Supporting Information:

Bridging Antimony Centers with Electron-Withdrawing Carborane Cages

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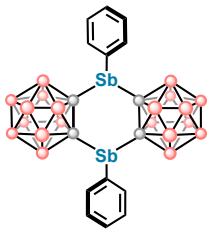
I. General Information and Synthetic Procedures/Characterization

i. General Consideration

Anhydrous manipulations and sample preparation were performed in an inert atmosphere of N_2 using glovebox. Anhydrous solvents were obtained through a Grubb's-type column. All other manipulations were performed in unpurified solvents unless otherwise stated. All commercially available chemicals were used as received. Diphenylantimony chloride ($SbPh_2Cl$) and dichlorophenylstibane ($SbPhCl_2$) were synthesized following previous procedures.[1] Tetrachloro-*o*-benzoquinone (*o*-chloranil) was purified from its protonated form via recrystallization in cyclohexane. *ortho*-Carborane was obtained from Boron Specialties. $SbCl_3$ and *o*-carborane were purified separately by sublimation at 90°C and transferred into the glovebox. Deuterated solvents were obtained from Cambridge Isotope Laboratories. NMR spectra were acquired on Bruker NEO 600 (supported by NIH S10OD028644 to UCLA) or Bruker 400 spectrometers and processed with MestReNova. ^{1}H, $^{13}C\{^{1}H\}$, ^{11}B, and $^{11}B\{^{1}H\}$ NMR data were collected at room temperature with the spectrometer locked to the ^{2}H signal of the stated solvent and are referenced to the residual ^{1}H and ^{13}C resonances of that solvent. Chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz; multiplicities are given as s, d, t, q, m, br.

ii. Experimental



Synthesis of 1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$ [1a]

In an N_2-filled glovebox, *o*-carborane (300 mg, 2.08 mmol) was dissolved in toluene followed by the dropwise addition of 2 equiv. of *n*-BuLi (2.5 M in hexanes, 1.66 mL, 4.16 mmol) to the stirred solution, resulting in the immediate precipitation of the dilithiated cage, $Li_2C_2B_{10}H_{10}$. After stirring for 4 hours, the white solid was collected by filtration, washed thoroughly with toluene, and resuspended in dichloromethane. The resulting suspension was transferred dropwise into a solution of $SbCl_2Ph$ (2.0 equiv.) in dichloromethane and heated at 40 ºC in a sealed vial. The mixture was allowed to stir for 12 hours before being passed through a pad of celite. Removal of volatiles under reduced pressure afforded a pale white residue, which was purified by three recrystallizations from hot benzene to give **1a** as a white crystalline solid (63% yield).

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ (ppm). 2.66 (m, 20H), 7.09 (m, 6H), 7.45 (d, 4H).

$^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 135.32, 130.01, 128.37.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). -13.75 (d, 2B), -8.20 (d, 9B), 2.77 (d, 5B), -2.14 (d, 4B).

$^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). -13.80, -9.37, -7.30, -3.00, 1.67.

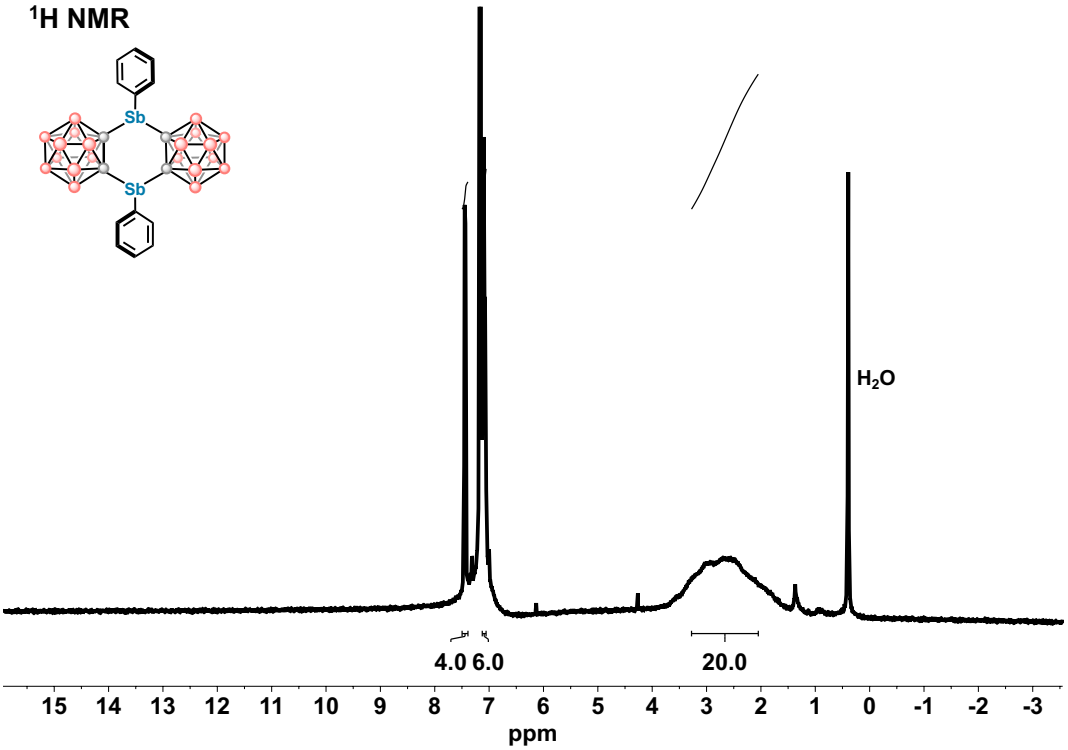


Figure S1 ^{1}H NMR spectrum of **[1a]** in $CDCl_3$

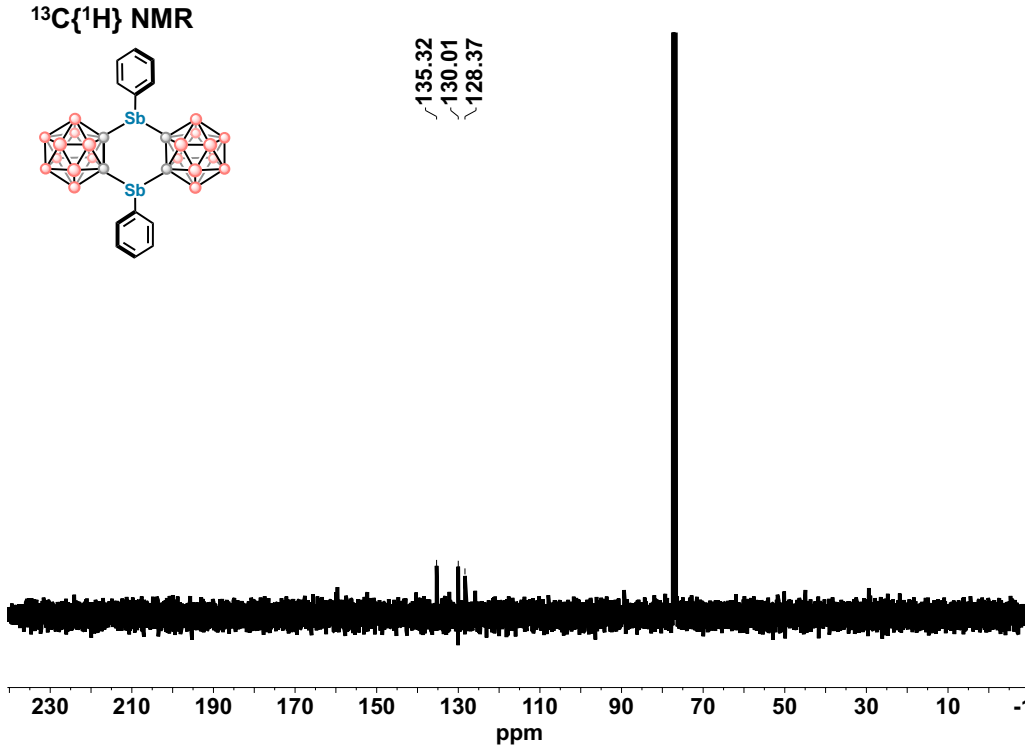


Figure S2 ^{13}C{^{1}H} NMR spectrum of **[1a]** in $CDCl_3$

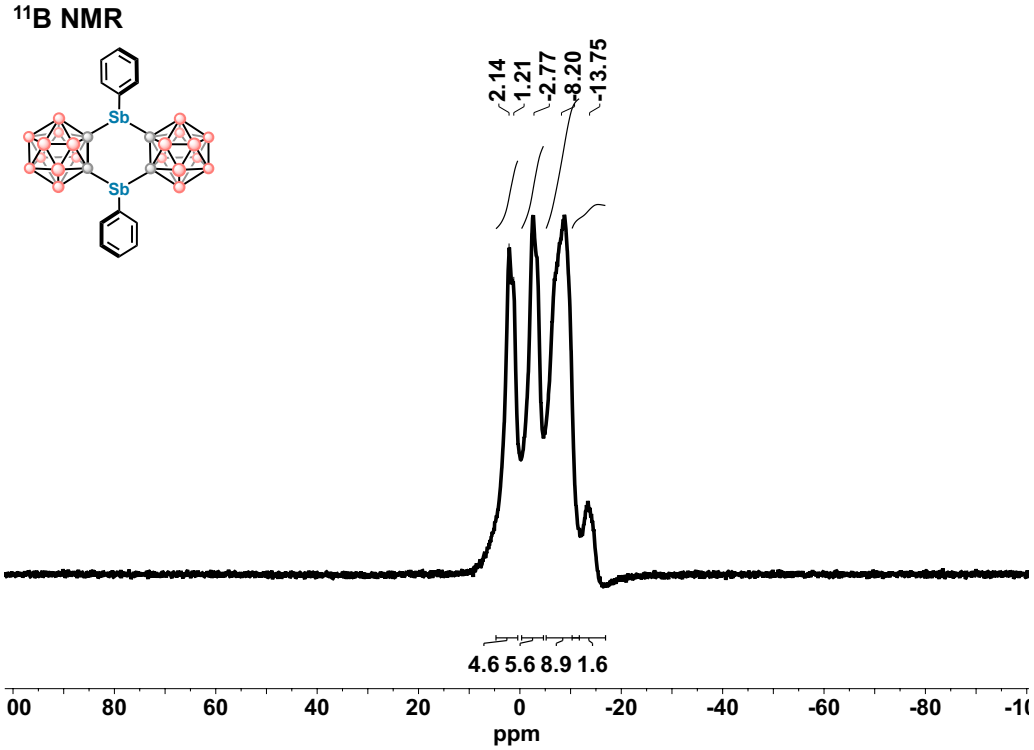


Figure S3 ^{11}B NMR spectrum of **[1a]** in $CDCl_3$

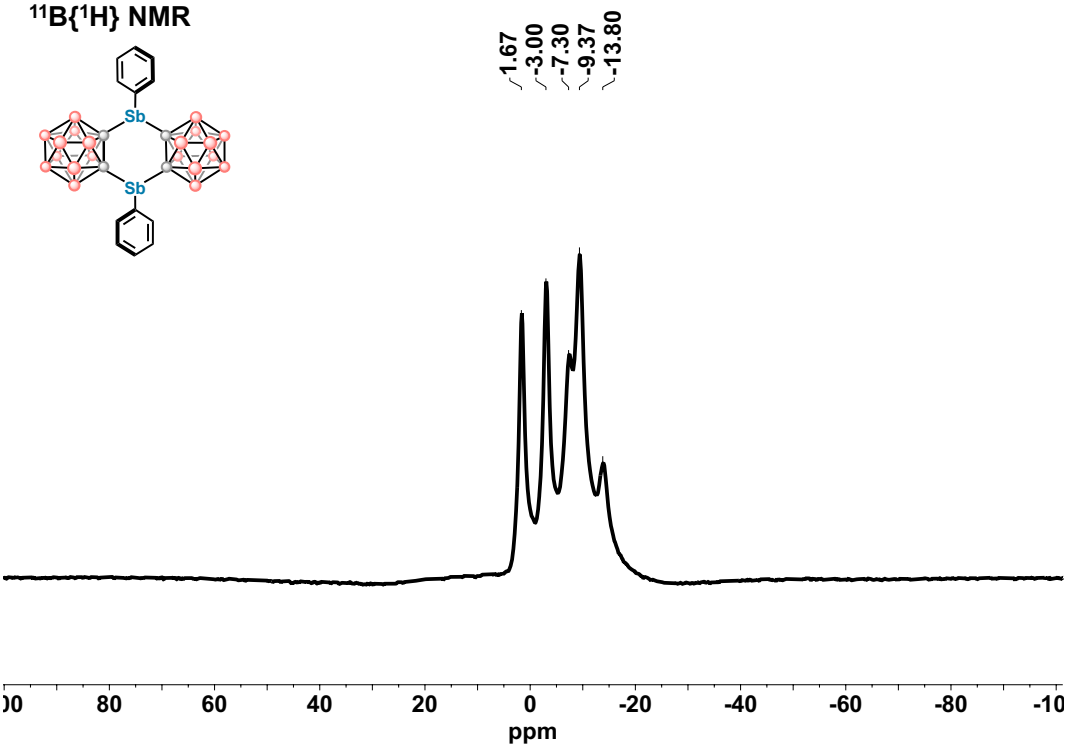
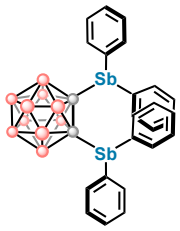


Figure S4 $^{11}B\{^1H\}$ NMR spectrum of **[1a]** in $CDCl_3$



Synthesis of 1,2-($SbPh_2$)$_2$-*ortho*-($C_2B_{10}H_{10}$) 2a

In an N_2-filled glovebox, *o*-carborane (300 mg, 2.08 mmol) was dissolved in toluene followed by the dropwise addition of 2 equiv. of *n*-BuLi (2.5 M in hexanes, 1.66 mL, 4.16 mmol) to the stirred solution, resulting in the immediate precipitation of the dilithiated cage, $Li_2C_2B_{10}H_{10}$. After stirring for 4 hours, the white solid was collected by filtration, washed thoroughly with toluene, and resuspended in dichloromethane. The resulting suspension was transferred dropwise into a solution of $SbClPh_2$ (2 equiv., 1.20 g, 3.84 mmol) in dichloromethane/THF mixture and stirred at 40 ºC in a sealed vial. The mixture was allowed to stir for 12 hours before being passed through a pad of celite. Removal of volatiles under reduced pressure afforded a pale white residue, which was purified by three recrystallizations from hot dry benzene to give **1a** as a white crystalline solid (86% yield).

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ (ppm) 2.79 (m, 10H), 7.09 (m, 12H), 7.57 (m, 8H)

^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 138.61, 137. 72, 130.27, 129.19, 68.09.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 2.07 (d, 2B), -4.11 (d, 2B), -8.30(d, 6B).

^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.67, -4.55, -8.75, -10.13.

