Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

For

Donor-acceptor stabilized silaformyl chloride

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Contents:

(1) Experimental details and physical data

All syntheses and manipulations were carried out under an inert atmosphere of dry nitrogen gas using glove-box or Schlenk-line techniques. The starting materials IPr·$SiCl_2$ (**1**),[1] IPr (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene),[2] and $H_2O{\cdot}B(C_6F_5)_3$[3] were prepared according to the reported methods. THF-d_8 was dried over K-mirror (potassium metal) and distilled under dry nitrogen prior to use. All other solvents were dried and purified by a MBRAUN solvent purification system (MB SPS 800). ^1H, ^{11}B, ^{13}C, ^{19}F, and ^{29}Si NMR spectra were recorded using a Bruker Avance DPX 200, Bruker Avance DPX 300 or Bruker Avance DRX 500 spectrometer. Elemental analyses were performed at the Institut für Anorganische Chemie, Universität Göttingen.

Synthesis of [IPr·SiH(Cl)=O·B(C_6F_5)$_3$] (3): To a 100 mL THF solution of IPr·$SiCl_2$ (**1**) (3.05 g, 6.26 mmol) and IPr (2.50 g, 6.43 mmol) was added drop by drop a 100 mL THF solution of $H_2O{\cdot}B(C_6F_5)_3$ (3.31 g, 6.24 mmol) at –78 ^{0}C. After 4 h, the reaction mixture was slowly warmed to room temperature and stirred overnight. White insoluble precipitate of IPr·HCl separated, which was removed by filtration. Removal of the volatiles under vacuum afforded white solid, which was dissolved in 50 mL toluene. Colorless upper layer was transferred in a flask, to separate oily compound, and concentrated to 30 mL by removal of the volatiles under vacuum. The resulting solution was stored at 4 ^{o}C in a freezer for one week to afford colorless crystals of **3** (1.59 g, 26 %). Elemental analysis (%) calcd for $C_{45}H_{37}BClF_{15}N_2OSi$: C 55.09, H 3.80, N 2.86; found: C 55.07, H 3.78, N 2.81. Mp 162 ºC (dec). ^1H NMR (500 MHz, THF-d_8, 25 ^{o}C): δ 1.18 (d, J = 6.89 Hz, 12 H, CHMe_2); 1.22 (d, J = 6.82 Hz, 12 H, CHMe_2); 2.42 (m, J = 6.84 Hz, 4 H, CHMe$_2$); 5.55 (br, 1 H, SiH); 7.40 (d, J = 7.50 Hz, 4 H, m-C_6H_3); 7.54 (t, J = 8.00 Hz, 2 H, p-C_6H_3); 8.17 (s, 2 H, NCH) . ^{11}B NMR (96 MHz, THF-d_8, 25 ^{o}C): δ –5.28. ^{13}C NMR (75 MHz, THF-d_8, 25 ^{o}C): δ 23.60, 24.85, 26.36, 30.06, 125.53, 127.20, 131.28, 133.00, 140.85, 146.18. ^{19}F NMR (282 MHz, THF-d_8, 25 ^{o}C): δ – 134.36 (d, 6 F, $J_{F\text{-}F}$ = 16 Hz, o-C_6F_5); – 163.94 (m, 3 F, $J_{F\text{-}F}$ = 20 Hz, p-C_6F_5); –167.79 (m, 6 F, m-C_6F_5) . $^{29}Si\{^1H\}$ NMR (99 MHz, THF-d_8, 25 ^{o}C): δ – 49.78 . ^{29}Si NMR (99 MHz, THF-d_8, 25 ^{o}C): δ – 49.8 (d, $J_{Si\text{-}H}$ = 344 Hz).

[IPrH]$^+$[ClB(C_6F_5)$_3$]$^-$ (4): To the oily compound, obtained in the above mentioned reaction, 15 mL of THF was added and the solution was kept at –35 ^{0}C. Colorless crystals of the imidazolium-borate salt [IPrH]$^+$[ClB(C_6F_5)$_3$]$^-$ (**4**) were also isolated (1.58 g, 27%). The

mechanism for the formation of **4** is not known. Compound **4** is air stable, soluble in common organic solvents, and has been characterized by elemental analysis and NMR spectroscopy. $[IPrH]^+[ClB(C_6F_5)_3]^-$ (**4**): Elemental analysis (%) calcd for $C_{45}H_{37}BClF_{15}N_2$: C 57.68, H 3.98, N 2.99; found: C 57.65, H 3.95, N 2.92. Mp 201 ºC. ^{1}H NMR (500 MHz, C_6D_6, 25 ^{o}C): δ 0.94 (d, J = 7.00 Hz, 12 H, CH*Me*$_2$); 0.97 (d, J = 7.00 Hz, 12 H, CH*Me*$_2$); 1.98 (m, J = 7.00 Hz, 4 H, C*H*Me$_2$); 6.69 (s, 2 *H*, NC*H*); 6.97 (d, J = 8.00 Hz, 4 H, *m*-C_6H_3); 7.24 (t, J = 8.00 Hz, 2 H, *p*-C_6H_3) . ^{11}B NMR (96 MHz, C_6D_6, 25 ^{o}C): δ –6.43. ^{13}C NMR (75 MHz, C_6D_6, 25 ^{o}C): δ 23.48, 23.66, 29.11, 124.84, 125.49, 129.39, 132.71, 137.38, 144.59. ^{19}F NMR (188 MHz, C_6D_6, 25 ^{o}C): δ – 131.66 (d, 6 F, $J_{F\text{-}F}$ = 17 Hz, *o*-C_6F_5); – 161.60 (m, 3 F, $J_{F\text{-}F}$ = 20 Hz, *p*-C_6F_5); –166.35 (m, 6 F, $J_{F\text{-}F}$ = 18 Hz, *m*-C_6F_5).

