655	1.03942
H	-1.45826	-1.75910	-2.34056
H	-1.59416	-0.13877	-2.60373

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$SiEt_3$-(Aniline-Anilide)

C	0.70801	-1.74819	-0.91630
C	1.14020	-3.06676	-0.84612
C	0.30629	-4.06611	-0.34943
C	-0.97330	-3.71948	0.07620
C	-1.41595	-2.40298	0.01632
C	-0.57990	-1.38971	-0.48149
N	-0.98815	-0.06208	-0.53957
Si	-2.45424	0.67464	0.07881
C	-2.15436	2.52471	-0.12426
C	-2.13218	2.98164	-1.58897
C	-3.97167	0.16038	-0.90872
C	-5.23593	0.90105	-0.45095
C	-2.69121	0.25710	1.90886
C	-1.36125	0.17311	2.66801
H	1.36325	-0.97700	-1.31398
H	2.14121	-3.31147	-1.19016
H	0.64527	-5.09467	-0.29810
H	-1.64072	-4.48277	0.46473
H	-2.41775	-2.15845	0.35830
H	-0.22257	0.56677	-0.76523
H	-2.92963	3.06989	0.42810
H	-1.20524	2.78091	0.36516
H	-1.37587	2.44011	-2.16567
H	-3.09787	2.79779	-2.07055
H	-1.91655	4.04988	-1.68037
H	-3.77766	0.35542	-1.97001

H	-4.11795	-0.92306	-0.82627
H	-5.45105	0.70839	0.60536
H	-5.12564	1.98462	-0.56844
H	-6.11650	0.59867	-1.02439
H	-3.24385	-0.68351	2.02045
H	-3.33084	1.03144	2.35197
H	-0.78301	1.09845	2.55989
H	-0.75127	-0.65058	2.28175
H	-1.50898	0.00575	3.73854
C	5.75472	0.75406	-0.24706
C	5.01031	-0.38795	0.03537
C	3.65385	-0.29889	0.32783
C	3.01612	0.94714	0.33539
C	3.76474	2.09446	0.04981
C	5.12097	1.99436	-0.23481
N	1.63384	1.04433	0.56571
H	6.81304	0.67970	-0.47108
H	5.48905	-1.36234	0.03603
H	3.07821	-1.19287	0.55250
H	3.27383	3.06398	0.04683
H	5.68615	2.89571	-0.45071
H	1.36362	1.89985	1.03517
H	1.24216	0.24101	1.04577

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$[SiPhH_2\text{-}(Aniline)_2]^+$

C	-1.363194	-4.848053	0.411899
C	-0.975343	-6.104977	-0.043337
C	0.345798	-6.521653	0.096992
C	1.283868	-5.680217	0.690591
C	0.912194	-4.419323	1.148636
C	-0.415608	-4.026945	1.010946
N	-0.812854	-2.679902	1.450742
Si	-0.121665	-1.343590	0.316904
C	-0.974440	-1.562190	-1.297317
C	-2.011714	-0.694370	-1.673375
C	-2.679779	-0.875954	-2.880255
C	-2.317297	-1.925146	-3.721165
C	-1.287201	-2.793753	-3.362417
C	-0.616296	-2.614038	-2.158727
H	-2.390099	-4.512868	0.292129
H	-1.708275	-6.754398	-0.508610
H	0.644725	-7.501590	-0.258014
H	2.314217	-6.000078	0.800960
H	1.645791	-3.761026	1.605529
H	-0.560903	-2.496819	2.479219
H	-1.834621	-2.618060	1.410786
H	1.322232	-1.617186	0.338853
H	-0.496837	-0.104383	1.027083
H	-2.294580	0.134740	-1.029308
H	-3.476132	-0.197794	-3.166783
H	-2.835457	-2.063924	-4.664300
H	-1.004066	-3.604574	-4.024792
H	0.189752	-3.293805	-1.890312
C	1.755405	-3.768192	4.369791
C	3.057697	-4.171841	4.091307
C	3.927240	-3.328723	3.402093
C	3.491503	-2.066156	3.005920
H	1.076259	-4.433394	4.895827
H	3.393112	-5.150252	4.418298
H	4.941774	-3.646245	3.189769
H	4.166683	-1.394317	2.486682
C	2.189482	-1.654204	3.280173
C	1.319647	-2.510573	3.956249
N	-0.054938	-2.138216	4.097623
H	1.852910	-0.663609	2.980900
H	-0.519017	-2.681071	4.821061
H	-0.155089	-1.153376	4.332447

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$SiPhH_2$-(Aniline-Anilide)

C	-1.803922	-5.218201	1.840803
C	-1.421463	-6.553455	1.815307
C	-0.278916	-6.952411	1.123484
C	0.460945	-5.990176	0.436959
C	0.086723	-4.651370	0.453012
C	-1.044483	-4.241194	1.177481
N	-1.394522	-2.898668	1.257121
Si	-0.503671	-1.536856	0.614935
C	-0.589078	-1.560770	-1.257752
C	0.275856	-0.769383	-2.025818
C	0.209434	-0.775305	-3.415883
C	-0.720834	-1.586385	-4.062293
C	-1.580032	-2.388797	-3.316549
C	-1.513555	-2.373566	-1.925381
H	-2.692124	-4.915721	2.390467
H	-2.020879	-7.287418	2.344985
H	0.020701	-7.994158	1.107315
H	1.344545	-6.282981	-0.122117
H	0.681816	-3.921010	-0.087877
H	-0.118494	-4.490972	4.017339
H	0.918986	-1.551463	1.013660
H	-1.199865	-0.359177	1.185366
H	1.017414	-0.142540	-1.534068
H	0.885190	-0.154159	-3.995496
H	-0.771299	-1.596675	-5.146657
H	-2.299515	-3.027952	-3.818775
H	-2.179906	-3.009010	-1.346559
C	2.602932	-3.413287	2.562792
C	3.303114	-2.237582	2.320128
C	2.904358	-1.035529	2.901144
C	1.782847	-1.027982	3.727943
C	1.077445	-2.199018	3.980052
C	1.486147	-3.415130	3.411430
N	0.846011	-4.606242	3.737476
H	2.920664	-4.348050	2.108568
H	4.169546	-2.262786	1.666035
H	3.454360	-0.120863	2.709682
H	1.451185	-0.100630	4.185496
H	0.212443	-2.186267	4.638272
H	-2.210344	-2.712154	1.823132
H	0.915264	-5.322579	3.023062

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(1-phenylethyl)aniline-BEt_3

B	1.94001	-0.68828	-0.16925
C	2.64812	-0.88525	1.28357
N	0.26859	-0.14003	-0.06788
C	-0.55952	-0.80810	1.01991
C	-0.03703	1.27063	-0.24515
C	0.58449	2.23505	0.54335
C	0.26804	3.57758	0.36587
C	-0.65616	3.96267	-0.60291
C	-1.98315	-1.00505	0.53225
C	-0.46515	-0.09051	2.35705
C	-2.96510	-0.02163	0.68421
C	-4.24625	-0.21824	0.17672
C	-4.56435	-1.39983	-0.48804
C	-3.59483	-2.38646	-0.64349
C	-2.31408	-2.18726	-0.13605
C	-1.26380	2.99739	-1.39910
C	-0.95757	1.65122	-1.21914
C	2.66352	0.40007	-1.13329
C	1.69791	-2.12836	-0.93785
C	2.78612	-3.19340	-0.75178
C	4.04188	-0.06537	-1.61832
C	3.19025	0.32035	2.06380
H	3.52357	-1.50538	1.04373
H	2.06062	-1.52855	1.95831
H	-0.05158	-0.58931	-0.92843
H	-0.09586	-1.79248	1.12614
H	1.32640	1.92994	1.27133
H	0.75760	4.32616	0.97976
H	-0.89382	5.01199	-0.74185
H	-0.88514	0.91622	2.32206
H	0.57205	-0.02191	2.68508
H	-1.02586	-0.66779	3.09594
H	-2.72935	0.90875	1.19149
H	-4.99801	0.55435	0.30189
H	-5.56466	-1.55189	-0.88020
H	-3.83551	-3.31315	-1.15414
H	-1.55961	-2.96180	-0.25328
H	-1.97887	3.28686	-2.16178
H	-1.44184	0.89301	-1.82929
H	2.78272	1.37543	-0.64291
H	2.03844	0.60257	-2.01857
H	0.74885	-2.60214	-0.63356
H	1.57888	-1.93469	-2.01721
H	2.61339	-4.07180	-1.38249
H	3.78023	-2.80553	-0.99358
H	2.82223	-3.53788	0.28650
H	4.55246	0.69968	-2.21231
H	3.96044	-0.96104	-2.24270
H	4.69721	-0.31630	-0.77568
H	3.89860	0.01553	2.84128
H	2.41018	0.89498	2.57661
H	3.71619	1.01480	1.39945

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[(1-phenylethyl)anilide-BEt_3]-

B	-0.21323	1.54414	-0.05413
C	1.40229	1.89697	-0.06507
C	-0.95206	2.31526	-1.32603
C	-0.85090	2.15582	1.33842
N	-0.41845	-0.08158	-0.15964
C	0.46792	-0.84133	-1.04072
C	-1.65048	-0.69429	0.05026
C	-2.27169	-1.54655	-0.89874
C	-3.48315	-2.18097	-0.64836
C	-4.15344	-2.00205	0.55698
C	1.84264	-1.06483	-0.40558
C	0.53450	-0.35934	-2.49770
C	1.90107	-1.37608	0.95753
C	3.11123	-1.66022	1.57699
C	4.29812	-1.64033	0.84420
C	4.25282	-1.33666	-0.51135
C	3.03445	-1.05612	-1.13016
C	-3.56075	-1.17694	1.51271
C	-2.34577	-0.55092	1.27597
C	-0.13472	1.72411	2.62420
C	-2.39135	1.88984	-1.63776
C	1.70222	3.39773	0.05204
H	1.92958	1.38116	0.75064
H	1.90034	1.54407	-0.97997
H	-0.36037	2.24422	-2.25351
H	-0.96661	3.39165	-1.09065
H	-0.78001	3.25153	1.26579
H	-1.92874	1.96577	1.42491
H	0.06477	-1.86248	-1.08716
H	-1.81307	-1.68434	-1.87271
H	-3.91370	-2.81329	-1.42185
H	-5.10170	-2.49395	0.75022
H	1.10301	0.56727	-2.59623
H	-0.47777	-0.16126	-2.85922
H	0.99013	-1.12095	-3.14192
H	0.97259	-1.36183	1.52079
H	3.13236	-1.89041	2.63873
H	5.24693	-1.85424	1.32800
H	5.16999	-1.30890	-1.09373
H	3.02267	-0.80429	-2.18609
H	-4.04163	-1.03517	2.47803
H	-1.89139	0.03262	2.06330
H	-0.66278	2.01052	3.54478
H	0.01792	0.63749	2.65219
H	0.86655	2.16780	2.67317
H	-2.89482	2.55967	-2.34927
H	-3.00238	1.85747	-0.72720
H	-2.43074	0.87993	-2.06074
H	1.32896	3.81013	0.99689
H	2.77745	3.61745	0.00710
H	1.22010	3.96413	-0.75322

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(1-phenylethyl)aniline-BPh_3

B	0.90697	0.59763	0.01000
C	1.77518	0.40084	-1.35029
C	0.07393	2.00020	-0.17274
C	1.79157	0.44679	1.37460
C	0.06618	3.06842	0.73438
C	-0.70781	4.21184	0.52385
C	-1.49468	4.32856	-0.61725
C	3.08206	-0.11359	1.32881
C	3.86693	-0.28917	2.46599
C	3.38789	0.09836	3.71376
C	2.87961	1.26148	-1.50144
C	3.65395	1.28604	-2.65389
C	3.34188	0.44635	-3.72284
C	2.24822	-0.40138	-3.61493
C	1.48206	-0.41925	-2.44677
C	-1.47397	3.30417	-1.56221
C	-0.69536	2.17412	-1.33846
C	2.11913	0.66083	3.80198
C	1.34688	0.83016	2.65357
N	-0.38322	-0.54415	0.02615
C	-1.35699	-0.33332	1.20137
C	-0.11949	-1.95738	-0.23183
C	-0.95913	-2.64620	-1.10719
C	-0.73967	-3.99625	-1.36157
C	0.31362	-4.65995	-0.73863
C	-1.13821	-1.32660	2.33245
C	-2.78451	-0.29081	0.69173
C	1.14578	-3.96563	0.13446
C	0.93543	-2.61380	0.39313
C	-3.34330	0.95282	0.37899
C	-3.55327	-1.44469	0.51007
C	-4.63969	1.04067	-0.11926
C	-5.39391	-0.11409	-0.30873
C	-4.84923	-1.35591	0.00899
H	0.69016	3.02315	1.62126
H	-0.68836	5.01600	1.25378
H	-2.09810	5.21608	-0.78090
H	3.48129	-0.43037	0.36929
H	4.85596	-0.72865	2.37484
H	3.99523	-0.03326	4.60391
H	3.13151	1.93537	-0.68457
H	4.49876	1.96507	-2.72348
H	3.94194	0.45992	-4.62741
H	1.98447	-1.05810	-4.43900
H	0.63944	-1.10374	-2.41683
H	-2.05614	3.39097	-2.47495
H	-0.66240	1.41048	-2.11709
H	1.72671	0.97310	4.76535
H	0.36397	1.27663	2.77763
H	-0.90935	-0.21075	-0.78555
H	-1.11915	0.66882	1.55690
H	-1.77710	-2.12199	-1.59495
H	-1.39046	-4.52459	-2.05021
H	0.48837	-5.71182	-0.93811
H	-0.10409	-1.30552	2.68033
H	-1.38582	-2.34975	2.04288
H	-1.78876	-1.03697	3.16148
H	1.97268	-4.47464	0.61818
H	1.58748	-2.07164	1.06679
H	-2.75520	1.85589	0.52776
H	-3.14146	-2.41832	0.75795
H	-5.05844	2.01343	-0.35596
H	-6.40552	-0.04743	-0.69602
H	-5.43658	-2.25835	-0.12699

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[(1-phenylethyl)anilide-BPh_3]-

B	-0.71745	-0.41688	0.08295
C	-0.75087	-0.15729	1.72243
C	0.01355	-1.88797	-0.07471
C	-2.23681	-0.52700	-0.56935
N	0.10559	0.71251	-0.68734
C	1.21582	0.44131	-1.60726
C	-0.26020	2.04888	-0.60090
C	-1.53083	2.44482	-0.10444
C	-1.90637	3.77633	-0.03915
C	-1.05359	4.80116	-0.45161
C	2.59708	0.42867	-0.94384
C	1.03113	-0.77217	-2.54542
C	0.20857	4.44305	-0.90688
C	0.60473	3.11056	-0.97364
C	-2.49164	-0.09170	-1.88111
C	-3.72938	-0.25105	-2.50085
C	-4.78210	-0.85312	-1.81702
C	-0.54164	-2.96192	-0.78478
C	0.11716	-4.18488	-0.91843
C	1.36756	-4.37395	-0.33796
C	-0.33115	1.00664	2.38730
C	-0.34791	1.12819	3.77815
C	-0.79295	0.07859	4.57335
C	-4.57326	-1.27633	-0.50749
C	-3.32735	-1.11057	0.09627
C	3.71985	-0.05380	-1.62505
C	5.15005	0.47731	0.24603
C	2.78103	0.94337	0.34208
C	-1.19837	-1.10112	3.95340
C	-1.16135	-1.20899	2.56647
C	1.93199	-3.33664	0.40380
C	1.25254	-2.13012	0.54322
C	4.04126	0.96457	0.93294
C	4.98250	-0.03195	-1.03843
H	1.23765	1.29511	-2.29675
H	-2.22249	1.69056	0.24346
H	-2.89551	4.01489	0.34356
H	-1.35893	5.84135	-0.39990
H	-0.02912	-0.94134	-2.73850
H	1.45601	-1.69140	-2.14093
H	1.51814	-0.56184	-3.50408
H	0.91926	5.21056	-1.20475
H	1.62402	2.90156	-1.27610
H	-1.69527	0.41498	-2.42193
H	-3.87479	0.10590	-3.51781

H	-5.75116	-0.98001	-2.29242
H	-1.50700	-2.83146	-1.26857
H	-0.34562	-4.98941	-1.48548
H	1.89063	-5.32035	-0.44932
H	0.01626	1.85973	1.81322
H	-0.01023	2.05393	4.23814
H	-0.81083	0.17103	5.65614
H	-5.38590	-1.73568	0.05078
H	-3.20712	-1.44025	1.12421
H	3.60759	-0.46515	-2.62368
H	6.13291	0.48910	0.70815
H	1.91205	1.29548	0.88841
H	-1.52711	-1.94704	4.55262
H	-1.42803	-2.16310	2.11624
H	2.90119	-3.46967	0.87822
H	1.69793	-1.34358	1.14727
H	4.15290	1.35746	1.93940
H	5.83642	-0.42181	-1.58572

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(1-phenylethyl)aniline-B(C_6F_5)Ph_2

B	-0.30136	-0.02509	0.50593
N	-0.89192	-0.86405	-0.93185
C	-1.55721	0.72505	1.21885
C	0.45806	-1.12396	1.42065
C	0.69723	1.18730	-0.01664
C	0.93914	1.69355	-1.28696
C	1.75066	2.78703	-1.57004
C	2.35787	3.46359	-0.52771
C	2.13319	3.02929	0.77199
C	1.31220	1.93371	0.99676
C	-1.99040	0.44342	2.51997
C	-3.07512	1.10681	3.09522
C	-3.75649	2.08573	2.38252
C	-3.32157	2.41988	1.10079
C	-2.23240	1.75945	0.54711
C	-0.25519	-2.16421	2.03822
C	0.36729	-3.14362	2.80992
C	1.74535	-3.10316	2.99940
C	2.48138	-2.07969	2.40832
C	1.84431	-1.11673	1.63248
F	1.11770	1.60030	2.27557
F	2.69613	3.67704	1.78931
F	3.13845	4.51375	-0.76491
F	1.92996	3.18749	-2.82889
F	0.36640	1.13488	-2.39657
C	-0.48697	-2.31196	-1.15488
C	1.01509	-2.50172	-1.12581
C	-1.03434	-2.82420	-2.49049
C	1.88512	-1.64394	-1.80023
C	3.25737	-1.87940	-1.78314
C	3.76999	-2.98771	-1.11580
C	2.90189	-3.86672	-0.47325
C	1.53367	-3.62425	-0.48018
C	-4.09851	0.27431	-2.47756
C	-2.73720	0.07855	-2.25548
C	-2.32178	-0.69005	-1.17566
C	-3.25079	-1.28199	-0.32618
C	-4.60639	-1.08596	-0.55564
C	-5.03428	-0.30514	-1.62849
H	-0.43479	-0.35321	-1.68538
H	-1.46290	-0.29728	3.11170
H	-3.38075	0.85953	4.10766
H	-4.60448	2.59912	2.82539
H	-3.82519	3.20132	0.53945
H	-1.90153	2.05247	-0.44818
H	-1.33740	-2.21014	1.92669
H	-0.22480	-3.92999	3.26922
H	2.23907	-3.85861	3.60296
H	3.55856	-2.03844	2.53977
H	2.45447	-0.35584	1.15312
H	-0.92472	-2.87882	-0.33045
H	-0.66746	-3.84074	-2.64696
H	-2.12486	-2.83329	-2.51867
H	-0.66428	-2.20707	-3.31701
H	1.50965	-0.78028	-2.34077
H	3.92497	-1.19408	-2.29538
H	4.84004	-3.16669	-1.09895
H	3.29149	-4.73128	0.05448
H	0.86301	-4.28695	0.06011
H	-4.42185	0.88283	-3.31532
H	-2.00019	0.54338	-2.90462
H	-2.91523	-1.86116	0.52728
H	-5.33123	-1.53314	0.11589
H	-6.09407	-0.14851	-1.79781

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[(1-phenylethyl)anilide-B(C_6F_5)Ph_2]-

B	-0.44011	0.58229	0.30449
N	1.01938	-0.00672	0.07973
C	-0.77248	1.80196	-0.77018
C	-0.50971	1.16886	1.85146
C	-1.63154	-0.56269	0.02374
C	-2.97340	-0.21089	0.20007
C	-4.05193	-1.04291	-0.06842
C	-3.82106	-2.30594	-0.59108
C	-2.51683	-2.69308	-0.83783
C	-1.46703	-1.82184	-0.54907
C	-0.34197	3.12333	-0.57505
C	-0.57359	4.13418	-1.50483
C	-1.26639	3.86449	-2.68083
C	-1.72466	2.57017	-2.90237
C	-1.48119	1.57235	-1.96149
C	-1.49866	0.89792	2.80971
C	-1.46046	1.42385	4.10046
C	-0.41327	2.25099	4.49322
C	0.60099	2.52425	3.57955
C	0.54814	1.98407	2.29696
F	-0.25840	-2.30366	-0.89155
F	-2.27533	-3.89755	-1.37261
F	-4.84138	-3.12786	-0.86385
F	-5.30986	-0.63545	0.14556

F	-3.29700	1.01942	0.62876
C	1.67796	-0.72181	1.17777
C	2.89093	-1.52109	0.71253
C	0.75267	-1.72550	1.88525
C	4.00552	-1.64658	1.54155
C	5.08998	-2.43958	1.17287
C	5.07275	-3.11888	-0.04119
C	3.96372	-2.99788	-0.87725
C	2.88145	-2.20853	-0.50416
C	2.45635	1.45621	-3.01452
C	1.62746	0.76175	-2.14652
C	1.90288	0.68386	-0.76887
C	3.09359	1.28395	-0.32215
C	3.93517	1.96249	-1.19951
C	3.62099	2.06779	-2.54985
H	0.19441	3.38260	0.33122
H	-0.21085	5.13962	-1.30614
H	-1.44957	4.64992	-3.40916
H	-2.27318	2.33289	-3.81075
H	-1.84403	0.56993	-2.17918
H	-2.32362	0.23755	2.55864
H	-2.25387	1.18105	4.80316
H	-0.38087	2.66492	5.49737
H	1.44090	3.15159	3.86799
H	1.36996	2.18752	1.61237
H	2.03212	-0.02821	1.96254
H	1.29808	-2.16742	2.72493
H	-0.14593	-1.24788	2.27513
H	0.47179	-2.52715	1.20059
H	4.02144	-1.10865	2.48766
H	5.95077	-2.51980	1.83104
H	5.91833	-3.73279	-0.33754
H	3.94449	-3.51952	-1.82993
H	2.01868	-2.09858	-1.15291
H	2.19840	1.50597	-4.06900
H	0.74060	0.25893	-2.51567
H	3.36564	1.21691	0.72710
H	4.84495	2.41711	-0.81572
H	4.27559	2.60309	-3.23083

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(1-phenylethyl)aniline-B(C_6F_5)$_2$Ph

B	0.52120	-0.18119	0.52647
N	0.26643	-1.29581	-0.73531
C	3.10360	-1.09856	3.37291
C	2.36476	-0.39887	2.41829
C	1.32349	-0.99180	1.69346
C	-1.03206	0.26449	0.89297
C	1.36021	1.14454	0.04157
C	-1.69108	1.29649	0.22113
C	-3.03315	1.60901	0.38044
C	-3.79934	0.88967	1.28197
C	-3.19570	-0.12487	2.00447
C	-1.85084	-0.41403	1.79851
C	1.36502	2.23426	0.91731
C	2.01991	3.43114	0.67165
C	2.71524	3.59529	-0.51913
C	2.73767	2.55332	-1.42888
C	2.06840	1.36953	-1.13200
C	1.07138	-2.34415	1.98382
C	1.80175	-3.05898	2.92302
C	2.82890	-2.43496	3.62806
F	3.39112	2.68589	-2.58259
F	2.13284	0.42807	-2.09869
F	-1.06805	2.01493	-0.73386
F	-3.59753	2.55385	-0.37085
F	-5.09264	1.15436	1.43270
F	-3.91189	-0.83893	2.87224
F	-1.39667	-1.45631	2.50553
F	0.71207	2.14756	2.08470
F	1.98610	4.42105	1.56067
F	3.34987	4.73406	-0.77823
C	-0.40082	-0.70248	-1.98991
C	1.32468	-2.28666	-1.00370
C	0.92931	-3.57159	-1.36573
C	1.88288	-4.55688	-1.59772
C	3.23449	-4.25701	-1.46076
C	-1.91894	-0.77719	-1.92302
C	0.08588	-1.31757	-3.30229
C	3.62162	-2.97553	-1.07997
C	2.67194	-1.98644	-0.84461
C	-2.63012	-1.81152	-1.31498
C	-4.02432	-1.80327	-1.30161
C	-4.72540	-0.77265	-1.91814
C	-4.02447	0.24855	-2.55631
C	-2.63508	0.24385	-2.55658
H	-0.46989	-1.84673	-0.29019
H	3.89924	-0.59220	3.91087
H	2.63157	0.63675	2.23785
H	0.27454	-2.87549	1.46622
H	1.56926	-4.10357	3.10561
H	3.40482	-2.98666	4.36437
H	-0.12625	0.35080	-1.98382
H	-0.12830	-3.80472	-1.46784
H	1.56629	-5.55530	-1.87923
H	3.98274	-5.02242	-1.63615
H	-0.34660	-0.72714	-4.11366
H	1.17205	-1.28628	-3.38720
H	-0.25633	-2.34784	-3.41919
H	4.67205	-2.74139	-0.94651
H	2.97977	-1.00981	-0.49660
H	-2.12187	-2.64178	-0.82631
H	-4.55905	-2.60548	-0.80389
H	-5.80980	-0.76290	-1.89799
H	-4.55897	1.06330	-3.03295
H	-2.09229	1.06404	-3.01869

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[(1-phenylethyl)anilide-B(C_6F_5)$_2$Ph]-

B	0.44276	0.03304	0.67928
N	-0.43417	1.33376	0.53930
C	3.12684	0.27678	3.63089

C	2.56319	0.14292	2.36217
C	1.18152	0.05306	2.15404
C	-0.52924	-1.30829	0.45155
C	1.53409	-0.18002	-0.56245
C	-1.20518	-1.44409	-0.76496
C	-2.02399	-2.51501	-1.09505
C	-2.17381	-3.55498	-0.19058
C	-1.49268	-3.49788	1.01171
C	-0.68368	-2.40077	1.30374
C	1.59136	0.50732	-1.77408
C	2.49039	0.19961	-2.79133
C	3.36712	-0.86175	-2.64155
C	3.32093	-1.60971	-1.47649
C	2.40611	-1.26737	-0.48870
C	0.39214	0.09754	3.31549
C	0.93218	0.22777	4.59008
C	2.31247	0.32238	4.75603
F	4.13801	-2.65985	-1.32657
F	2.37606	-2.08023	0.58043
F	-1.05657	-0.51914	-1.72358
F	-2.64351	-2.57110	-2.27851
F	-2.95136	-4.60247	-0.48281
F	-1.60979	-4.50607	1.88507
F	-0.05058	-2.47987	2.48042
F	0.75716	1.51607	-2.05561
F	2.50466	0.90847	-3.92657
F	4.23363	-1.16986	-3.61275
C	-1.80960	1.28058	1.04535
C	0.14625	2.59045	0.40082
C	-0.61590	3.75289	0.13560
C	-0.02369	4.99931	-0.02307
C	1.35525	5.16089	0.06137
C	-2.08295	2.20080	2.25981
C	-2.90291	1.42990	-0.01724
C	-2.61197	1.73421	-1.34829
C	-3.63402	1.86082	-2.28591
C	-4.96269	1.67752	-1.91420
C	-5.26363	1.35996	-0.59211
C	-4.24121	1.23883	0.34367
C	2.12566	4.02809	0.30954
C	1.54465	2.77946	0.48021
H	4.20643	0.34689	3.73626
H	3.23482	0.11966	1.50553
H	-0.68785	-0.00080	3.22482
H	0.27596	0.25035	5.45639
H	2.74391	0.42711	5.74761
H	-1.93604	0.26361	1.42831
H	-1.68935	3.67782	0.02129
H	-0.66132	5.85551	-0.22910
H	1.81518	6.13552	-0.06603
H	-2.92235	1.80766	2.84143
H	-1.20053	2.22415	2.90308
H	-2.32680	3.22447	1.97574
H	-1.57320	1.85256	-1.63796
H	-3.38614	2.09832	-3.31621
H	-5.75667	1.77295	-2.64898
H	-6.29490	1.20188	-0.28937
H	-4.48638	0.98147	1.37147
H	3.20689	4.11191	0.38412
H	2.18645	1.93654	0.68792

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(1-phenylethyl)aniline-B(C_6F_5)$_3$

B	-0.24404	0.04663	-0.00984
C	-1.04930	-2.10159	-1.47456
C	-0.03748	-1.33365	-0.89593
C	0.70956	1.30423	-0.46741
C	-1.77174	0.61763	-0.10178
C	-2.25307	0.85176	-1.39247
C	-3.48944	1.40862	-1.67542
C	-4.31241	1.79963	-0.62788
C	-3.86391	1.63831	0.67128
C	-2.61195	1.07753	0.89950
C	1.66535	1.30950	-1.48843
C	2.43567	2.42077	-1.81991
C	2.23160	3.62697	-1.17089
C	1.23231	3.70517	-0.21251
C	0.49082	2.57060	0.08817
C	1.22785	-1.91691	-0.99792
C	1.50651	-3.11615	-1.63274
C	0.46356	-3.81883	-2.22032
C	-0.81989	-3.30607	-2.13549
F	-1.49534	0.51943	-2.44867
F	-2.33745	-1.75973	-1.38925
F	-1.83663	-3.98253	-2.66390
F	0.69209	-4.97082	-2.83864
F	2.74700	-3.59551	-1.67633
F	2.27239	-1.33045	-0.37694
F	-0.47952	2.76393	0.99476
F	0.97650	4.86039	0.39826
F	2.95406	4.69547	-1.48413
F	3.35131	2.33566	-2.78201
F	1.89758	0.24086	-2.25420
F	-2.21869	1.06614	2.18370
F	-4.61268	2.04895	1.69476
F	-5.50234	2.33947	-0.87084
F	-3.88790	1.57813	-2.93462
N	0.28485	-0.58227	1.56206
C	1.16946	0.11719	2.63673
C	-0.66871	-1.52050	2.19383
C	-0.76668	-2.82307	1.70104
C	-1.63368	-3.73325	2.29899
C	-2.38723	-3.36398	3.40659
C	0.76424	1.50818	3.09711
C	2.62046	-0.00683	2.20467
C	-2.24650	-2.08229	3.92861
C	-1.38691	-1.16491	3.33420
C	3.27742	-1.21126	2.47671
C	3.30451	0.98855	1.50535
C	4.58099	-1.42864	2.04509
C	5.24836	-0.43486	1.33475
C	4.60924	0.77321	1.07133

H	0.99188	-1.20371	1.16969
H	1.05033	-0.55334	3.49147
H	-0.15893	-3.14457	0.86373
H	-1.70276	-4.73856	1.89776
H	-3.06213	-4.07391	3.87201
H	-0.31497	1.63005	3.15679
H	1.15034	2.29766	2.45740
H	1.19706	1.65347	4.09033
H	-2.80402	-1.78691	4.81081
H	-1.28019	-0.18100	3.76865
H	2.75550	-1.98989	3.03040
H	2.82388	1.93460	1.28133
H	5.07423	-2.36969	2.26420
H	6.26399	-0.59953	0.99069
H	5.12459	1.55320	0.52004

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[(1-phenylethyl)anilide-B(C_6F_5)$_3$]-