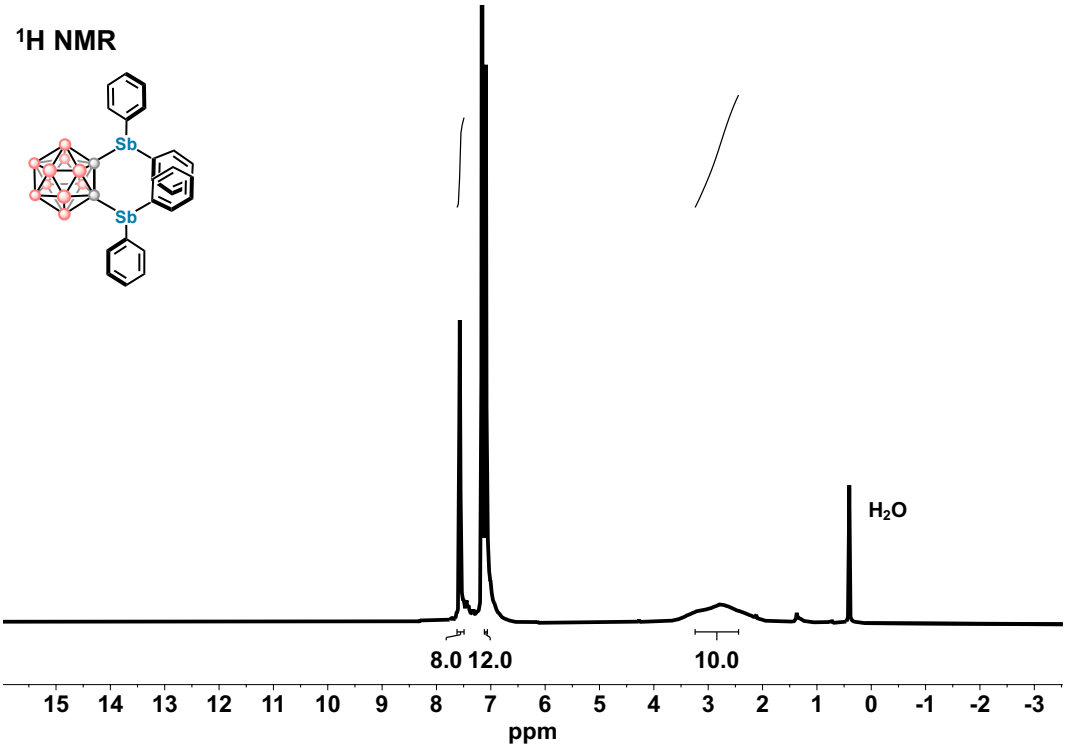


Figure S5 ^{1}H NMR spectrum of **[2a]** in C_6D_6

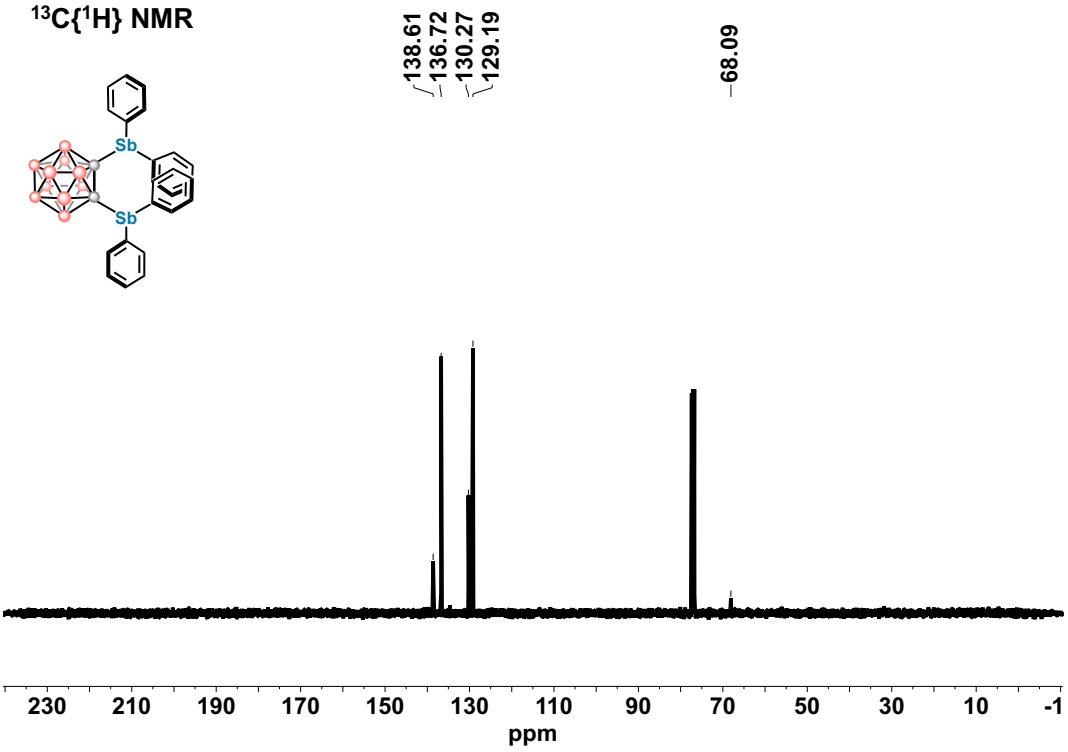


Figure S6 ^{13}C{^{1}H} NMR spectrum of **[2a]** in C_6D_6

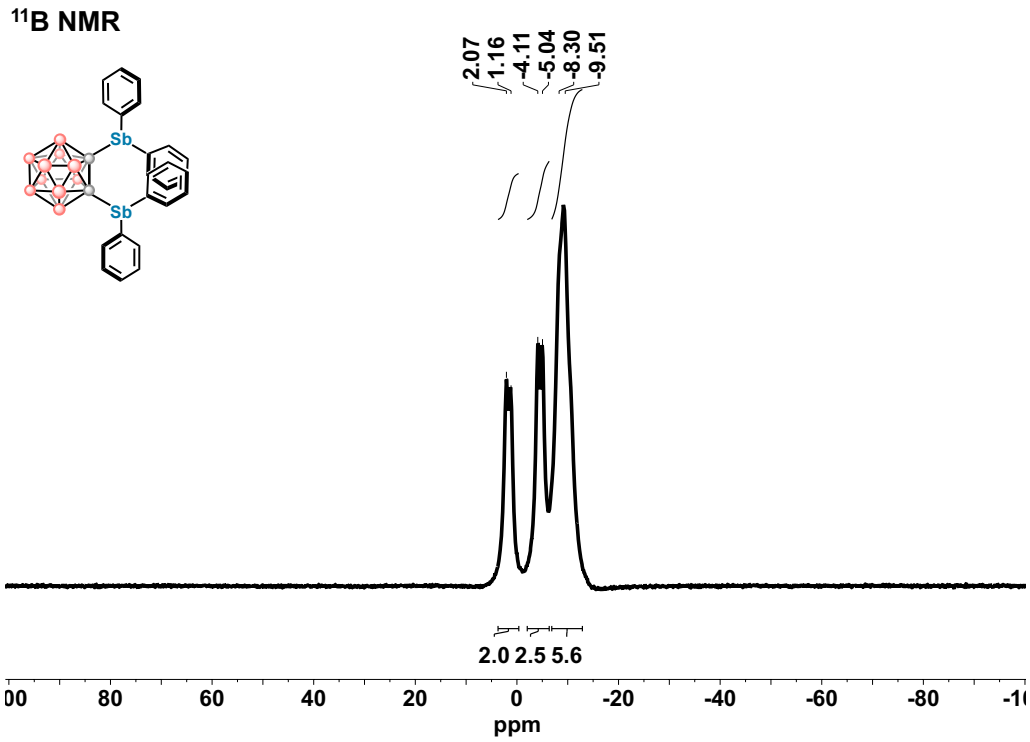


Figure S7 ^{11}B NMR spectrum of **[2a]** in C_6D_6

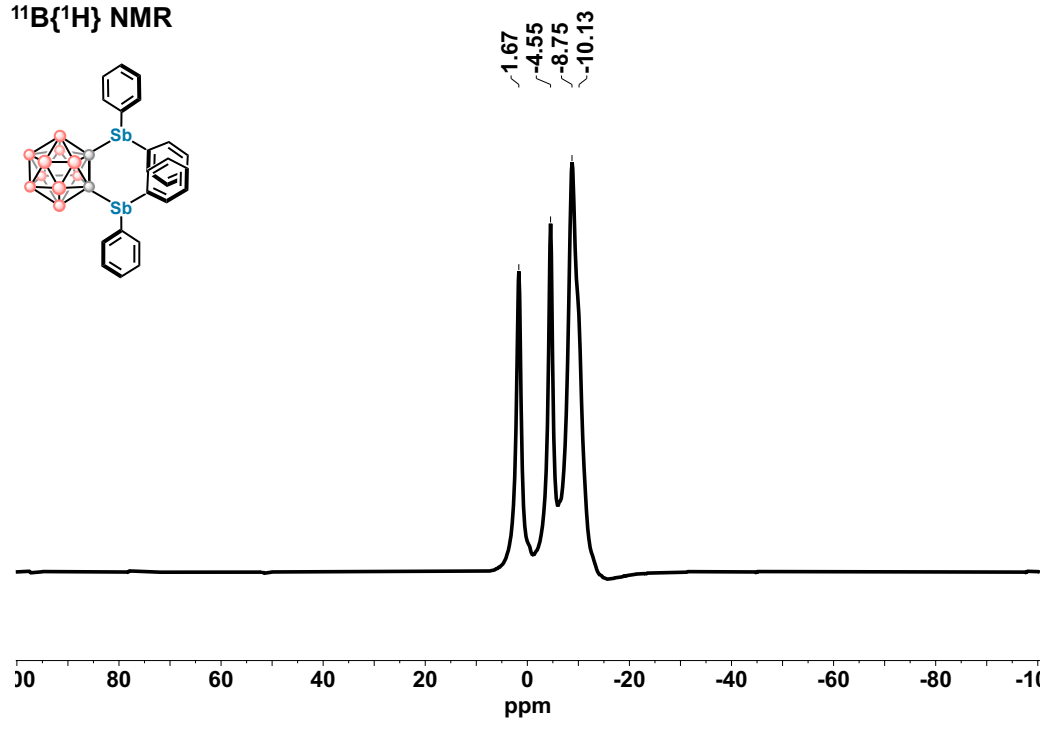
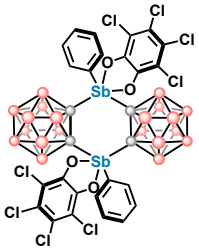


Figure S8 $^{11}B\{^1H\}$ NMR spectrum of **[2a]** in C_6D_6



Synthesis of *o*-$(C_2B_{10}H_{10})_2$(SbPh(diolate))$_2$ [1b]

In an N_2-filled glovebox, a dry sample of **1a** (100 mg, 1.47 mmol) was dissolved in dichloromethane to give a deep red solution. A concentrated solution of *o*-chloranil (2 equiv., 72.1 mg, 2.93 mmol) in 0.5 mL of dichloromethane was added dropwise to the vigorously stirring stibine solution. Within ~5 minutes, the reaction mixture underwent a distinct color change from deep red to bright orange, consistent with oxidation at antimony. Upon completion, the product began to precipitate as an orange solid. The volatiles were removed *in vacuo*, and the resulting solid was washed thoroughly with hexanes to remove residual oxidant and byproducts, affording the stiborane in quantitative yield**.**

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ (ppm) 2.32 (m, 20H), 7.73 (m, 4H), 7.86 (m, 4H) 7.96 (m, 2H)

^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 134.73, 128.19, 120.14, 184.06, 53.94, 5.74.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.73 (d, 4B), -4.26 (d, 6B), -9.63(d, 12B).

^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.67, -4.25, -9.67.