The molecular structure of **4** in the solid state was unambiguously determined by single crystal X-ray diffraction (Fig. S1). Compound **4** crystallizes in the monoclinic space group *P*2(1)/*n*. The molecular structure of **4** contains a well separated imidazolium cation and a borate $[ClB(C_6F_5)_3]^-$ anion (Fig. 2). The boron atom in compound **4** is four-coordinate with three C_6F_5 groups and one chlorine atom. The cationic imidazolium moiety features the bond lengths and angles as formerly observed in imidazolium chloride $[IPr{\cdot}H]^+Cl^-$.[4]

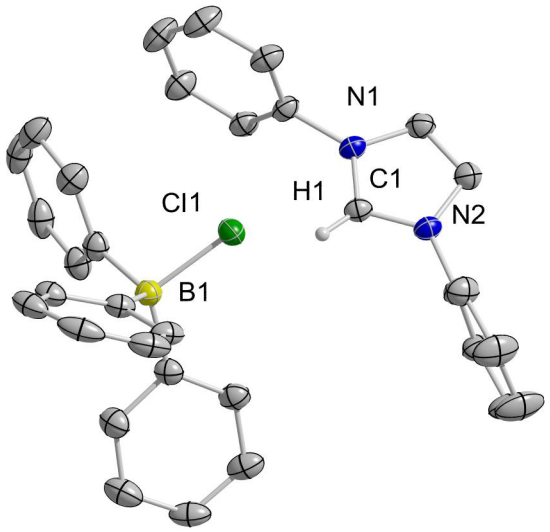


Fig. S1 Representation of the molecular structure of **4** with 50 % probability level for the displacement ellipsoids; isopropyl groups, H and F atoms are omitted for clarity: Selected bond lengths [Å] and angles [°]: N1–C1 1.3321(19), Cl1–B1 1.922 2(18), C1–H1 0.88(2); N1–C1–N2 108.75 (12).

(2) X-ray crystallography

Crystal data for **3** and **4** are summarized in Tables T1 and T2. For compound **4** a single crystal was measured on a Bruker three-circle diffractometer equipped with a SMART 6000 CCD area detector and a CuKα rotating anode. Integration was performed with SAINT.[5] Intensity data for compound **4** was corrected for absorption and scaled with SADABS.[6] Structure solution was accomplished by direct methods.[7] Subsequent least-squares refinement of positions and atomic displacement parameters for non-hydrogen atoms was carried out on F^2 with the program SHELXL-97.[7] Hydrogen-atom positions were freely refined, including isotropic treatment of atomic motion.

Compound **3** turned out to be twinned while being measured on the same Bruker three-circle diffractometer. Integration was also performed with SAINT,[5] whereas twinning required evoking the empirical absorption and scaling program TWINABS.[8] The structure was again solved by direct methods, and subsequently refined on F^2 by full-matrix least-squares methods with the program SHELXL-97.[7] Non-hydrogen atoms were refined anisotropically and hydrogen atoms were added using the riding model. The asymmetric unit of **3** contains two molecules, in which one molecule shows substantial disorder. Interestingly, most of the disorder is due to the imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ (**4**), which may be due the co-crystallization of **4** with **3**. Resolving the disorder required restraining bond lengths and thermal parameters. The contribution of the main component **3** was refined to 80% and that of the imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ (**4**) to 20% site occupancy (Fig. S2). Fig. S3 depicts both conformations, whereas Fig. S1 illustrates the imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ (**4**). Orientation and conformation of the salt in the structure of the product are very close to that found in the salt structure, but also to the product itself (see Fig. S3). This conformational similarity supports assignment of the salt being present, the use of restraints in the refinement and the mechanism of formation of the product. Despite the disorder structure **3** could be refinened to a R-Factor of 5.83%.

The crystal containing compound **3** consists of the (*S*) and (*R*) enantiomers, since it crystallizes in the common space group $P2_1/c$. Further potential disorder around the chiral center is conceivable in case of an enantiomeric excess of one of the two forms. Due to the comparably low remaining residual electron density around the silicon atom it was not necessary to be modelled.