B	-0.26198	0.01134	0.11726
C	-2.38224	-0.35412	-1.61700
C	-1.78197	0.31695	-0.55115
C	0.82563	1.20661	-0.36490
C	0.37002	-1.40147	-0.52850
C	0.66446	-2.57114	0.16310
C	1.32943	-3.66016	-0.40132
C	1.72656	-3.61544	-1.72290
C	1.44441	-2.47801	-2.46710
C	0.78591	-1.42258	-1.86222
C	2.19380	0.95204	-0.52715
C	3.12684	1.88068	-0.97009
C	2.71980	3.15985	-1.30304
C	1.37888	3.47295	-1.18121
C	0.48017	2.51000	-0.72969
C	-2.64016	1.24581	0.04872
C	-3.93216	1.52276	-0.37292
C	-4.45899	0.84177	-1.45755
C	-3.67335	-0.10795	-2.07967
F	0.31582	-2.75477	1.44789
F	-1.77584	-1.36446	-2.26353
F	-4.16474	-0.80509	-3.11197
F	-5.70012	1.09173	-1.88475
F	-4.67451	2.44043	0.25705
F	-2.25129	1.95091	1.11819
F	-0.77920	2.96154	-0.64011
F	0.95170	4.70122	-1.49765
F	3.60020	4.07210	-1.72334
F	4.42241	1.55731	-1.03755
F	2.73058	-0.23286	-0.21108
F	0.55521	-0.35652	-2.64787
F	1.81320	-2.41932	-3.75248
F	2.36139	-4.65106	-2.28140
F	1.58084	-4.75294	0.33064
N	-0.42621	-0.05697	1.67272
C	0.39623	0.69861	2.63128
C	-1.56584	-0.65418	2.20990
C	-2.25352	-1.67522	1.50924
C	-3.39415	-2.27458	2.01784
C	-3.91811	-1.90337	3.25541
C	0.03212	2.18236	2.76007
C	1.89735	0.45684	2.48471
C	-3.26371	-0.90312	3.96171
C	-2.12415	-0.28536	3.45484
C	2.37569	-0.84977	2.62310
C	2.82295	1.48399	2.29966
C	3.73529	-1.12661	2.55078
C	4.64846	-0.09598	2.33722
C	4.18717	1.20961	2.21184
H	0.18453	0.24827	3.60786
H	-1.87555	-2.01301	0.55247
H	-3.87454	-3.05609	1.43536
H	-4.81053	-2.37735	3.65064
H	0.63154	2.65093	3.54788
H	-1.02260	2.28740	3.01334
H	0.19286	2.72704	1.82724
H	-3.64936	-0.57317	4.92298
H	-1.68978	0.51818	4.03577
H	1.65973	-1.65197	2.76710
H	2.47893	2.50717	2.17787
H	4.08248	-2.15076	2.65147
H	5.71054	-0.30974	2.26472
H	4.88748	2.02056	2.03361

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[(1-phenylethyl)aniline-$SiEt_3$]$^+$

Si	-1.84226	-0.14670	0.04315
C	-2.44156	1.43465	-0.75945
C	-2.90371	-0.66643	1.50116
C	-1.47853	-1.55501	-1.13474
N	-0.23254	0.38800	0.96047
C	0.63286	-0.76345	1.55075
C	0.52231	1.46014	0.29867
C	0.90963	1.31816	-1.03049
C	1.62407	2.34441	-1.63881
C	1.94619	3.49709	-0.92483
C	1.18889	-0.29415	2.88990
C	1.69625	-1.26861	0.60489
C	1.54902	3.62986	0.40232
C	0.83088	2.60846	1.02003
C	1.53999	-2.51965	0.00473
C	2.87932	-0.55313	0.38196
C	2.52629	-3.03691	-0.83106
C	3.68647	-2.30642	-1.06684
C	3.86288	-1.06654	-0.45511
C	-3.96669	1.45642	-0.96723
C	-2.54695	-1.62544	-2.24363
C	-4.09942	-1.54332	1.08510
H	-1.92201	1.58195	-1.71296
H	-2.14499	2.28297	-0.12894
H	-2.29850	-1.21510	2.23493
H	-3.26438	0.23456	2.01491
H	-0.48343	-1.46474	-1.58110
H	-1.47159	-2.49364	-0.56794

H	-0.63556	0.82492	1.79747
H	-0.08654	-1.57114	1.72178
H	0.68284	0.40856	-1.57751
H	1.93315	2.23908	-2.67267
H	2.50379	4.29333	-1.40514
H	1.84610	0.57061	2.76743
H	0.38421	-0.03254	3.58556
H	1.77353	-1.09963	3.33729
H	1.79180	4.52714	0.96030
H	0.51449	2.71137	2.05546
H	0.64741	-3.10575	0.20628
H	3.03460	0.41441	0.85084
H	2.39197	-4.01249	-1.28531
H	4.45905	-2.70720	-1.71419
H	4.77311	-0.50136	-0.62336
H	-4.27403	2.39038	-1.44182
H	-4.50121	1.38070	-0.01595
H	-4.30490	0.63762	-1.60846
H	-2.34887	-2.46574	-2.91180
H	-3.55210	-1.76391	-1.83442
H	-2.55413	-0.71495	-2.84945
H	-4.70201	-1.81341	1.95437
H	-4.75551	-1.02660	0.37921
H	-3.76594	-2.47234	0.61379

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(1-phenylethyl)anilide-$SiEt_3$

Si	0.93519	-1.35292	-0.05931
C	1.17727	-1.30974	1.81538
C	2.58853	-1.82968	-0.86074
C	-0.35529	-2.67985	-0.46305
N	0.32932	0.19014	-0.69187
C	-0.95810	0.24992	-1.39960
C	0.98490	1.40172	-0.35539
C	2.36605	1.52378	-0.56426
C	3.05511	2.66588	-0.16939
C	2.37725	3.73593	0.40563
C	-2.18919	0.27345	-0.48996
C	-0.99006	1.37266	-2.44589
C	0.99738	3.64843	0.57142
C	0.30719	2.49827	0.20358
C	-0.30117	-3.89844	0.47217
C	2.91719	-3.32697	-0.78951
C	2.01549	-0.16204	2.39540
C	-3.46523	0.18748	-1.05803
C	-4.49003	0.22786	1.12624
C	-2.08757	0.31942	0.90146
C	-3.22743	0.30135	1.70375
C	-4.60454	0.16713	-0.26120
H	0.18958	-1.33076	2.29424
H	1.64437	-2.27104	2.07536
H	3.39509	-1.26275	-0.37997
H	2.56805	-1.50332	-1.90840
H	-1.35743	-2.24189	-0.40018
H	-0.22538	-3.00190	-1.50503
H	-1.02792	-0.68499	-1.97038
H	2.89602	0.71751	-1.05795
H	4.12674	2.72426	-0.33350
H	2.91219	4.63019	0.70681
H	-0.08795	1.32261	-3.06088
H	-1.04212	2.36225	-1.99014
H	-1.85951	1.25408	-3.09579
H	0.44822	4.47914	1.00401
H	-0.76442	2.44393	0.36046
H	-1.03779	-4.65252	0.18049
H	0.67985	-4.38131	0.47072
H	-0.52085	-3.60858	1.50370
H	3.88517	-3.54688	-1.24916
H	2.16362	-3.92767	-1.30802
H	2.96298	-3.67887	0.24651
H	2.18317	-0.29797	3.46808
H	2.99606	-0.09564	1.91319
H	1.52685	0.80607	2.25221
H	-3.56963	0.12294	-2.13816
H	-5.37812	0.21210	1.74951
H	-1.10371	0.37872	1.35797
H	-3.12343	0.34352	2.78348
H	-5.58417	0.09918	-0.72387

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[(1-phenylethyl)aniline-$SiPhH_2$]$^+$

Si	-0.21802	-0.60050	-1.50085
C	1.31582	-1.36714	-0.82874
N	-1.09949	0.12381	0.03656
C	-0.75888	1.59668	0.38752
C	-2.53766	-0.16989	0.14346
C	-1.44100	2.56209	-0.56346
C	-3.37605	0.02808	-0.94891
C	-4.73482	-0.23603	-0.81079
C	-5.24104	-0.69469	0.40373
C	0.74760	1.70953	0.48373
C	-4.39018	-0.88874	1.48795
C	-3.02944	-0.62279	1.36192
C	1.39584	1.09295	1.56059
C	1.50665	2.38954	-0.46951
C	2.77863	1.13624	1.67414
C	3.53028	1.81855	0.71737
C	2.89438	2.44880	-0.34685
C	2.58590	-0.90297	-1.19301
C	3.72751	-1.47303	-0.63681
C	3.60969	-2.50319	0.29224
C	2.35152	-2.97789	0.66174
C	1.21101	-2.41804	0.09850
H	-1.22788	-1.55897	-1.97406
H	-0.00956	0.52940	-2.41964
H	-0.64040	-0.40756	0.78697
H	-1.19118	1.72015	1.38710
H	-1.13497	3.57606	-0.29752
H	-2.52570	2.50298	-0.47308
H	-1.16312	2.38900	-1.60637
H	-2.98149	0.38567	-1.89635
H	-5.39659	-0.08641	-1.65636

H	-6.30029	-0.90323	0.50324
H	-4.78063	-1.24808	2.43331
H	-2.36092	-0.76978	2.20732
H	0.81258	0.58811	2.33037
H	1.02429	2.89317	-1.30131
H	3.26930	0.65321	2.51200
H	4.61003	1.86698	0.81075
H	3.47517	2.99372	-1.08346
H	2.68770	-0.08716	-1.90328
H	4.70821	-1.11060	-0.92641
H	4.50079	-2.94539	0.72536
H	2.26342	-3.79053	1.37470
H	0.23557	-2.81889	0.37384

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(1-phenylethyl)anilide-$SiPhH_2$

Si	1.24276	-1.48936	-0.83410
C	2.83835	-0.61835	-0.39273
N	-0.11926	-0.70001	-0.05298
C	0.06396	0.64056	0.53309
C	-1.34760	-1.37768	0.07064
C	-2.35210	-0.98697	0.97204
C	-3.53808	-1.70502	1.07089
C	-3.76875	-2.82909	0.28464
C	-1.04183	1.60975	0.12329
C	0.37273	0.59038	2.03320
C	-2.79180	-3.21184	-0.62828
C	-1.60828	-2.49376	-0.74442
C	3.38168	0.37152	-1.22397
C	4.57080	1.01506	-0.89170
C	5.24210	0.67115	0.27894
C	4.72543	-0.31738	1.11308
C	3.53557	-0.95641	0.77636
C	-1.54743	1.55762	-1.17954
C	-2.99525	3.43550	-0.73373
C	-1.53265	2.58666	0.98982
C	-2.50250	3.49375	0.56435
C	-2.51325	2.46068	-1.60551
H	1.11072	-1.47069	-2.31622
H	1.30898	-2.89742	-0.37839
H	0.97318	1.03693	0.06467
H	-2.22238	-0.10709	1.58710
H	-4.29155	-1.37282	1.77846
H	-4.69493	-3.38621	0.37177
H	1.19873	-0.10595	2.19506
H	-0.47631	0.25542	2.63256
H	0.69140	1.57107	2.39611
H	-2.95211	-4.07061	-1.27277
H	-0.89111	-2.79908	-1.50083
H	2.86917	0.64357	-2.14414
H	4.97538	1.78054	-1.54615
H	6.17068	1.16966	0.53860
H	5.25179	-0.59251	2.02152
H	3.14662	-1.73413	1.43035
H	-1.18793	0.78514	-1.85390
H	-3.75240	4.13913	-1.06414
H	-1.16820	2.64473	2.01022
H	-2.87369	4.24449	1.25496
H	-2.89646	2.40011	-2.61926

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BEt_3-$(PhNHMePh)_2$

B	2.82640	0.17578	-0.96121
C	4.32986	-0.46352	-0.96503
N	1.70583	-0.63658	0.10332
C	1.83060	-2.14688	0.02058
C	1.50301	-0.11698	1.45002
C	2.57974	0.09112	2.30831
C	2.35440	0.58906	3.58700
C	1.06214	0.89802	4.00671
C	0.48330	-2.83526	0.12480
C	2.83824	-2.71361	1.01153
C	-0.16475	-3.01857	1.35209
C	-1.37937	-3.69561	1.41342
C	-1.96649	-4.19618	0.25253
C	-1.33358	-4.01505	-0.97308
C	-0.11517	-3.34189	-1.03185
C	-0.00721	0.70926	3.13795
C	0.20974	0.19701	1.86146
C	2.77969	1.73198	-0.50962
C	2.06901	-0.05361	-2.42341
C	2.95612	-0.33176	-3.64256
C	3.45793	2.65468	-1.52834
C	5.33950	-0.13581	0.14516
N	-0.96314	1.09672	-1.15310
C	-2.12410	0.64601	-1.95223
C	-1.13939	2.33503	-0.46641
C	-0.42355	3.46745	-0.86794
C	-0.55351	4.67083	-0.18223
C	-1.42244	4.76980	0.89978
C	-3.23386	0.12223	-1.06354
C	-1.65354	-0.42856	-2.92957
C	-2.98261	-0.91151	-0.15666
C	-3.99376	-1.37366	0.67850
C	-5.27089	-0.81672	0.61055
C	-5.53054	0.20193	-0.29997
C	-4.51317	0.66909	-1.13045
C	-2.14794	3.64901	1.29580
C	-2.00606	2.43671	0.62866
H	4.75822	-0.04298	-1.88551
H	4.34110	-1.54802	-1.15735
H	0.83107	-0.40865	-0.38510
H	2.21260	-2.31751	-0.98982
H	3.58554	-0.11238	1.96421
H	3.19678	0.75189	4.25113
H	0.89394	1.29801	5.00113
H	2.51188	-2.58979	2.04597
H	3.81267	-2.23999	0.89332
H	2.94533	-3.78291	0.81449
H	0.28179	-2.63473	2.26431
H	-1.86660	-3.83693	2.37338
H	-2.91492	-4.72122	0.30396

H	-1.78319	-4.39969	-1.88266
H	0.38706	-3.21416	-1.98841
H	-1.01633	0.96813	3.44203
H	-0.61912	0.05561	1.17369
H	3.24486	1.89955	0.47064
H	1.73526	2.05584	-0.37797
H	1.31687	-0.86129	-2.38078
H	1.48599	0.85329	-2.65933
H	2.37016	-0.43651	-4.56222
H	3.67486	0.47863	-3.80333
H	3.53594	-1.25141	-3.51321
H	3.39112	3.71063	-1.24471
H	3.00935	2.55534	-2.52442
H	4.52178	2.41169	-1.63433
H	6.36904	-0.31253	-0.18334
H	5.20743	-0.74060	1.04962
H	5.27085	0.91492	0.44763
H	-0.17098	1.19250	-1.78469
H	-2.52826	1.49433	-2.52732
H	0.25097	3.39610	-1.71855
H	0.02196	5.53316	-0.50328
H	-1.53040	5.70890	1.43200
H	-1.24874	-1.28363	-2.37945
H	-0.87311	-0.04302	-3.59385
H	-2.49189	-0.77507	-3.53804
H	-1.98540	-1.34348	-0.09678
H	-3.78198	-2.17113	1.38375
H	-6.05781	-1.17642	1.26577
H	-6.52081	0.64237	-0.35813
H	-4.70901	1.48164	-1.82516
H	-2.82496	3.71212	2.14216
H	-2.55999	1.56525	0.96124

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[BEt_3-(PhNHMePh-PhNMePh)]-

B	-2.522432	-0.049814	-1.602729
C	-3.918036	0.555190	-2.255048
N	-2.516531	0.352637	-0.010166
C	-2.543947	1.807308	0.166305
C	-2.713946	-0.423725	1.110577
C	-3.141886	-1.776036	1.031946
C	-3.283580	-2.575731	2.156782
C	-3.031806	-2.092119	3.439828
C	-1.291862	2.453988	0.771197
C	-3.860175	2.304470	0.794268
C	-1.208233	3.847632	0.877049
C	-0.042888	4.472242	1.311113
C	1.076518	3.713454	1.644085
C	1.009350	2.326818	1.542024
C	-0.163218	1.708150	1.115120
C	-2.643014	-0.761501	3.551681
C	-2.488883	0.050463	2.435173
C	-2.437631	-1.661794	-1.961197
C	-1.146950	0.665190	-2.238102
C	-1.298918	1.354546	-3.600533
C	-2.144099	-1.929286	-3.445581
C	-5.184524	-0.110019	-1.701101
N	1.820563	-0.365949	-0.497895
C	2.913302	0.077282	-1.336330
C	1.665775	-1.702207	-0.135167
C	0.417007	-2.121613	0.355710
C	0.227470	-3.426914	0.777824
C	1.273381	-4.351267	0.721804
C	4.226929	0.198026	-0.571988
C	2.528505	1.436348	-1.929820
C	4.274439	0.176433	0.821521
C	5.487033	0.331657	1.489931
C	6.668160	0.506478	0.774871
C	6.631413	0.515547	-0.618048
C	5.419526	0.358452	-1.282352
C	2.506056	-3.942454	0.227628
C	2.712636	-2.631663	-0.201081
H	-3.909497	0.433602	-3.349005
H	-4.010686	1.644208	-2.110221
H	0.940617	0.088407	-0.718923
H	-2.553040	2.208961	-0.851452
H	-3.386439	-2.191134	0.068947
H	-3.617592	-3.602317	2.019818
H	-3.145452	-2.723410	4.314922
H	-4.015807	1.913069	1.800814
H	-4.686779	1.964821	0.165389
H	-3.895480	3.396509	0.842904
H	-2.059730	4.458778	0.590077
H	-0.005553	5.556254	1.376069
H	1.991338	4.197047	1.973344
H	1.875731	1.717031	1.779308
H	-0.216447	0.626639	1.052879
H	-2.443561	-0.333776	4.531699
H	-2.168581	1.071156	2.596174
H	-3.375541	-2.191513	-1.747218
H	-1.664946	-2.176321	-1.371672
H	-0.716191	1.407855	-1.548923
H	-0.369854	-0.114511	-2.333185
H	-0.357943	1.778294	-3.979713
H	-1.675654	0.663318	-4.362004
H	-2.022469	2.176230	-3.538489
H	-2.142427	-3.001817	-3.677682
H	-1.168600	-1.534592	-3.748708
H	-2.896448	-1.459717	-4.091212
H	-6.109835	0.409220	-1.985451
H	-5.153054	-0.156830	-0.604872
H	-5.276124	-1.142918	-2.055041
H	3.080404	-0.636022	-2.163432
H	-0.414573	-1.420202	0.377231
H	-0.753510	-3.709962	1.148736
H	1.124419	-5.373586	1.054015
H	2.329376	2.143663	-1.118265
H	1.623216	1.343003	-2.537274
H	3.337180	1.830788	-2.549549
H	3.352166	0.012688	1.369549
H	5.507605	0.308045	2.575387
H	7.612486	0.625449	1.297345

H	7.548158	0.640814	-1.186801
H	5.393536	0.358201	-2.370354
H	3.329837	-4.648903	0.169966
H	3.686243	-2.334351	-0.575584

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BPh_3-$(PhNHMePh)_2$

B	2.527656	0.429556	0.159025
C	3.259168	-0.049846	4.015293
C	3.408048	0.209836	2.652543
C	2.346776	0.081500	1.746097
C	1.833646	1.863406	-0.240229
C	4.077719	0.380048	-0.331621
C	2.306235	2.683949	-1.280155
C	1.640211	3.846312	-1.667802
C	0.459215	4.222919	-1.029824
C	-0.031059	3.437691	0.010699
C	0.660607	2.290921	0.397642
C	4.865834	1.501045	0.003980
C	6.219639	1.587122	-0.299620
C	6.853186	0.545880	-0.975655
C	6.112101	-0.575650	-1.321704
C	4.756437	-0.651256	-0.994642
C	1.121074	-0.342346	2.294059
C	0.958507	-0.610574	3.649532
C	2.032701	-0.461448	4.523620
H	4.111103	0.064447	4.679438
H	4.385225	0.512418	2.287435
H	3.220601	2.409453	-1.801333
H	2.040081	4.453853	-2.474712
H	-0.065192	5.123802	-1.334458
H	-0.945562	3.712438	0.530827
H	0.268425	1.716827	1.229877
H	4.394146	2.334525	0.519911
H	6.780975	2.471558	-0.012771
H	7.908019	0.609634	-1.223803
H	6.585028	-1.403314	-1.842485
H	4.233983	-1.564059	-1.255929
H	0.251558	-0.484245	1.650680
H	-0.007645	-0.945489	4.021323
H	1.915384	-0.670665	5.582404
N	1.489754	-0.684240	-0.646754
C	1.428475	-0.530991	-2.182508
C	1.460932	-2.076950	-0.181622
C	0.264682	-2.781353	-0.295030
C	0.181517	-4.099963	0.139998
C	1.296762	-4.717662	0.699069
C	-0.007544	-0.267778	-2.623668
C	2.064084	-1.685166	-2.948561
C	2.481617	-4.000787	0.835250
C	2.568588	-2.678691	0.405604
C	-0.852641	-1.295810	-3.057975
C	-2.170156	-1.028608	-3.422751
C	-2.661675	0.275360	-3.374594
C	-1.818603	1.309209	-2.972628
C	-0.504095	1.039629	-2.597358
H	0.586813	-0.298029	-0.337514
H	2.006066	0.374694	-2.378252
H	-0.600010	-2.279485	-0.711735
H	-0.758642	-4.635732	0.051690
H	1.237075	-5.744251	1.044698
H	1.898568	-1.508103	-4.014140
H	3.137663	-1.730414	-2.781210
H	1.631764	-2.653646	-2.689801
H	3.346376	-4.462544	1.299638
H	3.473145	-2.109734	0.575762
H	-0.484703	-2.315489	-3.116030
H	-2.809264	-1.838985	-3.760044
H	-3.690835	0.480314	-3.652986
H	-2.178506	2.332828	-2.938932
H	0.139727	1.855321	-2.286933
N	-2.035504	-0.189047	0.205361
C	-2.838047	-1.396818	0.567043
C	-2.486511	1.025805	0.813041
C	-2.096359	1.352659	2.115396
C	-2.549882	2.526179	2.711532
C	-3.391135	3.392907	2.016729
C	-4.323092	-1.200936	0.307460
C	-2.512381	-1.877230	1.975619
C	-5.162209	-0.567471	1.229091
C	-6.501025	-0.337699	0.926899
C	-7.022995	-0.736073	-0.301370
C	-6.197446	-1.366200	-1.227991
C	-4.858670	-1.594148	-0.921024
C	-3.778266	3.074952	0.717368
C	-3.337001	1.896290	0.124274
H	-2.122005	-0.075288	-0.804479
H	-2.501368	-2.171335	-0.132179
H	-1.406332	0.703229	2.645016
H	-2.228370	2.770076	3.718961
H	-3.737069	4.309529	2.482847
H	-2.801693	-1.144648	2.733126
H	-1.437180	-2.061783	2.064624
H	-3.049902	-2.805813	2.184820
H	-4.764343	-0.231830	2.182589
H	-7.137818	0.158439	1.652337
H	-8.067832	-0.556995	-0.533864
H	-6.596291	-1.685710	-2.185809
H	-4.212567	-2.086161	-1.644479
H	-4.438335	3.738128	0.167141
H	-3.670132	1.624458	-0.873665

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[BPh_3-(PhNHMePh-PhNMePh)]-

B	2.405180	0.238351	0.501412
N	1.900822	-0.410443	-0.860074
C	2.041236	-1.307065	4.142259
C	2.552072	-0.682018	3.004660
C	1.831014	-0.586059	1.805659
C	1.785100	1.782644	0.589137
C	4.051113	0.307821	0.509858
C	2.477008	2.904149	0.099367

C	1.921729	4.182215	0.072347
C	0.634829	4.394763	0.557209
C	-0.072930	3.314632	1.076201
C	0.500993	2.044185	1.091122
C	4.761007	1.149319	1.386982
C	6.152276	1.201146	1.416316
C	6.899309	0.406371	0.548449
C	6.231834	-0.431218	-0.339174
C	4.836923	-0.472609	-0.351475
C	0.555134	-1.182250	1.815981
C	0.029543	-1.808835	2.944058
C	0.771858	-1.872227	4.121107
C	1.700704	-1.763075	-1.059818
C	0.851377	-2.272753	-2.073181
C	0.658722	-3.639679	-2.249969
C	1.275768	-4.568498	-1.418146
C	2.110444	-4.088143	-0.408547
C	2.329758	-2.730156	-0.236283
C	1.902818	0.492561	-2.010517
C	0.560801	1.158592	-2.308551
C	2.545295	-0.067899	-3.294659
C	-0.643598	0.664400	-1.809958
C	-1.857446	1.270347	-2.130515
C	-1.879650	2.412314	-2.925603
C	-0.679518	2.939738	-3.399444
C	0.524738	2.314309	-3.095565
H	2.642365	-1.353741	5.047288
H	3.553858	-0.264783	3.051473
H	3.487730	2.771547	-0.282597
H	2.497388	5.013408	-0.328319
H	0.193064	5.387461	0.538540
H	-1.074239	3.458416	1.475977
H	-0.073299	1.224765	1.518570
H	4.197089	1.796482	2.057299
H	6.655992	1.868206	2.112003
H	7.985367	0.444546	0.562341
H	6.797680	-1.055803	-1.026456
H	4.337769	-1.140471	-1.049740
H	-0.032475	-1.170632	0.894976
H	-0.964223	-2.249319	2.917227
H	0.365006	-2.359736	5.002545
H	0.316854	-1.579463	-2.713432
H	0.001837	-3.979824	-3.048278
H	1.116145	-5.633326	-1.553365
H	2.615567	-4.785632	0.254595
H	2.999555	-2.392613	0.545455
H	2.572764	1.310009	-1.726422
H	2.684878	0.749905	-4.007677
H	3.527679	-0.483966	-3.055908
H	1.954613	-0.840921	-3.785578
H	-0.623024	-0.203716	-1.157164
H	-2.782426	0.849349	-1.745032
H	-2.823796	2.892333	-3.166982
H	-0.681524	3.844002	-4.001890
H	1.459595	2.739710	-3.455119
N	-2.962106	-0.636557	2.004978
C	-3.374005	-1.877341	1.311643
C	-3.707921	0.539789	1.759536
C	-4.975744	0.717708	2.328789
C	-5.710270	1.869313	2.062803
C	-5.184153	2.876217	1.255324
C	-3.537289	-1.735332	-0.196318
C	-4.606521	-2.503043	1.962601
C	-4.671342	-1.133548	-0.758412
C	-4.814054	-1.038831	-2.139161
C	-3.823000	-1.537229	-2.982689
C	-2.684643	-2.118363	-2.435006
C	-2.543846	-2.216683	-1.051800
C	-3.907566	2.722023	0.720401
C	-3.179541	1.562238	0.964583
H	-1.980835	-0.463016	1.799188
H	-2.536739	-2.565922	1.473913
H	-5.363637	-0.040956	3.000051
H	-6.693692	1.989503	2.508385
H	-5.758925	3.775241	1.056725
H	-5.505073	-1.906453	1.787341
H	-4.450156	-2.587301	3.041137
H	-4.782190	-3.497520	1.543352
H	-5.445411	-0.728806	-0.112306
H	-5.698688	-0.567545	-2.557104
H	-3.930968	-1.456785	-4.059828
H	-1.894175	-2.493098	-3.077241
H	-1.642739	-2.671966	-0.642348
H	-3.470060	3.492117	0.090961
H	-2.193624	1.439927	0.522456

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$B(C_6F_5)Ph_2$-$(PhNHMePh)_2$

B	1.878944	0.192423	0.246304
C	2.315019	-0.396087	4.140464
C	2.582630	-0.174564	2.790477
C	1.568510	-0.049859	1.831568
C	1.281027	1.566502	-0.406201
C	3.494177	0.195643	-0.062953
C	1.888591	2.189294	-1.510699
C	1.348331	3.325616	-2.111161
C	0.164408	3.876284	-1.624107
C	-0.452632	3.292857	-0.520588
C	0.110318	2.166101	0.075728
C	4.196119	1.263503	0.514385
C	5.551359	1.494776	0.333168
C	6.287450	0.647493	-0.485546
C	5.643464	-0.411348	-1.098165
C	4.280714	-0.598834	-0.879613
C	0.254400	-0.197866	2.314199
C	-0.029880	-0.419453	3.658419
C	1.004058	-0.512196	4.585911
F	6.318268	-1.237190	-1.898725
F	3.742089	-1.644786	-1.538062
F	3.552529	2.137083	1.294691
F	6.151514	2.526302	0.924504
F	7.587709	0.853326	-0.675526

H	3.138279	-0.481588	4.843454
H	3.622890	-0.112838	2.485541
H	2.812286	1.781685	-1.916607
H	1.851432	3.778885	-2.960337
H	-0.260761	4.760419	-2.089511
H	-1.365418	3.714733	-0.107669
H	-0.377292	1.762224	0.954258
H	-0.592903	-0.161795	1.628313
H	-1.063000	-0.528328	3.981217
H	0.789897	-0.684414	5.636012
N	0.904432	-1.025335	-0.495805
C	0.820593	-1.126272	-2.038981
C	0.849735	-2.327923	0.168985
C	-0.402716	-2.860866	0.457732
C	-0.504056	-4.098456	1.084407
C	0.649779	-4.800111	1.422314
C	-0.589614	-0.754165	-2.489896
C	1.223696	-2.490984	-2.592971
C	1.898664	-4.252590	1.140338
C	2.006749	-3.013134	0.515844
C	-1.594990	-1.721454	-2.620771
C	-2.871151	-1.369164	-3.053295
C	-3.172295	-0.040425	-3.348267
C	-2.182221	0.930143	-3.210800
C	-0.902408	0.575454	-2.788635
H	0.007444	-0.584543	-0.256162
H	1.513823	-0.364103	-2.403301
H	-1.288494	-2.282047	0.210707
H	-1.483649	-4.503687	1.317673
H	0.577123	-5.763408	1.915729
H	1.143368	-2.438756	-3.681653
H	2.240435	-2.762390	-2.331736
H	0.567213	-3.287346	-2.240164
H	2.800707	-4.787860	1.417036
H	2.977504	-2.581995	0.309672
H	-1.387431	-2.762979	-2.399560
H	-3.627920	-2.137414	-3.173978
H	-4.170351	0.231361	-3.677917
H	-2.397345	1.971569	-3.428890
H	-0.140931	1.342274	-2.696442
N	-2.737932	-0.004225	0.179000
C	-3.634620	-1.108249	0.629020
C	-3.117408	1.307228	0.600555
C	-2.777951	1.769372	1.876232
C	-3.156404	3.045358	2.284967
C	-3.870472	3.880011	1.427514
C	-5.099255	-0.882364	0.284203
C	-3.416644	-1.430753	2.103645
C	-5.897080	0.017963	1.000142
C	-7.222985	0.232511	0.638005
C	-7.777934	-0.452046	-0.441012
C	-6.998458	-1.356348	-1.155061
C	-5.670425	-1.565244	-0.791138
C	-4.203427	3.428011	0.152974
C	-3.835146	2.149739	-0.254356
H	-2.745337	-0.014272	-0.839342
H	-3.308041	-1.976254	0.041270
H	-2.186378	1.139430	2.533507
H	-2.875912	3.392891	3.274004
H	-4.158419	4.875501	1.748498
H	-3.726646	-0.602207	2.745978
H	-2.358381	-1.638407	2.292516
H	-4.007469	-2.306901	2.383307
H	-5.477205	0.568613	1.837169
H	-7.825147	0.938130	1.201368
H	-8.813406	-0.284350	-0.719277
H	-7.423814	-1.903785	-1.990362
H	-5.066148	-2.281113	-1.342113
H	-4.761758	4.067151	-0.523768
H	-4.119770	1.781455	-1.236148