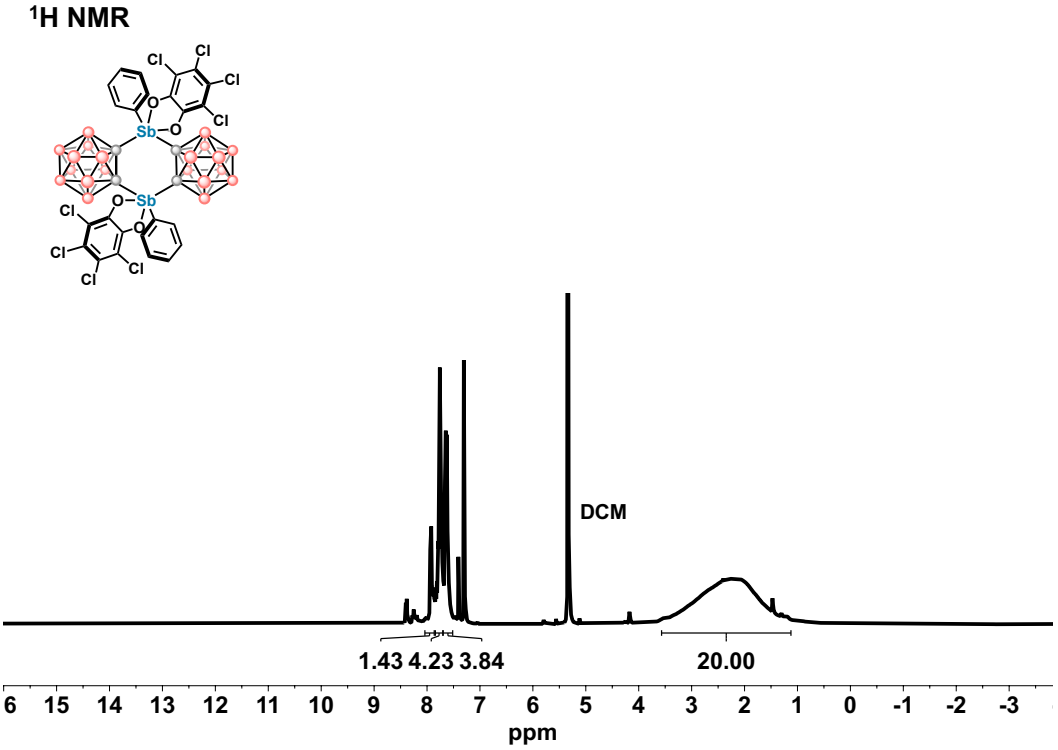


Figure S9 ^{1}H NMR spectrum of **[1b]** in C_6D_6

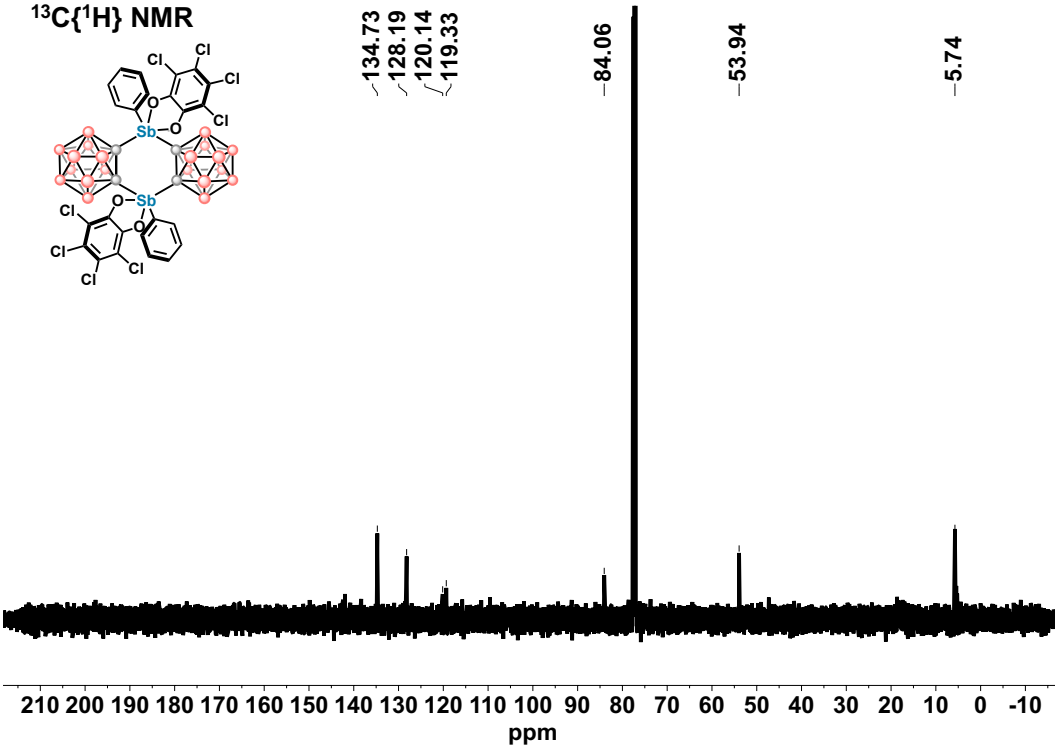


Figure S10 ^{13}C{^{1}H} NMR spectrum of **[1b]** in C_6D_6

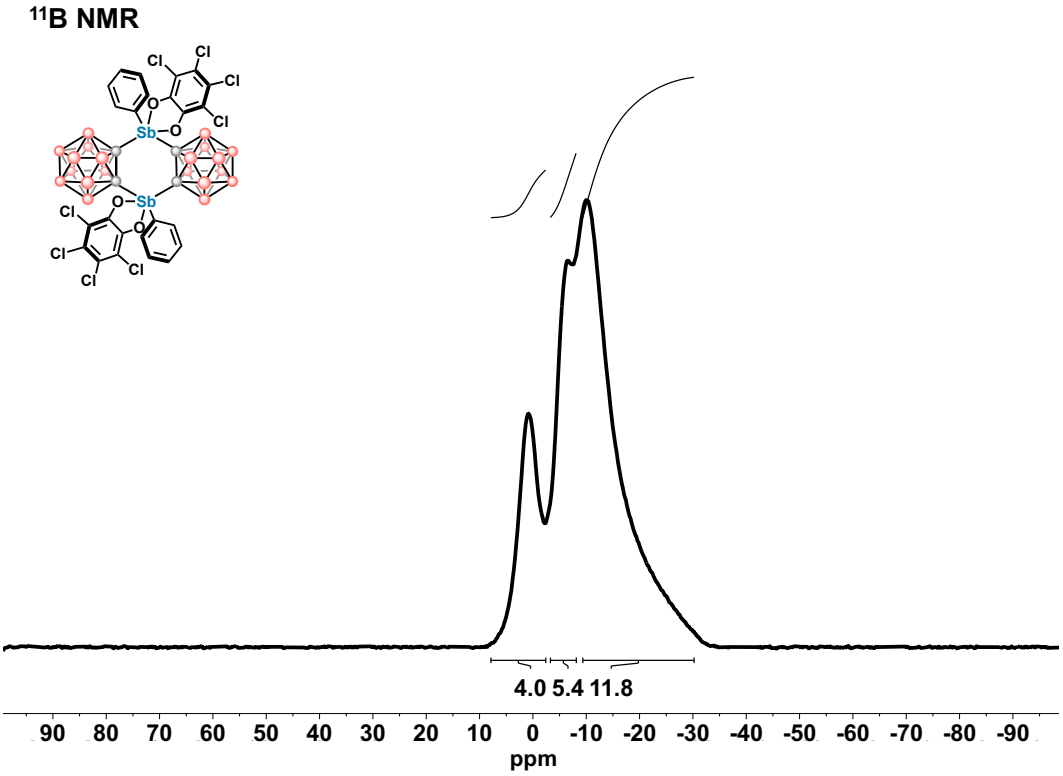


Figure S11 ^{11}B NMR spectrum of **[1b]** in C_6D_6

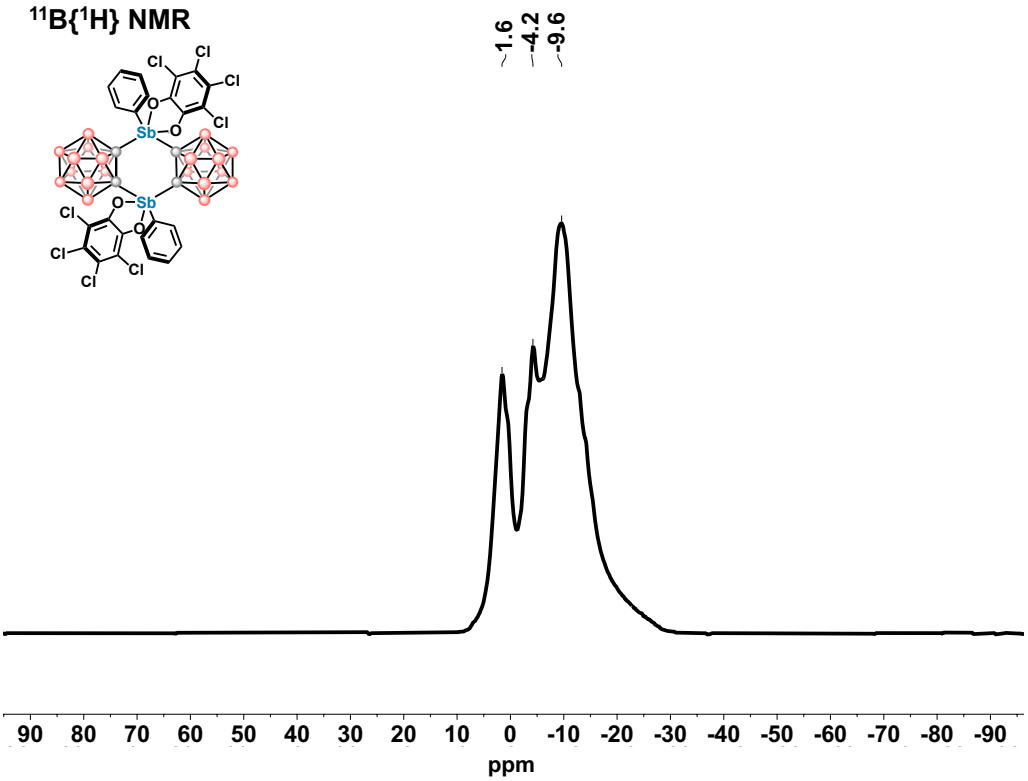
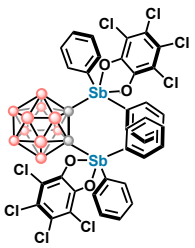


Figure S12 $^{11}B\{^1H\}$ NMR spectrum of **[1b]** in C_6D_6



Synthesis of *o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$ [2b]

In an N_2-filled glovebox, a dry sample of **2b** (100 mg, 1.44 mmol) was dissolved in dichloromethane. A concentrated solution of *o*-chloranil (2 equiv., 70.83 mg, 2.88 mmol) in 0.5 mL of dichloromethane was added dropwise to the vigorously stirring stibine solution. Over the course of ~5 minutes, the solution gradually shifted from deep red to a uniform deep orange, indicative of oxidation at antimony centers. No precipitation was observed at any point, and the oxidized stiborane remained fully dissolved throughout the reaction. Following complete consumption of starting material, the volatiles were removed *in vacuo*, and the resulting residue was washed with hexanes to remove excess oxidant and byproducts, furnishing the stiborane product in quantitative yield**.**

^{1}H NMR (600 MHz, $CDCl_3$, 25 °C): δ (ppm) 2.18 (m, 10H), 7.60 (m, 12H), 7.87 (d, 8H).

^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 142.90, 136.02, 134.96, 132.77, 129.84, 128.38, 122.87, 117.50.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 0.82 (bs, 2B), -5.71 (bs, 3B), -9.67 (bs, 5B).

^{11}B{^{1}H} NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.19, -5.72, -9.76.

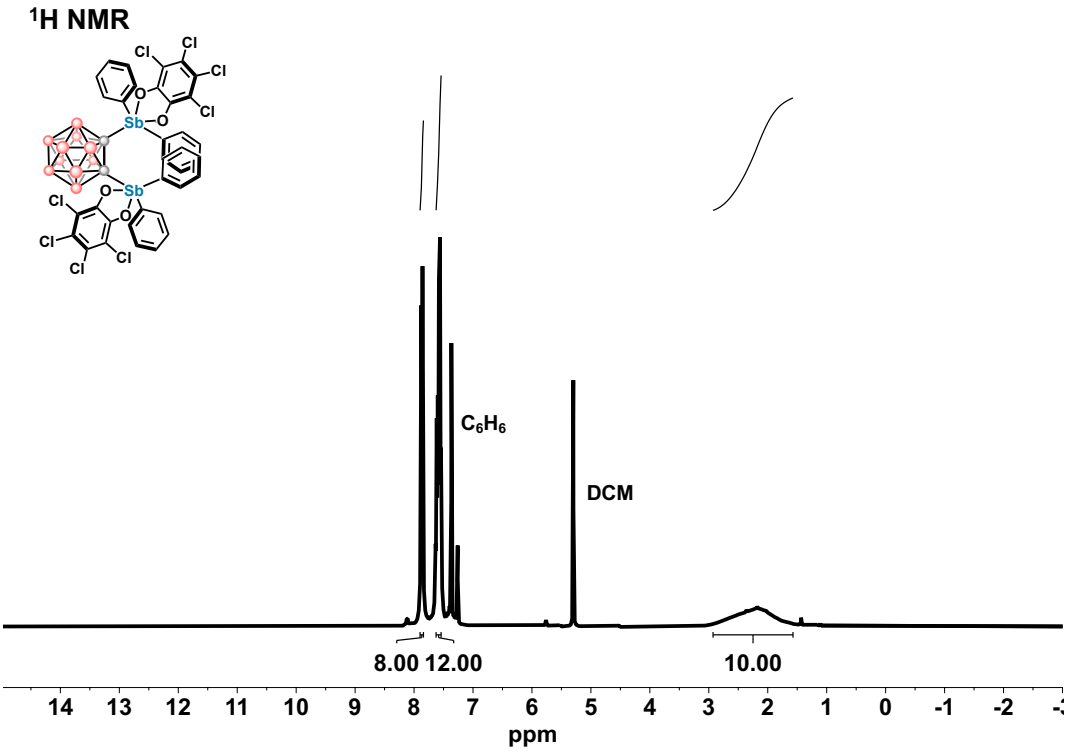


Figure S13 ^{1}H NMR spectrum of **[2b]** in $CDCl_3$

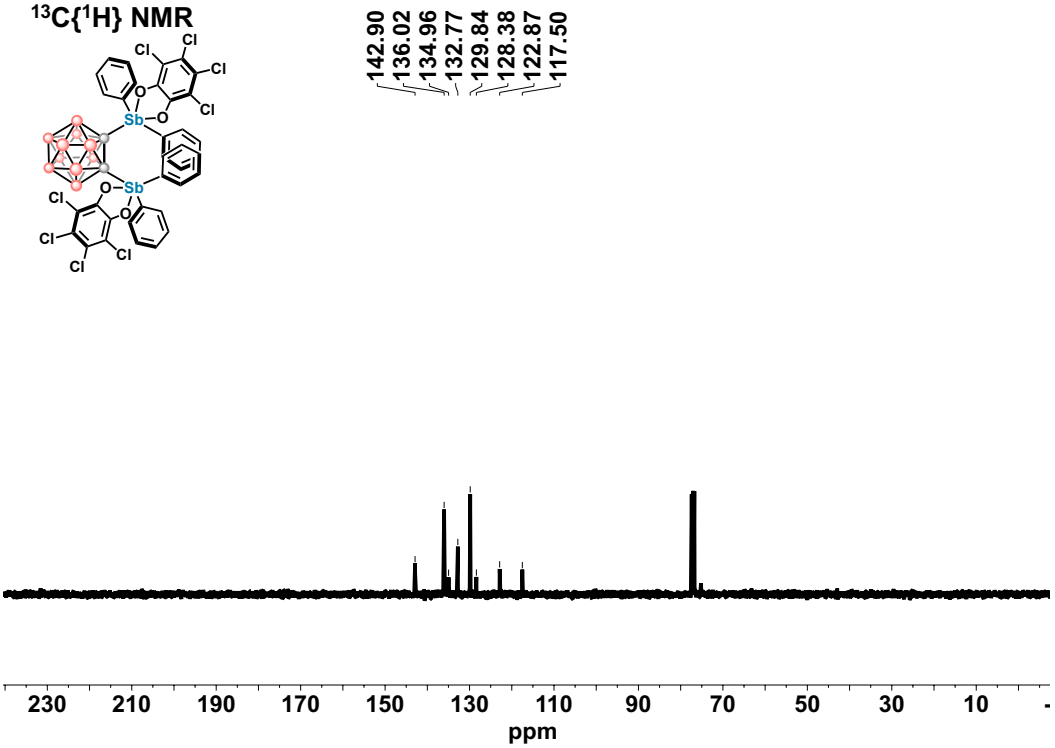


Figure S14 $^{13}C\{^{1}H\}$ NMR spectrum of **[2b]** in C_6D_6

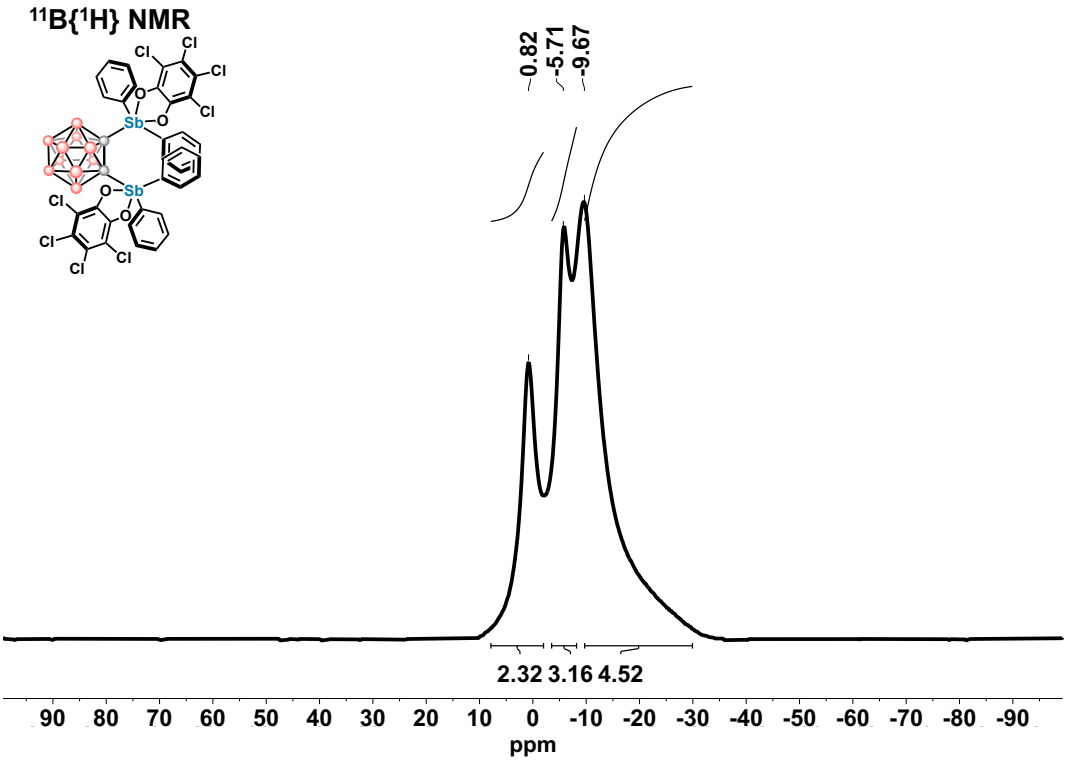


Figure S15 ^{11}B NMR spectrum of **[2b]** in C_6D_6

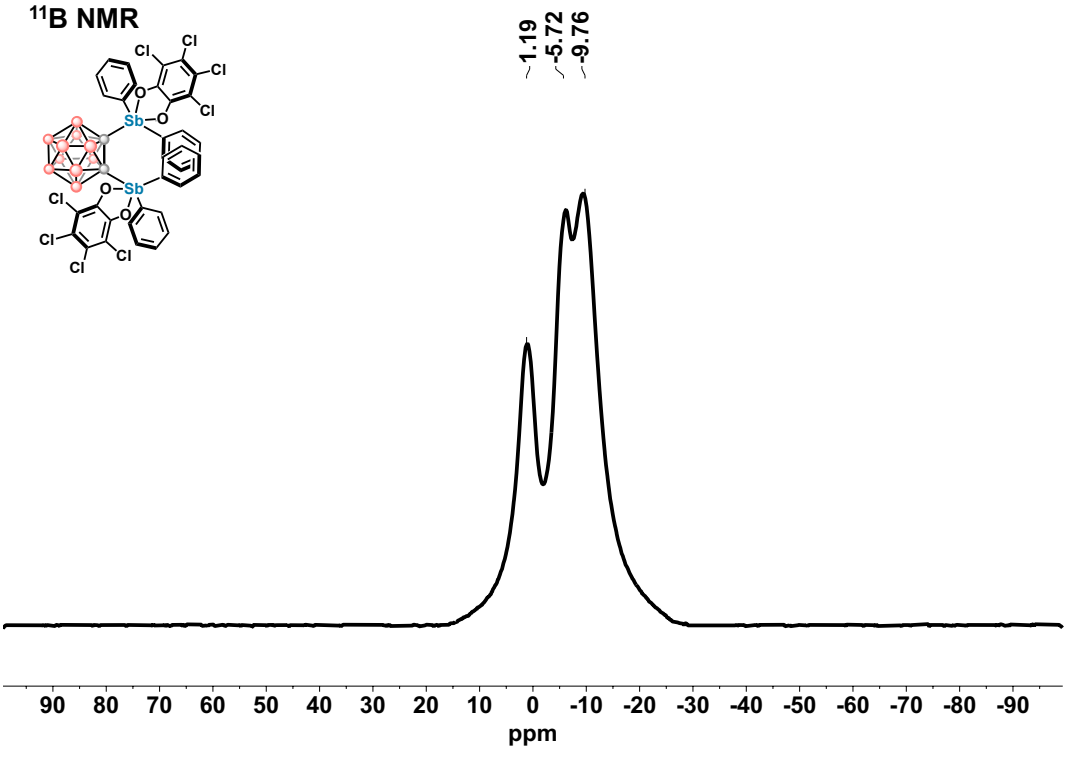
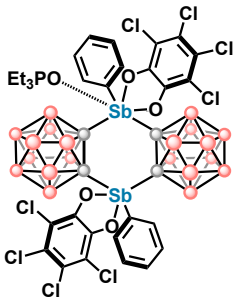


Figure S16 $^{11}B\{^1H\}$ NMR spectrum of **[2b]** in C_6D_6



Synthesis of [Et_3PO][*o*-($C_2B_{10}H_{10}$)$_2$($SbPh_2$(diolate))$_2$] [1c]

Stiborane **1b** (25 mg, 0.21 mmol) was dissolved in $CDCl_3$ in an N_2-filled glovebox. To this solution, Et_3PO (1 equiv., 2.86 mg, 0.21 mmol) was added, and the mixture was gently stirred to ensure homogeneity. The resulting solution was transferred to an NMR tube, and a ^{31}P NMR spectrum was recorded at room temperature. Coordination of Et_3PO to the antimony center resulted in a downfield shift relative to free Et_3PO, which appears at 50.0 ppm in $CDCl_3$, consistent with formation of the Lewis acid–base adduct **1c**.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 2.19 (bs, B), 6.04 (bs, B), 8.77 (bs, B).