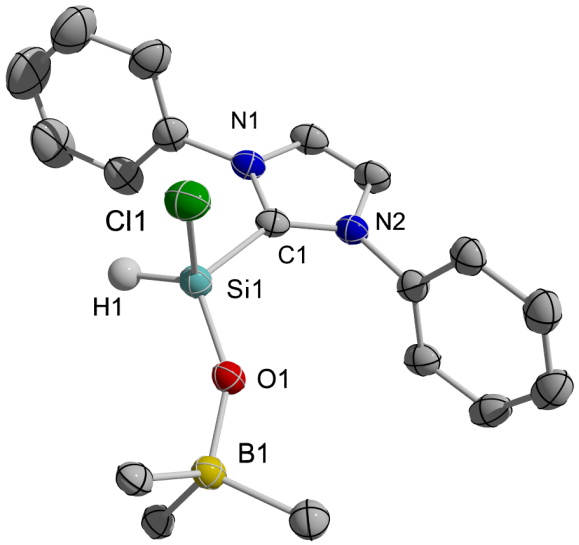


Fig. S2 Displacement ellipsoids structure of one molecule of **3** without disorder with ellipsoids at the 50% probability level; isopropyl groups and H atoms (except the one on the Si atom as located in the difference Fourier map) were omitted. Only *ipso*-C atoms of C_6F_5 groups are shown. The asymmetric unit contains two molecules of compound **3**. Only one molecule of **3** was non-disordered. The second molecule of **3** (80% occupancy) was disordered and superposed to a molecule of the imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ with 20% occupancy. The salt had the same conformation as in the structure determination of **4** and was modelled with restraints. Selected bond lengths [Å] and angles [°] with the values for the second molecule are given in the brackets: Si1−O1 1.568(15) [1.541(3)], Si1−C1 1.911(2) [1.903(4)], Si1−Cl1, 2.049(8) [2.0391(13)], O1−B1 1.492(3) [1.458(5)]; O1−Si1−C1 110.90(9) [109.44(14)], O1−Si1−Cl1 112.65(6) [111.51(11)], C1−Si1−Cl1 103.08(7) [106.59(12)].

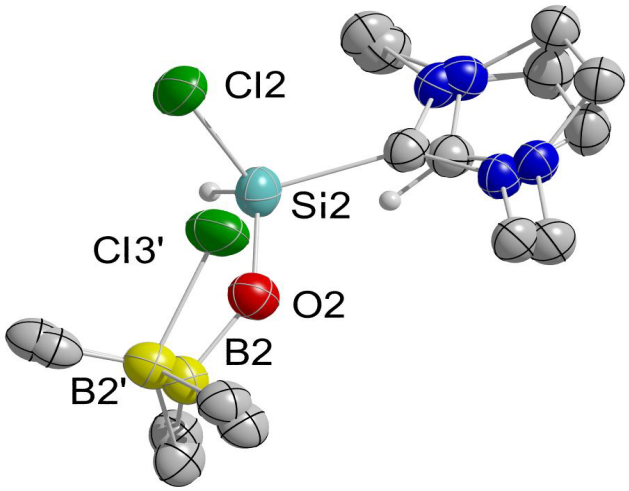


Fig. S3 Displacement ellipsoids structure of one molecule of **3** with disordered imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ (**4**) (ellipsoids are shown at 50% probability level; isopropyl groups and H atoms are omitted, and only *ipso*-C atoms of C_6F_5 groups are shown for clarity). The asymmetric unit contains two molecules of the compound **3**. One molecule of **3** was without any disorder (as shown in Fig. S2). The second molecule of **3** (80% occupancy) was disordered caused mainly by the disordered imidazolium-borate salt $[IPrH]^+[ClB(C_6F_5)_3]^-$ with 20% occupancy, which was modelled.

(3) Tables T1 and T2

Table T1: Crystal data and structure refinement for **3**

Identification code	**3**	
Empirical formula	$C_{45}H_{36.90}BClF_{15}N_2O_{0.90}Si_{0.90}$	
Formula weight	976.61	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/c$	
Unit cell dimensions	a = 19.5187(3) Å	α= 90°.
	b = 24.0524(4) Å	β= 90.6860(10)°
	c = 18.8976(3) Å	γ= 90°.
Volume	8871.3(2) Å^3	
Z	8	
Density (calculated)	1.462 mg/m^3	
Absorption coefficient	1.904 mm^{-1}	
F(000)	3982	
Crystal size	0.50 x 0.25 x 0.15 mm^3	
Theta range for data collection	2.26 to 72.40°.	
Index ranges	-24<=h<=24, 0<=k<=29,	
	0<=l<=21	
Reflections collected	17134	
Independent reflections	17134 [R(int) = 0.0305]	
Completeness to theta = 72.40°	97.5 %	
Absorption correction	semi-empirical from symmetry	
	equivalents	
Max. and min. transmission	0.753579 and 0.651098	
Refinement method	Full-matrix least-squares	
	on F^2	
Data / restraints / parameters	17134 / 7037 / 1759	
Goodness-of-fit on F^2	1.1	
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1577	
R indices (all data)	R1 = 0.0599, wR2 = 0.1595	
Largest diff. peak and hole	0.869 and -0.604 e.Å^{-3}	