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[B(C_6F_5)Ph_2-(PhNHMePh-PhNMePh)]-

B	-2.100413	0.124295	0.197213
N	-1.284818	1.135015	-0.732991
C	-3.339652	0.896602	3.898275
C	-3.275295	0.426332	2.583568
C	-2.181155	0.681190	1.748370
C	-1.325936	-1.388936	0.217287
C	-3.623265	-0.145899	-0.377644
C	-1.489955	-2.340169	-0.797440
C	-0.880983	-3.587861	-0.833252
C	-0.094303	-3.993697	0.230046
C	0.053459	-3.133903	1.300254
C	-0.540855	-1.873473	1.272085
C	-4.374454	-1.267764	0.017113
C	-5.673700	-1.495164	-0.424778
C	-6.279575	-0.599203	-1.304270
C	-5.563920	0.516114	-1.724176
C	-4.264023	0.730727	-1.263723
C	-1.148155	1.448847	2.314799
C	-1.198464	1.932245	3.615004
C	-2.302816	1.656487	4.422231
F	-2.281581	-2.107416	-1.866375
F	-1.053129	-4.397462	-1.887649
F	0.530279	-5.175670	0.208999
F	0.830623	-3.487328	2.326323
F	-0.276942	-1.146919	2.361764
C	-1.381987	2.524870	-0.547603
C	-0.398638	3.418950	-1.024136
C	-0.477324	4.793121	-0.819236
C	-1.537821	5.348266	-0.112294
C	-2.527601	4.490296	0.361419
C	-2.462620	3.120726	0.140718
C	-1.055107	0.650317	-2.115780
C	0.308941	0.023380	-2.420618
C	-1.357090	1.650487	-3.249446
C	1.518063	0.671664	-2.153982
C	2.739444	0.149529	-2.572386
C	2.776757	-1.056314	-3.267143
C	1.585474	-1.730761	-3.525318
C	0.367854	-1.193126	-3.112516

H	-4.211922	0.671749	4.507446
H	-4.118087	-0.141963	2.201211
H	-3.917919	-1.992886	0.690083
H	-6.213518	-2.377613	-0.090064
H	-7.291842	-0.772979	-1.658932
H	-6.015841	1.224401	-2.414389
H	-3.731471	1.614755	-1.603952
H	-0.274380	1.666736	1.709202
H	-0.378381	2.533677	4.000668
H	-2.351007	2.033112	5.440537
H	0.445157	3.034864	-1.581434
H	0.310652	5.429463	-1.215587
H	-1.595926	6.418280	0.059780
H	-3.378431	4.889898	0.906275
H	-3.260702	2.491978	0.513459
H	-1.788925	-0.142914	-2.263460
H	-1.409821	1.089620	-4.187275
H	-2.314670	2.151563	-3.088670
H	-0.587326	2.415355	-3.364779
H	1.520353	1.593643	-1.587128
H	3.655749	0.684884	-2.336550
H	3.725772	-1.476580	-3.585689
H	1.599706	-2.683513	-4.046968
H	-0.554532	-1.729292	-3.318758
N	1.833470	0.279925	1.012360
C	2.353344	1.634374	1.198632
C	2.573651	-0.896670	1.136314
C	3.330874	-1.199491	2.280875
C	4.032538	-2.396896	2.369461
C	3.968296	-3.342903	1.349824
C	3.519514	2.015845	0.290081
C	2.665512	1.968262	2.661292
C	4.719400	1.294460	0.273141
C	5.757373	1.666888	-0.576421
C	5.621183	2.769217	-1.418241
C	4.439373	3.504063	-1.397120
C	3.402537	3.130083	-0.545218
C	3.180855	-3.071411	0.233887
C	2.503586	-1.863913	0.119906
H	1.172686	0.241241	0.242598
H	1.513673	2.276394	0.902288
H	3.340873	-0.509763	3.115452
H	4.611681	-2.603074	3.265317
H	4.502809	-4.283385	1.434430
H	3.617443	1.535749	2.980140
H	1.861786	1.589873	3.299438
H	2.743661	3.052987	2.779572
H	4.837119	0.427341	0.914964
H	6.676546	1.088603	-0.583868
H	6.430554	3.052832	-2.084101
H	4.320396	4.366542	-2.046011
H	2.476694	3.702736	-0.530525
H	3.086308	-3.803417	-0.563617
H	1.883325	-1.668498	-0.751339

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$B(C_6F_5)_2Ph$-$(PhNHMePh)_2$

B	-1.66862	-0.24177	-0.32031
N	-0.71018	-1.44189	0.51875
C	-2.50363	-1.64357	-3.91759
C	-2.64931	-1.14768	-2.62113
C	-1.55043	-0.75578	-1.85370
C	-0.95735	1.22702	-0.04815
C	-3.22870	-0.04774	0.14265
C	-0.96402	1.81173	1.21744
C	-0.43582	3.05587	1.52736
C	0.03630	3.85862	0.50235
C	-0.05631	3.39207	-0.79736
C	-0.51479	2.10217	-1.04916
C	-3.94189	0.92080	-0.57531
C	-5.26123	1.26410	-0.31871
C	-5.94201	0.63544	0.71546
C	-5.28343	-0.32475	1.46298
C	-3.96011	-0.63260	1.16349
C	-0.28654	-0.89867	-2.44691
C	-0.12294	-1.38932	-3.73493
C	-1.24015	-1.76451	-4.48136
F	-5.91076	-0.94440	2.46250
F	-3.40371	-1.57793	1.94657
F	-1.54937	1.17866	2.25923
F	-0.41080	3.48006	2.79370
F	0.53852	5.06269	0.75695
F	0.28782	4.18899	-1.80785
F	-0.55301	1.78111	-2.34207
F	-3.34962	1.57373	-1.58277
F	-5.87711	2.19123	-1.04908
F	-7.20658	0.94978	0.97925
C	-0.59342	-1.55322	2.07076
C	-0.78856	-2.77237	-0.09233
C	0.38152	-3.37707	-0.53593
C	0.33309	-4.65296	-1.09088
C	-0.88430	-5.31701	-1.20154
C	0.83015	-1.23890	2.50459
C	-1.01973	-2.90584	2.64404
C	-2.05311	-4.69657	-0.76539
C	-2.01141	-3.42167	-0.21209
C	1.83857	-2.20834	2.40868
C	3.13366	-1.93295	2.83456
C	3.45169	-0.68018	3.35753
C	2.45305	0.28189	3.47605
C	1.15202	0.00471	3.05506
N	2.56038	-0.35515	-0.21822
C	3.59654	-1.32480	-0.67760
C	2.71054	1.00022	-0.63922
C	2.48140	1.37923	-1.96889
C	2.70185	2.69276	-2.36743
C	3.11173	3.65700	-1.44757
C	5.02290	-0.94464	-0.30196
C	3.47254	-1.64963	-2.16393
C	5.65871	0.18331	-0.83690
C	6.96171	0.50211	-0.46711

C	7.65979	-0.30421	0.42877
C	7.04895	-1.44140	0.94688
C	5.74202	-1.75321	0.58073
C	3.28578	3.29696	-0.11573
C	3.09745	1.97607	0.28285
H	0.21120	-1.07849	0.23191
H	-3.38251	-1.93523	-4.48466
H	-3.65093	-1.08025	-2.20352
H	0.59742	-0.61168	-1.87638
H	0.87256	-1.47603	-4.16380
H	-1.12269	-2.14697	-5.49048
H	-1.26054	-0.79585	2.46214
H	1.31890	-2.83054	-0.46954
H	1.24657	-5.11843	-1.44610
H	-0.92556	-6.30958	-1.63700
H	-0.92208	-2.82941	3.73021
H	-2.05066	-3.15282	2.40847
H	-0.38776	-3.72679	2.30248
H	-3.00687	-5.20397	-0.86294
H	-2.91831	-2.93089	0.12309
H	1.61330	-3.18971	2.00256
H	3.89623	-2.70138	2.76854
H	4.46671	-0.46392	3.67401
H	2.68001	1.25500	3.90040
H	0.38141	0.75719	3.17579
H	2.59866	-0.36187	0.79960
H	3.36124	-2.23975	-0.11809
H	2.11551	0.65427	-2.68690
H	2.51467	2.97266	-3.39886
H	3.25766	4.68440	-1.76251
H	3.78402	-0.80778	-2.78648
H	2.44064	-1.91612	-2.41545
H	4.12459	-2.49370	-2.40296
H	5.13722	0.82091	-1.54404
H	7.43513	1.38419	-0.88626
H	8.67673	-0.05250	0.71192
H	7.58866	-2.08875	1.63096
H	5.27470	-2.65235	0.97338
H	3.58132	4.04153	0.61685
H	3.27947	1.68262	1.31297

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[B(C_6F_5)$_2$Ph-(PhNHMePh-PhNMePh)]-

B	-1.53710	-0.33919	-0.38681
N	-0.72958	-1.30068	0.56541
C	-2.53078	-1.54469	-4.05912
C	-2.59394	-0.96462	-2.78942
C	-1.49680	-0.93554	-1.92220
C	-0.87665	1.20863	-0.31415
C	-3.14991	-0.10219	0.05097
C	-1.18133	2.10274	0.71457
C	-0.65986	3.38256	0.84324
C	0.17460	3.87757	-0.14299
C	0.45285	3.07303	-1.23157
C	-0.05675	1.77849	-1.29379
C	-3.88775	0.91541	-0.55894
C	-5.20892	1.21846	-0.26130
C	-5.87175	0.48636	0.71224
C	-5.19321	-0.53311	1.35418
C	-3.86873	-0.79967	1.01440
C	-0.31836	-1.52655	-2.41146
C	-0.23701	-2.11117	-3.66708
C	-1.35216	-2.12575	-4.50543
F	-5.81382	-1.25161	2.29804
F	-3.30992	-1.80618	1.71051
F	-2.03562	1.76552	1.70902
F	-0.95387	4.13031	1.91582
F	0.71930	5.09327	-0.03375
F	1.26775	3.51924	-2.18920
F	0.31527	1.11242	-2.38987
F	-3.32959	1.67454	-1.51792
F	-5.85117	2.20476	-0.89861
F	-7.14458	0.75809	1.01903
C	-0.76621	-2.69099	0.30531
C	0.33654	-3.51858	0.57821
C	0.33040	-4.88139	0.29816
C	-0.78048	-5.47398	-0.29173
C	-1.88453	-4.67424	-0.57782
C	-1.88454	-3.31881	-0.27476
N	2.49892	-0.14542	-0.97529
C	3.19896	-1.42209	-1.13561
C	3.12351	1.10675	-1.03702
C	3.83823	1.53538	-2.16733
C	4.43402	2.79193	-2.19114
C	4.29511	3.67086	-1.12005
C	4.31208	-1.68062	-0.12378
C	3.69953	-1.65863	-2.56305
C	5.39858	-0.80882	0.01930
C	6.39621	-1.06845	0.95435
C	6.33308	-2.20513	1.75856
C	5.26648	-3.08745	1.61362
C	4.26995	-2.82536	0.67580
C	3.53715	3.27526	-0.02105
C	2.96902	2.00826	0.02738
H	1.83665	-0.19473	-0.20600
H	-3.41351	-1.54504	-4.69369
H	-3.54602	-0.54803	-2.47512
H	0.56271	-1.51705	-1.77780
H	0.69533	-2.56713	-3.99171
H	-1.29956	-2.58658	-5.48813
H	1.22437	-3.07896	1.01541
H	1.21033	-5.47616	0.53088
H	-0.78601	-6.53359	-0.52726
H	-2.76635	-5.11027	-1.03863
H	-2.75796	-2.72490	-0.51297
H	2.42056	-2.17299	-0.94638
H	3.89491	0.89661	-3.03971
H	4.98496	3.09795	-3.07602
H	4.74613	4.65719	-1.15400
H	4.59737	-1.07276	-2.77595
H	2.91421	-1.39107	-3.27587
H	3.95843	-2.71398	-2.68778

H	5.45829	0.08449	-0.59433
H	7.22592	-0.37566	1.05821
H	7.11015	-2.40151	2.49090
H	5.20604	-3.97829	2.23141
H	3.43813	-3.51815	0.56144
H	3.38137	3.95372	0.81312
H	2.36870	1.71252	0.88318
C	-0.58163	-0.90017	1.98866
C	0.69048	-0.13020	2.36972
C	-0.70420	-2.04511	3.01215
C	1.96500	-0.68561	2.21678
C	3.10431	-0.06699	2.72384
C	2.99143	1.14472	3.40150
C	1.73417	1.72294	3.55584
C	0.59901	1.08753	3.05393
H	-1.41792	-0.22999	2.20734
H	-0.79821	-1.60002	4.00722
H	-1.57882	-2.66400	2.81402
H	0.18000	-2.68649	3.02051
H	2.08113	-1.62866	1.69605
H	4.07478	-0.53423	2.57790
H	3.87569	1.63901	3.79196
H	1.62920	2.67401	4.07015
H	-0.37570	1.54463	3.19600

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$B(C_6F_5)_3$-$(PhNHMePh)_2$

B	1.613725	-0.001725	0.128979
C	3.078629	3.019230	-2.043592
C	3.005217	1.902311	-1.213270
C	1.809709	1.263851	-0.895527
C	0.791572	-1.273811	-0.529189
C	3.060535	-0.622911	0.579012
C	0.619960	-2.446025	0.206016
C	-0.011350	-3.590873	-0.256298
C	-0.418159	-3.646812	-1.579108
C	-0.172026	-2.555025	-2.394102
C	0.384864	-1.397610	-1.861323
C	3.793219	-1.207244	-0.460828
C	5.016597	-1.834373	-0.296042
C	5.583564	-1.899022	0.970622
C	4.912504	-1.320559	2.032337
C	3.685591	-0.701728	1.810761
C	0.689039	1.859675	-1.463591
C	0.703209	2.971470	-2.282317
C	1.923970	3.560117	-2.583925
F	5.436131	-1.354099	3.257174
F	3.121446	-0.148706	2.901729
F	1.114434	-2.541946	1.460280
F	-0.196703	-4.631609	0.558410
F	-1.010557	-4.732971	-2.062104
F	-0.464279	-2.619267	-3.690891
F	0.559305	-0.413169	-2.747630
F	3.330337	-1.134907	-1.717290
F	5.655533	-2.363829	-1.336573
F	6.756595	-2.495706	1.154483
F	4.257131	3.583512	-2.303590
F	4.176845	1.508334	-0.696679
F	-0.523768	1.353791	-1.168537
F	-0.435026	3.475255	-2.763758
F	1.981701	4.631769	-3.367238
N	0.559515	0.652657	1.346405
C	0.321003	-0.028742	2.732755
C	0.669191	2.106007	1.490102
C	-0.464839	2.885229	1.296815
C	-0.372042	4.270561	1.416232
C	0.847343	4.862615	1.728605
C	-1.141387	-0.426729	2.875047
C	0.735125	0.827196	3.930639
C	1.978992	4.068880	1.915958
C	1.895834	2.686713	1.796663
C	-2.108353	0.514792	3.255202
C	-3.433928	0.138467	3.443966
C	-3.824914	-1.185364	3.247829
C	-2.870616	-2.130112	2.882607
C	-1.539463	-1.754747	2.698314
H	-0.332353	0.509248	0.848025
H	0.933260	-0.923228	2.717754
H	-1.397178	2.403540	1.013502
H	-1.252931	4.882315	1.251824
H	0.921667	5.941187	1.815578
H	0.572805	0.215552	4.821883
H	1.779729	1.119827	3.901420
H	0.132827	1.731372	4.025809
H	2.934077	4.528450	2.146369
H	2.774091	2.059285	1.919819
H	-1.829195	1.552107	3.411441
H	-4.165157	0.878008	3.750958
H	-4.862769	-1.471789	3.382109
H	-3.155768	-3.168055	2.741929
H	-0.806586	-2.508250	2.434799
N	-2.829288	0.277580	0.079551
C	-3.776772	1.422863	0.150094
C	-2.970411	-0.641065	-0.997462
C	-2.688711	-0.270779	-2.321189
C	-2.904659	-1.172168	-3.357107
C	-3.349341	-2.468304	-3.097896
C	-5.234598	1.010926	0.308604
C	-3.601078	2.418103	-0.995335
C	-5.908445	0.276106	-0.675342
C	-7.238464	-0.091552	-0.495078
C	-7.924440	0.279174	0.659290
C	-7.274057	1.032281	1.631428
C	-5.940689	1.391673	1.451679
C	-3.572125	-2.858128	-1.781879
C	-3.396064	-1.948612	-0.742227
H	-2.947666	-0.243973	0.945021
H	-3.497042	1.935226	1.080690
H	-2.286681	0.711858	-2.532101
H	-2.684355	-0.870390	-4.375931
H	-3.488589	-3.172085	-3.911191
H	-3.999677	2.020781	-1.931492

H	-2.546938	2.668772	-1.142788
H	-4.159721	3.328634	-0.763252
H	-5.395463	-0.012031	-1.587798
H	-7.743055	-0.666655	-1.264889
H	-8.962274	-0.008108	0.793665
H	-7.803285	1.344041	2.526488
H	-5.440688	1.995595	2.204943
H	-3.896983	-3.869919	-1.559965
H	-3.618859	-2.238086	0.281040

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[$B(C_6F_5)_3$-(PhNHMePh-PhNMePh)]-

B	1.564091	0.134700	0.055824
N	1.145902	0.474313	1.510054
C	1.530503	3.408044	-2.287042
C	1.938810	2.225812	-1.670258
C	1.115507	1.438444	-0.873330
C	0.811014	-1.272393	-0.491511
C	3.192526	-0.188129	-0.123557
C	1.236606	-2.532665	-0.060464
C	0.663842	-3.739191	-0.438335
C	-0.357399	-3.746536	-1.372396
C	-0.771325	-2.539055	-1.902963
C	-0.208834	-1.351459	-1.442859
C	3.664552	-0.675912	-1.341703
C	4.974853	-1.057661	-1.576332
C	5.902614	-0.955038	-0.548138
C	5.494665	-0.462564	0.677542
C	4.164508	-0.088464	0.862637
C	-0.177815	1.945241	-0.746008
C	-0.626006	3.115739	-1.328699
C	0.238217	3.863827	-2.114230
F	6.380433	-0.347944	1.674630
F	3.881868	0.388926	2.089367
F	2.272764	-2.668077	0.791590
F	1.105506	-4.890920	0.078235
F	-0.916696	-4.893458	-1.765509
F	-1.716452	-2.518590	-2.844002
F	-0.735827	-0.259007	-2.027067
F	2.827176	-0.755993	-2.388793
F	5.362622	-1.510672	-2.773966
F	7.174270	-1.316018	-0.746714
C	1.074703	1.812084	1.933069
C	-0.008404	2.277369	2.699159
C	-0.116553	3.614871	3.064974
C	0.842679	4.539737	2.659808
C	1.924611	4.096964	1.901881
C	2.049515	2.755303	1.560207
F	2.389831	4.114893	-3.029297
F	3.235903	1.932794	-1.859259
F	-1.100917	1.284951	-0.017154
F	-1.888371	3.533456	-1.144916
F	-0.172943	4.995605	-2.689787
C	1.223383	-0.568362	2.538496
C	0.021500	-1.505282	2.593794
C	1.505771	-0.052594	3.959589
C	-1.266578	-1.090212	2.256614
C	-2.350543	-1.955998	2.397594
C	-2.156132	-3.259031	2.850154
C	-0.869098	-3.691109	3.164953
C	0.205827	-2.816951	3.042790
H	-0.782988	1.571559	2.982747
H	-0.970544	3.941318	3.653731
H	0.748596	5.587062	2.928830
H	2.688425	4.800369	1.582172
H	2.905197	2.421101	0.981558
H	2.090007	-1.190381	2.296414
H	1.737855	-0.910241	4.597424
H	2.360149	0.627424	3.955528
H	0.648188	0.464530	4.394538
H	-1.412254	-0.092178	1.852262
H	-3.346108	-1.609468	2.132769
H	-3.000550	-3.935709	2.945372
H	-0.701749	-4.711220	3.498360
H	1.212964	-3.158829	3.271729
N	-3.698221	0.891089	-1.761582
C	-4.554333	1.826988	-0.993428
C	-4.046289	-0.484349	-1.663214
C	-5.020214	-1.023140	-2.510080
C	-5.373725	-2.365365	-2.411453
C	-4.745729	-3.193571	-1.483228
C	-4.586090	1.511426	0.496805
C	-5.945070	1.936357	-1.610419
C	-5.454744	0.553317	1.030819
C	-5.432123	0.248845	2.389185
C	-4.534297	0.893232	3.237194
C	-3.658025	1.840415	2.714950
C	-3.680810	2.142119	1.355130
C	-3.763507	-2.667424	-0.648566
C	-3.424718	-1.320503	-0.731813
H	-2.745970	1.000932	-1.420528
H	-4.065504	2.798080	-1.107493
H	-5.471377	-0.380356	-3.259462
H	-6.128085	-2.771800	-3.079020
H	-5.011105	-4.244226	-1.420655
H	-6.495993	0.994479	-1.551060
H	-5.855179	2.209895	-2.664857
H	-6.526440	2.701581	-1.088676
H	-6.145182	0.026852	0.377670
H	-6.109941	-0.502292	2.784112
H	-4.510143	0.650430	4.294933
H	-2.952224	2.347859	3.365746
H	-2.977220	2.864649	0.949866
H	-3.252831	-3.298444	0.074332
H	-2.663783	-0.902869	-0.076874

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[$SiEt_3$-$(PhNHMePh)_2$]$^+$

Si	-0.37318	-1.46311	1.28402
C	-0.71771	-0.69679	2.96676
C	1.47368	-1.74530	1.09583
C	-1.37527	-3.00200	0.88908

N	-0.87018	-0.02148	0.08971
C	-1.00349	-0.22350	-1.44577
C	-2.00719	0.76931	0.60030
C	-3.16337	0.13125	1.04086
C	-4.24174	0.89797	1.46898
C	-4.16884	2.28929	1.44664
C	0.23331	-0.93133	-1.96838
C	-2.31916	-0.84380	-1.86322
C	-3.01356	2.91467	0.98896
C	-1.92790	2.15508	0.55936
C	-2.44256	-2.20796	-2.13792
C	-3.43356	-0.01741	-2.04860
C	-3.66151	-2.74105	-2.54896
C	-4.76880	-1.91261	-2.70536
C	-4.65114	-0.54659	-2.46041
C	0.09370	-1.33129	4.10850
C	-1.59825	-3.86174	2.14719
C	1.88544	-3.12891	1.63390
N	2.17888	1.41235	-0.10483
C	3.21826	1.22744	-1.15230
C	1.52534	2.66589	-0.04141
C	1.02872	3.27738	-1.20094
C	0.32191	4.47381	-1.11156
C	0.08648	5.07141	0.12548
C	3.84384	-0.14111	-0.96746
C	4.26795	2.34128	-1.14567
C	4.54884	-0.44333	0.20191
C	5.09522	-1.70792	0.39507
C	4.94968	-2.68887	-0.58524
C	4.26760	-2.39250	-1.76128
C	3.72258	-1.12344	-1.95060
C	0.57752	4.46324	1.27906
C	1.29497	3.27393	1.19849
H	-1.78696	-0.74147	3.19600
H	-0.48012	0.37443	2.89916
H	1.81915	-1.64856	0.06368
H	1.99910	-0.96275	1.65783
H	-2.33747	-2.75516	0.43314
H	-0.83119	-3.58410	0.13467
H	-0.02903	0.58015	0.15204
H	-0.99465	0.81060	-1.81033
H	-3.23969	-0.95088	1.03320
H	-5.14371	0.40364	1.81216
H	-5.01329	2.88179	1.78106
H	1.13376	-0.40175	-1.65062
H	0.30576	-1.96550	-1.61969
H	0.19348	-0.94867	-3.05986
H	-2.94347	3.99678	0.96026
H	-1.03648	2.64475	0.18488
H	-1.58669	-2.86825	-2.04405
H	-3.34617	1.05019	-1.86160
H	-3.74050	-3.80215	-2.75961
H	-5.71628	-2.32760	-3.03219
H	-5.50429	0.10864	-2.59870
H	-0.12255	-0.83003	5.05449
H	1.17058	-1.25267	3.93403
H	-0.14663	-2.39013	4.23897
H	-2.17085	-4.75877	1.90229
H	-0.65391	-4.18817	2.59164
H	-2.15518	-3.31202	2.91192
H	2.96750	-3.25245	1.55272
H	1.61264	-3.26691	2.68408
H	1.41962	-3.93489	1.05880
H	2.58504	1.18816	0.80037
H	2.70500	1.22812	-2.12089
H	1.20297	2.82461	-2.17250
H	-0.04672	4.94095	-2.01891
H	-0.45884	6.00646	0.18749
H	4.78951	2.37341	-0.18428
H	3.80904	3.31750	-1.31806
H	5.00938	2.16039	-1.92697
H	4.68705	0.31591	0.96940
H	5.64379	-1.92645	1.30567
H	5.37935	-3.67402	-0.43712
H	4.16761	-3.14424	-2.53724
H	3.20056	-0.89334	-2.87624
H	0.41267	4.92077	2.24899
H	1.68883	2.81412	2.10194

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$SiEt_3$-(PhNHMePh-PhNMePh)

Si	-0.76758	-1.19782	1.21688
C	-0.47786	-0.14220	2.76863
C	0.80647	-2.17315	0.79926
C	-2.16788	-2.44085	1.54711
N	-1.16082	-0.03381	-0.07089
C	-1.56364	-0.34176	-1.46660
C	-1.68245	1.24147	0.33632
C	-2.80428	1.33639	1.16534
C	-3.30265	2.57877	1.54580
C	-2.70327	3.74517	1.07905
C	-0.87031	-1.57870	-2.02435
C	-3.08007	-0.41502	-1.62126
C	-1.60466	3.65856	0.22717
C	-1.09661	2.41697	-0.14330
C	-3.79292	-1.59375	-1.38903
C	-3.79305	0.73587	-1.96607
C	-5.18114	-1.62038	-1.49114
C	-5.87983	-0.46498	-1.83139
C	-5.18091	0.71468	-2.06989
C	0.54873	-0.71616	3.75383
C	-2.20373	-2.98360	2.98370
C	1.00975	-3.45392	1.62287
N	1.72053	1.04613	-1.41530
C	2.62840	0.27102	-2.28975
C	2.25496	1.87660	-0.39563
C	2.82492	3.11809	-0.70485
C	3.28588	3.95353	0.30758
C	3.15492	3.58841	1.64588
C	3.28280	-0.89804	-1.56934
C	3.66051	1.14669	-2.99279
C	4.15828	-0.69126	-0.49589

C	4.69218	-1.77219	0.19873
C	4.37649	-3.07680	-0.17844
C	3.53131	-3.29379	-1.26207
C	2.99053	-2.20894	-1.94939
C	2.56227	2.36948	1.96295
C	2.13058	1.51790	0.95181
H	-1.43549	0.01387	3.27950
H	-0.16105	0.85722	2.44920
H	0.79643	-2.45288	-0.25634
H	1.69093	-1.53063	0.90704
H	-3.12418	-1.95690	1.31459
H	-2.08134	-3.27697	0.83856
H	1.04530	0.40860	-0.99055
H	-1.22468	0.51083	-2.07277
H	-3.29521	0.42475	1.49675
H	-4.17051	2.63329	2.19547
H	-3.09279	4.71462	1.37237
H	0.21554	-1.45111	-2.01731
H	-1.10559	-2.48350	-1.45482
H	-1.19630	-1.73995	-3.05473
H	-1.12918	4.56107	-0.14397
H	-0.24382	2.34810	-0.81197
H	-3.26485	-2.50532	-1.12508
H	-3.25061	1.66253	-2.13759
H	-5.71680	-2.54693	-1.30936
H	-6.96193	-0.48554	-1.91247
H	-5.71539	1.62119	-2.33560
H	0.70654	-0.04016	4.59983
H	1.52136	-0.87569	3.27419
H	0.22615	-1.67872	4.16327
H	-3.03395	-3.68104	3.12981
H	-1.28235	-3.51352	3.24247
H	-2.32647	-2.17237	3.70821
H	1.92594	-3.96545	1.31214
H	1.09576	-3.24970	2.69389
H	0.17765	-4.15248	1.48610
H	1.97541	-0.15145	-3.06407
H	2.87586	3.43360	-1.74103
H	3.72790	4.91045	0.04772
H	3.50043	4.25231	2.43110
H	4.36948	1.57938	-2.28246
H	3.16930	1.95731	-3.53723
H	4.22537	0.53657	-3.70160
H	4.41353	0.32007	-0.19356
H	5.36061	-1.59607	1.03565
H	4.79395	-3.91814	0.36567
H	3.28752	-4.30595	-1.56991
H	2.32454	-2.38278	-2.79210
H	2.44162	2.06957	3.00002
H	1.69128	0.55648	1.19909

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$[SiPhH_2\text{-}(PhNHMePh)_2]^+$

Si	-2.11724	-1.91430	-1.06177
C	-2.76995	-0.38042	-1.84613
N	-0.93097	-1.57557	0.38813
C	-1.66208	-1.22778	1.68743
C	-0.01981	-2.73503	0.49031
C	-0.65791	-0.88633	2.78303
C	-0.33121	-3.83354	1.28523
C	0.54033	-4.92131	1.31283
C	1.70366	-4.91842	0.55081
C	-2.63733	-0.10040	1.43935
C	1.99313	-3.82504	-0.26144
C	1.12723	-2.73838	-0.30091
C	-2.18462	1.12421	0.93956
C	-3.98572	-0.25864	1.75530
C	-3.07301	2.17294	0.74577
C	-4.42063	2.01285	1.07024
C	-4.87557	0.80014	1.57770
C	-4.11406	-0.01039	-1.70576
C	-4.59102	1.14977	-2.30793
C	-3.72890	1.95596	-3.04667
C	-2.39090	1.59580	-3.20239
C	-1.91859	0.42727	-2.61583
N	1.28388	0.46705	0.18615
C	1.66829	0.81312	-1.22369
C	1.65279	1.39563	1.22128
C	0.98731	2.61473	1.38797
C	1.34513	3.46931	2.42688
C	2.34839	3.11420	3.32402
C	3.16513	0.70125	-1.43724
C	1.08775	2.14397	-1.68351
C	4.05033	1.64291	-0.90069
C	5.42297	1.48984	-1.06738
C	5.92898	0.40077	-1.77452
C	5.05656	-0.53695	-2.31764
C	3.68282	-0.38560	-2.14514
C	3.00127	1.89440	3.17213
C	2.66170	1.04554	2.12400
H	-1.22686	-2.66737	-1.96050
H	-3.13544	-2.75150	-0.40033
H	-0.32767	-0.73967	0.18508
H	-2.23450	-2.11989	1.95131
H	-0.11491	0.03048	2.53637
H	0.05741	-1.69390	2.95319
H	-1.20743	-0.70834	3.70960
H	-1.22763	-3.85840	1.89349
H	0.30139	-5.77344	1.93928
H	2.37729	-5.76720	0.58297
H	2.88940	-3.81310	-0.87219
H	1.33531	-1.90854	-0.96995
H	-1.13336	1.24610	0.69115
H	-4.34212	-1.20638	2.15152
H	-2.71816	3.11607	0.34220
H	-5.11400	2.83493	0.92681
H	-5.92175	0.67446	1.83556
H	-4.79007	-0.62002	-1.11253
H	-5.63387	1.42714	-2.19569
H	-4.10145	2.86243	-3.51238
H	-1.72331	2.21614	-3.79161
H	-0.87937	0.14130	-2.77083