$^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 2.42, -5.39, -8.93

$^{31}P\{^1H\}$ NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 71.64

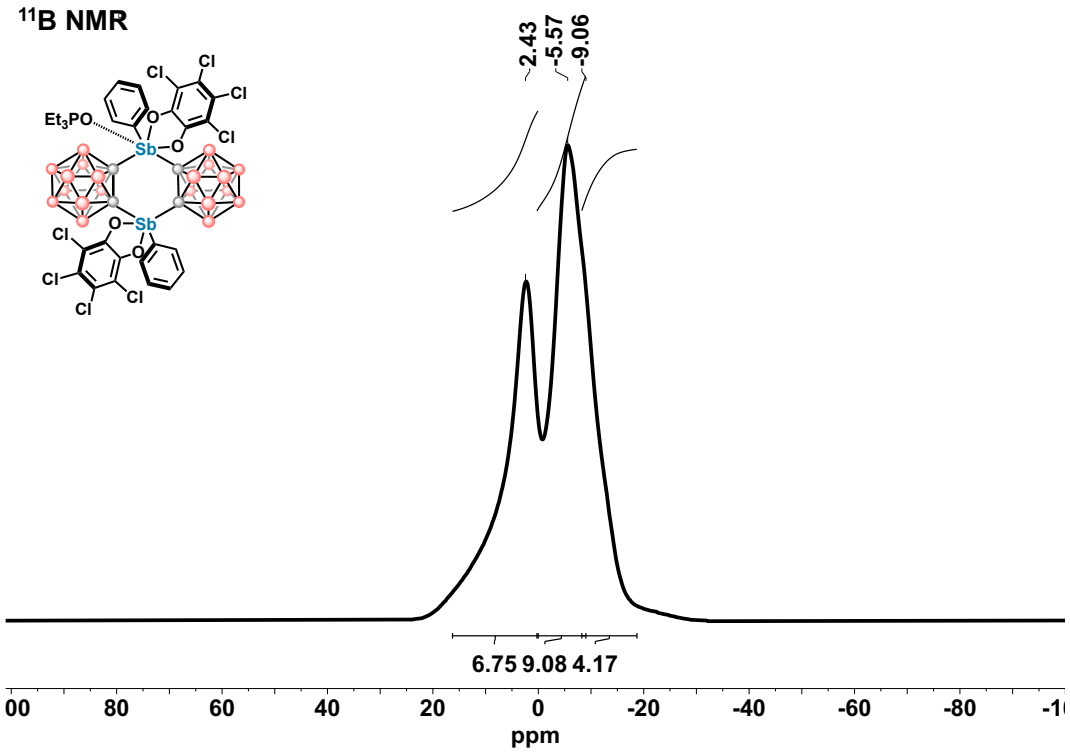


Figure S17 ^{11}B NMR spectrum of **[1c]** in $CDCl_3$

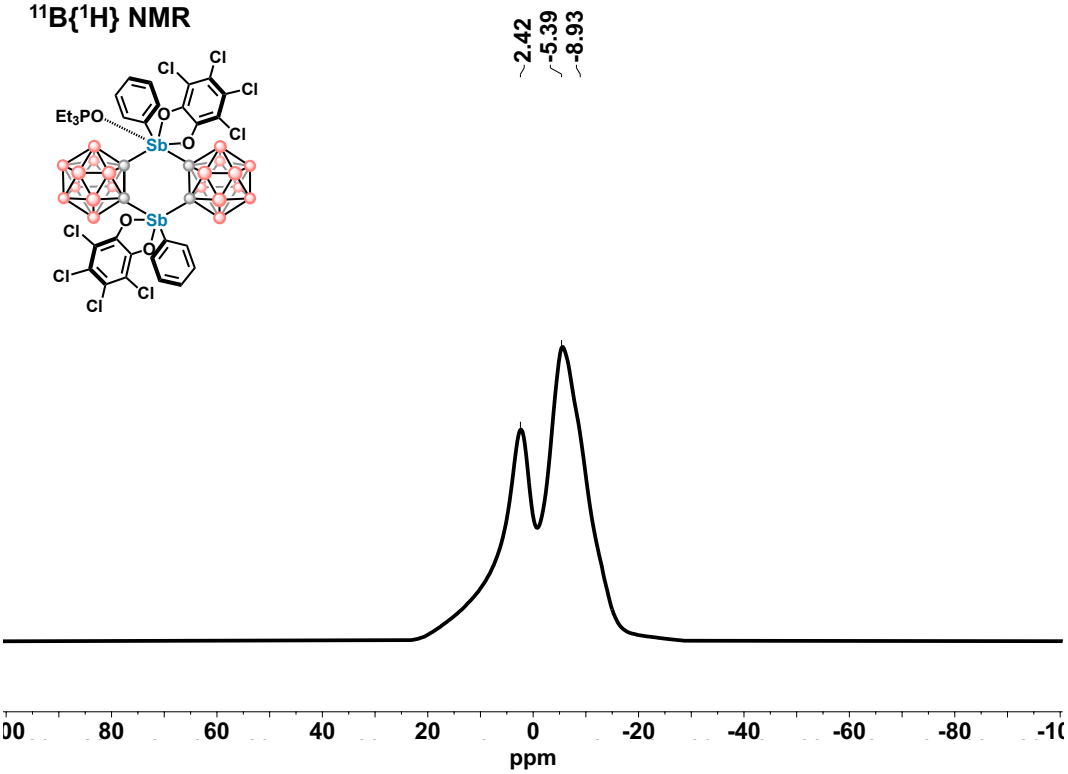


Figure S18 $^{11}B\{^1H\}$ NMR spectrum of **[1c]** in $CDCl_3$

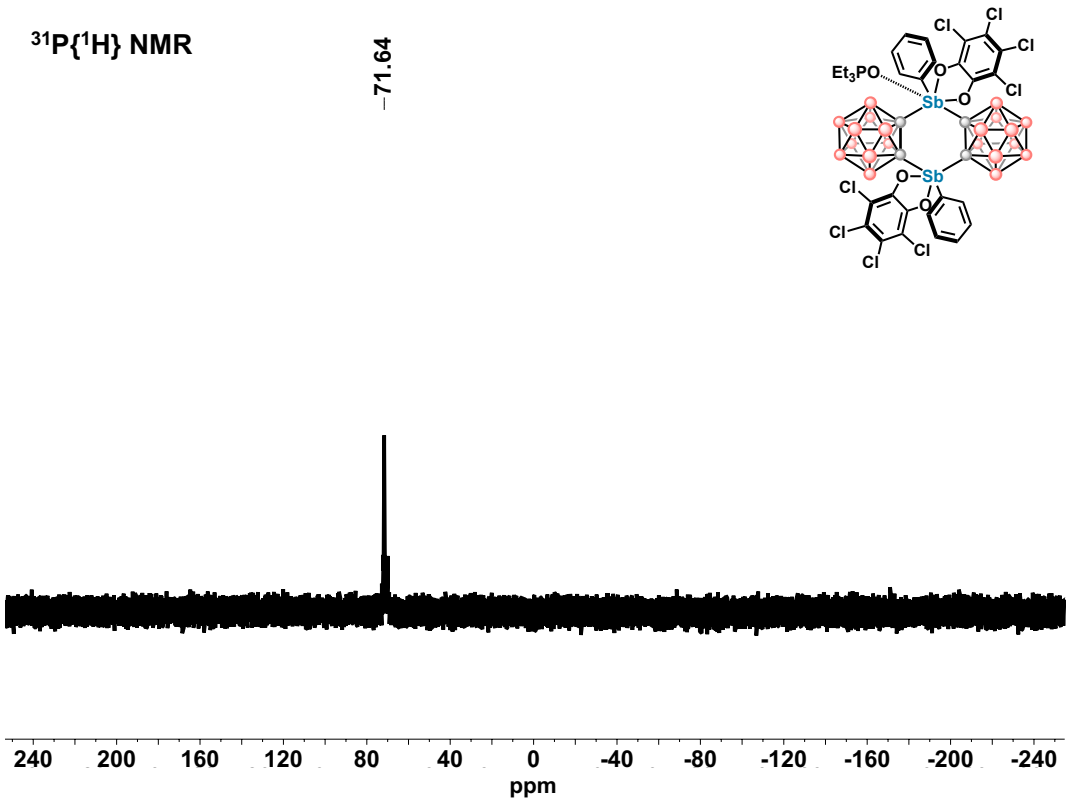
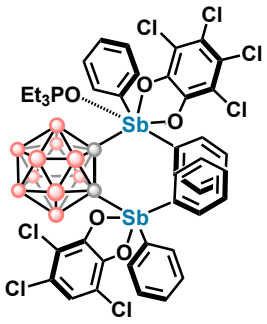


Figure S19 $^{31}P\{^{1}H\}$ NMR spectrum of **[1c]** in $CDCl_3$



Synthesis of [Et_3PO][[*o*-($C_2B_{10}H_{10}$)($SbPh_4$(diolate))$_2$] [2c]

Stiborane **2b** (25 mg, 0.21 mmol) was dissolved in $CDCl_3$ in an N_2-filled glovebox. To this solution, Et_3PO (1 equiv., 2.86 mg, 0.21 mmol) was added, and the mixture was gently stirred to ensure homogeneity. The resulting solution was transferred to an NMR tube, and a ^{31}P NMR spectrum was recorded at room temperature. Coordination of Et_3PO to the antimony center resulted in a downfield shift relative to free Et_3PO, which appears at 50.0 ppm in $CDCl_3$, consistent with formation of the Lewis acid–base adduct **2c**.

^{11}B NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.20 (s, 3B), -5.73 (s, 3B), 9.94 (s, 4B).

$^{11}B\{^1H\}$ NMR (192 MHz, $CDCl_3$, 25 °C): δ (ppm). 1.20, -5.73, 9.94.

$^{31}P\{^1H\}$ NMR (150 MHz, $CDCl_3$, 25 °C): δ (ppm). 66.5.

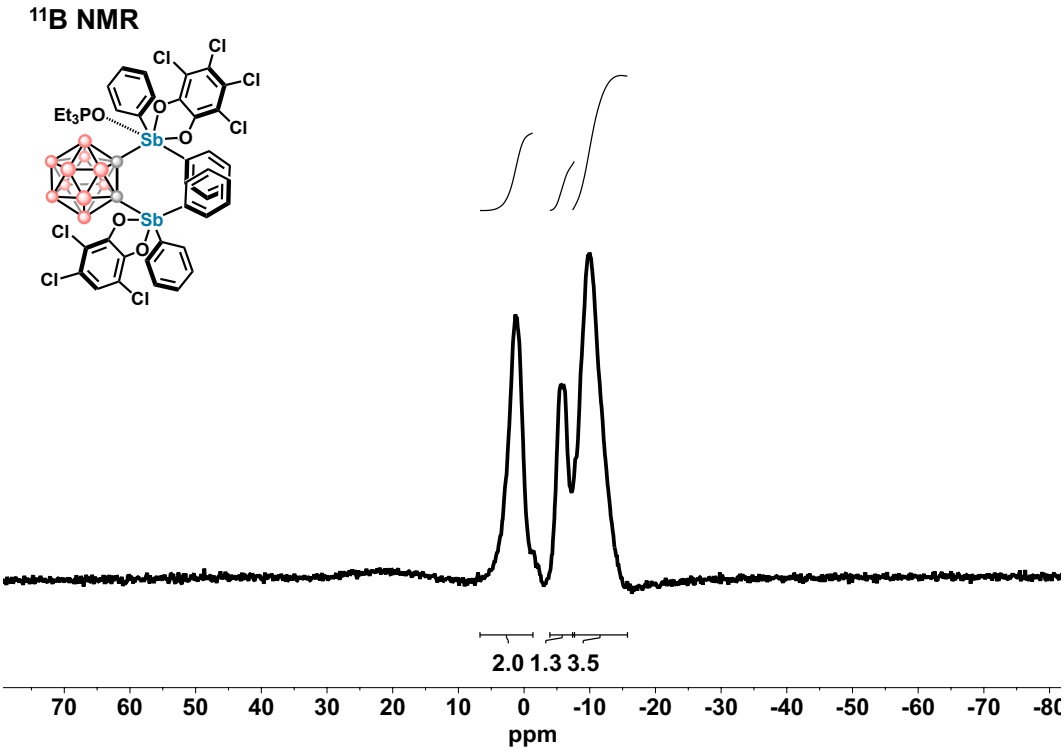


Figure S20 ^{11}B NMR spectrum of **[2c]** in $CDCl_3$

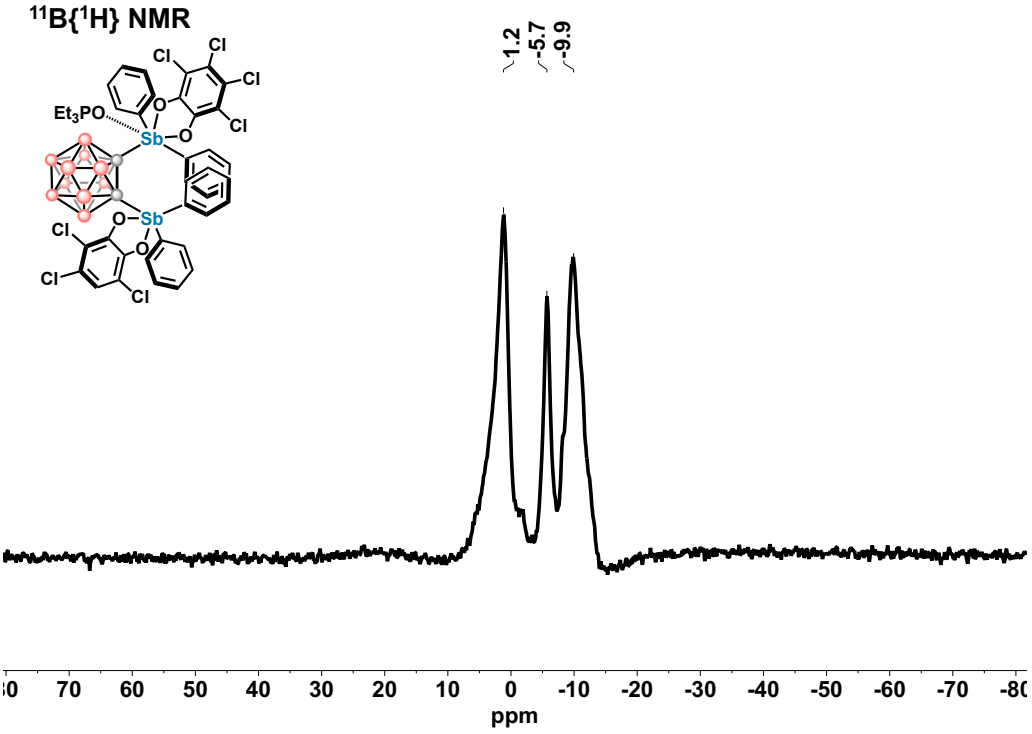


Figure S21 $^{11}B\{^1H\}$ NMR spectrum of **[2c]** in $CDCl_3$

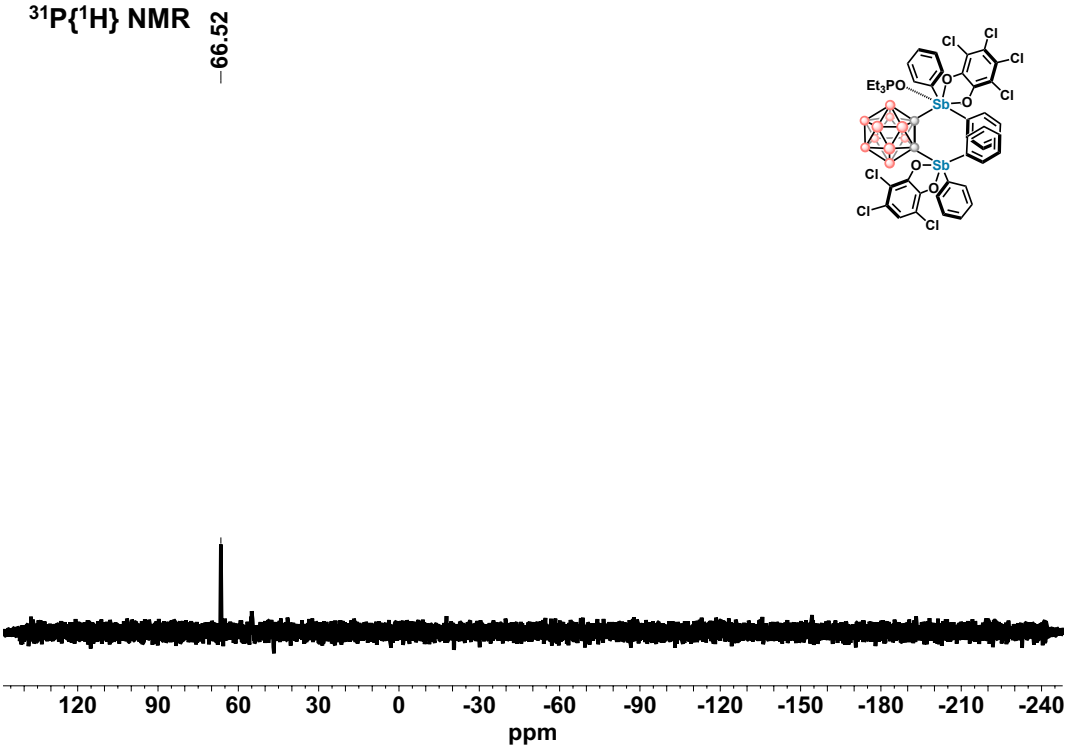
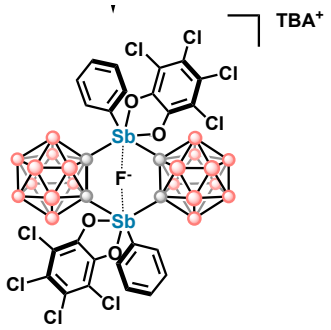


Figure S22 $^{31}P\{^{1}H\}$ NMR spectrum of **[2c]** in $CDCl_3$

Fluoride Anion Binding to 1b and 2b



Synthesis of [^{n}Bu$_4$N][μ^2-F$^-$][*o*-(C$_2$B$_{10}$H$_{10}$)$_2$(SbPh$_2$(diolate))$_2$] [1d]

In an N_2-filled glovebox, stiborane **1b** (50.0 mg, 48.4 μmol) was dissolved in dichloromethane to give a homogeneous deep orange solution. To this stirring solution, [nBu$_4$N][Ph$_3$SiF$_2$] (1 equiv., 26.2 mg, 48.4 μmol) was added in a single portion. The reaction mixture was allowed to stir at 25 °C for 10 minutes, during which the color remained orange and no precipitate formed. Clean formation of the fluoride adduct was observed by ^{19}F NMR spectroscopy, showing disappearance of free [Ph$_3$SiF$_2$]$^-$ and appearance of a new resonance corresponding to the Sb–F–Sb bridged species. Following completion, the solvent was removed in vacuo, and the resulting residue was washed with hexanes to remove excess salt and silane-derived byproducts, affording **1d** as a stable orange solid.