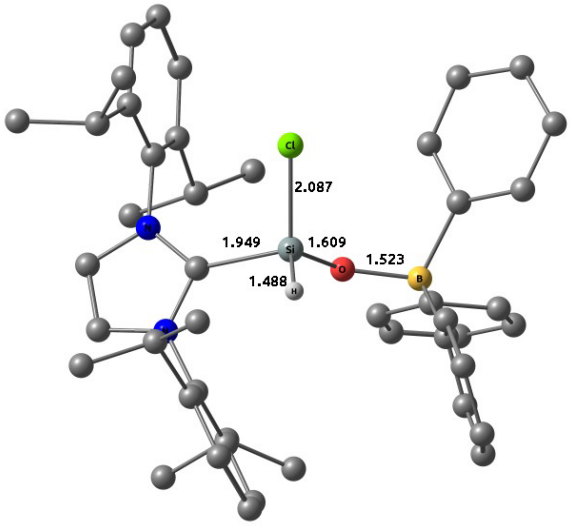
Table T2: Crystal data and structure refinement for **4**

Identification code	1 x	
Empirical formula	$C_{45}H_{37}BCl\,F_{15}N_2$	
Formula weight	937.03	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 12.3598(3) Å	α= 90°.
	b = 18.4204(4) Å	β= 97.7500(10)°
	c = 18.8960(4) Å	γ= 90°.
Volume	4262.80(17) $Å^3$	
Z	4	
Density (calculated)	1.460 mg/m^3	
Absorption coefficient	1.705 mm^{-1}	
F(000)	1912	
Crystal size	0.10 x 0.03 x 0.01 mm^3	
Theta range for data collection	3.37 to 72.36°.	
Index ranges	-15<=h<=10, -21<=k<=22, -23<=l<=21	
Reflections collected	37243	
Independent reflections	8000 [R(int) = 0.0222]	
Completeness to theta = 72.62°	94.80%	
Absorption correction	semi-empirical from symmetry equivalents	
Max. and min. transmission	0.4697 and 0.3963	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8000 / 0 / 725	
Goodness-of-fit on F^2	1.06	
Final R indices [I>2sigma(I)]	$R1$ = 0.0362, $wR2$ = 0.0972	
R indices (all data)	$R1$ = 0.0401, $wR2$ = 0.1040	
Largest diff. peak and hole	0.342 and -0.267 $e.Å^{-3}$	

(4) Theoretical details

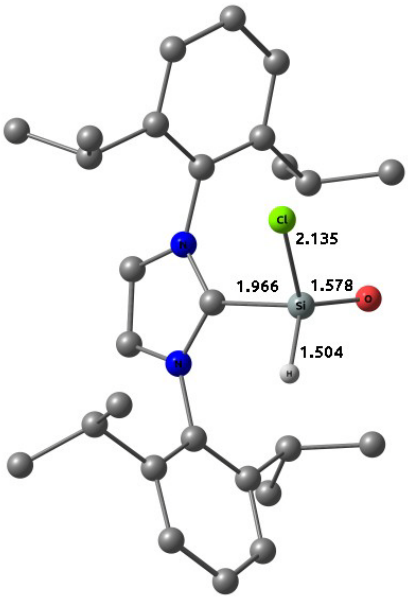
Geometry optimizations without symmetry constraints were carried out using the Gaussian 03 program package.[9] The calculations were performed using density functional theory at the BP86[10,11] level in conjunction with a def2-SVP basis set.[12] Improved single-point energies with a larger def2-TZVPP basis set[13] have been obtained using BP86/SVP optimized geometries. . The dispersion interactions were calculated with the D-3 model developed by Grimme et al.[14] The atomic partial charges were calculated with the NBO method.[15]

Fig. S4 Optimized geometries (BP86/TZVPP) of the molecules. Bond lengths in Å, bond angles in degree.