H	1.80599	-0.38393	0.39822
H	1.19784	0.02806	-1.83379
H	0.19322	2.90339	0.70923
H	0.82492	4.41456	2.53971
H	2.61647	3.78111	4.13576
H	1.56764	2.98970	-1.18773
H	0.00997	2.18652	-1.49372
H	1.25723	2.24851	-2.75809
H	3.66926	2.49658	-0.34725
H	6.10035	2.22627	-0.64815
H	6.99976	0.28895	-1.90718
H	5.44295	-1.37960	-2.88145
H	3.00240	-1.11047	-2.58945
H	3.78605	1.60457	3.86266
H	3.19338	0.10605	1.99153

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$SiPhH_2$-(PhNHMePh-PhNMePh)

Si	-2.22609	-0.10217	2.11763
C	-2.91576	-1.30711	0.86722
N	-1.00915	0.96550	1.40665
C	-1.50688	2.18659	0.72007
C	0.26167	0.99675	2.03575
C	-0.46424	2.84792	-0.18701
C	0.81889	2.16014	2.58280
C	2.09091	2.13504	3.14924
C	2.82121	0.95075	3.21280
C	-2.72079	1.81154	-0.11927
C	2.25981	-0.22071	2.70760
C	0.99942	-0.19406	2.12369
C	-2.56587	0.98650	-1.24039
C	-3.99610	2.26020	0.21853
C	-3.66914	0.61585	-1.99792
C	-4.94267	1.06536	-1.64929
C	-5.10535	1.88941	-0.54138
C	-4.28904	-1.48800	0.68443
C	-4.76998	-2.35725	-0.29429
C	-3.88043	-3.05626	-1.10407
C	-2.50554	-2.88831	-0.93496
C	-2.03532	-2.01986	0.04237
N	1.06361	0.01092	-1.43312
C	1.33901	-1.41689	-1.71585
C	2.11029	0.96147	-1.60638
C	2.43879	1.41538	-2.88927
C	3.43765	2.36731	-3.06657
C	4.09921	2.91090	-1.96766
C	2.26884	-2.06528	-0.70003
C	1.82337	-1.64624	-3.14409
C	3.61130	-1.68283	-0.59083
C	4.44040	-2.27359	0.35762
C	3.94715	-3.26276	1.20713
C	2.61619	-3.65692	1.10282
C	1.78789	-3.06089	0.15345
C	3.75298	2.48837	-0.68711
C	2.77633	1.51411	-0.50576
H	-1.52995	-0.82354	3.20549
H	-3.35292	0.68049	2.68918
H	0.70773	0.07977	-0.47975
H	-1.83878	2.92384	1.47003
H	-0.16882	2.17137	-0.99159
H	0.43798	3.15424	0.34220
H	-0.91631	3.73358	-0.64130
H	0.25712	3.08828	2.56111
H	2.50792	3.05225	3.55378
H	3.81298	0.94074	3.65181
H	2.80875	-1.15725	2.73322
H	0.58396	-1.10880	1.70857
H	-1.57764	0.61076	-1.49964
H	-4.12377	2.89619	1.09098
H	-3.53909	-0.04096	-2.85220
H	-5.80479	0.76793	-2.23814
H	-6.09303	2.24408	-0.26403
H	-4.99407	-0.92474	1.29131
H	-5.83994	-2.47949	-0.43191
H	-4.25517	-3.72912	-1.86915
H	-1.80762	-3.42999	-1.56778
H	-0.96251	-1.86791	0.15240
H	0.36238	-1.90822	-1.62245
H	1.88644	1.03339	-3.74085
H	3.68204	2.70405	-4.06926
H	4.86737	3.66403	-2.10891
H	2.81051	-1.20787	-3.31008
H	1.12126	-1.20951	-3.85907
H	1.89710	-2.72038	-3.33066
H	4.00995	-0.91657	-1.24894
H	5.47821	-1.96394	0.43051
H	4.59791	-3.72565	1.94225
H	2.22245	-4.43082	1.75420
H	0.75049	-3.38002	0.07037
H	4.25048	2.90650	0.18288
H	2.53020	1.16907	0.49361

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Benzyl-2-methyl-2-propanamine-BEt_3

N	0.565575	-0.640415	-0.150259
C	-0.531018	-0.425427	-1.145825
C	1.358904	-1.901362	-0.474950
C	0.447363	-3.120782	-0.270692
C	1.872818	-1.858242	-1.918540
C	2.543439	-2.053582	0.479444
C	-1.900351	-0.210241	-0.540682
C	-2.352813	-0.963203	0.545436
C	-3.635096	-0.776618	1.055014
C	-4.488856	0.156801	0.476139
C	-4.052606	0.900084	-0.617340
C	-2.768724	0.717585	-1.119873
B	1.355896	0.858547	0.322787
C	1.851058	0.636376	1.872788
C	2.559154	1.218117	-0.707805
C	0.193000	2.028509	0.339773
C	-0.051320	2.892375	-0.907833
C	3.336306	2.455920	-0.231485

C	0.803957	0.071413	2.844243
H	0.107438	-0.846029	0.739747
H	-0.597315	-1.296153	-1.800403
H	-0.249645	0.419187	-1.773218
H	0.980223	-4.026937	-0.571146
H	0.181385	-3.229596	0.787234
H	-0.476316	-3.071892	-0.854237
H	2.600447	-2.663266	-2.051933
H	2.367061	-0.910935	-2.135150
H	1.080337	-2.015944	-2.653810
H	2.220212	-2.042653	1.523148
H	3.015237	-3.020784	0.283715
H	3.286196	-1.270711	0.337118
H	-1.711274	-1.710101	1.007713
H	-3.965960	-1.365436	1.904312
H	-5.487020	0.304509	0.874679
H	-4.709812	1.631918	-1.075637
H	-2.429679	1.311792	-1.963263
H	2.110571	1.642189	2.229055
H	2.781377	0.064884	1.975699
H	2.170301	1.414266	-1.720515
H	3.293317	0.410561	-0.826101
H	0.512989	2.725105	1.128200
H	-0.772929	1.656988	0.706755
H	-0.820312	3.651872	-0.727950
H	0.860282	3.418107	-1.208664
H	-0.374342	2.325989	-1.787814
H	4.071936	2.795795	-0.967790
H	3.876504	2.236732	0.695045
H	2.669626	3.297660	-0.017155
H	-0.155100	0.594135	2.744940
H	1.111186	0.151436	3.891681
H	0.603276	-0.998863	2.676743

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[Benzyl-2-methyl-2-propanamide-BEt_3]-

N	-0.526397	-0.750738	-0.579733
C	-0.363424	-1.771923	0.430917
C	-1.468344	-1.171500	-1.628382
C	-0.884655	-2.379137	-2.393870
C	-2.873120	-1.554003	-1.093382
C	-1.692149	-0.074239	-2.674322
C	1.050083	-2.317224	0.605643
C	2.049652	-2.066098	-0.333772
C	3.318334	-2.622308	-0.188508
C	3.610928	-3.440145	0.900704
C	2.621341	-3.693134	1.848661
C	1.355512	-3.134636	1.698193
B	-0.411200	0.743942	-0.007230
C	0.177518	1.810351	-1.144282
C	-1.868529	1.285527	0.573213
C	0.719943	0.818110	1.228444
C	0.390666	0.363805	2.663641
C	-1.826225	2.659459	1.254529
C	1.448484	1.344543	-1.862193
H	-0.724607	-1.442649	1.417372
H	-0.972558	-2.659165	0.209289
H	-1.587120	-2.742118	-3.154878
H	0.043960	-2.078986	-2.890639
H	-0.648849	-3.216605	-1.729847
H	-3.545142	-1.817122	-1.920194
H	-3.304276	-0.710777	-0.548578
H	-2.840305	-2.413151	-0.416309
H	-0.745078	0.256245	-3.105563
H	-2.319444	-0.472700	-3.480999
H	-2.196222	0.791886	-2.243904
H	1.800306	-1.404476	-1.157743
H	4.086868	-2.410650	-0.927542
H	4.602154	-3.870152	1.015475
H	2.838649	-4.322270	2.708119
H	0.583850	-3.328430	2.442134
H	0.422042	2.746189	-0.617632
H	-0.563607	2.112227	-1.898044
H	-2.287542	0.554062	1.287091
H	-2.613573	1.345673	-0.236977
H	0.970109	1.887646	1.297654
H	1.665404	0.339563	0.933751
H	0.998178	0.889536	3.413507
H	-0.661123	0.548194	2.918671
H	0.576723	-0.704688	2.820040
H	-2.804323	2.992732	1.630251
H	-1.468913	3.426420	0.557052
H	-1.133927	2.661914	2.104621
H	2.237742	1.109054	-1.137889
H	1.857787	2.086375	-2.563169
H	1.265499	0.422135	-2.427707

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Benzyl-2-methyl-2-propanamine-BPh_3

N	-0.40460	-0.91445	-0.15888
C	-0.18892	-2.37779	-0.54423
C	0.48976	-2.42983	-1.91940
C	0.66254	-3.10027	0.49359
C	-1.54429	-3.08609	-0.67222
C	-1.38438	-0.71813	0.97555
C	-2.84543	-0.60047	0.59415
C	-3.28774	0.40618	-0.26842
C	-4.64132	0.53274	-0.56891
C	-5.57369	-0.32758	0.00346
C	-5.14553	-1.31367	0.88821
C	-3.79158	-1.44574	1.17888
B	0.88452	0.30174	-0.02077
C	1.39532	0.48031	1.51299
C	2.20779	-0.06109	-0.91466
C	3.22052	-0.86678	-0.35877
C	4.35645	-1.24236	-1.06836
C	4.54723	-0.78607	-2.37060
C	3.60580	0.07341	-2.92459
C	2.46668	0.43124	-2.20326
C	1.25205	-0.40061	2.59221
C	1.84762	-0.16745	3.83371
C	2.61709	0.97003	4.03737

C	2.79441	1.86234	2.98088
C	2.20045	1.61171	1.75014
C	-1.66330	3.66904	-1.53282
C	-1.22822	3.65873	-0.21136
C	-0.40138	2.63468	0.25165
C	0.01930	1.58065	-0.57332
C	-0.46025	1.61330	-1.89800
C	-1.27406	2.63506	-2.38110
H	-0.88449	-0.53168	-0.97665
H	0.41307	-3.45093	-2.30269
H	-0.01753	-1.77158	-2.63463
H	1.54122	-2.15471	-1.88365
H	0.86657	-4.11187	0.13095
H	0.14609	-3.19764	1.45322
H	1.61493	-2.59441	0.64919
H	-2.21253	-2.56270	-1.36387
H	-1.37186	-4.09305	-1.06093
H	-2.05732	-3.18619	0.28521
H	-1.25432	-1.54275	1.67783
H	-1.08164	0.19321	1.49327
H	-2.58041	1.11068	-0.69392
H	-4.96457	1.31936	-1.24332
H	-6.62847	-0.22454	-0.22961
H	-5.86435	-1.98182	1.35140
H	-3.46427	-2.21676	1.87276
H	3.12903	-1.19149	0.67453
H	5.10219	-1.87654	-0.59785
H	5.43164	-1.07215	-2.93157
H	3.75823	0.47694	-3.92148
H	1.77944	1.12969	-2.66541
H	0.67341	-1.31128	2.47851
H	1.70775	-0.88243	4.63939
H	3.08006	1.15752	5.00109
H	3.40384	2.75115	3.11544
H	2.37235	2.30974	0.93292
H	-2.30298	4.46722	-1.89621
H	-1.53712	4.44836	0.46718
H	-0.08314	2.65280	1.29037
H	-0.20971	0.80054	-2.57947
H	-1.61306	2.61695	-3.41270

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[Benzyl-2-methyl-2-propanamide-BPh_3]-

N	-0.39776	-0.77422	0.49174
C	-0.16170	-1.83727	1.50627
C	0.76481	-1.35616	2.62974
C	-1.48926	-2.23438	2.18299
C	0.47172	-3.13891	0.94375
C	-1.39375	-1.18183	-0.48232
C	-2.84808	-0.80689	-0.19681
C	-3.86827	-1.42443	-0.92634
C	-5.20366	-1.08418	-0.73342
C	-5.54706	-0.11280	0.20447
C	-4.54056	0.50697	0.94065
C	-3.20642	0.16190	0.74019
B	0.80581	0.11420	-0.05252
C	0.30824	1.06278	-1.31714
C	1.27118	1.27402	1.02318
C	0.42316	1.74547	2.03682
C	0.75723	2.82006	2.85844
C	1.97198	3.47958	2.68846
C	2.82774	3.05731	1.67379
C	2.47228	1.98487	0.85842
C	1.03869	1.23341	-2.50217
C	0.63803	2.11617	-3.50802
C	-0.52346	2.86544	-3.36346
C	-1.26608	2.73286	-2.19000
C	-0.84452	1.86039	-1.19349
C	3.96783	-2.80622	-1.35878
C	4.21633	-1.97699	-0.27019
C	3.27299	-1.02241	0.11645
C	2.04793	-0.85835	-0.54655
C	1.84177	-1.70472	-1.65349
C	2.76949	-2.65882	-2.05751
H	0.95292	-2.19388	3.31169
H	1.72464	-1.01078	2.24413
H	0.31559	-0.54204	3.20170
H	-1.29129	-2.95407	2.98547
H	-2.19206	-2.70036	1.48515
H	-1.97740	-1.35715	2.61708
H	1.53084	-3.00624	0.71763
H	0.38093	-3.93945	1.68825
H	-0.02256	-3.48353	0.03087
H	-1.16180	-0.72928	-1.45190
H	-1.38807	-2.26904	-0.66981
H	-3.60418	-2.18640	-1.65776
H	-5.97829	-1.57988	-1.31250
H	-6.58791	0.15533	0.36103
H	-4.79551	1.26429	1.67706
H	-2.41182	0.62662	1.31556
H	-0.52869	1.23868	2.18088
H	0.06666	3.14575	3.63350
H	2.24202	4.31621	3.32765
H	3.77227	3.57184	1.51114
H	3.14206	1.69653	0.04978
H	1.95251	0.66283	-2.64710
H	1.23911	2.21431	-4.40946
H	-0.84317	3.54872	-4.14605
H	-2.17202	3.31768	-2.04951
H	-1.42441	1.79485	-0.27637
H	4.69624	-3.55346	-1.66273
H	5.14643	-2.07461	0.28531
H	3.49415	-0.39575	0.97822
H	0.90816	-1.61511	-2.20793
H	2.55855	-3.29528	-2.91392

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Benzyl-2-methyl-2-propanamine-$B(C_6F_5)Ph_2$

N	0.16883	-1.41350	-0.23025
C	0.76106	-2.71155	-0.79875
C	1.89007	-3.23352	0.08134
C	-0.34224	-3.77477	-0.90500

C	1.26499	-2.43643	-2.22298
C	-0.74397	-1.63401	0.94043
C	-2.20647	-1.89768	0.63845
C	-2.87825	-1.41868	-0.48713
C	-4.24144	-1.65783	-0.65291
C	-4.95452	-2.37032	0.30446
C	-4.29339	-2.85112	1.43175
C	-2.93248	-2.61860	1.59153
H	-0.42394	-1.10571	-1.00074
H	2.35698	-4.08232	-0.42635
H	2.65107	-2.47235	0.25199
H	1.52582	-3.59198	1.04847
H	0.09667	-4.67347	-1.34569
H	-1.15918	-3.44394	-1.55340
H	-0.76625	-4.05475	0.06170
H	0.53059	-1.86203	-2.79801
H	2.20927	-1.89731	-2.24216
H	1.40580	-3.39647	-2.72685
H	-0.34997	-2.47214	1.51670
H	-0.66504	-0.75296	1.58236
H	-2.36257	-0.86212	-1.26263
H	-4.74362	-1.27889	-1.53700
H	-6.01571	-2.55259	0.17257
H	-4.83572	-3.41316	2.18504
H	-2.42157	-3.00064	2.47210
B	1.07424	0.03865	0.03694
C	1.84504	0.07088	1.47160
C	2.19981	0.29561	-1.12431
C	3.50259	-0.20676	-0.93274
C	4.50844	-0.06639	-1.88249
C	4.25756	0.62387	-3.06626
C	3.00265	1.18706	-3.26133
C	2.00102	1.02773	-2.30337
C	1.90502	-0.90601	2.46960
C	2.66682	-0.74581	3.63109
C	3.39705	0.41503	3.83337
C	3.36357	1.41125	2.85668
C	2.61120	1.23086	1.70640
C	-2.34505	3.00667	-0.31781
C	-1.60949	2.93481	0.85322
C	-0.57441	2.00989	0.97639
C	-0.18243	1.13857	-0.04538
C	-0.98368	1.24938	-1.18286
C	-2.03653	2.13500	-1.34994
F	-3.34533	3.87262	-0.43915
F	-1.91448	3.73686	1.87083
F	0.00052	1.98666	2.18136
F	-0.80737	0.38737	-2.22360
F	-2.75584	2.13272	-2.47167
H	3.74510	-0.70774	0.00024
H	5.49298	-0.48285	-1.69126
H	5.03734	0.74147	-3.81230
H	2.79705	1.76026	-4.16045
H	1.04813	1.50238	-2.50094
H	1.36232	-1.83771	2.36318
H	2.68378	-1.53821	4.37364
H	3.98888	0.54520	4.73391
H	3.93162	2.32664	2.99225
H	2.61447	2.01569	0.95239

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[Benzyl-2-methyl-2-propanamide-B(C_6F_5)Ph_2]-

N	0.83148	-0.47340	-0.77215
C	0.40469	-0.95562	-2.11105
C	1.62111	-1.46170	-2.91154
C	-0.62997	-2.11521	-2.05717
C	-0.22644	0.16060	-2.95422
C	1.60685	-1.47317	-0.05869
C	3.12327	-1.43682	-0.23367
C	3.87491	-2.56400	0.11173
C	5.26321	-2.56477	0.01768
C	5.93238	-1.42819	-0.43084
C	5.19547	-0.29989	-0.78121
C	3.80617	-0.30660	-0.68314
B	-0.07566	0.49681	0.06639
C	0.01362	2.06621	-0.42674
C	-1.65908	-0.08718	0.10152
C	-2.79106	0.43943	-0.51416
C	-4.04414	-0.17272	-0.50615
C	-4.21479	-1.37748	0.15120
C	-3.12164	-1.95602	0.77945
C	-1.89509	-1.31023	0.73320
C	-0.82278	3.04814	0.13056
C	-0.66824	4.40276	-0.13770
C	0.35988	4.83799	-0.97462
C	1.22327	3.89599	-1.52164
C	1.04768	2.53948	-1.24284
C	1.43241	1.13754	4.25773
C	0.10343	0.78792	4.05199
C	-0.37031	0.54672	2.76105
C	0.44811	0.64879	1.62831
C	1.77868	1.03486	1.87231
C	2.27250	1.26125	3.15163
F	-2.74314	1.58106	-1.22344
F	-5.08707	0.39374	-1.12802
F	-5.40982	-1.97940	0.17432
F	-3.26456	-3.13251	1.40457
F	-0.88061	-1.97502	1.31410
H	1.30688	-1.71909	-3.92922
H	2.38964	-0.68587	-2.97044
H	2.07542	-2.35293	-2.46790
H	-0.62431	-2.66978	-3.00273
H	-1.64352	-1.73658	-1.90725
H	-0.41508	-2.82390	-1.25203
H	0.50866	0.91907	-3.23053
H	-0.62139	-0.28187	-3.87638
H	-1.04679	0.66385	-2.44196
H	1.42324	-1.37719	1.01401
H	1.29008	-2.50104	-0.30128
H	3.35577	-3.45556	0.45897
H	5.82399	-3.45473	0.29057
H	7.01568	-1.42385	-0.50896

H	5.70487	0.59252	-1.13440
H	3.22192	0.56365	-0.96449
H	-1.61600	2.73468	0.80873
H	-1.34491	5.12561	0.31194
H	0.48825	5.89615	-1.18677
H	2.03898	4.21529	-2.16653
H	1.73191	1.81433	-1.67607
H	1.80831	1.31902	5.26111
H	-0.57254	0.69651	4.89899
H	-1.41804	0.27979	2.64388
H	2.44562	1.16788	1.02411
H	3.31342	1.54449	3.28631

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Benzyl-2-methyl-2-propanamine-B(C_6F_5)$_2$Ph

N	-0.13028	-0.95547	-1.58505
C	-1.17291	-1.68126	-2.47224
C	-1.91329	-2.78441	-1.71704
C	-0.40981	-2.35495	-3.62326
C	-2.21166	-0.69445	-3.02218
C	0.39462	0.24946	-2.35079
C	1.85871	0.57554	-2.18627
C	2.83105	-0.32538	-2.62345
C	4.18272	-0.03240	-2.47715
C	4.57392	1.18560	-1.92638
C	3.60924	2.11043	-1.53364
C	2.25748	1.80605	-1.66075
H	0.65832	-1.60644	-1.52061
H	-2.65799	-3.20077	-2.40117
H	-2.42954	-2.42048	-0.83321
H	-1.25044	-3.59544	-1.41789
H	-1.11803	-2.92762	-4.22704
H	0.09622	-1.65623	-4.29346
H	0.33149	-3.06124	-3.23165
H	-2.76909	-0.20765	-2.22066
H	-1.78523	0.07403	-3.66842
H	-2.92304	-1.26411	-3.62501
H	0.23075	0.05449	-3.40885
H	-0.22070	1.10128	-2.07974
H	2.53070	-1.27786	-3.05738
H	4.92987	-0.75240	-2.79361
H	5.62789	1.41322	-1.80660
H	3.90867	3.06428	-1.11154
H	1.50582	2.51308	-1.32692
B	-0.44654	-0.63395	0.05991
C	0.92572	0.04730	0.68022
C	-1.78257	0.33532	0.11268
C	-1.74333	1.70385	-0.16968
C	-2.84560	2.54570	-0.19279
C	-4.09916	2.03116	0.09890
C	-4.20766	0.68652	0.40837
C	-3.07138	-0.11870	0.41458
C	0.96692	1.11280	1.57626
C	2.14352	1.60281	2.13546
C	3.35189	0.98819	1.85102
C	3.35964	-0.12849	1.02798
C	2.16124	-0.57630	0.50010
C	-0.48971	-4.08055	2.88284
C	0.07062	-4.25377	1.62310
C	0.04889	-3.21155	0.69766
C	-0.54687	-1.97584	0.97843
C	-1.07424	-1.82297	2.27169
C	-1.05651	-2.85010	3.20706
F	-0.57539	2.31517	-0.45001
F	-2.70626	3.83717	-0.48448
F	-5.17224	2.81300	0.08352
F	-5.39817	0.16658	0.69885
F	-3.31913	-1.39975	0.72242
F	-0.15471	1.72836	1.97969
F	2.11120	2.64813	2.96148
F	4.48501	1.44973	2.37300
F	4.50486	-0.75210	0.75441
F	2.24784	-1.68436	-0.27190
H	-0.47478	-4.88832	3.60745
H	0.53534	-5.19854	1.35756
H	0.52865	-3.38727	-0.26263
H	-1.50288	-0.86391	2.55778
H	-1.48321	-2.68898	4.19231

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[Benzyl-2-methyl-2-propanamide-B(C_6F_5)$_2$Ph]-

N	-0.17604	-1.32068	-1.07705
C	0.30676	-1.73947	-2.40803
C	1.28302	-0.71776	-3.00833
C	0.98597	-3.12814	-2.38428
C	-0.85546	-1.83331	-3.42380
C	-1.30050	-2.09476	-0.57859
C	-2.71455	-1.52730	-0.73727
C	-3.74562	-2.10820	0.00862
C	-5.04655	-1.62078	-0.05644
C	-5.34307	-0.53087	-0.87284
C	-4.32518	0.05692	-1.61836
C	-3.02531	-0.43980	-1.55095
B	0.45471	-0.45716	0.07258
C	0.90339	-1.32997	1.40262
C	1.89258	0.37374	-0.18388
C	3.06319	-0.34438	-0.44282
C	4.33828	0.19420	-0.51813
C	4.51919	1.54492	-0.26775
C	3.41157	2.30446	0.05476
C	2.14919	1.71458	0.11029
C	1.17898	-0.68000	2.61583
C	1.65127	-1.35966	3.73265
C	1.87350	-2.73522	3.66868
C	1.61891	-3.40619	2.47735
C	1.14520	-2.70715	1.36668
C	-3.11448	2.22588	0.73180
C	-2.19594	2.47497	-0.27905
C	-1.08288	1.66119	-0.39340
C	-0.77909	0.60677	0.46555
C	-1.74153	0.39239	1.44539
C	-2.88969	1.17012	1.59342

F	-1.66615	-0.65146	2.28921
F	-3.78369	0.89099	2.55006
F	-4.21380	2.97980	0.84606
F	-2.42946	3.46239	-1.15625
F	-0.29387	1.90174	-1.45931
F	3.00354	-1.66860	-0.66339
F	5.39325	-0.57580	-0.81360
F	5.73664	2.09556	-0.32723
F	3.56128	3.60535	0.33587
F	1.18905	2.56112	0.51853
H	1.33611	-0.86743	-4.09235
H	0.93026	0.29781	-2.81132
H	2.29319	-0.82987	-2.62083
H	1.36285	-3.38817	-3.38088
H	0.27732	-3.91101	-2.09119
H	1.82085	-3.13697	-1.68571
H	-1.23111	-0.83960	-3.68067
H	-0.49068	-2.29978	-4.34556
H	-1.69462	-2.43027	-3.05772
H	-1.31185	-3.10301	-1.02047
H	-1.17880	-2.26928	0.49728
H	-3.51159	-2.94042	0.66982
H	-5.82708	-2.07968	0.54388
H	-6.35339	-0.13528	-0.91476
H	-4.53522	0.92424	-2.23886
H	-2.22021	0.04450	-2.09227
H	1.01311	0.39613	2.68028
H	1.84778	-0.81976	4.65566
H	2.24282	-3.27407	4.53706
H	1.79276	-4.47748	2.40955
H	0.95840	-3.24300	0.43773

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Benzyl-2-methyl-2-propanamine-B(C_6F_5)$_3$

N	0.199544	-0.423542	1.771280
C	-0.746985	-0.275488	2.988326
C	-1.491723	1.061833	2.972616
C	0.123056	-0.282841	4.253510
C	-1.784073	-1.410154	3.044403
C	0.906285	-1.769312	1.798624
C	2.415340	-1.713472	1.741408
C	3.171120	-0.981741	2.660009
C	4.559648	-0.969372	2.582154
C	5.211471	-1.699945	1.592139
C	4.468233	-2.447343	0.683889
C	3.078570	-2.453395	0.761104
H	0.933303	0.270626	1.937773
H	-2.203780	1.043193	3.802783
H	-2.056291	1.227858	2.058939
H	-0.817747	1.903266	3.131884
H	-0.522341	-0.118352	5.119585
H	0.659040	-1.220789	4.417977
H	0.845545	0.539512	4.223624
H	-2.656861	-1.185868	2.431149
H	-1.393419	-2.381621	2.734755
H	-2.123325	-1.506716	4.079322
H	0.612719	-2.280347	2.714702
H	0.535387	-2.358366	0.967426
H	2.680458	-0.401012	3.435456
H	5.132952	-0.385523	3.294508
H	6.294195	-1.683432	1.527176
H	4.967370	-3.015134	-0.094528
H	2.496521	-3.015047	0.033674
B	-0.365771	0.016155	0.243374
C	0.731990	-0.478067	-0.879980
C	-1.864553	-0.629976	0.040358
C	-2.066132	-2.000209	-0.133347
C	-3.306012	-2.610952	-0.242363
C	-4.453394	-1.833954	-0.193491
C	-4.321845	-0.463262	-0.047603
C	-3.053933	0.100764	0.052685
C	0.460784	-1.148845	-2.073138
C	1.438431	-1.446798	-3.018606
C	2.747690	-1.039901	-2.813939
C	3.059553	-0.319390	-1.670784
C	2.051386	-0.041169	-0.762586
C	-0.070642	4.403581	-0.644094
C	0.507262	3.929095	0.520889
C	0.395284	2.579786	0.837392
C	-0.299690	1.653379	0.070524
C	-0.828558	2.181425	-1.108937
C	-0.746694	3.515943	-1.471508
F	-1.460131	1.364561	-1.963545
F	-1.292883	3.949982	-2.604464
F	0.025629	5.688024	-0.970267
F	1.178267	4.755677	1.321371
F	1.032334	2.213439	1.978962
F	-1.021017	-2.845784	-0.202893
F	-3.400241	-3.930202	-0.392847
F	-5.653192	-2.393025	-0.291043
F	-5.404994	0.308684	-0.009587
F	-3.057860	1.435336	0.202380
F	-0.776245	-1.534849	-2.399137
F	1.118684	-2.106890	-4.129519
F	3.689883	-1.329755	-3.704986
F	4.310562	0.074802	-1.445842
F	2.410880	0.682273	0.314757

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[Benzyl-2-methyl-2-propanamide-B(C_6F_5)$_3$]-

N	0.44716	0.07691	1.77504
C	0.12275	-0.46259	3.11434
C	-0.71521	0.50253	3.98222
C	-0.62352	-1.80131	3.03024
C	1.41661	-0.76765	3.90199
C	1.33515	1.22835	1.79194
C	2.82159	1.02669	1.48405
C	3.57715	2.15163	1.13610
C	4.92635	2.04550	0.81624
C	5.55126	0.80006	0.83410
C	4.81026	-0.32702	1.17708
C	3.46001	-0.21172	1.50088

B	-0.21623	-0.09201	0.38188
C	-0.99834	1.28494	-0.19933
C	-1.47651	-1.16923	0.17364
C	-1.58130	-2.17270	-0.78991
C	-2.73623	-2.92416	-1.00566
C	-3.88075	-2.66535	-0.27582
C	-3.85279	-1.64288	0.65990
C	-2.68153	-0.92336	0.83499
C	-1.35980	1.34506	-1.54495
C	-2.09642	2.37200	-2.11456
C	-2.52666	3.42004	-1.31336
C	-2.20971	3.40731	0.03306
C	-1.47110	2.34927	0.55841
C	3.53567	-1.11583	-1.88728
C	3.00520	0.15507	-2.00100
C	1.79642	0.45197	-1.37597
C	1.07021	-0.45585	-0.61679
C	1.67179	-1.70693	-0.51204
C	2.85715	-2.06194	-1.13216
F	1.12783	-2.64574	0.28649
F	3.38659	-3.28265	-0.96906
F	4.69969	-1.42389	-2.46901
F	3.66163	1.09072	-2.69679
F	1.39960	1.73287	-1.50122
F	-2.40258	2.36543	-3.41785
F	-0.99198	0.35560	-2.37781
F	-3.23914	4.42448	-1.83575
F	-2.62446	4.40829	0.82057
F	-1.23177	2.42981	1.87781
F	-0.57491	-2.48628	-1.61532
F	-2.75085	-3.88549	-1.93610
F	-4.99404	-3.37749	-0.47376
F	-4.95153	-1.35508	1.36758
F	-2.75346	0.07340	1.73514
H	-0.92243	0.03886	4.95396
H	-0.18409	1.44036	4.17357
H	-1.65970	0.74148	3.49932
H	-0.53179	-2.31787	3.99185
H	-0.19013	-2.43324	2.25157
H	-1.68730	-1.67058	2.83966
H	2.11053	0.07682	3.92179
H	1.16084	-1.01451	4.93809
H	1.93666	-1.62835	3.47288
H	0.99355	1.97295	1.06177
H	1.27285	1.74887	2.75764
H	3.08640	3.12209	1.09329
H	5.48699	2.93240	0.53506
H	6.59995	0.70814	0.56840
H	5.27632	-1.30885	1.16961
H	2.87035	-1.09422	1.72068