^{11}B NMR (193 MHz, C$_6$D$_6$, 25 °C) δ (ppm): 0.61 (s, 5B), -8.60 (s, 15B).

^{11}B{^{1}H} NMR (193 MHz, C$_6$D$_6$, 25 °C) δ (ppm): 0.96, -7.08, -10.00

^{19}F NMR (151 MHz, C$_6$D$_6$, 25 ºC) δ (ppm): -53.83

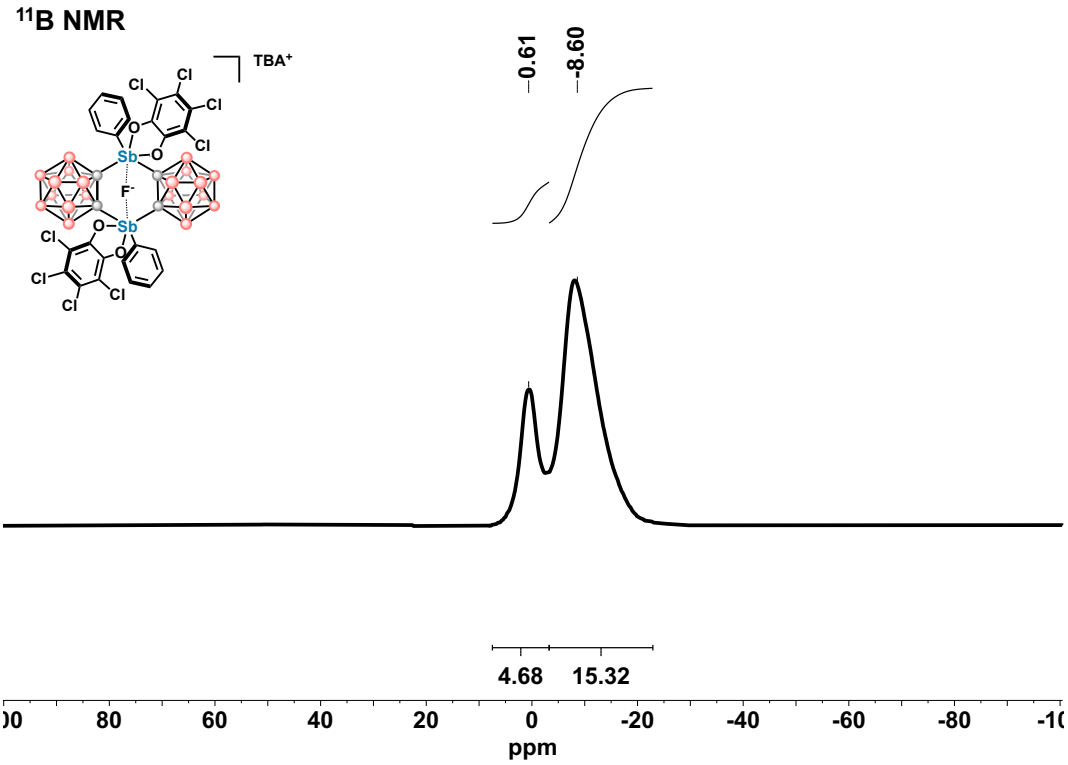


Figure S23 ^{11}B NMR spectrum of **[1d]** in C_6D_6

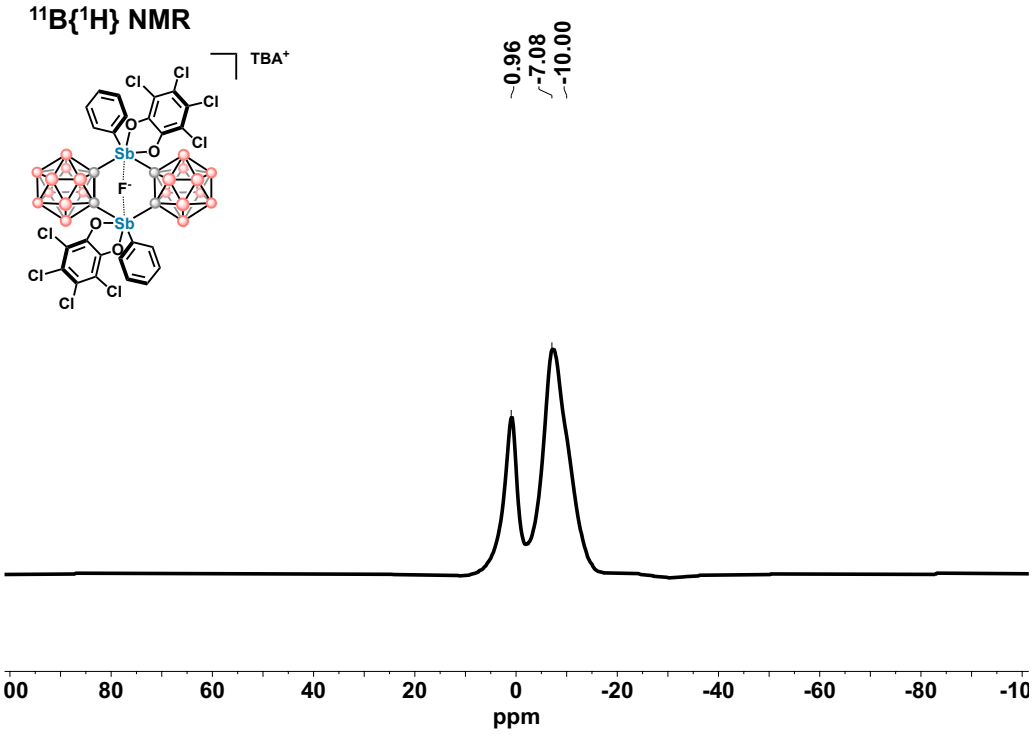


Figure S24 $^{11}B\{^1H\}$ NMR spectrum of **[1d]** in C_6D_6

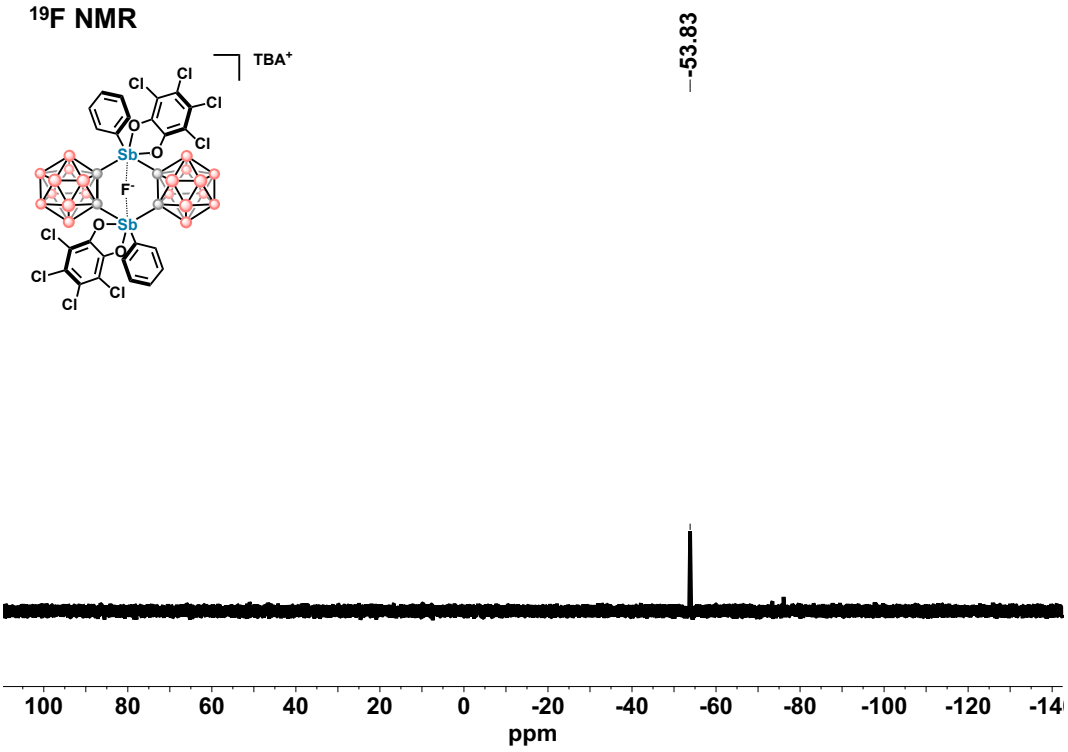
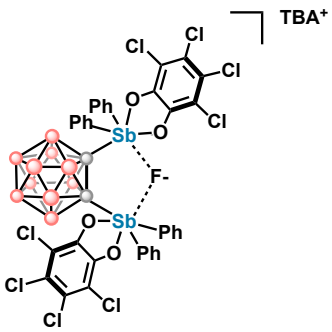


Figure S25 ^{19}F NMR spectrum of **[1d]** in C_6D_6



Synthesis of [^{n}Bu$_4$N][μ^2-F$^-$][*o*-($C_2B_{10}H_{10}$)($SbPh_4$(diolate))$_2$] [2d]

In an N_2-filled glovebox, stiborane **2b** (50.0 mg, 42.2 μmol) was dissolved in 0.5 mL dichloromethane to afford a homogeneous orange solution. To this stirring solution, [nBu$_4$N][Ph_3SiF_2] (1.0 equiv., 22.8 mg, 42.2 μmol) was added in a single portion. The reaction mixture was allowed to stir at 25 °C for 10 minutes, during which no precipitate was observed and the solution remained uniformly orange. Formation of the fluoride adduct was confirmed by ^{19}F NMR spectroscopy**,** which showed disappearance of the free [Ph_3SiF_2]$^-$ signal and appearance of a new resonance at approximately −77 ppm, consistent with an Sb–F interaction. The volatiles were then removed *in vacuo*, and the resulting residue was washed with hexanes to remove excess salt and silane-derived byproducts, affording **2d** as an orange solid suitable for further characterization.

^{11}B NMR (193 MHz, C_6D_6, 25 °C) δ (ppm): 0.31 (s, 2B), -9.10 (s, 6B).