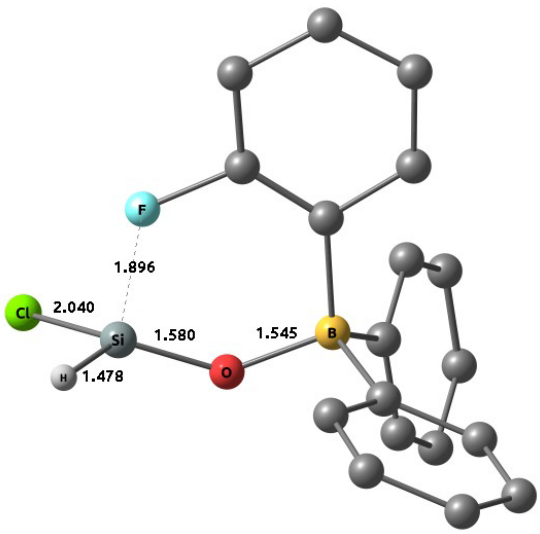


3

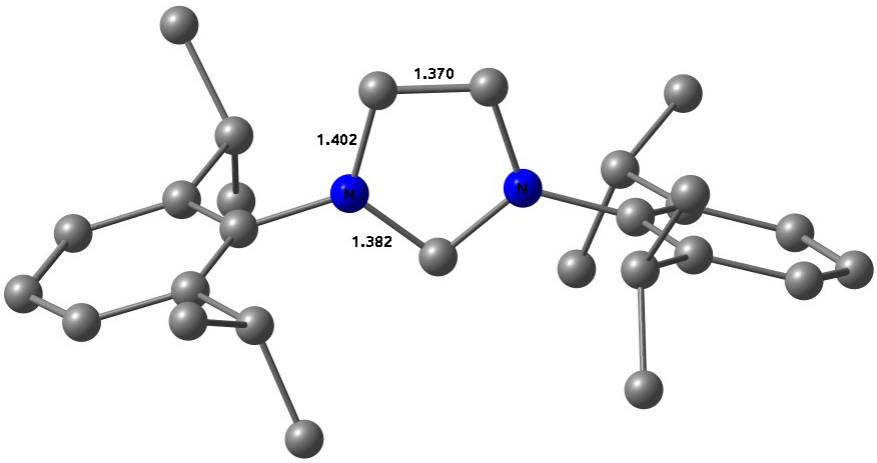
α(O-Si-C) = 107.4, α(O-Si-Cl) = 115.7, α(C-Si-Cl) = 105.5, θ(C-Si.O-B) = 169.7



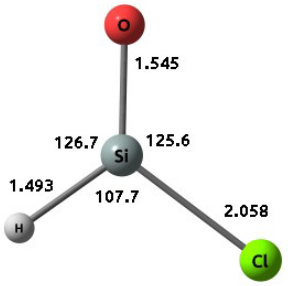
IPr→SiH(Cl)O



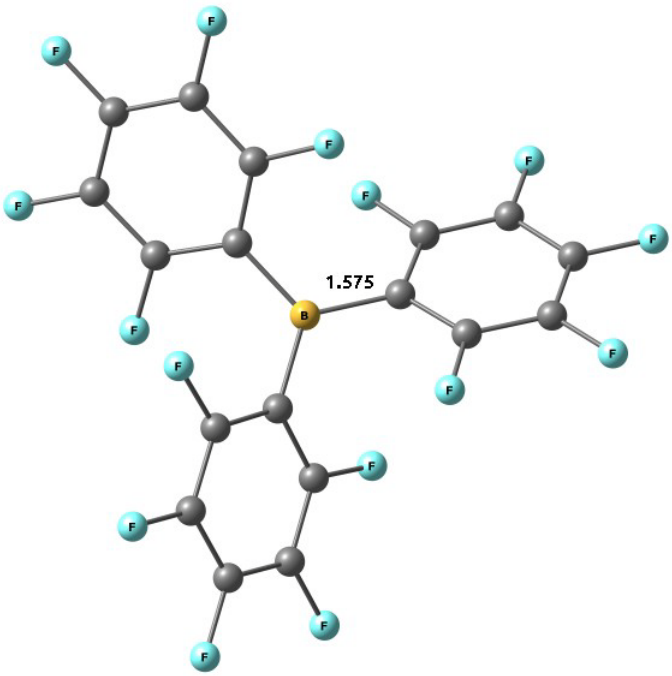
SiH(Cl)O→B(C_6F_5)$_3$



IPr



SiH(Cl)O



$B(C_6F_5)_3$

Table T3. Calculated cartesian coordinates and energies [a.u.] of the complexes.

3
E(RB-P86) = -4191.26953011

C	-2.73160700	-3.11643200	1.13614300
C	-3.46804900	-2.16333200	0.38255300
C	-4.32478800	-2.51149300	-0.69658900
C	-4.38651000	-3.87490200	-1.04730600
C	-3.64192800	-4.83773700	-0.35328700
C	-2.83323100	-4.46233100	0.72722600
N	-3.41838500	-0.75911700	0.78590300
C	-2.55450000	0.21855200	0.36741700
N	-2.96929500	1.37084400	0.98500800
C	-4.08158900	1.11931800	1.77208600
C	-4.36100900	-0.21840900	1.64886200
C	-2.39320900	2.70291200	0.83245700
C	-2.84765400	3.50902500	-0.24647400
C	-2.29969400	4.80330400	-0.35155400
C	-1.35437800	5.26915700	0.57236600
C	-0.93857400	4.45180600	1.63165200
C	-1.44862700	3.14687100	1.79655300
C	-3.91640400	3.04778000	-1.24029900
C	-5.29090000	3.65704800	-0.87805300
C	-1.03291100	2.29931000	2.99947600
C	0.45524600	2.44605100	3.36728900
Si	-1.07111500	0.20759400	-0.89663300
Cl	-1.57331600	-1.22113900	-2.33205200
C	-5.20647100	-1.49476900	-1.42711500
C	-6.65772200	-1.56027100	-0.89481300