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[Benzyl-2-methyl-2-propanamine-$SiEt_3$]$^+$

N	0.10434	0.68649	0.01176
C	0.13885	2.19339	0.37107
C	-1.28245	2.60486	0.76304
C	1.06933	2.37240	1.56889
C	0.64034	3.03274	-0.80134
C	-0.85003	0.37725	-1.12753
C	-2.17034	-0.18124	-0.64826
C	-2.23951	-1.15254	0.35459
C	-3.47090	-1.66014	0.76110
C	-4.64283	-1.20984	0.16097
C	-4.58084	-0.24760	-0.84384
C	-3.35138	0.26725	-1.24198
Si	1.73486	-0.34618	-0.08364
C	1.22604	-1.96363	-0.90485
C	2.21941	-0.69048	1.69487
C	3.00879	0.56996	-1.10240
C	2.10939	-3.14709	-0.46591
C	4.20088	-0.35151	-1.42676
C	1.08711	-1.27555	2.55399
H	-0.34260	0.27258	0.84042
H	-1.26752	3.64708	1.08976
H	-1.98748	2.52617	-0.06732
H	-1.66168	1.99735	1.59196
H	0.99434	3.40499	1.91636
H	2.11479	2.19197	1.30696
H	0.78975	1.72294	2.40459
H	-0.02130	3.00274	-1.66908
H	0.67827	4.07352	-0.47029
H	1.64635	2.75075	-1.11224
H	-1.01663	1.29588	-1.68697
H	-0.35747	-0.32042	-1.80739
H	-1.33734	-1.53640	0.82881
H	-3.51192	-2.41208	1.54157
H	-5.60150	-1.60670	0.47610
H	-5.49097	0.10948	-1.31320
H	-3.30981	1.02437	-2.02099
H	0.17628	-2.20646	-0.70127
H	1.29800	-1.84009	-1.99308
H	3.02756	-1.43066	1.62224
H	2.66503	0.18099	2.18040
H	3.36457	1.45922	-0.57097
H	2.55402	0.91845	-2.03754
H	1.84731	-4.04525	-1.02845
H	3.17250	-2.95468	-0.63408
H	1.97836	-3.37437	0.59532
H	4.96796	0.19773	-1.97578
H	3.89464	-1.19692	-2.04857
H	4.66936	-0.74813	-0.52085
H	1.45622	-1.58245	3.53462
H	0.28334	-0.55142	2.73798
H	0.63808	-2.15845	2.08582

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Benzyl-2-methyl-2-propanamide-$SiEt_3$

N	0.03575	0.74016	0.06126
C	-0.07979	2.20855	-0.13645
C	0.59269	2.62833	-1.44679
C	-1.55538	2.62745	-0.24823
C	0.57835	2.97500	1.02307

C	-0.91368	0.19140	1.03155
C	-2.22984	-0.30375	0.45059
C	-2.34845	-0.65382	-0.89382
C	-3.55092	-1.15054	-1.39175
C	-4.64903	-1.30422	-0.55027
C	-4.53883	-0.95508	0.79390
C	-3.33686	-0.45791	1.28750
Si	1.50499	-0.24308	-0.01484
C	2.74287	0.27827	-1.35270
C	2.35363	-0.22615	1.69049
C	0.92781	-2.00308	-0.42754
C	3.70785	-0.84805	-1.75710
C	1.80213	-3.13218	0.13510
C	3.82801	-0.64814	1.73592
H	0.35398	3.67446	-1.65945
H	1.67917	2.54772	-1.39813
H	0.22649	2.01513	-2.27579
H	-1.60576	3.70621	-0.42195
H	-2.12971	2.41293	0.65623
H	-2.04029	2.11703	-1.08424
H	1.65582	2.78018	1.04716
H	0.43359	4.05453	0.91201
H	0.15592	2.67707	1.98825
H	-0.45797	-0.65911	1.55757
H	-1.12807	0.91588	1.82960
H	-1.48946	-0.51265	-1.54362
H	-3.63052	-1.41620	-2.44146
H	-5.58649	-1.68870	-0.93898
H	-5.39165	-1.06500	1.45656
H	-3.25568	-0.18077	2.33660
H	2.18937	0.59711	-2.24153
H	3.31733	1.15157	-1.01832
H	1.77283	-0.85948	2.37450
H	2.25703	0.79159	2.08890
H	-0.10255	-2.13752	-0.07840
H	0.86918	-2.08374	-1.52160
H	4.41130	-0.50494	-2.52134
H	4.29698	-1.21367	-0.91187
H	3.16494	-1.70203	-2.17277
H	1.40104	-4.11672	-0.12309
H	2.82636	-3.08678	-0.24736
H	1.86120	-3.07933	1.22727
H	4.23323	-0.58293	2.75028
H	4.44401	-0.00720	1.09689
H	3.96480	-1.67915	1.39606

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[Benzyl-2-methyl-2-propanamine-$SiPhH_2$]$^+$

N	0.599472	-1.007492	0.320256
C	0.742710	-2.115956	1.381383
C	-0.611394	-2.247340	2.083820
C	1.158834	-3.412500	0.695986
C	1.788317	-1.682801	2.414033
C	1.881551	-0.624661	-0.394807
C	1.761540	0.768352	-0.961105
C	1.764524	0.992764	-2.338508
C	1.633169	2.287390	-2.837658
C	1.490776	3.361085	-1.962270
C	1.496622	3.144578	-0.584518
C	1.639575	1.854134	-0.087729
Si	-0.833094	-1.172205	-0.945408
C	-1.980021	0.218272	-0.571647
C	-3.121532	-0.004475	0.215896
C	-3.976515	1.046411	0.530438
C	-3.700123	2.328614	0.060504
C	-2.574039	2.563061	-0.726662
C	-1.717063	1.515376	-1.043871
H	-0.507933	-2.939204	2.922176
H	-0.946146	-1.285346	2.488156
H	-1.389506	-2.646825	1.431415
H	1.229231	-4.201001	1.448950
H	2.140451	-3.322850	0.223117
H	0.430184	-3.736323	-0.052193
H	2.810308	-1.717756	2.033428
H	1.582601	-0.677725	2.798872
H	1.742141	-2.371125	3.260555
H	2.695762	-0.672850	0.328552
H	2.064920	-1.364243	-1.176349
H	1.877466	0.157082	-3.023717
H	1.643499	2.454910	-3.909110
H	1.388296	4.368189	-2.351855
H	1.404341	3.980843	0.099754
H	1.675765	1.697292	0.989856
H	-0.124753	-1.114990	-2.231645
H	-1.420174	-2.498203	-0.711047
H	-3.354213	-1.003842	0.576650
H	-4.859260	0.865463	1.133915
H	-4.369270	3.147426	0.303427
H	-2.366670	3.560827	-1.098547
H	-0.847191	1.709373	-1.667585
H	0.328951	-0.170171	0.851352

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Benzyl-2-methyl-2-propanamide-$SiPhH_2$

N	0.194144	-1.518670	-0.819908
C	0.707486	-1.556632	0.570904
C	0.011377	-0.469770	1.396691
C	0.414840	-2.925472	1.204875
C	2.217148	-1.281729	0.608663
C	0.962925	-2.245842	-1.819838
C	2.039206	-1.441625	-2.536103
C	3.072374	-2.112015	-3.194472
C	4.041313	-1.408528	-3.902385
C	3.990205	-0.017455	-3.959644
C	2.965996	0.658771	-3.303656
C	1.996999	-0.049677	-2.596563
Si	-1.348442	-0.862603	-1.265518
C	-2.808054	-1.715850	-0.445301
C	-2.898889	-3.115405	-0.427461
C	-3.985868	-3.758901	0.155578
C	-5.007286	-3.007724	0.734995
C	-4.935690	-1.617845	0.730649

C	-3.842832	-0.980867	0.145816
H	0.391497	-0.487977	2.421680
H	0.204028	0.521285	0.975254
H	-1.071802	-0.628530	1.448503
H	0.817155	-2.975504	2.221801
H	0.871062	-3.735584	0.627288
H	-0.664193	-3.099066	1.248635
H	2.788445	-2.034574	0.058348
H	2.445560	-0.304204	0.176192
H	2.562489	-1.295334	1.646849
H	0.280638	-2.635583	-2.585598
H	1.427843	-3.133146	-1.370175
H	3.117564	-3.198152	-3.149015
H	4.840122	-1.945030	-4.404926
H	4.746529	0.534595	-4.508119
H	2.921509	1.742908	-3.338978
H	1.210004	0.478435	-2.065268
H	-1.491658	0.584817	-0.957259
H	-1.413158	-1.046444	-2.735952
H	-2.100155	-3.710021	-0.868192
H	-4.038664	-4.843169	0.160634
H	-5.856045	-3.506961	1.191926
H	-5.727737	-1.031127	1.185504
H	-3.792418	0.106003	0.154486

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BEt_3-(tBuNHBn)$_2$

N	0.42971	1.37609	0.74845
C	1.79253	1.33316	1.38252
C	-0.62303	1.79979	1.77442
C	-0.75743	0.69869	2.83406
C	-0.22991	3.12092	2.45075
C	-1.99172	1.95975	1.11271
C	2.53901	0.01883	1.29210
C	2.01978	-1.15531	1.84608
C	2.78028	-2.32093	1.87805
C	4.06112	-2.34095	1.33286
C	4.57947	-1.18270	0.76104
C	3.82630	-0.01215	0.74956
B	0.45965	2.11327	-0.87039
C	-0.84785	1.45325	-1.64171
C	0.35111	3.73367	-0.77296
C	1.88481	1.65440	-1.55422
C	3.10404	2.59191	-1.47891
C	0.23230	4.33946	-2.18147
C	-0.67460	1.02366	-3.10412
N	-0.52247	-1.99547	-0.57159
C	0.35019	-2.89408	-1.36638
C	1.62347	-2.11352	-1.69019
C	-0.32336	-3.31772	-2.68146
C	0.70481	-4.12662	-0.53357
C	-1.71150	-2.63997	-0.00149
C	-2.84800	-1.66736	0.20868
C	-3.40446	-0.99528	-0.88509
C	-4.46642	-0.11387	-0.71430
C	-5.00119	0.09690	0.55625
C	-4.46526	-0.57580	1.64976
C	-3.39385	-1.45006	1.47433
H	0.19280	0.40631	0.49779
H	1.69292	1.56459	2.44290
H	2.38399	2.13290	0.94315
H	-1.53594	0.98079	3.54878
H	-1.06136	-0.24409	2.36484
H	0.16497	0.53723	3.39935
H	-1.10571	3.51004	2.97696
H	0.09014	3.86784	1.72518
H	0.55965	2.99757	3.19576
H	-2.31092	1.03999	0.61979
H	-2.72323	2.18307	1.89493
H	-2.00335	2.77264	0.38860
H	1.01564	-1.16845	2.25654
H	2.36947	-3.21697	2.33296
H	4.64957	-3.25239	1.35373
H	5.57391	-1.18609	0.32668
H	4.23780	0.89031	0.30707
H	-1.69008	2.15961	-1.61573
H	-1.23247	0.58483	-1.09207
H	1.22508	4.17732	-0.26973
H	-0.52559	4.08014	-0.21064
H	1.68877	1.52675	-2.62638
H	2.18539	0.65044	-1.22725
H	3.98481	2.14424	-1.95439
H	2.90764	3.53648	-1.99455
H	3.40186	2.87055	-0.46191
H	0.26605	5.43387	-2.16990
H	-0.71586	4.04752	-2.64577
H	1.02908	3.99171	-2.84732
H	-0.31108	1.84760	-3.72773
H	-1.62165	0.68091	-3.53972
H	0.04807	0.20692	-3.21375
H	-0.82273	-1.25032	-1.19883
H	2.29310	-2.71507	-2.31290
H	2.14983	-1.83394	-0.77421
H	1.38490	-1.19709	-2.23986
H	0.33503	-3.97377	-3.25917
H	-1.25895	-3.85938	-2.51076
H	-0.54217	-2.43606	-3.29525
H	1.46636	-4.71689	-1.05095
H	1.10684	-3.81719	0.43432
H	-0.16212	-4.77325	-0.36672
H	-2.08726	-3.45550	-0.64065
H	-1.44382	-3.09696	0.95851
H	-2.99857	-1.16388	-1.88128
H	-4.87863	0.40655	-1.57272
H	-5.83124	0.78285	0.69041
H	-4.87696	-0.41878	2.64184
H	-2.97672	-1.97470	2.33032

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[BEt_3-(tBuNHBn-tBuNBn)]-

N	2.73901	0.31295	0.39413
C	2.19908	-0.32510	1.57372

C	3.82063	1.25503	0.72156
C	3.27229	2.41157	1.58648
C	5.00862	0.59891	1.47020
C	4.40110	1.91496	-0.53438
C	0.71556	-0.08481	1.83238
C	0.06481	1.03024	1.29939
C	-1.25367	1.32294	1.64052
C	-1.96209	0.48023	2.49817
C	-1.33286	-0.65335	3.01347
C	-0.00551	-0.92652	2.68574
B	2.72307	-0.61471	-0.91374
C	2.46997	0.27763	-2.29680
C	4.11375	-1.50861	-1.06633
C	1.42144	-1.67615	-0.86281
C	1.50402	-2.98644	-0.05296
C	4.11475	-2.49781	-2.23935
C	1.31288	1.27560	-2.19514
N	-2.87849	-1.03892	-0.49424
C	-3.19305	-2.45104	-0.24328
C	-1.84602	-3.16501	-0.14675
C	-3.98114	-3.00716	-1.43360
C	-3.98533	-2.67258	1.05604
C	-3.96869	-0.09002	-0.38624
C	-3.50574	1.31137	-0.72514
C	-2.37706	1.52307	-1.51793
C	-1.91548	2.81427	-1.76006
C	-2.59007	3.91113	-1.22881
C	-3.73092	3.70912	-0.45397
C	-4.18004	2.41607	-0.20138
H	-2.12748	-0.74705	0.13377
H	2.69287	0.03759	2.48651
H	2.38147	-1.40940	1.58909
H	4.08032	3.08694	1.89409
H	2.54263	2.98774	1.00791
H	2.77121	2.05690	2.49252
H	5.79985	1.33337	1.66741
H	5.42645	-0.21050	0.86735
H	4.70495	0.18038	2.43511
H	3.61645	2.40649	-1.11364
H	5.13489	2.67258	-0.23368
H	4.90016	1.19023	-1.17770
H	0.62205	1.64795	0.60230
H	-1.73397	2.20479	1.22466
H	-2.99522	0.70216	2.75484
H	-1.87442	-1.32177	3.67873
H	0.48636	-1.80430	3.10192
H	2.22783	-0.42803	-3.10657
H	3.36457	0.80668	-2.65630
H	4.31325	-2.06837	-0.13562
H	4.99292	-0.85701	-1.19266
H	1.26558	-1.96960	-1.91199
H	0.48780	-1.15768	-0.58895
H	0.91307	-3.79769	-0.50013
H	2.53512	-3.35210	0.02468
H	1.13032	-2.87346	0.97215
H	5.04532	-3.07715	-2.32155
H	3.97696	-1.96922	-3.18994
H	3.29128	-3.21707	-2.15831
H	0.41036	0.77600	-1.82227
H	1.05855	1.75646	-3.15220
H	1.53568	2.07109	-1.47262
H	-1.98036	-4.24480	-0.02506
H	-1.27328	-2.78791	0.70884
H	-1.25208	-2.97311	-1.04453
H	-4.14888	-4.08200	-1.30888
H	-4.96160	-2.52924	-1.53137
H	-3.42077	-2.84023	-2.35701
H	-4.09056	-3.74246	1.26483
H	-3.46136	-2.20506	1.89645
H	-4.99172	-2.24450	0.99448
H	-4.76201	-0.38803	-1.08627
H	-4.43703	-0.05736	0.61442
H	-1.84049	0.66252	-1.90299
H	-1.01187	2.95228	-2.34638
H	-2.22336	4.91742	-1.40735
H	-4.25877	4.55813	-0.02903
H	-5.04927	2.25767	0.43382

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BPh_3-$(tBuNHBn)_2$

N	0.97098	-0.94375	-0.72285
C	0.74199	-0.91953	-2.23453
C	0.13701	0.44015	-2.60889
C	2.03617	-1.17573	-2.99641
C	-0.29660	-1.98115	-2.60794
C	1.17658	-2.33075	-0.15187
C	-0.05128	-3.06380	0.35235
C	-0.74706	-2.60673	1.47739
C	-1.79667	-3.35028	2.00878
C	-2.16928	-4.56067	1.43031
C	-1.47508	-5.03121	0.31948
C	-0.42155	-4.28950	-0.20767
B	2.02638	0.17850	0.13830
C	3.52536	-0.41674	0.36068
C	2.21159	1.61753	-0.62655
C	3.22787	1.78031	-1.58716
C	3.41013	2.96410	-2.29539
C	2.59466	4.06361	-2.03797
C	1.63458	3.96482	-1.03714
C	1.46028	2.76796	-0.34121
C	4.16089	-1.47814	-0.29619
C	5.50069	-1.80346	-0.07293
C	6.25888	-1.06728	0.82736
C	5.66430	0.00602	1.48930
C	4.33266	0.32101	1.24933
C	-0.53246	0.40356	3.80824
C	0.75753	-0.11156	3.89679
C	1.58010	-0.16019	2.76908
C	1.14717	0.29074	1.51454
C	-0.17143	0.78279	1.45975
C	-0.99934	0.85815	2.57549
N	-3.11481	0.05841	-0.81039

C	-4.13620	-0.92020	-1.23888
C	-5.55503	-0.55524	-0.76550
C	-3.76329	-2.26300	-0.61134
C	-4.10755	-1.02162	-2.76544
C	-3.31557	1.44017	-1.27732
C	-3.07924	2.44580	-0.17615
C	-3.99087	2.54046	0.88196
C	-3.78322	3.44182	1.92032
C	-2.65057	4.25559	1.91949
C	-1.74063	4.17019	0.87091
C	-1.95953	3.27576	-0.17626
H	0.06002	-0.64927	-0.35819
H	-0.24285	0.37661	-3.63313
H	-0.71746	0.65746	-1.95606
H	0.85253	1.25769	-2.55852
H	1.83891	-1.05087	-4.06509
H	2.40120	-2.19708	-2.85092
H	2.81798	-0.47428	-2.70844
H	-1.21544	-1.82992	-2.03349
H	-0.53526	-1.87666	-3.67018
H	0.06108	-2.99948	-2.45145
H	1.67730	-2.93488	-0.91016
H	1.87213	-2.22243	0.68096
H	-0.44814	-1.68558	1.96488
H	-2.31632	-2.98023	2.88749
H	-2.98764	-5.13859	1.84780
H	-1.74489	-5.98037	-0.13227
H	0.13211	-4.68072	-1.05755
H	3.91696	0.95988	-1.77079
H	4.20028	3.03343	-3.03739
H	2.72851	4.99102	-2.58626
H	1.02128	4.82787	-0.78849
H	0.72163	2.74687	0.45201
H	3.61579	-2.07673	-1.01844
H	5.94760	-2.63545	-0.60962
H	7.29977	-1.31778	1.00659
H	6.24345	0.60373	2.18707
H	3.89783	1.18031	1.75643
H	-1.16737	0.44858	4.68783
H	1.12803	-0.48270	4.84797
H	2.58007	-0.57333	2.86974
H	-0.58450	1.11548	0.50750
H	-2.00037	1.27162	2.47631
H	-3.06632	0.05395	0.20722
H	-6.26908	-1.32602	-1.07171
H	-5.90558	0.39485	-1.17916
H	-5.58392	-0.48741	0.32782
H	-4.45926	-3.04387	-0.93264
H	-2.74826	-2.57090	-0.87700
H	-3.81195	-2.20073	0.48047
H	-4.79870	-1.79763	-3.10690
H	-4.40668	-0.07940	-3.23527
H	-3.10104	-1.27118	-3.11204
H	-2.64096	1.65125	-2.11658
H	-4.33550	1.58676	-1.65673
H	-4.87330	1.90363	0.88072
H	-4.50201	3.51022	2.73079
H	-2.47996	4.95224	2.73358
H	-0.85329	4.79638	0.86867
H	-1.23947	3.20602	-0.98911

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[BPh_3-(tBuNHBn-tBuNBn)]-

N	0.89700	-0.47872	-0.99957
C	0.42119	0.24135	-2.20197
C	-0.30106	1.54908	-1.81767
C	1.54237	0.58644	-3.20248
C	-0.62487	-0.59416	-2.96220
C	1.20265	-1.90148	-1.21478
C	0.20060	-2.98214	-0.77364
C	0.28280	-3.51704	0.52083
C	-0.51465	-4.58523	0.92120
C	-1.41407	-5.16699	0.03101
C	-1.49926	-4.66625	-1.26364
C	-0.69725	-3.59448	-1.65663
B	1.87379	0.15758	0.09153
C	3.49787	-0.07925	-0.19238
C	1.73170	1.80485	0.27981
C	2.58116	2.68586	-0.41715
C	2.46689	4.07155	-0.33579
C	1.49545	4.64493	0.48065
C	0.66566	3.80750	1.21909
C	0.79201	2.42246	1.12079
C	4.07111	-0.66638	-1.32922
C	5.45235	-0.76898	-1.51627
C	6.32841	-0.28169	-0.55464
C	5.80000	0.31982	0.58781
C	4.42255	0.41833	0.74946
C	0.51050	-1.93025	3.85343
C	1.86257	-1.92445	3.52788
C	2.31102	-1.25738	2.38399
C	1.44113	-0.58635	1.51122
C	0.07931	-0.62788	1.86818
C	-0.38362	-1.26562	3.01403
N	-3.14560	-0.15307	-0.05350
C	-3.97020	-1.36868	-0.06669
C	-5.34905	-1.05372	0.52570
C	-3.25701	-2.36534	0.84448
C	-4.13233	-1.97087	-1.47127
C	-3.56363	0.95948	-0.88830
C	-3.27924	2.30764	-0.24904
C	-3.08712	2.42879	1.12679
C	-2.88418	3.68095	1.70220
C	-2.85909	4.82480	0.90972
C	-3.03193	4.70870	-0.46758
C	-3.24082	3.45836	-1.03928
H	-2.17199	-0.39349	-0.24399
H	-0.98925	1.84297	-2.62073
H	-0.87600	1.41025	-0.89822
H	0.37845	2.38309	-1.65067
H	1.14560	1.16581	-4.04600
H	2.00261	-0.32047	-3.61184

H	2.32016	1.17629	-2.71195
H	-1.42711	-0.91541	-2.28831
H	-1.06492	0.00653	-3.76518
H	-0.18761	-1.47958	-3.42924
H	1.44383	-2.10815	-2.26999
H	2.11801	-2.14026	-0.66372
H	0.99596	-3.09812	1.22275
H	-0.42369	-4.96173	1.93616
H	-2.03724	-6.00118	0.34091
H	-2.18532	-5.11273	-1.97879
H	-0.76215	-3.24923	-2.68332
H	3.36296	2.27144	-1.04943
H	3.14095	4.70406	-0.90904
H	1.39532	5.72513	0.54963
H	-0.09218	4.23191	1.87211
H	0.11998	1.81017	1.71489
H	3.42279	-1.05267	-2.10962
H	5.84052	-1.23089	-2.42134
H	7.40361	-0.35951	-0.69299
H	6.46560	0.72185	1.34822
H	4.03422	0.92033	1.63459
H	0.15626	-2.44726	4.74152
H	2.57584	-2.44759	4.16107
H	3.37183	-1.29497	2.15237
H	-0.64551	-0.16570	1.20086
H	-1.44672	-1.26261	3.24262
H	-5.90024	-1.98391	0.69717
H	-5.95858	-0.43060	-0.13637
H	-5.23099	-0.53176	1.47972
H	-3.75761	-3.33860	0.82991
H	-2.22212	-2.51297	0.52058
H	-3.24084	-1.98790	1.87107
H	-4.78719	-2.84936	-1.44618
H	-4.56941	-1.24279	-2.16397
H	-3.16056	-2.28725	-1.86224
H	-3.11172	0.94056	-1.89300
H	-4.64705	0.89177	-1.04578
H	-3.08325	1.52408	1.72607
H	-2.72752	3.76012	2.77438
H	-2.68388	5.79815	1.35828
H	-2.99123	5.59199	-1.09800
H	-3.36083	3.36707	-2.11691

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$B(C_6F_5)Ph_2$-$(tBuNHBn)_2$

N	0.39335	0.50417	-0.96788
C	-0.71886	1.48040	-1.38777
C	-0.16845	2.60426	-2.25689
C	-1.80135	0.71712	-2.15737
C	-1.38080	2.03932	-0.12406
C	0.87147	-0.39952	-2.08726
C	0.20197	-1.75220	-2.23762
C	0.36147	-2.75298	-1.27408
C	-0.15513	-4.03008	-1.47636
C	-0.82308	-4.33745	-2.65737
C	-0.97136	-3.35741	-3.63491
C	-0.46111	-2.08002	-3.42436
B	1.76774	0.97525	-0.01767
C	3.04267	1.45873	-0.91247
C	1.50151	2.19625	1.04836
C	1.67723	3.52645	0.61647
C	1.47758	4.62122	1.44927
C	1.13259	4.42775	2.78485
C	1.02241	3.12926	3.26509
C	1.20866	2.04192	2.41105
C	3.10058	1.76403	-2.27552
C	4.24995	2.28503	-2.87807
C	5.39074	2.51590	-2.12505
C	5.36642	2.22963	-0.75921
C	4.21492	1.72390	-0.17647
C	2.30595	-2.97173	2.13062
C	3.28563	-2.52980	1.25683
C	3.12696	-1.31767	0.58553
C	2.02517	-0.47654	0.75658
C	1.05593	-1.00205	1.61570
C	1.16782	-2.19769	2.30925
F	2.44448	-4.12481	2.77693
F	4.36811	-3.27610	1.05046
F	4.09826	-1.03600	-0.28657
F	-0.13253	-0.36586	1.75110
F	0.19526	-2.62134	3.11755
N	-3.57966	-0.85893	0.53354
C	-3.50917	-2.33486	0.57148
C	-2.19161	-2.67932	1.26174
C	-3.48053	-2.85901	-0.86616
C	-4.66911	-2.98013	1.34526
C	-4.88175	-0.28945	0.18166
C	-4.82034	1.21908	0.14071
C	-4.98109	1.91806	-1.05544
C	-4.90764	3.30977	-1.08526
C	-4.66812	4.01981	0.08784
C	-4.51429	3.33232	1.29064
C	-4.59841	1.94416	1.31455
H	-0.11026	-0.10394	-0.31710
H	-0.97571	3.32119	-2.43192
H	0.65475	3.12770	-1.77241
H	0.16530	2.24566	-3.23553
H	-2.61064	1.41988	-2.37249
H	-2.22296	-0.09301	-1.55014
H	-1.44546	0.32296	-3.11022
H	-1.69613	1.22348	0.53370
H	-0.74016	2.72225	0.42796
H	-2.28390	2.57765	-0.42519
H	0.77155	0.15360	-3.02156
H	1.93938	-0.55921	-1.92641
H	0.91826	-2.54870	-0.36668
H	-0.01872	-4.78773	-0.71092
H	-1.21924	-5.33475	-2.81860
H	-1.47860	-3.58711	-4.56623
H	-0.56320	-1.33100	-4.20517
H	2.01068	3.71359	-0.40018
H	1.61299	5.62595	1.05998

H	0.98134	5.27619	3.44508
H	0.79549	2.95330	4.31255
H	1.12858	1.05483	2.84846
H	2.23524	1.61321	-2.91037
H	4.24218	2.50930	-3.94075
H	6.28609	2.91849	-2.58816
H	6.24620	2.41034	-0.14893
H	4.21284	1.53208	0.89531
H	-3.30876	-0.50145	1.44875
H	-2.02661	-3.76089	1.27110
H	-2.18343	-2.32501	2.29758
H	-1.36019	-2.20713	0.73229
H	-3.36003	-3.94687	-0.87168
H	-4.40694	-2.62710	-1.40103
H	-2.64039	-2.41961	-1.41305
H	-4.74631	-2.55670	2.35306
H	-5.62768	-2.83692	0.83786
H	-4.50542	-4.05737	1.44340
H	-5.16592	-0.66259	-0.80772
H	-5.68132	-0.59084	0.87825
H	-5.16369	1.36490	-1.97328
H	-5.03714	3.83785	-2.02490
H	-4.60569	5.10288	0.06776
H	-4.33296	3.87929	2.21013
H	-4.49262	1.41662	2.26033

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[B(C_6F_5)Ph_2-(tBuNHBn-tBuNBn)]-

N	-1.62407	0.33861	1.57042
C	-0.95819	0.58222	2.86160
C	-1.76919	1.54769	3.75398
C	-0.77163	-0.72020	3.67504
C	0.45951	1.13828	2.65908
C	-2.75566	-0.56644	1.61900
C	-2.50918	-2.02749	1.23365
C	-1.23181	-2.55858	1.06714
C	-1.04831	-3.87132	0.64091
C	-2.14957	-4.68235	0.37655
C	-3.43272	-4.16532	0.54300
C	-3.60626	-2.85055	0.96491
B	-1.54622	1.10715	0.20321
C	-2.97623	1.84574	-0.18696
C	-0.54083	2.40049	-0.00437
C	-0.67995	3.55017	0.79760
C	0.00251	4.73479	0.55173
C	0.83508	4.84322	-0.56273
C	0.95434	3.74972	-1.41089
C	0.28436	2.55752	-1.12706
C	-3.89831	2.24558	0.78804
C	-5.03215	2.99873	0.47901
C	-5.27998	3.37975	-0.83490
C	-4.37620	3.00272	-1.82888
C	-3.25002	2.25755	-1.50086
C	-0.52639	-2.41824	-2.47477
C	-1.83792	-1.99713	-2.35162
C	-2.12973	-0.86658	-1.59169
C	-1.17899	-0.10160	-0.91804
C	0.11722	-0.59761	-1.05383
C	0.46180	-1.70131	-1.81924
F	-0.21614	-3.49801	-3.19908
F	-2.81297	-2.68890	-2.95119
F	-3.44096	-0.59496	-1.48933
F	1.14705	-0.04252	-0.37391
F	1.74372	-2.11072	-1.90217
N	4.09744	-1.34444	0.19936
C	3.71612	-2.55173	0.95238
C	3.92015	-3.73190	-0.00127
C	2.25195	-2.52030	1.41177
C	4.64490	-2.71865	2.15849
C	3.99061	-0.07800	0.91815
C	4.49463	1.06452	0.06688
C	3.75730	2.24023	-0.06560
C	4.26635	3.31044	-0.80126
C	5.50578	3.20663	-1.42378
C	6.23561	2.02261	-1.31667
C	5.73195	0.95988	-0.57630
H	3.48544	-1.28405	-0.61440
H	-1.25831	1.73293	4.70661
H	-1.91990	2.50616	3.25363
H	-2.75617	1.12715	3.98117
H	-0.40102	-0.46544	4.67380
H	-0.03615	-1.37898	3.20693
H	-1.69794	-1.28625	3.80064
H	0.94410	0.58690	1.84832
H	0.47195	2.19570	2.40006
H	1.04216	1.00829	3.57865
H	-3.23828	-0.55971	2.60961
H	-3.53418	-0.21514	0.93258
H	-0.38578	-1.90031	1.23090
H	-0.04053	-4.25350	0.49583
H	-2.01008	-5.70224	0.03097
H	-4.29982	-4.78268	0.32547
H	-4.60975	-2.44042	1.06143
H	-1.37363	3.51970	1.63411
H	-0.13447	5.58537	1.21469
H	1.36016	5.77113	-0.77466
H	1.58036	3.81201	-2.29770
H	0.40365	1.73668	-1.82768
H	-3.72135	1.95326	1.82217
H	-5.72358	3.28619	1.26793
H	-6.16145	3.96439	-1.08409
H	-4.55157	3.29651	-2.86104
H	-2.54606	1.98880	-2.28857
H	3.66424	-4.67585	0.49074
H	4.96229	-3.77214	-0.33079
H	3.28051	-3.62196	-0.88189
H	1.98360	-3.43055	1.96033
H	2.05318	-1.66444	2.06581
H	1.59602	-2.43915	0.54003
H	5.68801	-2.61389	1.84380
H	4.43980	-1.98119	2.93975
H	4.50776	-3.71080	2.59954