^{11}B{^{1}H} NMR (193 MHz, C_6D_6, 25 °C) δ (ppm): 0.51, 8.59

^{19}F NMR (151 MHz, C_6D_6, 25 ºC) δ (ppm): -59.40

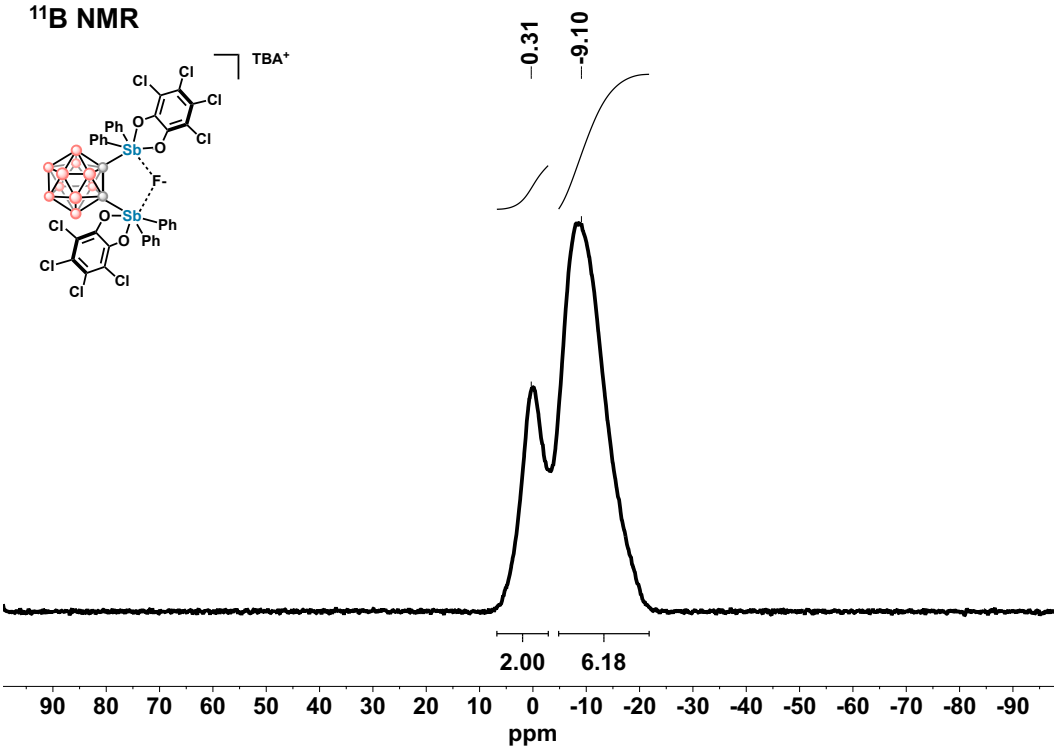


Figure S26 ^{11}B NMR spectrum of **[2d]** in C_6D_6

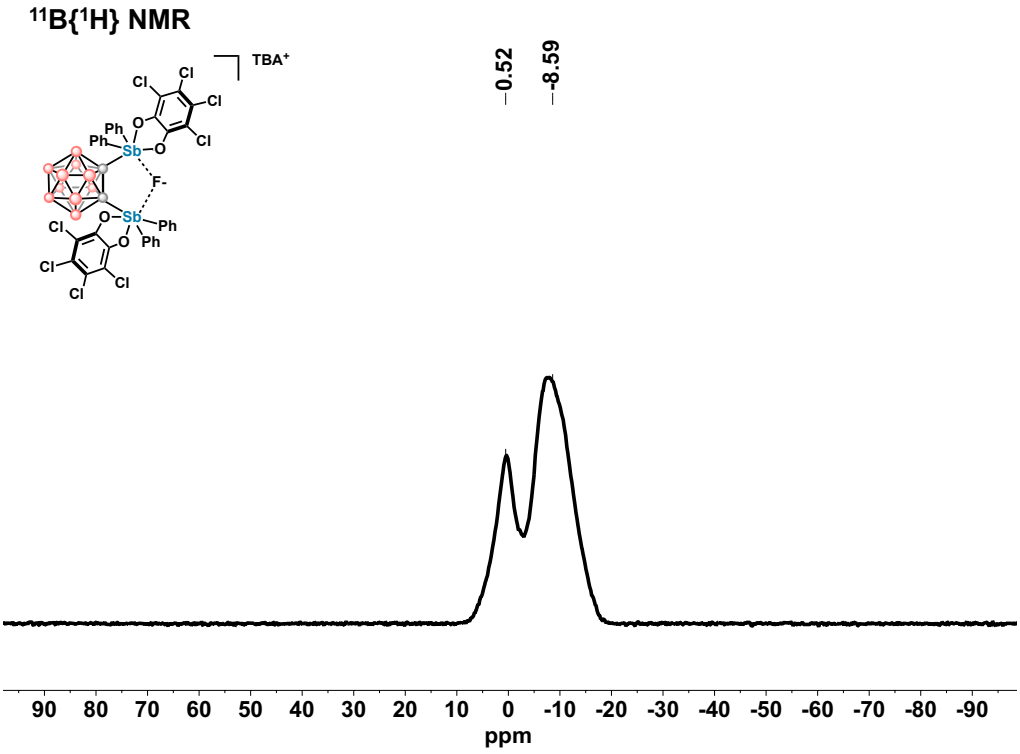


Figure S27 ^{11}B{^{1}H} NMR spectrum of **[2d]** in C_6D_6

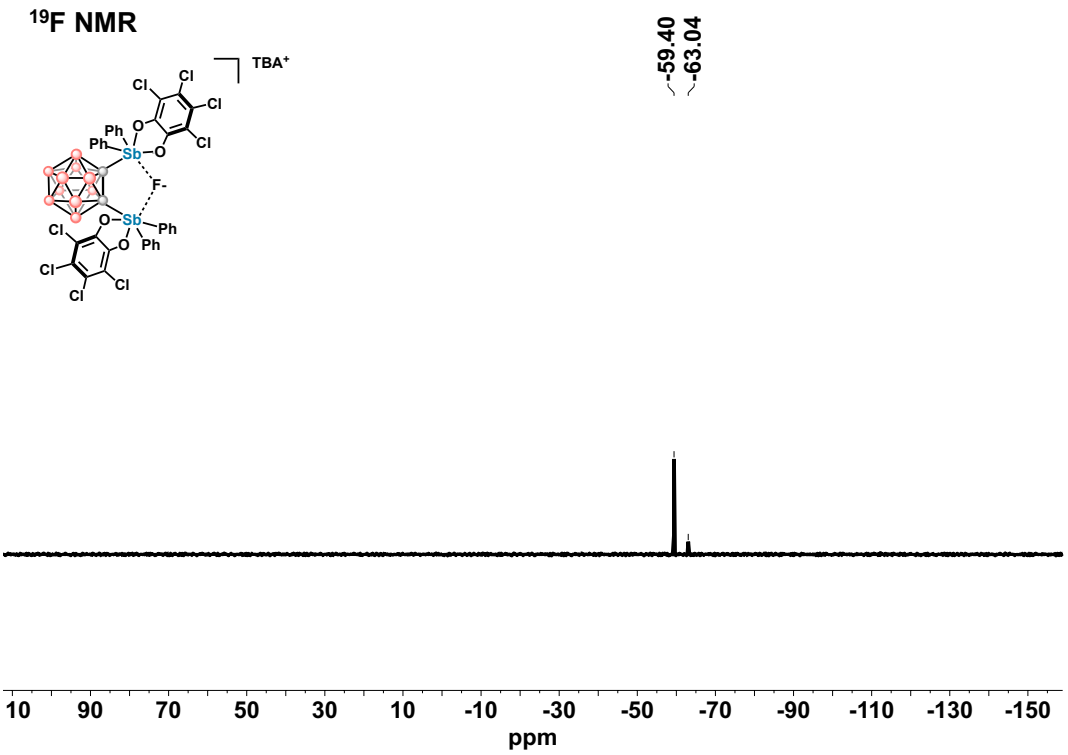
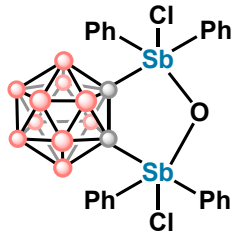


Figure S28 ^{19}F NMR spectrum of **[2d]** in C_6D_6



Synthesis of *o*-($C_2B_{10}H_{10}$)($SbPh_2Cl$)$_2$O [2e]

Stiborane **2b** (100 mg, 0.84 mmol) was dissolved in CH_2Cl_2 (2–3 mL) on the bench to give a homogeneous orange solution. To this stirring solution, a 1:1 mixture of CH_2Cl_2/H_2O (~2 mL total) was added, followed by slow addition of 1.0 equiv. of aqueous HCl (1 M). Upon introduction of the acidic aqueous layer, the reaction mixture immediately turned cloudy and colorless crystalline material began to form. The biphasic mixture was stirred at 25 °C for 10 minutes to ensure complete conversion. The resulting colorless crystals were collected by filtration, washed with cold hexanes and a small amount of water, and dried under vacuum to afford **2e** as a colorless crystalline solid in quantitative yield.

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ (ppm). 2.65 (m, 10H), 7.43 (m, 12H), 7.96 (m, 8H).

.

^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 25 °C): δ (ppm). 139.09, 134.58, 132.21, 129.46, 72.02.

^{11}B NMR (192 MHz, C_6D_6, 25 °C): δ (ppm). 0.35 (bs, 2B), -6.65 (bs, 4B), -10.87 (bs, 4B).

^{11}B{^{1}H} NMR (192 MHz, C_6D_6, 25 °C): δ (ppm). 0.12, -6.17, -10.25.

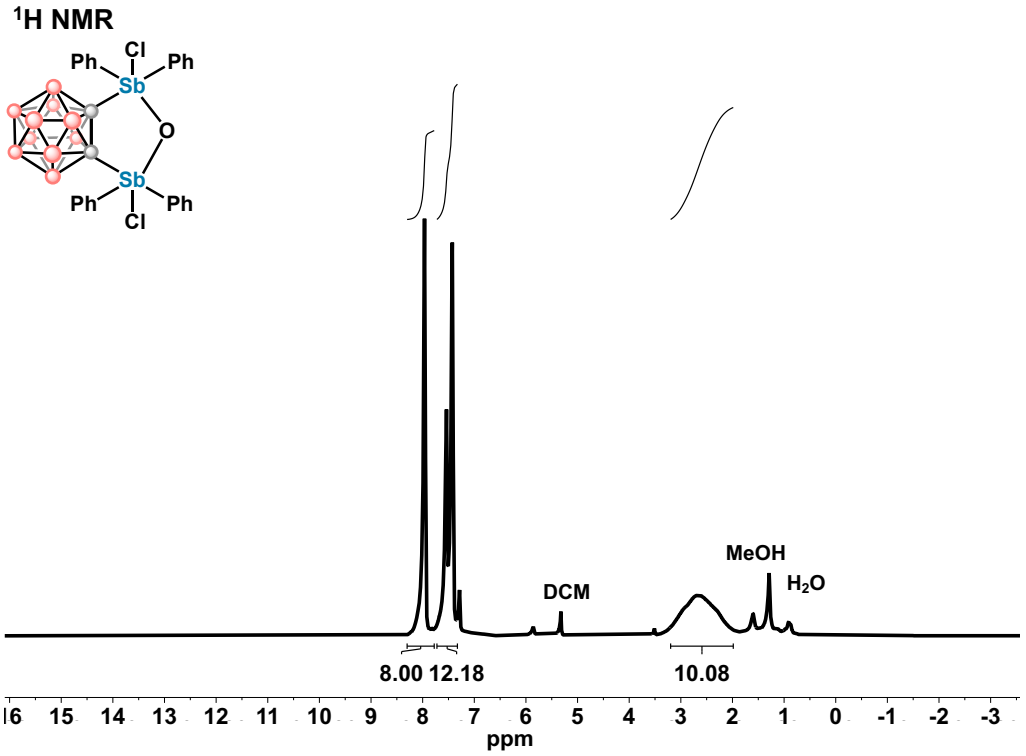


Figure S29 ^{1}H NMR spectrum of **[2e]** in C_6D_6

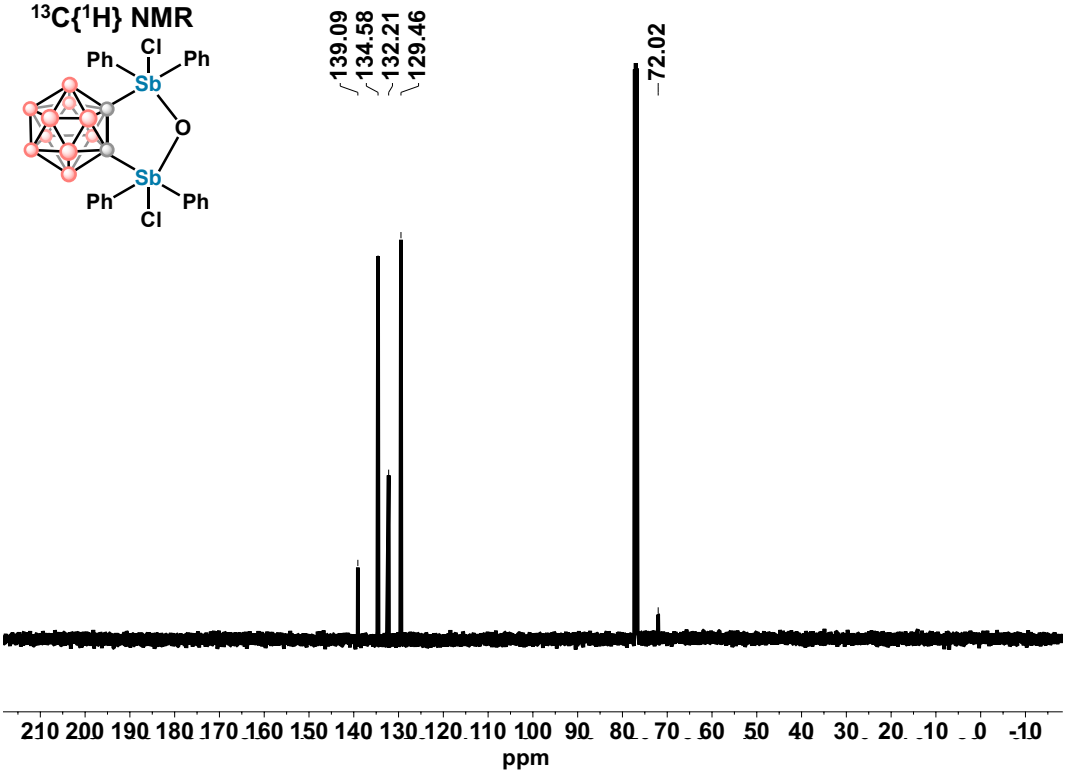


Figure S30 ^{13}C{^{1}H} NMR spectrum of **[2e]** in C_6D_6

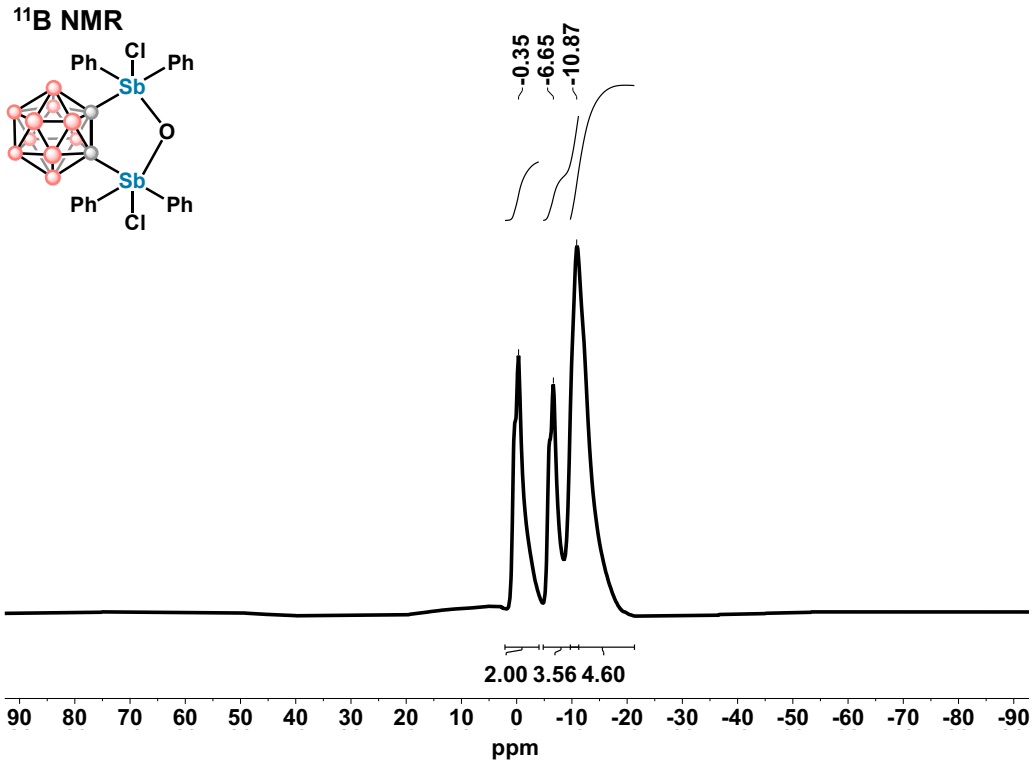


Figure S31. ^{11}B NMR spectrum of **[2e]** in C_6D_6

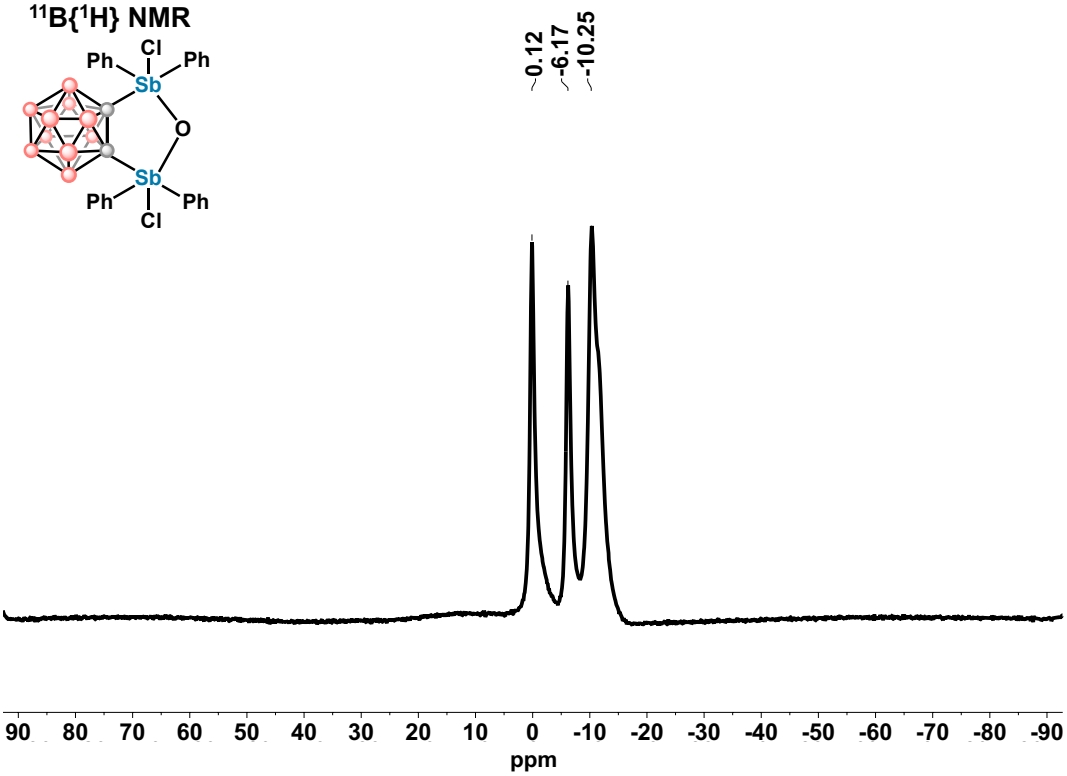


Figure S32. $^{11}B\{^1H\}$ NMR spectrum of **[2e]** in C_6D_6

II. Variable Temperature NMR of 1a

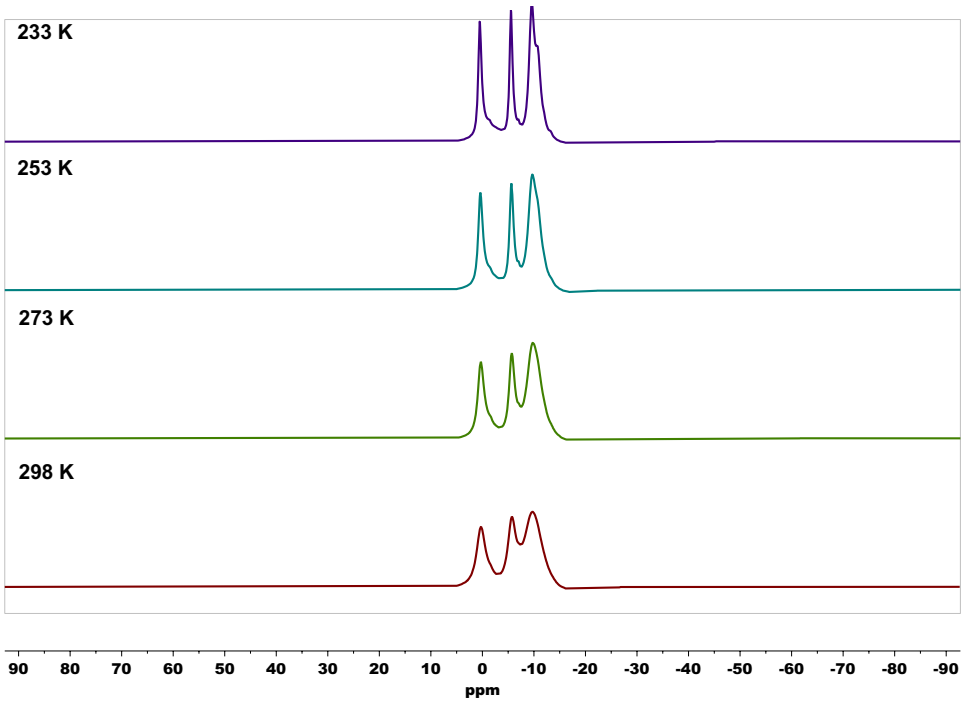


Figure S33. $^{11}B\{^{1}H\}$ NMR spectrum of **[2a]** in $CDCl_3$ at 233K, 253K, 273K, 298K.