C	-1.92911600	-2.74056800	2.38269900
C	-2.83612900	-2.76309600	3.63715400
C	-5.18803400	-1.66030900	-2.95969500
C	-0.69285900	-3.62795900	2.61932900
C	-1.91658600	2.62896000	4.22672600
C	-3.54578300	3.35334900	-2.70560600
O	0.27115600	-0.08568100	-0.06015600
H	-5.14767100	-0.83436500	2.09343200
H	-4.57342100	1.91144900	2.34375200
H	-5.02874400	-4.18613600	-1.88516000
H	-3.69681400	-5.89552200	-0.65508400
H	-2.26339800	-5.22977100	1.27075000
H	-0.19491400	4.82973200	2.34860000
H	-0.93488000	6.28163100	0.46411900
H	-2.61774900	5.45707900	-1.17779400
H	-1.55377800	-1.70609100	2.24529800
H	-4.81346000	-0.47911800	-1.20528000
H	-1.19137300	1.23352900	2.73477500
H	-4.01216700	1.94378800	-1.15392800
H	-7.29244900	-0.79517600	-1.38924900
H	-7.10677900	-2.55532800	-1.09782500
H	-6.71262700	-1.39115400	0.20021600
H	-5.76931300	-0.84415100	-3.43698600
H	-4.15551200	-1.62799200	-3.35810200
H	-5.65385700	-2.61645700	-3.27730900
H	-0.08016900	-3.19084500	3.43267300
H	-0.97374000	-4.65532400	2.93540900
H	-0.05888800	-3.69793000	1.71596500

H	-2.25849800	-2.45578600	4.53352700
H	-3.70752000	-2.08264400	3.55045400
H	-3.22852100	-3.78619700	3.81899200
H	-1.63166700	1.99078000	5.08880200
H	-1.78721300	3.68907300	4.53163600
H	-2.99689200	2.46909900	4.03238800
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H	1.12347900	2.28065400	2.50088300
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H	-5.60501300	3.39105600	0.15246900
H	-5.26175500	4.76524100	-0.94125700
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H	-2.55267400	2.93931000	-2.97277300
H	-1.20197900	1.53971600	-1.54674400
B	1.78244000	-0.07516200	-0.24557600
C	2.49807100	-0.48206400	1.19378900
C	2.20429800	-1.27357400	-1.32312300
C	2.15806800	1.45676400	-0.77140900
C	3.15813700	-1.16801600	-2.35405800
C	3.50323100	-2.23497900	-3.20656500
C	2.89092200	-3.48697700	-3.03377800
C	1.94231000	-3.65017100	-2.01110800
C	1.63390500	-2.55344200	-1.18756500
F	3.80950700	-0.00939700	-2.58623900
F	4.41510400	-2.06938900	-4.17852000
F	3.20739700	-4.51419800	-3.83603000

F	1.34965100	-4.84310000	-1.82586900
F	0.72515100	-2.79238900	-0.20868100
C	2.80367600	2.45715900	-0.02367200
C	3.02260800	3.76761300	-0.49521100
C	2.57109500	4.12705200	-1.77443300
C	1.90506000	3.17031500	-2.56008100
C	1.71898100	1.87969100	-2.04029000
F	3.24543900	2.22148500	1.23426300
F	3.64187500	4.67857900	0.27396700
F	2.75873200	5.37218200	-2.23639300
F	1.45091900	3.50193400	-3.78016500
F	1.05255200	1.00796500	-2.84419700
C	3.89523400	-0.66339500	1.24882600
C	4.59506500	-1.08133000	2.39392300
C	3.87880100	-1.34922600	3.57384200
C	2.48781600	-1.17160700	3.57673100
C	1.83522800	-0.74787300	2.40296800
F	4.64408200	-0.40345800	0.15575100
F	5.92886400	-1.22863300	2.37458300
F	4.51719600	-1.75338500	4.68179700
F	1.77908400	-1.41217200	4.69940100
F	0.48947200	-0.59627200	2.53301300

IPr→SiH(Cl)O

E(RB-P86) = -1984.58874986

C	-3.15843300	1.38671800	-0.08505500
C	-2.57207500	0.12472100	-0.36633300
C	-3.26149400	-1.10705800	-0.21190600

C	-4.58403200	-1.03940000	0.27466600
C	-5.18650100	0.18787700	0.58171600
C	-4.48300400	1.38671900	0.39655300
N	-1.19656300	0.09106300	-0.82963300
C	-0.09887200	0.04006900	-0.01246200
N	0.97723100	-0.02170700	-0.85641100
C	0.55475100	-0.00830700	-2.18219800
C	-0.81538400	0.06418800	-2.16712400
C	2.37889700	-0.07875900	-0.47054700
C	3.10717300	1.13888200	-0.41536200
C	4.47250800	1.05628400	-0.07743100
C	5.07843400	-0.17828500	0.19361500
C	4.33075600	-1.36108200	0.12603600
C	2.96072400	-1.34691000	-0.20991200
C	2.47925200	2.49715300	-0.73480300
C	2.73892500	3.54253300	0.36882500
C	2.18866200	-2.65977000	-0.34811200
C	2.39558600	-3.60703400	0.84885300
C	-2.65281500	-2.46343200	-0.57528600
C	-3.42199500	-3.10219600	-1.75430500
C	-2.41160000	2.70878100	-0.27448000
C	-2.11062100	3.39059500	1.07810600
C	2.95321300	3.01159200	-2.11296700
C	2.54198800	-3.34403800	-1.68898600
C	-2.56714000	-3.41275700	0.63916400
C	-3.16874800	3.65759700	-1.22829200
H	1.26743100	-0.05152200	-3.01115900
H	-1.54928300	0.09534600	-2.97807800