H	2.97384	0.15864	1.26242
H	4.62266	-0.14105	1.81267
H	2.77283	2.31949	0.39203
H	3.67681	4.21748	-0.88942
H	5.89914	4.03962	-1.99924
H	7.19820	1.93028	-1.81192
H	6.27872	0.02507	-0.49358

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$B(C_6F_5)_2Ph\text{-}(tBuNHBn)_2$

N	0.25817	-0.84054	0.34827
C	-0.16771	-2.25822	-0.11791
C	-0.15404	-2.35210	-1.64470
C	-1.61973	-2.52789	0.32324
C	0.74684	-3.33561	0.46997
C	0.53106	-0.77753	1.83151
C	-0.62947	-1.09124	2.74392
C	-0.53086	-2.12421	3.67574
C	-1.60327	-2.43325	4.51062
C	-2.78589	-1.70648	4.42096
C	-2.87928	-0.64924	3.51594
C	-1.80348	-0.33394	2.69332
B	1.46835	0.00650	-0.50263
C	1.69743	1.47798	0.22871
C	2.82759	-0.92313	-0.46180
C	3.61120	-0.99481	0.69469
C	4.72736	-1.80349	0.84669
C	5.14119	-2.59519	-0.21432
C	4.42885	-2.54416	-1.39958
C	3.31209	-1.71777	-1.50336
C	2.91673	2.15407	0.24397
C	3.06370	3.47091	0.66690
C	1.95619	4.19406	1.08437
C	0.71406	3.57888	1.06643
C	0.62684	2.26487	0.63714
C	0.17972	1.69372	-4.41195
C	-0.77635	1.36419	-3.45700
C	-0.39324	0.78806	-2.24723
C	0.94885	0.49451	-1.96098
C	1.89367	0.87532	-2.92524
C	1.52306	1.45772	-4.13285
F	3.31416	-0.23660	1.76533
F	5.40696	-1.81678	1.99186
F	6.20641	-3.37979	-0.09675
F	4.81508	-3.28278	-2.43792
F	2.71684	-1.75549	-2.70482
F	4.04032	1.56056	-0.18284
F	4.26360	4.04795	0.66374
F	2.08332	5.45415	1.48868
F	-0.38064	4.24184	1.44320
F	-0.62402	1.74119	0.61948
N	-3.38492	0.65566	-0.19906
C	-3.93866	2.03149	-0.09905
C	-3.63356	2.53826	1.31243
C	-5.45703	2.08505	-0.32674
C	-3.22096	2.92771	-1.11070
C	-3.82378	-0.12513	-1.36256
C	-5.09154	-0.94173	-1.18296
C	-5.28583	-1.72337	-0.03998
C	-6.43510	-2.49448	0.10795
C	-7.40762	-2.50087	-0.88859
C	-7.22141	-1.73249	-2.03393
C	-6.07175	-0.96060	-2.17623
H	-0.57655	-0.26244	0.19420
H	-0.42369	-3.37820	-1.90874
H	0.81184	-2.13059	-2.08667
H	-0.89190	-1.68606	-2.09513
H	-2.02323	-3.33539	-0.29399
H	-1.71232	-2.82168	1.36850
H	-2.24021	-1.64196	0.15758
H	1.79686	-3.18063	0.21624
H	0.64411	-3.41478	1.55404
H	0.43715	-4.29565	0.04900
H	0.89026	0.22914	2.03814
H	1.36496	-1.44732	2.03407
H	0.39013	-2.69769	3.74635
H	-1.51373	-3.24368	5.22651
H	-3.62580	-1.95026	5.06306
H	-3.79091	-0.06079	3.46249
H	-1.88121	0.49103	1.99184
H	-0.11601	2.14209	-5.35507
H	-1.82767	1.56210	-3.64785
H	-1.17947	0.59001	-1.51792
H	2.95123	0.72203	-2.72181
H	2.28566	1.72938	-4.85641
H	-3.66396	0.15487	0.64373
H	-4.05778	3.53623	1.45265
H	-2.55760	2.60094	1.48469
H	-4.08263	1.88112	2.06773
H	-5.82228	3.10643	-0.18244
H	-5.72865	1.77442	-1.33990
H	-5.98126	1.42773	0.37524
H	-2.14111	2.88981	-0.94751
H	-3.42662	2.62364	-2.14193
H	-3.56059	3.96212	-1.00264
H	-3.94411	0.55070	-2.21496
H	-3.01406	-0.81107	-1.64851
H	-4.53507	-1.74105	0.74906
H	-6.56949	-3.09442	1.00246
H	-8.30436	-3.10051	-0.77228
H	-7.97428	-1.72848	-2.81567
H	-5.93378	-0.35696	-3.07019

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$[B(C_6F_5)_2Ph\text{-}(tBuNHBn\text{-}tBuNBn)]^-$

N	0.41702	-0.96048	0.30576
C	0.11032	-2.33919	-0.19183
C	0.27639	-2.47587	-1.71366
C	-1.36827	-2.71169	0.06968
C	0.99252	-3.42563	0.46289
C	0.53704	-0.90981	1.76213
C	-0.70006	-1.21183	2.59359

C	-0.60922	-2.08062	3.68171
C	-1.71557	-2.34981	4.48796
C	-2.93747	-1.74554	4.21486
C	-3.03782	-0.86719	3.13478
C	-1.93170	-0.59969	2.33666
B	1.45371	-0.05064	-0.43955
C	1.59722	1.45822	0.29708
C	2.96680	-0.79700	-0.45972
C	3.69130	-0.91791	0.72967
C	4.84699	-1.66764	0.88288
C	5.36938	-2.34176	-0.21142
C	4.72522	-2.22697	-1.42860
C	3.56692	-1.45713	-1.52868
C	2.77346	2.20373	0.38415
C	2.83646	3.52162	0.82632
C	1.67755	4.18521	1.18945
C	0.47404	3.50664	1.09633
C	0.46601	2.19158	0.65336
C	-0.05617	1.80882	-4.20566
C	-0.93244	1.21375	-3.30090
C	-0.42976	0.57326	-2.17124
C	0.94169	0.49033	-1.89911
C	1.79653	1.11508	-2.81733
C	1.31387	1.75575	-3.95586
F	3.30189	-0.24891	1.83106
F	5.47721	-1.73304	2.06210
F	6.48264	-3.07278	-0.09235
F	5.22591	-2.84659	-2.50460
F	3.05313	-1.40688	-2.77243
F	3.96014	1.69306	0.01117
F	4.01063	4.16084	0.89048
F	1.71757	5.45299	1.61155
F	-0.66925	4.12774	1.41620
F	-0.76039	1.63728	0.57137
N	-3.54897	0.79481	-0.43211
C	-4.24375	2.07526	-0.20591
C	-3.81543	2.57291	1.17672
C	-5.75771	1.85497	-0.21311
C	-3.84958	3.11848	-1.26332
C	-3.96949	0.00288	-1.57897
C	-5.02016	-1.03485	-1.22789
C	-4.96688	-1.69814	0.00039
C	-5.89934	-2.68256	0.31074
C	-6.90115	-3.01562	-0.59970
C	-6.96211	-2.35684	-1.82418
C	-6.02589	-1.37219	-2.13301
H	-2.55216	0.98733	-0.49267
H	0.13668	-3.53004	-1.97487
H	1.25004	-2.16709	-2.08077
H	-0.47859	-1.90142	-2.25246
H	-1.63514	-3.59002	-0.52939
H	-1.58160	-2.94713	1.11320
H	-2.01622	-1.88050	-0.23068
H	2.05708	-3.22910	0.29948
H	0.81360	-3.50155	1.53953
H	0.75477	-4.40184	0.02751
H	0.84548	0.10235	2.03408
H	1.34566	-1.55352	2.14652
H	0.34338	-2.56241	3.89264
H	-1.62100	-3.03756	5.32366
H	-3.80456	-1.95580	4.83418
H	-3.98850	-0.39291	2.90217
H	-2.03313	0.05380	1.47850
H	-0.43489	2.31211	-5.09081
H	-2.00674	1.25130	-3.47296
H	-1.10077	0.10105	-1.45787
H	2.86900	1.11043	-2.62768
H	2.00888	2.22319	-4.64882
H	-4.28784	3.53473	1.40291
H	-2.73202	2.70429	1.22537
H	-4.10705	1.84740	1.94174
H	-6.26553	2.78769	0.05208
H	-6.12263	1.53957	-1.19586
H	-6.03305	1.08303	0.51160
H	-2.76812	3.29147	-1.23140
H	-4.11162	2.78352	-2.27267
H	-4.35681	4.07280	-1.08537
H	-4.33749	0.61090	-2.42315
H	-3.08711	-0.52968	-1.95723
H	-4.18823	-1.42360	0.70586
H	-5.84087	-3.19159	1.26842
H	-7.63054	-3.78195	-0.35504
H	-7.74217	-2.60460	-2.53823
H	-6.07872	-0.85308	-3.08784

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$B(C_6F_5)_3$-(tBuNHBn)$_2$

N	1.00189	0.36623	1.74346
C	1.40184	-0.44905	3.00729
C	1.33250	-1.96239	2.78619
C	0.38682	-0.10552	4.10844
C	2.82489	-0.10470	3.46884
C	1.27195	1.83688	2.01032
C	0.28524	2.80316	1.40878
C	-1.06242	2.74858	1.76473
C	-1.97174	3.64526	1.21345
C	-1.53116	4.62640	0.32764
C	-0.17913	4.70942	-0.00251
C	0.72533	3.79770	0.53299
B	1.48092	-0.16885	0.22004
C	0.98168	0.90451	-0.92992
C	3.10929	-0.38553	0.25802
C	4.00404	0.68732	0.27791
C	5.38032	0.56539	0.39820
C	5.94689	-0.69747	0.48181
C	5.11661	-1.80441	0.42655
C	3.74219	-1.62880	0.30344
C	1.74262	1.39891	-1.98823
C	1.22577	2.24053	-2.97126
C	-0.11752	2.57549	-2.96395
C	-0.93795	2.04411	-1.97848
C	-0.37349	1.22538	-1.01828

C	-0.94967	-3.53696	-1.47209
C	-1.37918	-2.94455	-0.29722
C	-0.61037	-1.93978	0.27910
C	0.60726	-1.49855	-0.22326
C	0.98167	-2.12404	-1.41513
C	0.24983	-3.12347	-2.03697
F	2.10005	-1.72868	-2.03705
F	0.67129	-3.66962	-3.17360
F	-1.69040	-4.47004	-2.06316
F	-2.53783	-3.30994	0.24904
F	-1.16139	-1.37622	1.38973
F	3.56405	1.95616	0.16134
F	6.15623	1.64622	0.42104
F	7.26087	-0.84175	0.59951
F	5.63518	-3.02815	0.48369
F	3.04219	-2.77383	0.24964
F	3.02996	1.07697	-2.14693
F	2.01632	2.70328	-3.93698
F	-0.62002	3.37364	-3.89883
F	-2.24030	2.32457	-1.97254
F	-1.22548	0.71722	-0.09812
N	-3.68728	0.70058	1.60860
C	-4.50475	-0.05157	2.58122
C	-4.89305	-1.47019	2.12639
C	-5.76023	0.75330	2.91582
C	-3.62946	-0.17747	3.83244
C	-4.30414	1.16997	0.36719
C	-4.81464	0.10466	-0.58550
C	-6.16024	0.02332	-0.94115
C	-6.61890	-1.00694	-1.76094
C	-5.73253	-1.97118	-2.23102
C	-4.38111	-1.88862	-1.89763
C	-3.92936	-0.85086	-1.09138
H	-0.01782	0.27961	1.70211
H	1.74253	-2.43439	3.68324
H	1.92214	-2.30157	1.93954
H	0.30769	-2.31251	2.67418
H	0.54930	-0.77800	4.95424
H	0.46748	0.91510	4.48823
H	-0.63608	-0.26580	3.75332
H	3.58027	-0.49530	2.78615
H	2.99568	0.96348	3.60845
H	2.97574	-0.58439	4.43952
H	1.24714	1.97485	3.08965
H	2.27872	2.05798	1.67567
H	-1.43744	1.98011	2.43960
H	-3.02024	3.55955	1.48055
H	-2.23960	5.32443	-0.10628
H	0.16808	5.47296	-0.69120
H	1.77413	3.83368	0.25078
H	-2.87937	0.12907	1.36834
H	-5.33784	-2.02165	2.96196
H	-4.00602	-2.01661	1.78920
H	-5.61257	-1.45985	1.30545
H	-6.28435	0.29452	3.75894
H	-5.49542	1.78094	3.18466
H	-6.45489	0.77865	2.07061
H	-2.74559	-0.78519	3.60424
H	-3.30178	0.80988	4.17163
H	-4.16953	-0.67372	4.64415
H	-5.11869	1.85779	0.61790
H	-3.53989	1.76251	-0.14474
H	-6.85830	0.76617	-0.56131
H	-7.67068	-1.06131	-2.02413
H	-6.09044	-2.78199	-2.85707
H	-3.68540	-2.64220	-2.25655
H	-2.87432	-0.77802	-0.83791

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[B(C_6F_5)$_3$-(tBuNHBn-tBuNBn)]-

N	-1.299817	1.657380	-0.637612
C	-1.889086	2.152152	-1.913047
C	-1.759000	1.134259	-3.056632
C	-1.142347	3.414824	-2.381468
C	-3.398356	2.510533	-1.809171
C	-1.254305	2.689763	0.385736
C	-0.006170	3.566405	0.489971
C	1.211751	3.261056	-0.115710
C	2.331844	4.064134	0.087293
C	2.247878	5.202612	0.884296
C	1.031972	5.529442	1.481235
C	-0.078964	4.715114	1.284909
B	-1.504671	0.189499	-0.189710
C	-0.990401	-0.070655	1.385743
C	-3.116204	-0.238342	-0.335012
C	-4.048107	0.456688	0.433360
C	-5.420565	0.305246	0.337290
C	-5.937554	-0.590415	-0.588744
C	-5.063538	-1.310078	-1.383070
C	-3.690042	-1.127945	-1.233554
C	-1.696046	-0.652828	2.437826
C	-1.141190	-0.922946	3.687229
C	0.189264	-0.637783	3.933125
C	0.950743	-0.089827	2.912702
C	0.350939	0.166662	1.689102
C	1.236169	-2.969205	-1.922271
C	1.426956	-1.646979	-2.274544
C	0.588535	-0.660335	-1.760703
C	-0.517860	-0.923460	-0.961500
C	-0.659848	-2.274778	-0.637084
C	0.178728	-3.285171	-1.081816
F	-1.658596	-2.657372	0.174837
F	0.007911	-4.552677	-0.687948
F	2.066078	-3.920445	-2.354907
F	2.457731	-1.315498	-3.065316
F	0.969023	0.594621	-2.078294
F	-3.624577	1.364472	1.330489
F	-6.252387	1.011991	1.111432
F	-7.258557	-0.752435	-0.709955
F	-5.543578	-2.176235	-2.283268
F	-2.935208	-1.857995	-2.077517
F	-2.978054	-1.025822	2.321049

F	-1.887166	-1.472580	4.651557
F	0.732498	-0.895145	5.124848
F	2.246073	0.169079	3.117051
F	1.168203	0.648139	0.734117
N	3.833902	1.125333	-0.690700
C	4.818495	1.059135	-1.778204
C	5.381565	-0.345844	-2.055407
C	5.978222	2.009038	-1.459653
C	4.085074	1.571057	-3.022023
C	4.199224	0.686723	0.649094
C	4.328216	-0.811677	0.889208
C	5.512158	-1.363271	1.379727
C	5.636922	-2.736135	1.583058
C	4.570582	-3.582141	1.294948
C	3.376270	-3.044724	0.817855
C	3.255637	-1.671465	0.627180
H	2.957867	0.696423	-0.981188
H	-2.326931	1.508959	-3.915351
H	-2.160904	0.153016	-2.802826
H	-0.721118	1.017479	-3.367890
H	-1.522046	3.716720	-3.363722
H	-1.276581	4.258389	-1.698067
H	-0.071971	3.213308	-2.467006
H	-4.027926	1.626805	-1.935677
H	-3.652761	2.969258	-0.849533
H	-3.668162	3.219204	-2.600044
H	-2.110852	3.378196	0.304156
H	-1.383754	2.229648	1.368879
H	1.279128	2.380404	-0.742080
H	3.270448	3.765183	-0.370827
H	3.121083	5.829060	1.042592
H	0.949407	6.417017	2.102794
H	-1.025492	4.969674	1.759361
H	6.014904	-0.328695	-2.950012
H	4.571989	-1.060820	-2.219151
H	5.986935	-0.705180	-1.219048
H	6.650907	2.080017	-2.320442
H	5.597163	3.007755	-1.226386
H	6.571299	1.655955	-0.609964
H	3.242719	0.917102	-3.262901
H	3.695853	2.577249	-2.838164
H	4.758159	1.600058	-3.884736
H	5.139954	1.172541	0.929823
H	3.434775	1.079243	1.325242
H	6.353422	-0.706119	1.591654
H	6.570221	-3.144741	1.959697
H	4.665953	-4.653218	1.443609
H	2.536126	-3.696802	0.593233
H	2.315042	-1.261510	0.269465

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$[SiEt_3\text{-}(tBuNHBn)_2]^+$

N	1.20460	-0.78579	0.81622
C	0.21660	-0.92913	2.00631
C	-0.05112	0.47892	2.53929
C	-1.08601	-1.50680	1.46322
C	0.78676	-1.82925	3.09927
C	2.53626	-0.18601	1.23301
C	2.72656	1.23550	0.75919
C	2.55914	1.59677	-0.58137
C	2.79856	2.90405	-0.99674
C	3.20120	3.86642	-0.07555
C	3.35518	3.51956	1.26430
C	3.11977	2.21173	1.67756
Si	1.39883	-2.24865	-0.43109
C	3.02313	-1.94611	-1.34409
C	-0.04216	-2.07944	-1.61591
C	1.50656	-3.88388	0.47945
C	2.98147	-2.46096	-2.79536
C	1.86541	-5.01312	-0.50619
C	-0.20000	-0.66278	-2.19170
N	-1.91699	1.89250	-0.26598
C	-1.37591	3.22074	-0.64990
C	-0.38328	3.61198	0.44664
C	-2.45785	4.30546	-0.75515
C	-0.64202	3.08589	-1.98527
C	-3.04339	1.40306	-1.07826
C	-3.58803	0.12508	-0.48728
C	-4.19357	0.14439	0.77335
C	-4.64968	-1.03005	1.36335
C	-4.51035	-2.24625	0.69537
C	-3.93349	-2.27408	-0.57146
C	-3.47936	-1.09344	-1.15841
H	0.74745	-0.06221	0.23922
H	-0.77327	0.41152	3.35673
H	0.84635	0.96737	2.92741
H	-0.48083	1.10364	1.75028
H	-1.84026	-1.47994	2.25309
H	-0.98413	-2.54865	1.14963
H	-1.47275	-0.90906	0.63143
H	1.67374	-1.41654	3.58427
H	0.02121	-1.92688	3.87303
H	1.01500	-2.83167	2.73802
H	2.59350	-0.21591	2.31891
H	3.33389	-0.83103	0.85823
H	2.23430	0.86522	-1.31703
H	2.66703	3.16798	-2.04079
H	3.38972	4.88425	-0.39945
H	3.66064	4.26600	1.98945
H	3.25029	1.94589	2.72360
H	3.31650	-0.89229	-1.35171
H	3.81618	-2.46867	-0.79280
H	0.17451	-2.78471	-2.42920
H	-0.98215	-2.41342	-1.16611
H	0.56668	-4.12402	0.98570
H	2.28052	-3.82390	1.25405
H	3.96385	-2.36477	-3.26219
H	2.69322	-3.51414	-2.85397
H	2.27111	-1.89105	-3.40040
H	1.87979	-5.97630	0.00757
H	2.85505	-4.86275	-0.94575
H	1.14000	-5.08924	-1.32204

H	-0.90096	-0.65504	-3.03095
H	-0.58835	0.04704	-1.44802
H	0.74939	-0.27125	-2.57697
H	-2.26064	1.97749	0.69139
H	0.08853	4.57095	0.21613
H	0.40621	2.86048	0.54514
H	-0.89261	3.71435	1.41271
H	-1.99557	5.28471	-0.90725
H	-3.13634	4.13183	-1.59431
H	-3.05115	4.35390	0.16482
H	0.11759	2.30111	-1.92000
H	-1.32651	2.84400	-2.80371
H	-0.14602	4.02748	-2.23907
H	-3.85713	2.13899	-1.15277
H	-2.68620	1.21130	-2.09528
H	-4.32541	1.09189	1.29242
H	-5.12636	-0.99684	2.33784
H	-4.87183	-3.16228	1.15071
H	-3.84950	-3.21259	-1.11091
H	-3.04347	-1.11748	-2.15380

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$SiEt_3$-(tBuNHBn-tBuNBn)

N	1.69409	-0.61238	0.85901
C	0.77328	-0.95190	1.97235
C	0.18676	0.33041	2.57966
C	-0.39276	-1.79901	1.46115
C	1.49307	-1.76331	3.06585
C	2.78066	0.29091	1.22650
C	2.61923	1.75089	0.82429
C	1.56838	2.20490	0.03053
C	1.48876	3.54850	-0.33862
C	2.45599	4.45277	0.08587
C	3.50846	4.00737	0.88423
C	3.58645	2.66823	1.24668
Si	1.95294	-1.62161	-0.56306
C	3.27275	-0.74705	-1.61391
C	0.42712	-1.81085	-1.66599
C	2.60050	-3.34105	-0.09040
C	3.21172	-1.06702	-3.11496
C	3.12882	-4.16665	-1.27111
C	-0.22762	-0.47316	-2.02652
N	-2.96532	1.42589	-0.06716
C	-2.78388	2.78526	-0.60104
C	-2.09766	3.58264	0.50948
C	-4.15709	3.39543	-0.89255
C	-1.91665	2.82146	-1.86947
C	-3.58317	0.43963	-0.94542
C	-3.57080	-0.91730	-0.27988
C	-3.95264	-1.04341	1.05932
C	-3.93901	-2.28643	1.68262
C	-3.53117	-3.41986	0.97996
C	-3.14438	-3.30207	-0.35153
C	-3.16781	-2.05627	-0.97704
H	-2.05803	1.06954	0.23337
H	-0.49000	0.08070	3.40239
H	0.96040	0.99774	2.97029
H	-0.38000	0.88433	1.82427
H	-1.08576	-1.99979	2.28221
H	-0.05918	-2.76809	1.07609
H	-0.95523	-1.28523	0.67591
H	2.31433	-1.20703	3.52583
H	0.79321	-2.03066	3.86379
H	1.90051	-2.68650	2.64261
H	2.94083	0.26439	2.31050
H	3.73210	-0.05693	0.80326
H	0.81457	1.49053	-0.29098
H	0.66386	3.88863	-0.95808
H	2.39183	5.49732	-0.20113
H	4.26783	4.70512	1.22337
H	4.41125	2.32292	1.86699
H	3.18358	0.33744	-1.47585
H	4.26412	-1.01747	-1.22567
H	0.78117	-2.30445	-2.58131
H	-0.31522	-2.48605	-1.22738
H	1.81169	-3.90048	0.42864
H	3.40095	-3.19993	0.64860
H	4.03711	-0.59391	-3.65478
H	3.26570	-2.14235	-3.31063
H	2.28048	-0.70481	-3.56056
H	3.44969	-5.16490	-0.95882
H	3.98990	-3.67902	-1.73868
H	2.36504	-4.29657	-2.04535
H	-0.97398	-0.57462	-2.82226
H	-0.73499	-0.04129	-1.15560
H	0.51188	0.26401	-2.36275
H	-1.93225	4.61950	0.20110
H	-1.12108	3.14740	0.75262
H	-2.71310	3.57381	1.41281
H	-4.05206	4.45634	-1.13739
H	-4.64668	2.90856	-1.74133
H	-4.80288	3.29916	-0.01523
H	-0.93925	2.36263	-1.68026
H	-2.38657	2.28422	-2.69899
H	-1.75224	3.85360	-2.19680
H	-4.62139	0.74539	-1.12534
H	-3.10209	0.35049	-1.93340
H	-4.24394	-0.15002	1.60300
H	-4.24086	-2.37244	2.72209
H	-3.51272	-4.38834	1.46962
H	-2.82061	-4.17789	-0.90559
H	-2.85848	-1.96541	-2.01557

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$[SiPhH_2$-$(tBuNHBn)_2]^+$

N	0.87412	1.65937	0.67997
C	0.16187	2.59295	1.69617
C	-0.24249	1.72898	2.89161
C	1.09029	3.73196	2.12060
C	-1.09311	3.18587	1.04597
C	0.93672	2.27277	-0.70602
C	1.62584	1.41960	-1.73892

C	2.84005	1.81963	-2.30272
C	3.42710	1.06325	-3.31554
C	2.80881	-0.10267	-3.76159
C	1.59594	-0.50650	-3.20390
C	1.00320	0.26076	-2.20824
Si	2.61527	1.11142	1.23241
C	2.97261	-0.66312	0.87824
C	2.80277	-1.58266	1.92710
C	3.04475	-2.93839	1.73002
C	3.47532	-3.38906	0.48436
C	3.67867	-2.48475	-0.55717
C	3.43391	-1.13046	-0.36202
N	-1.54188	-0.51868	0.42020
C	-1.19442	-1.93518	0.75929
C	-0.06152	-2.35170	-0.17798
C	-2.37043	-2.90176	0.56093
C	-0.70752	-1.97888	2.20675
C	-2.82951	-0.05311	1.00303
C	-3.98479	-0.07362	0.02675
C	-5.16155	-0.76813	0.30479
C	-6.21660	-0.76772	-0.60431
C	-6.10444	-0.07260	-1.80477
C	-4.93555	0.62907	-2.09132
C	-3.88654	0.62998	-1.17816
H	0.24352	0.82651	0.60757
H	-0.77638	2.35173	3.61308
H	-0.90476	0.91790	2.57774
H	0.61792	1.29663	3.40651
H	0.51415	4.42135	2.74279
H	1.46177	4.30593	1.26724
H	1.93818	3.39224	2.71824
H	-0.85685	3.99153	0.34723
H	-1.68046	2.42554	0.52478
H	-1.72036	3.61034	1.83315
H	-0.09144	2.45280	-1.02015
H	1.44172	3.23600	-0.60762
H	3.32048	2.73296	-1.96203
H	4.36352	1.38730	-3.75641
H	3.26525	-0.69010	-4.55117
H	1.10642	-1.40854	-3.55575
H	0.04591	-0.03662	-1.79039
H	3.45539	2.11140	0.55240
H	2.61330	1.29847	2.68940
H	2.48330	-1.24074	2.90902
H	2.90749	-3.63820	2.54749
H	3.66717	-4.44577	0.32860
H	4.03288	-2.83389	-1.52149
H	3.60431	-0.43754	-1.17927
H	-1.68395	-0.51057	-0.59084
H	0.29191	-3.35459	0.07541
H	0.78894	-1.66831	-0.10778
H	-0.40806	-2.37510	-1.21861
H	-2.03226	-3.93009	0.71632
H	-3.18682	-2.71682	1.26369
H	-2.77394	-2.82389	-0.45373
H	-0.38668	-2.99089	2.46960
H	0.14604	-1.30660	2.33713
H	-1.49072	-1.68580	2.91305
H	-3.07380	-0.65930	1.87900
H	-2.70491	0.96846	1.37740
H	-5.25503	-1.31362	1.24035
H	-7.12563	-1.31353	-0.37486
H	-6.92536	-0.07381	-2.51363
H	-4.84591	1.18081	-3.02123
H	-2.98203	1.19461	-1.40469

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$SiPhH_2$-(tBuNHBn-tBuNBn)

N	1.13990	1.95410	0.77683
C	0.03812	2.46925	1.62498
C	-0.19823	1.49390	2.78753
C	0.37783	3.85526	2.19337
C	-1.26243	2.55993	0.80604
C	1.33993	2.62904	-0.51255
C	1.92479	1.70229	-1.55919
C	3.13296	2.00533	-2.18717
C	3.66490	1.15703	-3.15716
C	2.98656	-0.00670	-3.50595
C	1.78018	-0.31841	-2.87937
C	1.25225	0.52727	-1.90948
Si	2.61258	1.26696	1.43492
C	2.81233	-0.57820	1.16274
C	2.35997	-1.50762	2.10978
C	2.53660	-2.87710	1.91781
C	3.16966	-3.34008	0.76733
C	3.62752	-2.43254	-0.18571
C	3.45326	-1.06592	0.01373
N	-1.50233	-0.99904	0.25884
C	-1.30613	-2.44754	0.05957
C	-0.06131	-2.59413	-0.81395
C	-2.51706	-3.02799	-0.67395
C	-1.09019	-3.18950	1.38801
C	-2.70497	-0.59674	0.97571
C	-3.83157	-0.14081	0.06428
C	-5.14239	-0.11764	0.54555
C	-6.18570	0.34345	-0.25083
C	-5.93000	0.78535	-1.54709
C	-4.62714	0.75967	-2.03622
C	-3.58384	0.29942	-1.23578
H	-0.66754	-0.61482	0.69768
H	-1.10022	1.77918	3.33646
H	-0.32865	0.46921	2.42115
H	0.63042	1.49604	3.49857
H	-0.44638	4.24564	2.79947
H	0.56609	4.56769	1.38379
H	1.27280	3.80388	2.82226
H	-1.28382	3.43506	0.15160
H	-1.39585	1.66408	0.19046
H	-2.12154	2.65084	1.47757
H	0.37447	2.98165	-0.88332
H	1.98777	3.51658	-0.42609
H	3.66579	2.90989	-1.90510