III. Gutmann Beckett Titration

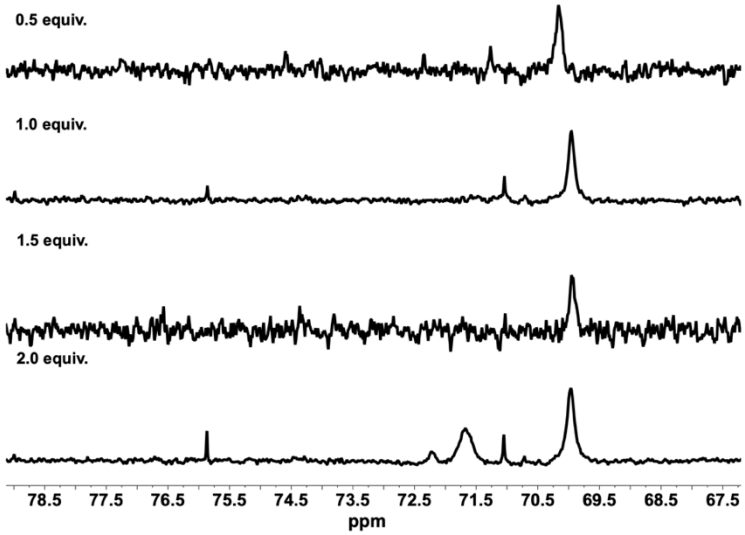
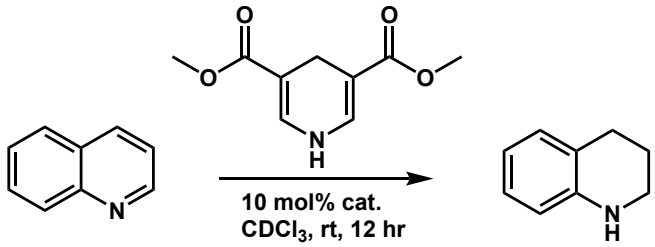


Figure S34. Gutmann–Beckett titration of **1b**. $^{31}P\{^{1}H\}$ NMR spectra recorded in $CDCl_3$ showing the progressive coordination shift upon addition of 0.5, 1.0, 1.5, and 2.0 equivalents of Et_3PO to **1b**.

IV. Hydrogenation of quinoline using a Hantzch ester and stiborane catalyst.



This reaction was prepared inside of a N_2 filled glovebox. Dry $CDCl_3$ solution (0.7 mL), antimony-based catalyst (0.008 mmol), Hantzsch ester (50 mg, 0.20 mmol), and quinoline (9 μL, 0.08 mmol) was added to a J-Young NMR tube. The tube was then sealed and the formation of the products was monitored by ^1H NMR in situ. The yield of the product was calculated based on the integration of two resonances: 6.4 ppm (d, 1H) and 6.5 ppm (t, 1H). The amount of the unreacted substrate was calculated based on the integration of two resonances: 8.1 ppm (d, 1H) and 8.2 ppm (d, 1H).

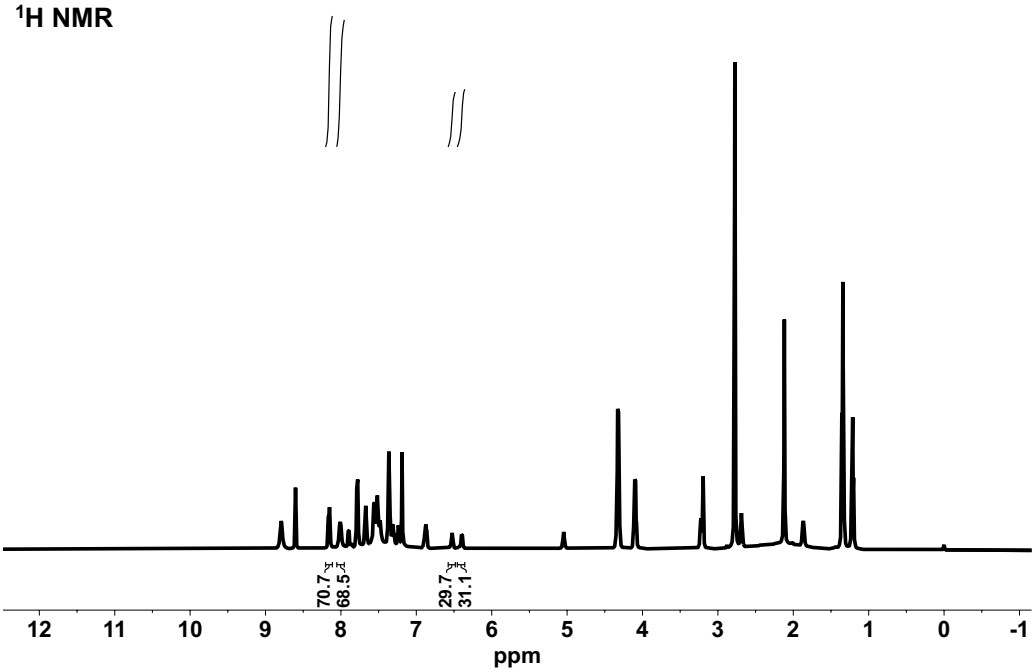


Figure S35. ^1H NMR spectrum of hydrogenation reaction using quinoline and Hantzsch ester with **2b** as the catalyst in $CDCl_3$.

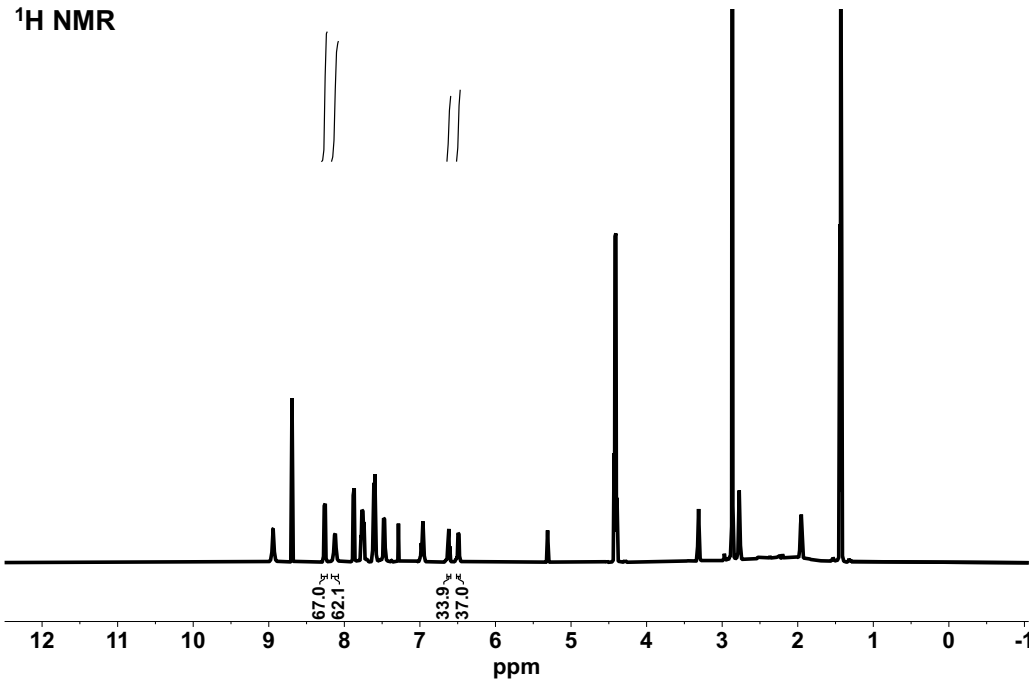


Figure S36. ^{1}H NMR spectrum of hydrogenation reaction using quinoline and Hantzsch ester with **1b** as the catalyst in $CDCl_3$.

V. Optimized Structures and Computational Details

All geometry optimizations of structures were achieved using B3LYP[2]D3[3]/LANL2Dz[4]def2-SVP[5] method, in gas phase as implemented in Gaussian16[6]. A split-valence basis set was employed, using LANL2Dz to handle the antimony centers and def2-SVP for all other atoms within the system. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as intermediates (no imaginary frequencies), as well as obtaining the thermochemistry: enthalpy (DH) and free energy (DG) at the temperature of 298 K. All structural figures were generated with CYLview.[7] Distances in structural figures are shown in Å and energies are in kJ/mol. Single point energy corrections were carried out further with the following method.

i) B2PLYPD3[8]/def2qzvpp-def2tzvp//B3LYP-D3/LANL2Dz-def2svp

For FIA, HIA and electron affinity (EA) calculations, Gibbs free energy and enthalpy corrections, as well as all entropic values, were obtained from the above-mentioned frequency calculations and used alongside the calculated Single Point electronic energies. The B2PLYPD3 method was benchmarked against reference FIA values[9] (see Table S5 for detailed benchmarking). Only the SCF portion of the B2PLYPD3 was used when performing the FIA, HIA, and EA calculations, the MP2 correction was not included in the electronic energies. For FIA and HIA calculations, isodesmic anchors were used according to the scheme outlined by Greb[10], with single point energy corrections calculated using the CCSD(t)[11]/aug-cc-pvtz[12] method in gas phase as implemented in Gaussian16. All EA values were calculated according to the relationship that the adiabatic electron affinity in gas phase is equal to the negative of the change of enthalpy at 0 K, as outlined by Chiu[13] (see Figure S49).

Figure S35. HOMO & LUMO orbitals of 1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. Constructed using an Isovalue of 0.0

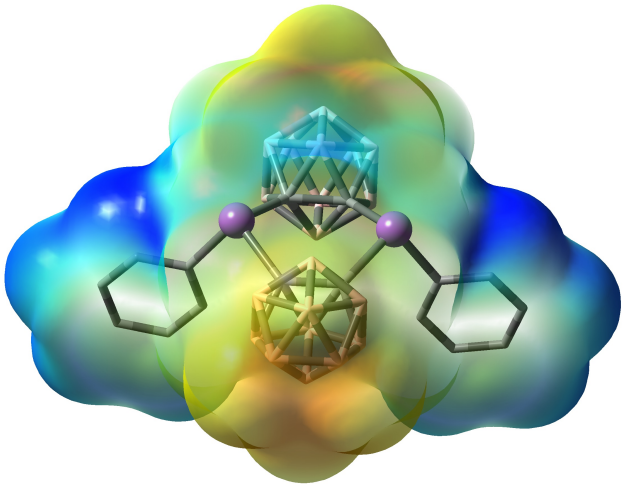


Figure S36. Electrostatic Potential Map of 1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

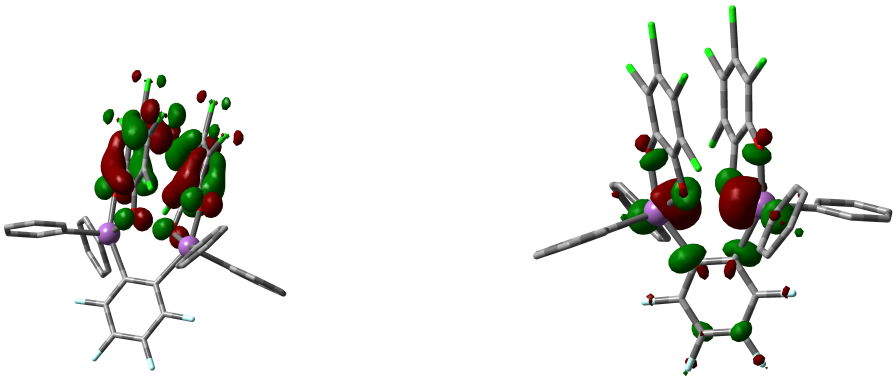


Figure S37. HOMO & LUMO orbitals of *o*-$(C_6F_4)(SbPh_2(diolate))_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. HOMO orbitals constructed using an Isovalue of 0.04, LUMO orbitals constructed using an Isovalue of 0.05.

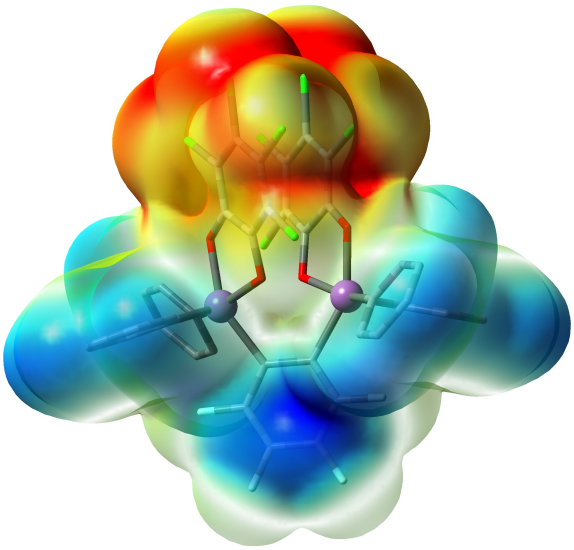


Figure S38. Electrostatic Potential Map of *o*-(C_6F_4)($SbPh_2$(diolate))$_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

HOMO ***LUMO***

Figure S39. HOMO & LUMO orbitals of *o*-($C_2B_{10}H_{10}$)($SbPh_2Cl)_2O$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. HOMO orbitals constructed using an Isovalue of 0.04, LUMO orbitals constructed using an Isovalue of 0.05.

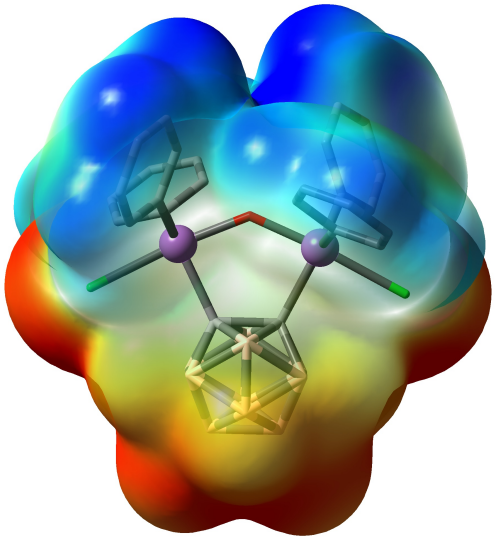


Figure S40. Electrostatic Potential Map of *o*-$(C_2B_{10}H_{10})(SbPh_2Cl)_2O$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

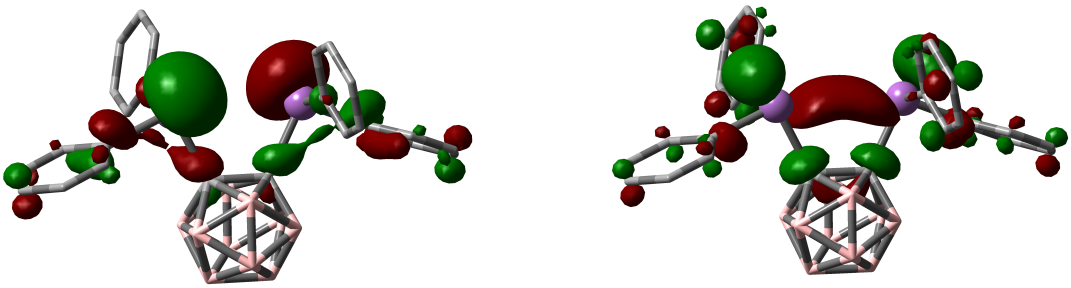


Figure S41. HOMO & LUMO orbitals of 1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. Constructed using an Isovalue of 0.04.