H	5.06974400	1.97950000	-0.01796200
H	6.14590100	-0.21811900	0.46311700
H	4.81720000	-2.32487000	0.34077700
H	-5.14983200	-1.97344300	0.41702700
H	-6.21847500	0.21135900	0.96646000
H	-4.97022600	2.34512100	0.63588200
H	1.10678200	-2.41608000	-0.34770200
H	1.37931300	2.35520200	-0.79192400
H	-1.61120900	-2.29048800	-0.91826100
H	-1.43486300	2.48112200	-0.75139400
H	2.46118500	3.97530100	-2.36285900
H	4.05074800	3.18205100	-2.11957400
H	2.72522100	2.29176000	-2.92654600
H	2.20495600	4.48754200	0.13485900
H	2.38514600	3.17509100	1.35220000
H	3.81778700	3.79011300	0.45741000
H	1.82521100	-4.54450900	0.68134700
H	3.46050900	-3.89036300	0.98976600
H	1.99310300	-3.13605900	1.76738300
H	1.94182700	-4.26863100	-1.82258700
H	2.34889600	-2.68443300	-2.56153000
H	3.61488800	-3.63127000	-1.72278500
H	-2.93334100	-4.04962000	-2.06380200
H	-4.46919200	-3.34489400	-1.47446700
H	-3.46096400	-2.43157900	-2.63872100
H	-2.19042600	-4.40504200	0.31191400
H	-1.85697400	-3.01425300	1.39552200
H	-3.56249500	-3.57368900	1.10565300

H	-2.57649000	4.57912800	-1.40841500
H	-3.36723000	3.18032000	-2.21035100
H	-4.14614800	3.97153100	-0.80514600
H	-1.55723300	4.33979600	0.91847900
H	-3.04664100	3.63444100	1.62369100
H	-1.49475200	2.74272500	1.73379200
Si	-0.18060100	-0.35129000	1.91262900
O	0.00398000	-1.91220200	2.05090300
H	-1.45221800	0.32751400	2.34070200
Cl	1.31383000	0.93682400	2.72727800

SiH(Cl)O→B(C_6F_5)$_3$

E(RB-P86) = -3032.00386075

F	-2.27292200	1.09968200	1.57092200
F	-3.22440400	3.60842900	1.36387800
F	-1.91499000	5.46980300	-0.18739800
F	0.38330500	4.76146700	-1.51043900
F	1.36742300	2.27772600	-1.30908000
F	2.41432900	1.55545500	1.31534100
F	5.02885400	1.08285700	0.84520400
F	5.79007600	-1.04232900	-0.72241700
F	3.87587500	-2.69418700	-1.80271800
F	1.27594700	-2.26298200	-1.32912200
F	-3.74499700	-3.30972100	0.20694800
F	-3.95400700	-3.01338900	-2.53881200
F	-0.31790200	0.00304500	-2.48607000
F	-2.21648300	-1.34742100	-3.84843600
F	-1.90376800	-2.03406600	1.62857600

C	-3.01642500	-2.35322200	-1.85770300
C	-2.91321500	-2.51069800	-0.46509700
C	-1.89945400	-1.77823500	0.16616400
C	-2.11845000	-1.49542300	-2.52636600
C	-1.13861100	-0.80082500	-1.79538100
C	-0.97123100	-0.92165000	-0.39691400
C	3.51250400	-1.64424500	-1.05143000
C	4.49257700	-0.80561400	-0.49677700
C	2.15286500	-1.38067300	-0.79327100
C	4.09991200	0.28219900	0.30389200
C	2.73130800	0.50641300	0.52800600
C	1.70770200	-0.29407000	-0.01982000
C	-0.36276100	1.57311000	0.19288000
C	-1.55147800	1.98763300	0.82136500
C	-2.09039800	3.28112700	0.72723300
C	-1.42692400	4.23016400	-0.07024900
C	-0.24819500	3.86438900	-0.74263000
C	0.25036200	2.55301600	-0.61219600
B	0.15579600	0.02134800	0.39347600
O	0.10057200	-0.29453600	1.90515100
Cl	-0.02207900	-2.65559000	3.90779400
H	-1.92159700	-0.47168400	3.68790100
Si	-0.84458400	-1.09167500	2.88810100