H	4.60775	1.40457	-3.63454
H	3.39609	-0.67163	-4.25983
H	1.25664	-1.23142	-3.14385
H	0.32360	0.27010	-1.40052
H	3.75927	1.94572	0.77900
H	2.68835	1.50945	2.89633
H	1.87259	-1.15973	3.01949
H	2.18151	-3.58078	2.66478
H	3.30686	-4.40619	0.61472
H	4.11983	-2.78773	-1.08589
H	3.81632	-0.36910	-0.73944
H	0.20100	-3.64789	-0.94983
H	0.79968	-2.08644	-0.36220
H	-0.25152	-2.14863	-1.79489
H	-2.34382	-4.08574	-0.89389
H	-3.43041	-2.95423	-0.07520
H	-2.68630	-2.49467	-1.61333
H	-0.88379	-4.24990	1.21051
H	-0.23455	-2.76225	1.92034
H	-1.97018	-3.12879	2.03554
H	-3.08910	-1.38836	1.63634
H	-2.45282	0.23834	1.63900
H	-5.34629	-0.46823	1.55516
H	-7.19953	0.35205	0.13741
H	-6.74240	1.14162	-2.17239
H	-4.42104	1.09671	-3.04758
H	-2.56549	0.25764	-1.61040

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Phenylphosphine-BEt_3

C	-1.667526	-2.549894	0.085804
C	-1.855880	-3.740054	-0.610360
C	-0.794972	-4.320294	-1.299794
C	0.455034	-3.706116	-1.298193
C	0.646228	-2.511502	-0.611764
C	-0.414570	-1.930252	0.091675
P	-0.161354	-0.333723	0.931462
B	0.341430	1.384284	-0.143787
C	0.889413	2.383030	1.016173
C	-0.142578	2.905522	2.020398
C	1.474531	0.891445	-1.195846
C	2.844640	0.548544	-0.602105
C	-1.059172	1.844307	-0.823754
C	-1.583941	0.966822	-1.964501
H	-2.498809	-2.102143	0.622836
H	-2.831652	-4.214392	-0.610696
H	-0.942548	-5.249240	-1.840636
H	1.282949	-4.154150	-1.837487
H	1.620519	-2.030461	-0.625719
H	0.727871	-0.671715	1.972877
H	1.734360	1.943126	1.564968
H	1.321313	3.242442	0.479240
H	0.296081	3.592765	2.750666
H	-0.954290	3.436337	1.514215
H	-0.606048	2.089880	2.591975
H	1.601916	1.718696	-1.911414
H	1.117183	0.050975	-1.807863
H	3.547500	0.170415	-1.351978
H	2.773220	-0.214056	0.187297
H	3.302367	1.425724	-0.135302
H	-0.879580	2.859071	-1.212994
H	-1.852388	1.971223	-0.072943
H	-2.519743	1.347020	-2.386778
H	-1.773857	-0.062063	-1.632014
H	-0.857135	0.903077	-2.780031
H	-1.348554	-0.238070	1.682133

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[Phenylphosphide-BEt_3]-

C	-1.609184	-2.452221	0.173226
C	-1.892558	-3.574061	-0.599154
C	-0.907083	-4.150925	-1.397984
C	0.367764	-3.587720	-1.401753
C	0.650281	-2.472760	-0.620254
C	-0.331713	-1.863956	0.183476
P	0.118863	-0.420854	1.223508
H	-2.396602	-2.006268	0.775692
H	-2.894521	-3.996776	-0.583285
H	-1.128571	-5.023180	-2.006248
H	1.151349	-4.023344	-2.017023
H	1.654980	-2.056227	-0.627109
H	-1.201036	-0.200255	1.711682
B	0.339159	1.223019	-0.035533
C	0.855560	2.412031	0.973163
C	-0.167531	2.898421	2.004606
C	1.478502	0.861137	-1.153773
C	2.899469	0.645374	-0.623058
C	-1.082875	1.633183	-0.738995
C	-1.540563	0.751655	-1.905342
H	1.766613	2.105814	1.508119
H	1.155187	3.272069	0.347563
H	0.212509	3.705073	2.646601
H	-1.074411	3.270159	1.514261
H	-0.476717	2.078480	2.664928
H	1.502942	1.691893	-1.881531
H	1.181514	-0.018942	-1.743690
H	3.613314	0.344936	-1.402691
H	2.916177	-0.126515	0.157296
H	3.288288	1.559179	-0.159758
H	-0.985804	2.670909	-1.109840
H	-1.890749	1.671572	0.007617
H	-2.501947	1.070103	-2.332383
H	-1.647586	-0.292761	-1.593181
H	-0.805317	0.764184	-2.718199

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Phenylphosphine-BPh_3

C	-2.506128	-1.117461	-2.392745
C	-2.920419	-2.363779	-2.851643
C	-1.985311	-3.372849	-3.064596
C	-0.635278	-3.135692	-2.817153
C	-0.211873	-1.893895	-2.354186

C	-1.151208	-0.875419	-2.146626
P	-0.628425	0.709720	-1.427940
B	0.228767	0.693804	0.455723
C	0.706640	2.229616	0.633855
C	2.021060	2.563391	0.988973
C	1.406653	-0.386930	0.180479
C	1.416452	-1.660781	0.764955
C	-0.970884	0.237651	1.440684
C	-1.711812	-0.940647	1.233850
C	2.415792	3.886102	1.184483
C	1.501312	4.921866	1.021639
C	0.184841	4.621771	0.678867
C	-0.198429	3.296651	0.496169
C	2.378170	-2.614752	0.432189
C	3.366815	-2.319452	-0.501252
C	-2.740302	-1.326529	2.089233
C	-3.057361	-0.542507	3.195565
C	-2.334679	0.622527	3.432647
C	-1.313693	1.004323	2.564228
C	3.398879	-1.052531	-1.082926
C	2.434862	-0.108810	-0.740753
H	-3.240152	-0.336066	-2.218490
H	-3.973239	-2.545191	-3.040486
H	-2.308983	-4.345365	-3.420934
H	0.095059	-3.921767	-2.977574
H	0.841847	-1.724897	-2.149653
H	0.226583	1.266166	-2.396676
H	2.750796	1.769671	1.123505
H	0.654009	-1.914094	1.495363
H	-1.471304	-1.584707	0.390005
H	3.441493	4.106984	1.464976
H	1.807870	5.952957	1.167664
H	-0.543165	5.419037	0.561645
H	-1.242230	3.082085	0.267974
H	2.352208	-3.592887	0.903412
H	4.112516	-3.062768	-0.765832
H	-3.291127	-2.241929	1.893500
H	-3.856792	-0.839624	3.867407
H	-2.566953	1.239552	4.295721
H	-0.765817	1.920367	2.766142
H	4.173954	-0.801673	-1.801147
H	2.480203	0.877321	-1.201252
H	-1.775810	1.501172	-1.618319

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[Phenylphosphide-BPh_3]-

C	-2.632447	-1.022825	-2.061693
C	-3.116389	-2.299264	-2.334206
C	-2.239291	-3.326257	-2.673581
C	-0.873902	-3.055021	-2.747719
C	-0.393821	-1.774732	-2.491277
C	-1.262367	-0.729799	-2.131757
P	-0.569665	0.930393	-1.756566
H	-3.324815	-0.241440	-1.760725
H	-4.183145	-2.495873	-2.263256
H	-2.613623	-4.325856	-2.875352
H	-0.175579	-3.846722	-3.005793
H	0.674900	-1.582542	-2.546769
H	-1.824902	1.519238	-1.434707
B	0.208962	0.695813	0.146414
C	0.769637	2.173235	0.562774
C	1.987359	2.331606	1.243884
C	1.443696	-0.351131	-0.050088
C	1.607810	-1.529992	0.690748
C	-0.971368	0.185054	1.143274
C	-1.545057	-1.097742	1.025411
C	2.457188	3.578023	1.655157
C	1.716311	4.727508	1.394950
C	0.501897	4.607817	0.723377
C	0.046720	3.354515	0.320128
C	2.681787	-2.398336	0.483100
C	3.644108	-2.109074	-0.477507
C	-2.589035	-1.528593	1.839587
C	-3.106972	-0.688165	2.823021
C	-2.558272	0.581604	2.974670
C	-1.514014	1.000837	2.151052
C	3.525808	-0.931184	-1.216094
C	2.450021	-0.076945	-0.998188
H	2.585738	1.447795	1.453116
H	0.875501	-1.778583	1.453964
H	-1.164772	-1.779114	0.268339
H	3.406916	3.651810	2.180104
H	2.079136	5.702378	1.710093
H	-0.091583	5.493962	0.510765
H	-0.910883	3.289257	-0.193483
H	2.764046	-3.305304	1.077676
H	4.478768	-2.784649	-0.645619
H	-3.001592	-2.525164	1.700183
H	-3.921968	-1.019588	3.461497
H	-2.942579	1.251439	3.740911
H	-1.104689	1.997204	2.296865
H	4.274828	-0.680531	-1.963654
H	2.374257	0.839301	-1.581355

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Phenylphosphine-B(C_6F_5)Ph_2

C	-2.352008	-1.362900	-2.398510
C	-2.685381	-2.643226	-2.828663
C	-1.684528	-3.577398	-3.081893
C	-0.346734	-3.232914	-2.905621
C	-0.002836	-1.955105	-2.477591
C	-1.009223	-1.015048	-2.225552
P	-0.558049	0.627715	-1.601526
B	0.140778	0.737779	0.300410
C	0.545816	2.287298	0.509453
C	1.785552	2.663651	1.042886
C	1.333697	-0.343328	0.123820
C	1.201127	-1.670017	0.558990
C	-1.008096	0.302064	1.362413
C	-2.376926	0.251332	1.145835
C	2.096541	3.999941	1.286523
C	1.170654	4.998956	0.999882

C	-0.075686	4.650379	0.485389
C	-0.378472	3.312247	0.253349
C	2.169770	-2.633284	0.288198
C	3.307229	-2.295520	-0.440363
C	-3.308146	-0.064832	2.127321
C	-2.865568	-0.336244	3.412183
C	-1.505399	-0.282786	3.690075
C	-0.615421	0.039714	2.675003
C	3.468429	-0.985341	-0.886407
C	2.493909	-0.030146	-0.605739
F	-2.883857	0.531789	-0.078459
F	-4.610442	-0.101624	1.845580
F	-3.734819	-0.641572	4.371418
F	-1.073455	-0.533858	4.924255
F	0.680891	0.094996	2.999331
H	-3.135183	-0.641159	-2.191045
H	-3.728165	-2.909504	-2.964658
H	-1.947722	-4.575597	-3.416357
H	0.435367	-3.959633	-3.098429
H	1.043304	-1.695371	-2.334690
H	0.495395	1.024990	-2.439515
H	-1.596363	1.453683	-2.061216
H	0.309927	-1.963978	1.107816
H	2.032483	-3.650942	0.641034
H	4.063262	-3.044137	-0.655746
H	4.353249	-0.706830	-1.450945
H	2.636145	0.987848	-0.964357
H	2.514553	1.894846	1.284275
H	3.064201	4.261093	1.704363
H	1.413764	6.040482	1.185179
H	-0.812560	5.419206	0.273386
H	-1.372085	3.056172	-0.115153

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[Phenylphosphide-B(C_6F_5)Ph_2]-

C	-2.258087	-1.519824	-2.048956
C	-2.471256	-2.869740	-2.316043
C	-1.436061	-3.661455	-2.806857
C	-0.183577	-3.089218	-3.015511
C	0.030108	-1.742896	-2.735862
C	-1.003449	-0.926216	-2.252592
P	-0.765489	0.863951	-1.865715
B	0.023422	0.781498	0.027044
C	0.517494	2.293689	0.396167
C	1.679630	2.534285	1.147535
C	1.206403	-0.323298	-0.057546
C	1.016095	-1.667993	0.295526
C	-1.102772	0.380178	1.165182
C	-2.488195	0.414221	1.039624
C	2.062839	3.819233	1.527524
C	1.285371	4.917854	1.170752
C	0.119002	4.710326	0.438575
C	-0.252725	3.420963	0.064759
C	1.992795	-2.640406	0.091092
C	3.214256	-2.298237	-0.480743
C	-3.373452	0.109603	2.070350
C	-2.880407	-0.231682	3.317023
C	-1.507382	-0.258697	3.509692
C	-0.664171	0.053401	2.451787
C	3.437606	-0.971139	-0.845272
C	2.449975	-0.012406	-0.636459
F	-3.077075	0.764285	-0.118874
F	-4.697501	0.154394	1.870542
F	-3.713585	-0.524591	4.322727
F	-1.015988	-0.572054	4.715753
F	0.646655	0.033169	2.733160
H	-3.075829	-0.911592	-1.674615
H	-3.452873	-3.303364	-2.143465
H	-1.601981	-4.714076	-3.018397
H	0.640546	-3.697275	-3.378976
H	1.025128	-1.322320	-2.859732
H	0.505235	0.964389	-2.495310
H	0.059260	-1.972170	0.716413
H	1.791901	-3.672219	0.368575
H	3.979351	-3.052389	-0.644405
H	4.384281	-0.683167	-1.296645
H	2.639760	1.014594	-0.943924
H	2.294386	1.688630	1.444825
H	2.971159	3.962588	2.108004
H	1.581686	5.921708	1.463371
H	-0.504146	5.555984	0.157639
H	-1.171494	3.278310	-0.500870

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Phenylphosphine-B(C_6F_5)$_2$Ph

C	-2.324540	-1.476245	-2.394182
C	-2.603608	-2.766738	-2.832644
C	-1.563958	-3.651973	-3.103423
C	-0.241760	-3.247333	-2.938025
C	0.047924	-1.959369	-2.501032
C	-0.997043	-1.069444	-2.227291
P	-0.639417	0.603725	-1.622809
B	0.102692	0.737508	0.263070
C	0.581971	2.274625	0.501169
C	1.759367	2.614871	1.168540
C	1.280395	-0.353482	0.078845
C	1.137124	-1.671701	0.528491
C	-1.024241	0.343582	1.360798
C	-2.388567	0.194978	1.160984
C	2.111710	3.930200	1.457438
C	1.265376	4.967271	1.096103
C	0.071488	4.677707	0.450256
C	-0.240123	3.353241	0.184186
C	2.095816	-2.645823	0.256098
C	3.227463	-2.323625	-0.486688
C	-3.289841	-0.106278	2.175108
C	-2.821462	-0.259623	3.470503
C	-1.464533	-0.108617	3.728921
C	-0.604265	0.192065	2.682493
C	3.397730	-1.017390	-0.944458
C	2.435060	-0.053206	-0.662663
F	2.618464	1.680123	1.576205

F	-2.917487	0.341489	-0.073313
F	3.252692	4.199874	2.087793
F	1.591820	6.226504	1.366891
F	-0.757847	5.660450	0.103591
F	-1.420131	3.125736	-0.427327
F	-4.588337	-0.243681	1.912383
F	-3.663234	-0.547460	4.457740
F	-1.008857	-0.247410	4.971347
F	0.690044	0.345858	2.979602
H	-3.138715	-0.792870	-2.177227
H	-3.634547	-3.078337	-2.961945
H	-1.784574	-4.658201	-3.444561
H	0.571481	-3.934574	-3.146000
H	1.082391	-1.654732	-2.368200
H	-1.743281	1.345203	-2.059775
H	0.250011	-1.949732	1.092253
H	1.954516	-3.658739	0.620396
H	3.975687	-3.079937	-0.701935
H	4.282146	-0.750723	-1.514940
H	2.587735	0.963607	-1.022408
H	0.371866	1.065554	-2.481085

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[Phenylphosphide-B(C_6F_5)$_2$Ph]-

C	-1.873940	-1.734002	-1.727767
C	-1.845336	-3.110468	-1.931889
C	-0.837130	-3.688850	-2.699103
C	0.138247	-2.872393	-3.267260
C	0.113720	-1.497369	-3.052567
C	-0.885595	-0.900521	-2.270265
P	-0.877124	0.893780	-1.843946
H	-2.661513	-1.294375	-1.122187
H	-2.610259	-3.735786	-1.480077
H	-0.808633	-4.763895	-2.848642
H	0.934675	-3.309540	-3.863637
H	0.899910	-0.876361	-3.475039
H	0.368300	1.161786	-2.471208
B	-0.090559	0.782660	0.041086
C	0.479398	2.259120	0.420959
C	1.692663	2.455687	1.096384
C	1.047000	-0.387341	-0.072338
C	0.841463	-1.719266	0.292333
C	-1.214147	0.454807	1.200738
C	-2.597995	0.508582	1.091296
C	2.125499	3.721574	1.482441
C	1.347933	4.843391	1.206264
C	0.132389	4.678157	0.547885
C	-0.290012	3.405809	0.169594
C	1.722871	-2.753365	0.000881
C	2.894131	-2.482421	-0.685735
C	-3.470433	0.318165	2.161521
C	-2.963196	0.069006	3.423021
C	-1.586928	0.003947	3.591678
C	-0.760609	0.198822	2.496944
C	3.152074	-1.178153	-1.074586
C	2.238168	-0.176789	-0.770050
F	-0.273243	-2.096360	0.941307
F	-3.202176	0.732623	-0.090900
F	1.450707	-4.008736	0.375500
F	3.759738	-3.462193	-0.973244
F	-4.795832	0.378860	1.978661
F	-3.783349	-0.112435	4.464445
F	-1.080768	-0.243528	4.806175
F	0.557722	0.108988	2.733598
F	4.274296	-0.897806	-1.751602
F	2.545891	1.042782	-1.241613
H	2.311299	1.592712	1.330539
H	3.074094	3.832906	2.001745
H	1.683689	5.833128	1.503626
H	-0.490187	5.542147	0.329372
H	-1.248324	3.294676	-0.335244

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Phenylphosphine-B(C_6F_5)$_3$

C	-1.835185	-1.860763	-1.738457
C	-1.779635	-3.212557	-2.061976
C	-0.772337	-3.693655	-2.894827
C	0.176829	-2.820998	-3.421517
C	0.126264	-1.466738	-3.107509
C	-0.879139	-0.985008	-2.262974
P	-0.781475	0.716182	-1.649530
B	-0.053431	0.757052	0.246770
C	0.550590	2.239112	0.511697
C	1.758812	2.484610	1.159762
C	1.027254	-0.441077	0.042630
C	0.760636	-1.769161	0.373187
C	-1.201994	0.468541	1.352384
C	-2.572089	0.398685	1.161848
C	2.199776	3.765405	1.471619
C	1.416052	4.862877	1.143759
C	0.199840	4.667432	0.504598
C	-0.200694	3.371280	0.217648
C	1.600580	-2.823439	0.035145
C	2.772146	-2.568879	-0.661498
C	-3.485689	0.199457	2.190263
C	-3.021861	0.072404	3.489742
C	-1.655427	0.137921	3.736402
C	-0.785174	0.334167	2.675540
C	3.078515	-1.264665	-1.023781
C	2.205479	-0.244169	-0.676015
F	2.562354	1.478857	1.512490
F	-0.374670	-2.107666	0.997777
F	-3.097223	0.495238	-0.081980
F	3.365547	3.948459	2.086020
F	1.828398	6.091411	1.435363
F	-0.563941	5.708857	0.181443
F	-1.391200	3.224317	-0.402574
F	1.281141	-4.073590	0.360705
F	3.583331	-3.565640	-0.997725
F	-4.790651	0.133192	1.934511
F	-3.874386	-0.115323	4.490977
F	-1.200920	0.013782	4.979935

F	0.522941	0.387675	2.953389
F	4.183291	-1.009014	-1.721609
F	2.507885	0.981511	-1.135881
H	-2.606927	-1.492087	-1.071372
H	-2.517463	-3.892564	-1.650417
H	-0.724770	-4.751339	-3.131233
H	0.962290	-3.193832	-4.070249
H	0.879527	-0.792006	-3.504858
H	-1.945309	1.383511	-2.043665
H	0.192188	1.294176	-2.478390

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[Phenylphosphide-$B(C_6F_5)_3$]-

C	-1.816958	-1.783720	-1.752443
C	-1.753309	-3.156594	-1.973974
C	-0.734467	-3.697961	-2.753692
C	0.215203	-2.849048	-3.317816
C	0.156908	-1.478117	-3.084105
C	-0.851316	-0.919007	-2.286394
P	-0.896681	0.873367	-1.845839
H	-2.612329	-1.373625	-1.137047
H	-2.498994	-3.807441	-1.526395
H	-0.678039	-4.769861	-2.916868
H	1.018938	-3.257560	-3.924481
H	0.924477	-0.831499	-3.502260
H	0.353111	1.169145	-2.454369
B	-0.110948	0.761110	0.048720
C	0.492799	2.238450	0.433681
C	1.735437	2.484856	1.016413
C	0.996999	-0.429552	-0.063074
C	0.748866	-1.751570	0.301813
C	-1.232224	0.479251	1.215120
C	-2.615392	0.462595	1.092594
C	2.177241	3.754072	1.375705
C	1.349571	4.849106	1.192515
C	0.085885	4.654230	0.658369
C	-0.314696	3.370365	0.311764
C	1.592089	-2.813977	-0.006397
C	2.763669	-2.578656	-0.703366
C	-3.481484	0.282126	2.169204
C	-2.968390	0.121202	3.443511
C	-1.592088	0.135681	3.623343
C	-0.770406	0.315778	2.522258
C	3.061331	-1.281119	-1.092003
C	2.183699	-0.255237	-0.775941
F	2.588661	1.490326	1.289706
F	-0.371972	-2.090736	0.962202
F	-3.216599	0.596390	-0.101065
F	3.388581	3.926451	1.917982
F	1.758644	6.074476	1.536817
F	-0.737202	5.697610	0.501074
F	-1.569500	3.253749	-0.147499
F	1.278599	-4.060543	0.363832
F	3.591608	-3.584795	-1.007538
F	-4.806386	0.268158	1.981811
F	-3.785192	-0.048612	4.488174
F	-1.082430	-0.019200	4.850647
F	0.550413	0.322445	2.759636
F	4.182289	-1.036631	-1.783405
F	2.516238	0.960941	-1.243000

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[Phenylphosphine-$SiEt_3$]$^+$

C	-1.613519	-2.635996	0.076306
C	-1.764997	-3.798455	-0.672835
C	-0.680029	-4.328383	-1.366417
C	0.563375	-3.700343	-1.317690
C	0.726462	-2.533686	-0.579632
C	-0.365452	-2.006427	0.119434
P	-0.169183	-0.473207	1.049830
Si	0.349024	1.466744	-0.169363
C	0.962150	2.627564	1.165784
C	-0.061376	2.921611	2.272431
C	1.650525	0.876758	-1.378746
C	3.008586	0.568949	-0.730965
C	-1.300127	1.915402	-0.931881
C	-1.847990	0.866250	-1.911239
H	-2.460518	-2.230913	0.622257
H	-2.729879	-4.291741	-0.707954
H	-0.802228	-5.236995	-1.945802
H	1.407585	-4.119336	-1.853752
H	1.699498	-2.050840	-0.542407
H	0.748946	-0.698072	2.089338
H	1.889843	2.228557	1.592365
H	1.246564	3.560087	0.660458
H	0.337777	3.642143	2.988627
H	-0.987018	3.339004	1.867524
H	-0.321319	2.020725	2.839953
H	1.764634	1.665437	-2.133686
H	1.263619	0.006513	-1.922784
H	3.709995	0.164680	-1.463597
H	2.926771	-0.163423	0.081667
H	3.459323	1.469097	-0.305908
H	-1.149127	2.871759	-1.450109
H	-2.026030	2.123758	-0.137335
H	-2.788175	1.202323	-2.352599
H	-2.042627	-0.092420	-1.418501
H	-1.148184	0.677529	-2.729769
H	-1.373607	-0.308607	1.749890

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Phenylphosphide-$SiEt_3$

C	-1.739775	-2.175347	0.319191
C	-2.233718	-3.058822	-0.636866
C	-1.359815	-3.716144	-1.498681
C	0.011096	-3.489496	-1.394617
C	0.503265	-2.596946	-0.446694
C	-0.366571	-1.920710	0.418053
P	0.191211	-0.654584	1.637757
Si	0.393137	1.048346	0.130511
C	0.708067	2.630187	1.116356
C	-0.479354	3.034145	1.998953

C	1.800792	0.756369	-1.097508
C	3.197966	0.738135	-0.469579
C	-1.252686	1.172714	-0.801806
C	-1.293406	0.388373	-2.121215
H	-2.426440	-1.675112	0.997366
H	-3.302225	-3.237523	-0.704767
H	-1.743159	-4.406823	-2.242612
H	0.699507	-4.004822	-2.057197
H	1.573405	-2.416640	-0.380868
H	1.566339	-1.004035	1.652180
H	1.607102	2.500688	1.731307
H	0.941564	3.432299	0.403223
H	-0.276688	3.953836	2.555046
H	-1.379283	3.203587	1.399258
H	-0.713978	2.250723	2.725992
H	1.740046	1.553593	-1.851342
H	1.607467	-0.179308	-1.636337
H	3.977792	0.582102	-1.220401
H	3.291729	-0.063020	0.270999
H	3.417182	1.680883	0.041306
H	-1.443220	2.236502	-0.997464
H	-2.064506	0.841413	-0.142052
H	-2.271576	0.474612	-2.603518
H	-1.093230	-0.676425	-1.967135
H	-0.545492	0.765628	-2.825337

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[Phenylphosphine-$SiPhH_2$]$^+$

C	-0.289014	-3.850554	0.431850
C	0.185011	-5.151200	0.309428
C	1.482896	-5.465427	0.709282
C	2.317053	-4.483173	1.237628
C	1.857486	-3.177426	1.371079
C	0.554112	-2.868795	0.968414
P	-0.034310	-1.172818	1.088338
Si	-0.444381	-0.211756	-0.982149
C	-1.460195	-1.523124	-1.784655
C	-2.821650	-1.658586	-1.465863
C	-3.552624	-2.734042	-1.959330
C	-2.931098	-3.679545	-2.775396
C	-1.583441	-3.550316	-3.105296
C	-0.847205	-2.478862	-2.609451
H	-1.301095	-3.610923	0.115041
H	-0.462593	-5.919665	-0.097794
H	1.845024	-6.483106	0.611399
H	3.324577	-4.731859	1.551383
H	2.508212	-2.415709	1.790099
H	0.888424	-0.474358	1.879067
H	-1.206020	-1.147751	1.859161
H	0.916467	-0.044016	-1.520660
H	-1.128042	1.046114	-0.631932
H	-3.318428	-0.920700	-0.839532
H	-4.605220	-2.831363	-1.716711
H	-3.504042	-4.515172	-3.163500
H	-1.107776	-4.281322	-3.750044
H	0.204871	-2.389791	-2.867275

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Phenylphosphide-$SiPhH_2$

C	-0.398967	-4.088781	1.056119
C	0.194964	-5.242286	0.550636
C	1.547964	-5.245553	0.224151
C	2.305698	-4.090298	0.408102
C	1.709416	-2.934433	0.903836
C	0.348044	-2.919044	1.231766
P	-0.547792	-1.403824	1.790745
Si	-0.599990	-0.492877	-0.291244
C	-1.474088	-1.683623	-1.439036
C	-2.818088	-1.492288	-1.786792
C	-3.481003	-2.398560	-2.610124
C	-2.806347	-3.514030	-3.099002
C	-1.470111	-3.720780	-2.763907
C	-0.809701	-2.812679	-1.942205
H	-1.456809	-4.090929	1.304362
H	-0.401822	-6.138077	0.411412
H	2.012686	-6.144447	-0.167909
H	3.362411	-4.086861	0.159771
H	2.303744	-2.032884	1.026756
H	0.587470	-0.665105	2.214219
H	0.789982	-0.259825	-0.760638
H	-1.339421	0.794124	-0.256736
H	-3.353815	-0.623053	-1.413028
H	-4.521674	-2.233750	-2.870881
H	-3.321283	-4.221446	-3.741580
H	-0.941289	-4.590473	-3.141221
H	0.231803	-2.992457	-1.681674

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BEt_3-$(PPhH_2)_2$

C	-0.55341	1.44509	0.72916
C	-1.53583	2.42178	0.85606
C	-2.09916	3.00132	-0.27768
C	-1.68491	2.59782	-1.54452
C	-0.70287	1.62084	-1.67844
C	-0.12958	1.04163	-0.54143
P	1.19577	-0.19762	-0.69139
B	2.96877	-0.12412	0.38826
C	3.56243	-1.62380	0.15612
C	4.06582	-1.96385	-1.25040
C	3.83251	1.05578	-0.31644
C	3.33666	2.48793	-0.09309
C	2.53850	0.17309	1.92514
C	1.69214	-0.90049	2.61839
H	-0.12364	0.99304	1.61773
H	-1.86450	2.72524	1.84479
H	-2.86137	3.76718	-0.17452
H	-2.12293	3.04536	-2.43083
H	-0.38629	1.30381	-2.66760
H	0.50973	-1.42047	-0.52836
H	1.36874	-0.22976	-2.08766
H	4.40641	-1.70947	0.85870
H	2.85171	-2.39838	0.47909

H	4.84716	-1.26769	-1.56930
H	4.48044	-2.97515	-1.31119
H	3.26428	-1.90422	-1.99853
H	4.85349	0.96725	0.08756
H	3.94433	0.88023	-1.39608
H	3.95900	3.22957	-0.60429
H	2.30905	2.62209	-0.45582
H	3.33009	2.74334	0.97095
H	2.04486	1.14949	2.02270
H	3.48312	0.28471	2.48020
H	2.22234	-1.85688	2.65757
H	0.74796	-1.08762	2.08465
H	1.42717	-0.62999	3.64638
C	-1.88802	-1.97923	0.73781
C	-2.27164	-1.52708	1.99931
C	-3.22544	-0.52109	2.12067
C	-3.78151	0.04299	0.97480
C	-3.37762	-0.38765	-0.28428
C	-2.43832	-1.41535	-0.41739
P	-1.88878	-1.89448	-2.10926
H	-1.16149	-2.78445	0.65873
H	-1.82936	-1.97204	2.88532
H	-3.53143	-0.17574	3.10290
H	-4.51696	0.83703	1.06020
H	-3.79261	0.08549	-1.17093
H	-1.25916	-3.11165	-1.74889
H	-3.08734	-2.52645	-2.52772

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[BEt_3-($PPhH_2$-PPhH)]-

C	1.84878	2.30091	0.92715
C	1.60345	3.65165	0.70209
C	0.30962	4.10365	0.44826
C	-0.73398	3.17965	0.43217
C	-0.48564	1.82895	0.65286
C	0.81415	1.34906	0.89127
P	1.19058	-0.42072	1.19856
H	2.86375	1.96802	1.13227
H	2.42989	4.35794	0.72551
H	0.11812	5.15799	0.26970
H	-1.75312	3.50690	0.23739
H	-1.31398	1.12562	0.62612
H	-0.12332	-0.87381	0.88774
B	2.24093	-1.14571	-0.43763
C	2.41603	-2.74349	-0.08934
C	1.13573	-3.58560	-0.13707
C	1.44227	-0.95886	-1.85677
C	1.32292	0.46360	-2.41271
C	3.69329	-0.38963	-0.48420
C	4.62029	-0.62055	0.71316
H	3.13395	-3.16572	-0.81502
H	2.88176	-2.88187	0.89742
H	0.67384	-3.54661	-1.13099
H	1.30296	-4.64468	0.10073
H	0.39057	-3.21070	0.57754
H	1.96812	-1.57921	-2.60647
H	0.43319	-1.39389	-1.79273
H	0.84809	0.49761	-3.40529
H	0.73675	1.10464	-1.74540
H	2.30940	0.92968	-2.51544
H	3.56527	0.69393	-0.62716
H	4.21140	-0.73304	-1.39745
H	4.86881	-1.68268	0.81826
H	4.13364	-0.32094	1.64974
H	5.56784	-0.06922	0.63947
C	-3.92131	0.17297	0.25827
C	-3.85408	1.13853	-0.74430
C	-2.94601	0.99880	-1.79003
C	-2.11726	-0.11952	-1.84156
C	-2.20027	-1.09407	-0.85221
C	-3.09027	-0.94978	0.21769
P	-3.12475	-2.26395	1.50686
H	-4.61068	0.30677	1.08769
H	-4.49674	2.01277	-0.69276
H	-2.86951	1.76695	-2.55301
H	-1.38254	-0.22523	-2.63321
H	-1.53364	-1.95281	-0.89263
H	-3.83777	-1.52136	2.48300
H	-1.85439	-1.98601	2.07323