IPr

E(RB-P86) = -1159.17128849

C	-0.68332500	-0.04507800	1.87170800
N	-1.06830700	-0.06973400	0.52408800

C	0.00001200	0.00000500	-0.34955600
N	1.06833600	0.06973800	0.52408600
C	0.68335600	0.04507000	1.87170600
C	-2.44714700	-0.14818000	0.10019400
H	-1.40251200	-0.09366500	2.69639900
H	1.40254700	0.09364400	2.69639500
C	2.44717600	0.14819000	0.10019000
C	-3.21715400	1.04272600	0.04234500
C	-4.56789300	0.93391900	-0.35120700
C	-5.12907500	-0.30700900	-0.67941000
C	-4.34549200	-1.46908100	-0.62204500
C	-2.99208800	-1.41865400	-0.23026700
C	-2.62794800	2.41543800	0.36911500
H	-5.18885100	1.84252200	-0.40676700
H	-6.18551900	-0.37036300	-0.98602600
H	-4.79554700	-2.43810900	-0.88747400
C	-2.13403900	-2.68353500	-0.22196900
C	3.21718500	-1.04271400	0.04232100
C	4.56792300	-0.93389600	-0.35123600
C	5.12910000	0.30703800	-0.67941600
C	4.34552000	1.46911200	-0.62201900
C	2.99211600	1.41867400	-0.23024000
C	2.62798800	-2.41543100	0.36909500
H	5.18888700	-1.84249400	-0.40680700
H	6.18554400	0.37040000	-0.98603200
H	4.79558100	2.43814500	-0.88741400
C	2.13404500	2.68353900	-0.22190300
H	-1.27720100	-2.49313900	0.45897000

C	-2.87608900	-3.92289200	0.31273500
C	-1.54764800	-2.93491400	-1.63001000
C	-3.30692400	3.05165000	1.60060200
H	-1.55694400	2.26739000	0.61719800
C	-2.68268200	3.35421100	-0.85472100
C	2.68270700	-3.35421100	-0.85473700
C	3.30698700	-3.05164400	1.60056900
H	1.55699000	-2.26738700	0.61720200
H	1.27740600	2.49323000	0.45931300
C	2.87619200	3.92301600	0.31238500
C	1.54724500	2.93468200	-1.62981800
H	-2.82824000	4.02113200	1.85434100
H	-4.38450500	3.25035300	1.41709000
H	-3.23592700	2.39347000	2.49125800
H	-2.19650500	4.32552500	-0.62319800
H	-2.16024700	2.90660100	-1.72417500
H	-3.72861500	3.57051500	-1.16034400
H	-0.89417600	-3.83337100	-1.62828600
H	-2.35794100	-3.10335800	-2.37157900
H	-0.94545800	-2.06338600	-1.95949800
H	-2.17395300	-4.77748400	0.40747100
H	-3.32441700	-3.73740900	1.31103200
H	-3.69027000	-4.25124000	-0.36800900
H	2.82831300	-4.02112900	1.85431300
H	4.38456600	-3.25034000	1.41703600
H	3.23600300	-2.39346800	2.49123000
H	2.19650300	-4.32551100	-0.62321000
H	2.16029400	-2.90659800	-1.72420200

H	3.72863900	-3.57054800	-1.16034300
H	2.17402800	4.77757400	0.40722400
H	3.32485800	3.73771100	1.31056300
H	3.69012600	4.25132800	-0.36867100
H	0.89372500	3.83310500	-1.62803700
H	2.35732400	3.10307000	-2.37163400
H	0.94501100	2.06307500	-1.95901200

SiH(Cl)O

E(RB-P86) = -825.333269864

Si	0.00000000	0.71675300	0.00000000
O	1.46877400	1.19579300	0.00000000
H	-1.21928400	1.57881100	0.00000000
Cl	-0.61946500	-1.24586500	0.00000000

$B(C_6F_5)_3$

E(RB-P86) = -2206.62822252

B	-0.00035800	-0.00192400	0.00005900
C	1.29023900	-0.90460900	-0.00105400
C	-1.42829900	-0.66650900	0.00098600
C	0.13715200	1.56716700	0.00028300
C	-2.50472600	-0.13294500	0.74840000
C	-3.78240100	-0.71507900	0.76932700
C	-4.02090300	-1.86996100	-0.00008200
C	-2.98408800	-2.43321200	-0.76844100
C	-1.71462700	-1.83340800	-0.74623500
F	-2.32381200	0.95926300	1.51051200
F	-4.76700800	-0.19034200	1.50566000

F	-5.22957300	-2.43100600	-0.00093100
F	-3.21823900	-3.52397700	-1.50492100
F	-0.76294600	-2.40081300	-1.50698000
C	2.44365200	-0.56580900	-0.74738300
C	3.60052700	-1.36137500	-0.76820700
C	3.63375800	-2.54097200	-0.00001700
C	2.51427800	-2.91587400	0.76732100
C	1.36855000	-2.10436000	0.74497700
F	2.45614400	0.54204700	-1.50832200
F	4.66201000	-1.01538300	-1.50341000
F	4.72631400	-3.30384000	0.00081800
F	2.55459000	-4.03142100	1.50279200
F	0.33214500	-2.49830100	1.50462100
C	-0.73262600	2.39786100	-0.74501300
C	-0.61921000	3.79730500	-0.76682500
C	0.38786900	4.41447600	-0.00026800
C	1.27160200	3.63115700	0.76659600
C	1.13845400	2.23346000	0.74559700
F	-1.70070400	1.85628800	-1.50406100
F	-1.44923900	4.54478200	-1.50119700
F	0.50479400	5.74186000	-0.00062500
F	2.21949800	4.22227800	1.50077600
F	1.99675500	1.53142300	1.50525900

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