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BPh_3-($PPhH_2$)$_2$

C	2.164066	-2.413635	-0.395414
C	3.317385	-3.191603	-0.412665
C	4.318528	-2.945970	-1.349505
C	4.166900	-1.920392	-2.278762
C	3.015833	-1.138916	-2.270519
C	2.009969	-1.382883	-1.331077
P	0.572240	-0.277515	-1.231639
B	0.484883	0.899022	0.458320
C	-0.924638	1.691301	0.373232
C	-1.718105	1.847450	1.519872
C	1.787309	1.856475	0.350552
C	3.095921	1.344132	0.266554
C	0.514940	-0.286848	1.564317
C	-0.544728	-1.212618	1.612662
C	-2.862267	2.643701	1.521679
C	-3.261936	3.299994	0.359432
C	-2.503937	3.150581	-0.800394
C	-1.353220	2.363249	-0.783241
C	4.209256	2.173565	0.161784
C	4.049896	3.556777	0.145899
C	-0.530733	-2.306237	2.472302
C	0.552820	-2.502764	3.328580
C	1.598731	-1.584911	3.325158
C	1.576035	-0.494032	2.455033
C	2.769695	4.093532	0.237738
C	1.661540	3.254014	0.333256
H	1.395476	-2.602265	0.349477
H	3.434354	-3.988018	0.314798
H	5.217760	-3.553424	-1.354630
H	4.944941	-1.725181	-3.009257

H	2.906590	-0.331201	-2.988450
H	0.586567	0.336581	-2.496724
H	-0.531313	-1.139631	-1.356347
H	-1.424724	1.339749	2.435139
H	3.254287	0.268401	0.293671
H	-1.402372	-1.073483	0.955177
H	-3.441846	2.754460	2.433901
H	-4.151461	3.922533	0.357132
H	-2.799229	3.658366	-1.714450
H	-0.756084	2.300469	-1.692579
H	5.202033	1.737778	0.096357
H	4.914909	4.208250	0.067249
H	-1.365048	-3.002358	2.470408
H	0.574385	-3.356298	3.999413
H	2.438995	-1.718124	4.000353
H	2.402901	0.209776	2.470027
H	2.630766	5.170759	0.233805
H	0.672502	3.697865	0.401963
C	-3.834061	-0.230802	-0.215107
C	-4.109646	-0.911584	0.968646
C	-3.876111	-2.280565	1.062682
C	-3.340672	-2.965082	-0.027207
C	-3.055483	-2.283886	-1.207369
C	-3.319463	-0.913060	-1.319986
P	-2.883384	-0.032074	-2.878819
H	-4.015106	0.838385	-0.273434
H	-4.501979	-0.362518	1.818946
H	-4.098093	-2.810376	1.983684
H	-3.143289	-4.030377	0.041068
H	-2.636168	-2.827743	-2.051458
H	-3.724028	1.089791	-2.696832
H	-3.785940	-0.717353	-3.731933

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[BPh_3-(PPhH2-PPhH)]-

C	2.08341	-2.67123	-0.58824
C	3.02442	-3.61565	-0.18666
C	4.37200	-3.44595	-0.49892
C	4.76870	-2.32484	-1.22356
C	3.82342	-1.38837	-1.63356
C	2.46480	-1.53682	-1.32082
P	1.29232	-0.20775	-1.82865
B	0.90051	0.72869	-0.03601
C	-0.30966	1.80211	-0.30025
C	-0.97349	2.35497	0.81279
C	2.28801	1.47922	0.36406
C	3.42377	0.76731	0.79727
C	0.36030	-0.36587	1.04744
C	-0.84834	-1.03482	0.77647
C	-1.99243	3.29487	0.68643
C	-2.40946	3.70995	-0.57952
C	-1.77795	3.18273	-1.70113
C	-0.74246	2.25432	-1.55624
C	4.63190	1.39558	1.09059
C	4.75376	2.77713	0.96142
C	-1.42958	-1.94110	1.65350
C	-0.79799	-2.23192	2.86444
C	0.39313	-1.58474	3.17234
C	0.95203	-0.66185	2.28299
C	3.65161	3.51170	0.53321
C	2.44917	2.86957	0.24183
H	1.04095	-2.79767	-0.30836
H	2.70390	-4.48192	0.38580
H	5.10570	-4.18062	-0.17899
H	5.81675	-2.17871	-1.47125
H	4.13842	-0.51291	-2.19569
H	0.13825	-1.04284	-1.87829
H	-0.67615	2.02474	1.80648
H	3.36143	-0.31326	0.90017
H	-1.35341	-0.82069	-0.16225
H	-2.46999	3.70153	1.57533
H	-3.21425	4.43199	-0.68665
H	-2.08856	3.49394	-2.69566
H	-0.25282	1.87548	-2.45163
H	5.48186	0.80082	1.41680
H	5.69391	3.27276	1.18944
H	-2.37982	-2.40596	1.39610
H	-1.23626	-2.94293	3.55989
H	0.89150	-1.78903	4.11738
H	1.86779	-0.15279	2.57044
H	3.72773	4.59119	0.42382
H	1.60493	3.46686	-0.09445
C	-3.74865	0.31287	-0.11318
C	-4.35925	0.47989	1.12683
C	-5.25544	-0.47238	1.60259
C	-5.54964	-1.59251	0.82740
C	-4.94677	-1.75611	-0.41632
C	-4.02881	-0.81344	-0.89226
P	-3.23515	-1.07838	-2.53563
H	-3.02620	1.04886	-0.45569
H	-4.10611	1.35157	1.72246
H	-5.72065	-0.34690	2.57565
H	-6.24919	-2.33948	1.19132
H	-5.18621	-2.62883	-1.01992
H	-2.25957	-2.01984	-2.11361
H	-2.33715	0.01538	-2.45981

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$B(C_6F_5)Ph$-$(PPhH_2)_2$

C	0.78332	3.36636	-1.56261
C	1.02809	4.69212	-1.21865
C	0.40639	5.25132	-0.10532
C	-0.46225	4.48510	0.66772
C	-0.71474	3.15920	0.33143
C	-0.09191	2.59784	-0.79005
P	-0.39237	0.85345	-1.18904
H	1.27829	2.93089	-2.42438
H	1.70581	5.28701	-1.82169
H	0.60000	6.28549	0.16035
H	-0.94500	4.91591	1.53856
H	-1.38621	2.56289	0.94504
H	-1.78253	0.71890	-1.05553

H	-0.23782	0.80654	-2.58514
B	0.42966	-0.52511	0.04425
C	-0.09849	-1.96542	-0.46693
C	-0.53942	-2.93364	0.44609
C	-0.22438	0.05183	1.40847
C	0.49594	0.84962	2.30814
C	2.05140	-0.46157	-0.00940
C	2.83544	0.10928	-1.00098
C	-0.89898	-4.21469	0.03292
C	-0.83564	-4.56143	-1.31509
C	-0.39860	-3.61852	-2.24326
C	-0.03037	-2.34457	-1.81599
C	-0.11601	1.45311	3.40461
C	-1.47982	1.28028	3.62690
C	4.22418	0.06893	-1.01308
C	4.88748	-0.58841	0.01102
C	4.15130	-1.19253	1.02228
C	2.76530	-1.12522	0.98833
C	-2.22125	0.49040	2.74959
C	-1.59798	-0.11346	1.66021
F	2.25586	0.74692	-2.04547
F	4.91475	0.64632	-1.99614
F	6.21638	-0.64319	0.02377
F	4.78121	-1.83249	2.00561
F	2.10445	-1.73808	1.97708
H	-0.59380	-2.67843	1.50107
H	1.55652	1.01997	2.13927
H	-1.22607	-4.94639	0.76624
H	-1.11595	-5.55898	-1.63896
H	-0.33275	-3.87913	-3.29543
H	0.34764	-1.63693	-2.55385
H	0.47172	2.06565	4.08170
H	-1.96008	1.75319	4.47804
H	-3.28514	0.33947	2.90945
H	-2.19517	-0.72425	0.98453
C	-3.74774	-0.90556	-1.42164
C	-3.59268	-2.19962	-0.93226
C	-4.13515	-2.54520	0.30295
C	-4.84483	-1.59827	1.03782
C	-5.00001	-0.30486	0.54473
C	-4.43641	0.06302	-0.68190
P	-4.65929	1.80221	-1.25152
H	-3.31603	-0.64757	-2.38598
H	-3.02578	-2.92935	-1.50237
H	-3.99731	-3.54964	0.68995
H	-5.27794	-1.86496	1.99689
H	-5.56348	0.42638	1.11919
H	-4.01724	1.65254	-2.50715
H	-3.50189	2.35353	-0.63260

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[B(C_6F_5)Ph-($PPhH_2$-PPhH)]-

C	1.50371	3.04977	-1.59893
C	1.98149	4.29445	-1.19724
C	1.27476	5.05179	-0.26625
C	0.09236	4.54436	0.26624
C	-0.37655	3.29462	-0.12820
C	0.31432	2.52208	-1.07463
P	-0.29342	0.87045	-1.63772
H	2.05928	2.47371	-2.33239
H	2.90813	4.67590	-1.61793
H	1.64444	6.02493	0.04450
H	-0.46231	5.11392	1.00707
H	-1.27697	2.89235	0.33073
H	-1.60282	1.04765	-1.11641
B	0.29165	-0.36343	-0.10064
C	-0.27105	-1.85810	-0.44298
C	-0.73197	-2.72256	0.56321
C	-0.33653	0.31939	1.22755
C	0.38560	1.19597	2.05061
C	1.93120	-0.51590	-0.01236
C	2.85155	-0.25337	-1.02252
C	-1.12712	-4.03134	0.29130
C	-1.06701	-4.52823	-1.00908
C	-0.59869	-3.69935	-2.02744
C	-0.21058	-2.39114	-1.74220
C	-0.21199	1.90732	3.09055
C	-1.57222	1.76636	3.34612
C	4.22337	-0.45421	-0.90082
C	4.73608	-0.97086	0.27608
C	3.86335	-1.28296	1.30723
C	2.50199	-1.06618	1.13843
C	-2.31954	0.89598	2.55165
C	-1.70707	0.18808	1.52181
F	2.45440	0.20929	-2.22271
F	5.05044	-0.16632	-1.91438
F	6.05127	-1.17599	0.41380
F	4.34375	-1.80362	2.44388
F	1.72645	-1.43427	2.16839
H	-0.78163	-2.35570	1.58524
H	1.44385	1.35670	1.85188
H	-1.48036	-4.66777	1.09952
H	-1.37282	-5.54850	-1.22504
H	-0.53536	-4.07311	-3.04658
H	0.15883	-1.76026	-2.54834
H	0.38720	2.58690	3.69162
H	-2.04442	2.32448	4.15019
H	-3.38455	0.76377	2.73116
H	-2.31612	-0.47767	0.91282
C	-3.77169	-0.69315	-1.36431
C	-3.68580	-2.02629	-0.97282
C	-4.33817	-2.45934	0.17847
C	-5.09364	-1.56100	0.92731
C	-5.18977	-0.23080	0.52717
C	-4.51210	0.22225	-0.60918
P	-4.60221	2.01745	-1.00737
H	-3.21688	-0.35722	-2.23608
H	-3.06758	-2.71637	-1.53898
H	-4.23545	-3.49224	0.49651
H	-5.60325	-1.89201	1.82748
H	-5.78091	0.46801	1.11496
H	-3.81435	1.97759	-2.18352

H	-3.51650	2.42587	-0.18828

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$B(C_6F_5)_2Ph\text{-}(PPhH_2)_2$

C	-2.45183	-2.23113	-1.90672
C	-3.46240	-3.18700	-1.88878
C	-3.32752	-4.33627	-1.11413
C	-2.17490	-4.53580	-0.35932
C	-1.15800	-3.58622	-0.37490
C	-1.29474	-2.42555	-1.14397
P	0.03075	-1.18137	-1.11906
H	-2.56337	-1.34252	-2.51952
H	-4.35620	-3.03207	-2.48374
H	-4.11915	-5.07820	-1.10237
H	-2.06350	-5.43368	0.23945
H	-0.25554	-3.74205	0.20948
H	0.18551	-0.84775	-2.47033
H	1.17257	-1.94007	-0.84011
B	-0.20349	0.35553	0.21614
C	0.68323	1.62025	-0.29163
C	0.40520	2.90152	0.18464
C	0.37087	-0.28531	1.58681
C	-0.21773	-1.42205	2.16557
C	-1.79906	0.67782	0.19856
C	-2.47721	0.86416	-1.00027
C	1.19632	4.00964	-0.09317
C	2.34009	3.85926	-0.86568
C	2.66870	2.60260	-1.34910
C	1.83890	1.53097	-1.05564
C	0.28089	-1.99554	3.33098
C	1.38159	-1.42729	3.97246
C	-3.83449	1.12251	-1.10660
C	-4.57876	1.25995	0.05562
C	-3.94627	1.12874	1.28332
C	-2.58318	0.85475	1.33764
C	1.97431	-0.29191	3.42867
C	1.47933	0.26001	2.24609
F	-0.64782	3.11030	0.98368
F	-1.80033	0.74349	-2.16640
F	0.87829	5.20873	0.38919
F	3.11498	4.90627	-1.13011
F	3.77727	2.42319	-2.06615
F	2.23513	0.33419	-1.54787
F	-4.41613	1.23299	-2.30128
F	-5.88221	1.51372	-0.00659
F	-4.64928	1.27990	2.40400
F	-2.05065	0.78475	2.55797
H	-1.10850	-1.85161	1.70971
H	-0.20351	-2.87087	3.75395
H	1.76399	-1.86049	4.89148
H	2.82587	0.16856	3.92144
H	1.96829	1.14002	1.83848
C	3.76985	-2.35673	-1.35072
C	3.14416	-3.55900	-1.67577
C	2.48414	-4.29404	-0.69263
C	2.44709	-3.81138	0.61471
C	3.06005	-2.60278	0.93703
C	3.74259	-1.86838	-0.03968
P	4.48477	-0.23566	0.39184
H	4.28495	-1.79532	-2.12537
H	3.18006	-3.92498	-2.69704
H	2.00144	-5.23306	-0.94459
H	1.93585	-4.37079	1.39335
H	3.00215	-2.23336	1.95688
H	5.32413	-0.70357	1.43432
H	5.50896	-0.26313	-0.58613

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$[B(C_6F_5)_2Ph\text{-}(PPhH_2\text{-}PPhH)]\text{-}$

C	-2.48782	0.49918	2.81901
C	-3.72807	0.61580	3.43920
C	-4.45967	1.79619	3.33363
C	-3.93495	2.85740	2.60022
C	-2.70035	2.73329	1.96897
C	-1.95140	1.54883	2.05562
P	-0.28797	1.37244	1.27905
H	-1.91695	-0.41699	2.93853
H	-4.11995	-0.21793	4.01520
H	-5.42544	1.88963	3.82144
H	-4.49230	3.78609	2.51179
H	-2.31306	3.56099	1.38090
H	-0.19726	2.72673	0.87400
B	-0.65339	0.55957	-0.60733
C	0.79203	-0.07649	-1.06720
C	0.98208	-1.35342	-1.59574
C	-1.12906	1.79244	-1.54217
C	-2.37885	2.40440	-1.32851
C	-1.77240	-0.62423	-0.42555
C	-1.66183	-1.57227	0.58969
C	2.23154	-1.88603	-1.90134
C	3.37076	-1.12081	-1.71242
C	3.23727	0.17680	-1.24220
C	1.97340	0.65525	-0.92720
C	-2.78829	3.52529	-2.03857
C	-1.95493	4.08382	-3.00878
C	-2.58261	-2.57793	0.83881
C	-3.68122	-2.70801	0.00455
C	-3.81823	-1.83030	-1.05680
C	-2.86841	-0.83315	-1.26271
C	-0.72096	3.49425	-3.25350
C	-0.32171	2.36926	-2.52991
F	-0.05418	-2.17001	-1.84727
F	-0.60295	-1.54153	1.42434
F	2.34187	-3.12681	-2.38783
F	4.57840	-1.61501	-1.99781
F	4.32146	0.93679	-1.08006
F	1.92901	1.91241	-0.45443
F	-2.41869	-3.41803	1.86759
F	-4.58621	-3.66932	0.21518
F	-4.85445	-1.96480	-1.89358
F	-3.06627	-0.08807	-2.35761
H	-3.04826	1.98204	-0.58206

H	-3.76274	3.96424	-1.83918
H	-2.26927	4.96075	-3.56796
H	-0.06101	3.90818	-4.01184
H	0.64696	1.92930	-2.75308
C	5.38483	-0.61350	1.48413
C	6.24736	0.48046	1.42230
C	5.75696	1.76306	1.63874
C	4.40268	1.95090	1.91242
C	3.54401	0.85979	1.98596
C	4.03094	-0.43682	1.77682
P	2.93352	-1.92379	1.81708
H	5.76367	-1.61488	1.29638
H	7.29801	0.32870	1.19314
H	6.42404	2.61809	1.58008
H	4.00822	2.95179	2.05886
H	2.48375	1.01244	2.18021
H	1.83186	-1.34521	1.14080
H	2.36266	-1.69319	3.09583

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$B(C_6F_5)_3$-$(PPhH_2)_2$

C	-2.88115	-2.10541	1.59499
C	-4.18322	-2.59235	1.60399
C	-5.20521	-1.85521	2.19989
C	-4.92377	-0.63200	2.80045
C	-3.62243	-0.13858	2.79733
C	-2.59605	-0.87261	2.19540
P	-0.97350	-0.09083	1.98171
B	-0.48871	0.29237	0.00816
C	-0.05821	1.85804	0.03224
C	-0.47069	2.81084	-0.89385
C	-1.89523	-0.03920	-0.72791
C	-2.13136	-1.09644	-1.60027
C	0.75210	-0.65663	-0.43532
C	0.93482	-1.95792	0.01993
C	0.01078	4.11463	-0.90224
C	0.95525	4.50848	0.03623
C	1.39638	3.59355	0.98126
C	0.87561	2.30947	0.95513
C	-3.40506	-1.43390	-2.05315
C	-4.50341	-0.70173	-1.63342
C	1.93403	-2.80793	-0.42216
C	2.81296	-2.36381	-1.39961
C	2.67817	-1.07828	-1.89504
C	1.66173	-0.25914	-1.41310
C	-4.31806	0.36970	-0.76768
C	-3.03295	0.67806	-0.36104
F	-1.34825	2.49523	-1.85049
F	-1.13702	-1.88168	-2.03369
F	0.08891	-2.47074	0.94508
F	-0.41581	4.98665	-1.81222
F	1.42796	5.75017	0.03215
F	2.30614	3.94153	1.89012
F	1.31851	1.45773	1.90960
F	-3.57326	-2.46337	-2.88092
F	-5.72418	-1.02384	-2.04743
F	2.07555	-4.02711	0.09945
F	3.78464	-3.15905	-1.83263
F	3.51825	-0.63259	-2.82494
F	1.58092	0.95382	-1.97283
F	-5.36394	1.06993	-0.33480
F	-2.89961	1.68663	0.52286
H	-2.09616	-2.67108	1.10606
H	-4.40189	-3.54441	1.13205
H	-6.22217	-2.23306	2.19019
H	-5.71712	-0.05309	3.26054
H	-3.41490	0.83102	3.23961
H	-0.02020	-0.78482	2.73935
H	-1.12429	1.09802	2.70685
C	4.96144	-1.92105	0.79322
C	5.78881	-1.53613	-0.25665
C	5.77210	-0.21884	-0.71252
C	4.93399	0.71171	-0.10741
C	4.10210	0.32499	0.94280
C	4.10361	-0.99596	1.40025
P	2.92077	-1.47049	2.73434
H	4.96181	-2.95596	1.12582
H	6.43321	-2.26907	-0.73090
H	6.40452	0.07676	-1.54309
H	4.91308	1.73798	-0.46012
H	3.44329	1.05361	1.40349
H	2.78589	-2.83443	2.37015
H	3.85741	-1.74141	3.76411

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$[B(C_6F_5)_3$-$(PPhH_2$-$PPhH)]$-

C	-1.59879	-2.62822	2.14648
C	-2.61913	-3.42474	2.65847
C	-3.62010	-2.86250	3.44524
C	-3.58763	-1.49583	3.71129
C	-2.57969	-0.69851	3.17802
C	-1.56818	-1.24317	2.37331
P	-0.14720	-0.25421	1.73442
B	-0.55425	0.37211	-0.22639
C	0.92309	0.26126	-0.93167
C	1.25097	-0.45540	-2.07780
C	-1.08287	1.92160	-0.16240
C	-2.21344	2.25071	0.58847
C	-1.63776	-0.68503	-0.83036
C	-1.32445	-2.04353	-0.84552
C	2.55202	-0.58596	-2.55866
C	3.59395	0.04789	-1.90406
C	3.31468	0.82560	-0.78857
C	2.00998	0.89983	-0.33175
C	-2.69964	3.53578	0.76041
C	-2.04749	4.59508	0.14527
C	-2.19792	-3.05431	-1.20517
C	-3.47845	-2.72043	-1.61980
C	-3.83723	-1.38509	-1.66490
C	-2.92393	-0.40486	-1.28434
C	-0.93401	4.33094	-0.62958
C	-0.48412	3.01994	-0.77649

F	0.31214	-1.08046	-2.80674
F	-0.09242	-2.43794	-0.46712
F	2.80059	-1.31229	-3.65358
F	4.84917	-0.07142	-2.34490
F	4.30288	1.47074	-0.16692
F	1.80362	1.66652	0.75369
F	-1.82550	-4.33716	-1.14387
F	-4.34698	-3.67152	-1.97596
F	-5.05950	-1.04280	-2.08819
F	-3.36999	0.85528	-1.40679
F	-2.91249	1.27684	1.18735
F	-3.79010	3.76677	1.50071
F	-2.49436	5.84569	0.29414
F	-0.30084	5.33650	-1.24525
F	0.58167	2.88871	-1.58191
H	-0.80808	-3.09088	1.56379
H	-2.62326	-4.49035	2.44710
H	-4.41385	-3.48252	3.85122
H	-4.35851	-1.04339	4.32891
H	-2.58387	0.36823	3.37593
H	-0.48469	0.94227	2.41718
C	5.69148	-1.17523	0.91196
C	6.45518	-0.17945	1.52018
C	5.87782	0.65337	2.47142
C	4.53397	0.49446	2.80838
C	3.77374	-0.50324	2.20878
C	4.35070	-1.35480	1.25763
P	3.38711	-2.67569	0.39499
H	6.13709	-1.81467	0.15441
H	7.49652	-0.04997	1.24068
H	6.46736	1.43596	2.93983
H	4.07151	1.15728	3.53344
H	2.71875	-0.60939	2.45385
H	2.20490	-1.92210	0.19137
H	2.87101	-3.31062	1.55555

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$[SiEt_3\text{-}(PPhH_2)_2]^+$

C	2.15957	0.69832	-1.18540
C	3.29370	1.20447	-1.80978
C	4.41817	1.53182	-1.05316
C	4.41335	1.35635	0.32817
C	3.28179	0.85386	0.96400
C	2.15425	0.52999	0.20418
P	0.68540	-0.15290	0.99682
Si	-0.08514	-2.12236	0.02103
C	-1.30145	-2.74398	1.30510
C	-2.54053	-1.84675	1.44552
C	-0.89630	-1.65753	-1.60051
C	-1.73385	-2.83436	-2.13497
C	1.49570	-3.11469	-0.14566
C	2.32102	-3.23773	1.14290
H	1.27905	0.45084	-1.77334
H	3.30230	1.33947	-2.88575
H	5.30288	1.92260	-1.54401
H	5.29025	1.60952	0.91357
H	3.28166	0.71824	2.04156
H	-0.29151	0.84245	1.16630
H	1.08194	-0.42504	2.31525
H	-1.60264	-3.75384	0.99774
H	-0.79518	-2.86834	2.26921
H	-2.27701	-0.81914	1.72725
H	-3.09518	-1.79264	0.50368
H	-3.21965	-2.22975	2.21002
H	-1.53998	-0.78175	-1.46041
H	-0.12595	-1.38276	-2.33012
H	-1.12478	-3.72964	-2.29298
H	-2.54319	-3.09278	-1.44609
H	-2.19119	-2.57435	-3.09155
H	2.10116	-2.67786	-0.94861
H	1.19974	-4.11059	-0.50087
H	1.72225	-3.61380	1.97772
H	2.74760	-2.27235	1.43734
H	3.15824	-3.92470	1.00524
C	-0.35298	3.39473	0.71737
C	-0.37729	2.90950	-0.58940
C	-1.42449	2.09094	-1.01159
C	-2.48171	1.77277	-0.14611
C	-2.44200	2.25918	1.16639
C	-1.38313	3.06082	1.59623
P	-3.86280	0.73093	-0.79671
H	0.45939	4.03419	1.04625
H	0.41856	3.17044	-1.27990
H	-1.43825	1.72281	-2.03577
H	-3.25356	2.03298	1.85210
H	-1.37566	3.44089	2.61280
H	-4.60495	0.66142	0.40584
H	-4.63617	1.78003	-1.34814

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$SiEt_3\text{-}(PPhH_2\text{-}PPhH)$

C	3.01368	0.82562	-1.40407
C	4.14547	1.59841	-1.16084
C	4.06913	2.70641	-0.32104
C	2.85209	3.03737	0.26941
C	1.72193	2.25910	0.03478
C	1.78882	1.13637	-0.79953
P	0.32210	0.07019	-1.13458
Si	0.84799	-1.59573	0.32264
C	-0.73416	-2.61299	0.54244
C	-1.03945	-3.50797	-0.66531
C	2.19630	-2.67538	-0.44480
C	2.54115	-3.88971	0.42879
C	1.44592	-0.90650	1.97601
C	0.40233	-0.05391	2.70426
H	3.07869	-0.02618	-2.07731
H	5.08689	1.33806	-1.63459
H	4.94994	3.31165	-0.13339
H	2.78160	3.90455	0.91893
H	0.77430	2.52692	0.49633
H	-0.55597	0.71708	-0.22886
H	-0.65202	-3.21878	1.45418

H	-1.56429	-1.91476	0.71423
H	-1.03474	-2.93483	-1.59898
H	-0.28931	-4.29813	-0.77048
H	-2.01791	-3.99078	-0.57879
H	1.86298	-3.00348	-1.43691
H	3.09295	-2.06535	-0.60654
H	2.94499	-3.57933	1.39714
H	1.65686	-4.50530	0.62655
H	3.28799	-4.53204	-0.04660
H	2.35417	-0.31800	1.79577
H	1.74516	-1.75478	2.60581
H	-0.53077	-0.60827	2.85768
H	0.15407	0.83930	2.12305
H	0.75873	0.27499	3.68508
C	-2.21943	2.85091	1.00317
C	-2.48087	2.88904	-0.36555
C	-3.03318	1.78127	-1.00081
C	-3.30355	0.60880	-0.28598
C	-3.04740	0.58408	1.08823
C	-2.51476	1.70046	1.73011
P	-3.98486	-0.83192	-1.21246
H	-1.79710	3.71755	1.50211
H	-2.25876	3.78402	-0.93778
H	-3.24094	1.82218	-2.06685
H	-3.25806	-0.31392	1.66330
H	-2.31926	1.66455	2.79748
H	-4.02389	-1.73347	-0.11841
H	-2.74094	-1.32553	-1.68903

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$[SiPhH_2\text{-}(PPhH_2)_2]^+$

C	-0.298651	-3.544977	0.279696
C	0.327729	-4.780191	0.158516
C	1.690637	-4.903806	0.423402
C	2.438469	-3.796708	0.815392
C	1.825408	-2.556422	0.948444
C	0.458705	-2.436522	0.678078
P	-0.322795	-0.820187	0.771625
Si	-0.835126	-0.032236	-1.337015
C	-1.771591	-1.468379	-2.021970
C	-3.108656	-1.682624	-1.648983
C	-3.773024	-2.836806	-2.050526
C	-3.108515	-3.784574	-2.828651
C	-1.784322	-3.579636	-3.210723
C	-1.115258	-2.428514	-2.806603
H	-1.359705	-3.450070	0.061092
H	-0.251846	-5.645742	-0.143151
H	2.171778	-5.872005	0.334084
H	3.492194	-3.901606	1.047508
H	2.405117	-1.700430	1.282110
H	0.508651	0.009233	1.533259
H	-1.494549	-0.914747	1.533561
H	0.490783	0.193674	-1.939421
H	-1.607942	1.197719	-1.083699
H	-3.639602	-0.944445	-1.051500
H	-4.807848	-2.994008	-1.766180
H	-3.629335	-4.682053	-3.145590
H	-1.274627	-4.314130	-3.824870
H	-0.080193	-2.280857	-3.103389
C	1.033538	-4.702222	3.872496
C	2.083062	-5.613435	3.770361
C	3.399902	-5.184755	3.908400
C	3.667404	-3.836838	4.144562
C	2.621270	-2.924305	4.234512
C	1.293831	-3.351386	4.110342
P	-0.052182	-2.101999	4.149494
H	0.009431	-5.051396	3.775301
H	1.867662	-6.663119	3.597012
H	4.215023	-5.897963	3.844189
H	4.691192	-3.497693	4.265704
H	2.840845	-1.874962	4.419238
H	0.027569	-1.709857	5.505491
H	-1.136922	-2.988800	4.340450

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$SiPhH_2$-(PPhH2-PPhH)

C	-0.721113	-3.678084	1.058163
C	-0.484011	-5.025988	0.797805
C	0.792260	-5.458847	0.448205
C	1.837294	-4.539146	0.379735
C	1.606775	-3.196827	0.663031
C	0.322120	-2.748006	0.994680
P	0.081519	-0.948253	1.309420
Si	-0.121807	-0.434588	-0.892446
C	-1.306561	-1.561303	-1.803801
C	-2.581729	-1.105744	-2.165467
C	-3.489418	-1.945770	-2.805325
C	-3.133741	-3.260738	-3.092633
C	-1.870906	-3.731833	-2.740379
C	-0.965197	-2.889497	-2.103143
H	-1.726751	-3.343563	1.297658
H	-1.305023	-5.734549	0.850544
H	0.973969	-6.507672	0.236189
H	2.839476	-4.870058	0.125543
H	2.433896	-2.491362	0.637140
H	-1.313311	-0.998131	1.556536
H	1.247406	-0.555095	-1.452356
H	-0.595842	0.966882	-1.024130
H	-2.869581	-0.079681	-1.948502
H	-4.471505	-1.574329	-3.080675
H	-3.839587	-3.917777	-3.591262
H	-1.590498	-4.757320	-2.960010
H	0.013615	-3.276291	-1.825954
C	1.637785	-4.759559	3.832062
C	2.982028	-4.978063	3.541674
C	3.871345	-3.908338	3.495793
C	3.410640	-2.616272	3.737912
C	2.065512	-2.397171	4.019925
C	1.166416	-3.468030	4.078986
P	-0.608843	-3.094361	4.400627
H	0.949559	-5.599642	3.853858
H	3.332267	-5.986822	3.344831

H	4.918956	-4.079813	3.269121	H	-0.586422	-3.241784	5.813226
H	4.096497	-1.775828	3.697628	H	-1.105413	-4.402335	4.177353
H	1.707027	-1.383315	4.178109				