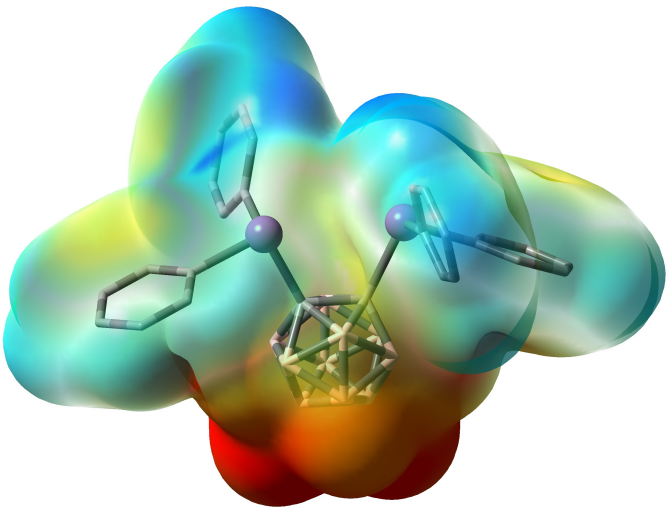


Figure S42. Electrostatic Potential Map of 1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

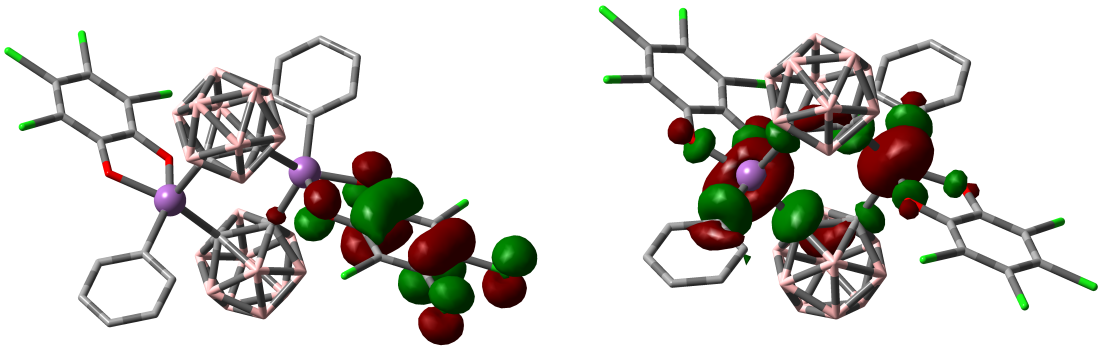


Figure S43. HOMO & LUMO orbitals of *o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. Constructed using an Isovalue of 0.04.

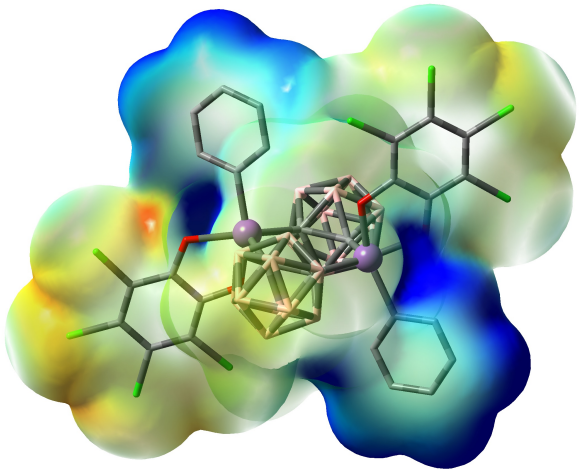


Figure S44. Electrostatic Potential Map of *o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

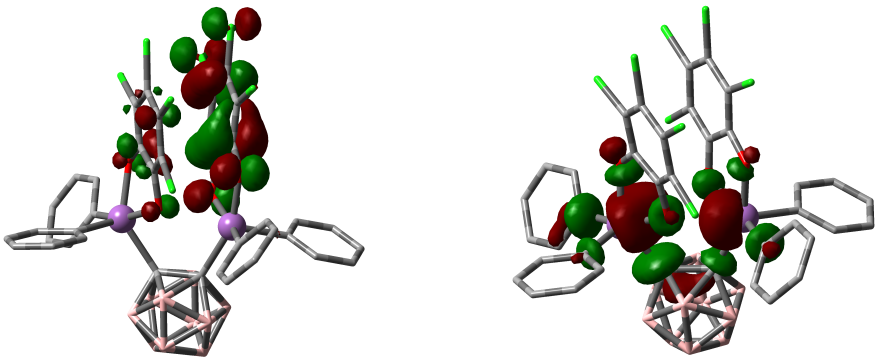


Figure S45. HOMO & LUMO orbitals of *o*-$(C_2B_{10}H_{10})(SbPh_2(diolate))_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory. Constructed using an Isovalue of 0.04.

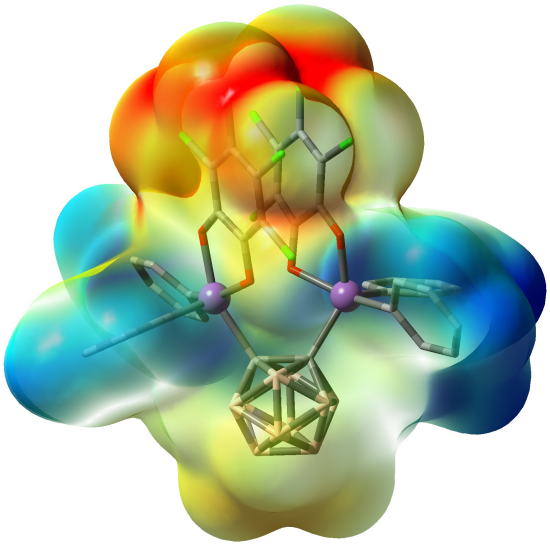


Figure S46. Electrostatic Potential Map of *o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$ calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

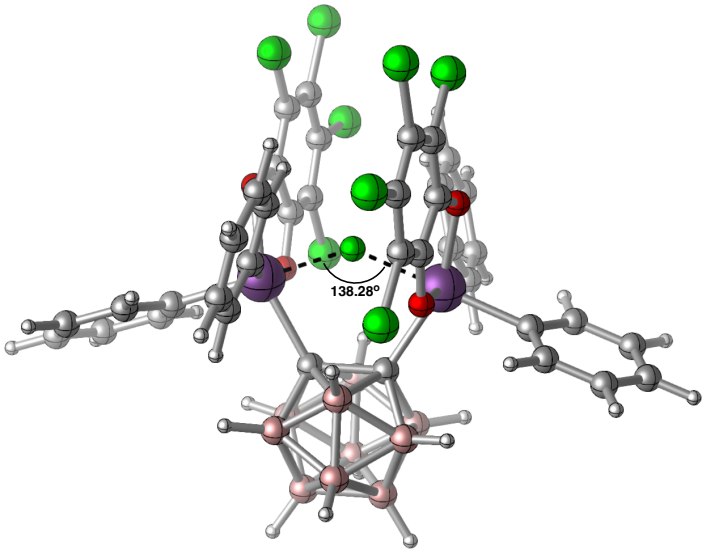


Figure S47. Vertex angle of *o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$ between the fluoride anion and metal centers is shown. Bond lengths represented by dashed lines are both 2.14 angstroms.

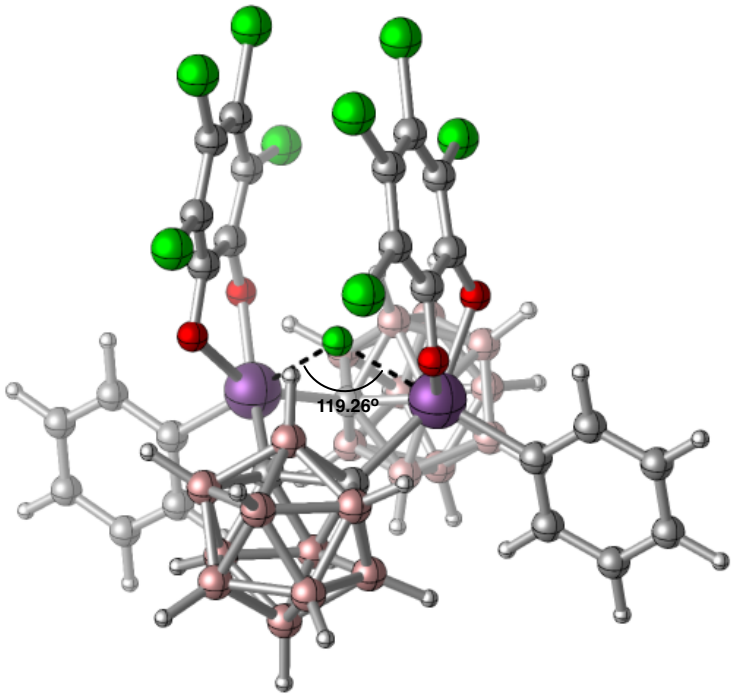


Figure S48. Vertex angle of *o*-$(C_2B_{10}H_{10})_2$(SbPh(diolate))$_2$ between the fluoride anion and metal centers is shown. Bond lengths represented by dashed lines are both 2.16 angstroms.

$$EA = -\Delta_g H^{0\,K} = -\Delta_g G^o - 0.00027\ eV - T\Delta_g S$$

Equation S1. Adiabatic electron affinity gas phase values were calculated using the relationship shown. All electron affinity values were calculated in eV at 298.15K. The 0.00027 eV term in the equation arises from the free energy of the electron computed from Boltzmann statistics.[13]

Structure	HOMO	LUMO	Gap
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$	-6.56	-1.78	4.78
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$	-7.47	-1.695	5.51
***o*-$(C_6F_4)(SbPh_2(diolate))_2$**	-5.65	-2.12	3.53
***o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$**	-6.32	-3.13	3.19
***o*-$(C_2B_{10}H_{10})(SbPh_2(diolate))_2$**	-5.71	-2.53	3.19
***o*-$(C_2B_{10}H_{10})(SbPh_2Cl)_2O$**	-7.41	-1.92	5.49

Table S1. HOMO & Lumo Gas Phase Values calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory, values are reported in eV.

Structure	Electronic Energy (a.u.)	Enthalpic Correction (a.u.)	FIA/HIA Value (kJ/mol)
Fluoride	-99.749537	0.00236	-
$SiFMe_3$	-508.437142	0.122589	941.433411
$SiMe_3$	-408.326245	0.117442	-
Hydride	-0.526562	0.00236	-
$SiHMe_3$	-409.212591	0.1272	925.189443

Table S2. Isodesmic anchor calculations reported in kJ/mol, calculated at the CCSD(t)/aug-cc-pvtz//B3LYP-D3/LANL2Dz-def2svp level of theory.

Structure	Electronic Energy (a.u.)	Enthalpic Correction (a.u.)	FIA Value (kJ/mol)
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$	-1834.794459	0.552338	248.73055
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$	-1702.546974	0.523157	282.56613
***o*-$(C_6F_4)(SbPh_2(diolate))_2$**	-6569.090449	0.56901	387.32077
***o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$**	-6139.748777	0.647185	448.22097
***o*-$(C_2B_{10}H_{10})(SbPh_2(diolate))_2$**	-6272.045228	0.677463	449.72502
***o*-$(C_2B_{10}H_{10})(SbPh_2Cl)_2O$**	-2830.048882	0.564397	308.27881

Table S3. FIA gas phase values reported in kJ/mol, calculated at the B2PLYPD3/def2qzvpp-def2tzvp//B3LYP-D3/LANL2Dz-def2svp level of theory using a 941.433411 kJ/mol TMS anchor.

Structure	Electronic Energy (a.u.)	Enthalpic Correction (a.u.)	HIA Value (kJ/mol)
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$	-1735.549435	0.554978	183.91003
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$	-1603.315039	0.525124	253.87782
***o*-$(C_6F_4)(SbPh_2(diolate))_2$**	-6469.855792	0.573232	345.56574
***o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$**	-6040.524090	0.650344	435.43209
***o*-$(C_2B_{10}H_{10})(SbPh_2(diolate))_2$**	-6172.804439	0.681221	393.08776

Table S4. HIA gas phase values reported in kJ/mol, calculated at the B2PLYPD3/def2qzvpp-def2tzvp//B3LYP-D3/LANL2Dz-def2svp level of theory using a 925.189443 kJ/mol TMS anchor.

Structure	**Method 1** (B2PLYPD3/def2qzvpp-def2tzvp//B3LYP-D3/LANL2Dz-def2svp)	**Method 2** (B2PLYPD3/def2qzvpp//B3LYP-D3/LANL2Dz-def2svp)	**Method 3** (pbe1pbe-D3BJ/def2qzvpp//B3LYP-D3/LANL2Dz-def2svp)	**Reference FIA Value***
SbH_5	211.6048	226.7906	348.05466	219
SbF_5	493.06627	507.37787	611.42644	496
$SbCl_5$	432.41985	447.33269	562.516	438
$SbBr_5$	419.48139	432.22556	548.92379	413

Table S5. FIA gas phase values reported in kJ/mol for different levels of theory, calculated using a 941.433411 kJ/mol TMS anchor. *Values taken from Greb[10].

Structure (Anionic)	Electronic Energy (a.u.)	$\Delta_g G^o$ (eV)	$T\Delta_g S$ (eV)	Electron Affinity (eV)
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$	-1734.9687	-0.649509	0.0831257	0.5661133
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$	-1602.7333	-1.282049	0.0323453	1.2494337
***o*-$(C_6F_4)(SbPh_2(diolate))_2$**	-6469.2527	-1.748507	0.0604374	1.6878000
***o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$**	-6039.9282	-2.819999	0.039688	2.7800415
***o*-$(C_2B_{10}H_{10})(SbPh_2(diolate))_2$**	-6172.2063	-2.397728	0.0843667	2.3130914
***o*-$(C_2B_{10}H_{10})(SbPh_2Cl)_2O$**	-2730.2428	-1.804671	0.0838238	1.7205769

Table S6. Electron affinity gas phase values reported in eV, calculated at the B2PLYPD3/def2qzvpp-def2tzvp//B3LYP-D3/LANL2Dz-def2svp level of theory.

Table S7. Cartesian coordinates (xyz format) and energies of all the structures calculated at the B3LYP-D3/LANL2Dz-def2svp level of theory.

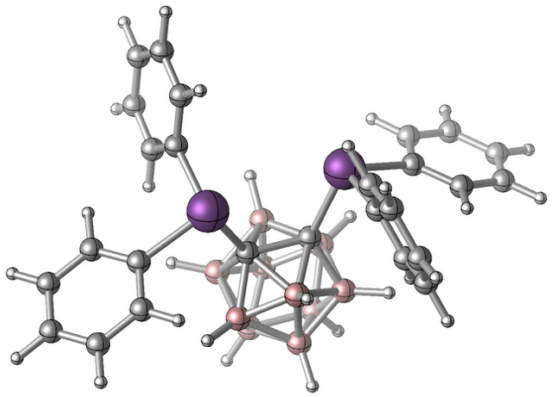
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$

E(scf) = -1267.44317231 a.u.

Sb	1.839359	-0.372956	-0.830776	B	1.311549	-1.062786	2.504703
Sb	-1.839361	0.372980	-0.830760	B	-1.311541	1.062713	2.504737
C	0.831681	-0.100295	1.167223	B	1.542733	0.695071	2.504609
C	-0.831678	0.100260	1.167228	B	-1.542725	-0.695144	2.504593
C	3.753157	-0.960722	-0.017925	B	0.181741	1.421545	1.610044
C	-3.753156	0.960723	-0.017886	B	-0.181736	-1.421593	1.610004

B	0.188952	1.439861	3.386284	H	-3.379955	-4.685834	-0.040400
B	-0.188942	-1.439960	3.386243	C	-2.760463	-2.644366	-0.367956
C	2.264245	1.698873	-1.282292	H	-2.954492	-2.363511	0.667833
C	-2.264249	-1.698835	-1.282337	C	-4.829912	0.079965	0.166697
B	0.882863	-0.114304	3.947888	H	-4.733107	-0.977266	-0.086981
B	-0.882851	0.114189	3.947893	C	-6.047742	0.545876	0.674449
C	4.829915	-0.079971	0.166677	H	-6.876208	-0.152939	0.817749
H	4.733109	0.977267	-0.086972	C	-6.205675	1.896290	0.998097
C	3.929348	-2.321158	0.291677	H	-7.156952	2.257220	1.397570
H	3.111913	-3.034242	0.145747	C	-5.144421	2.785455	0.802663
C	5.144424	-2.785478	0.802569	H	-5.261535	3.844147	1.048296
H	5.261539	-3.844177	1.048173	C	-3.929347	2.321150	0.291754
C	6.205679	-1.896319	0.998022	H	-3.111913	3.034238	0.145840
H	7.156958	-2.257260	1.397481	C	2.005700	2.111454	-2.601101
C	6.047746	-0.545896	0.674411	H	1.605695	1.402796	-3.333841
H	6.876214	0.152914	0.817726	C	2.760463	2.644376	-0.367886
C	-2.005711	-2.111377	-2.601159	H	2.954497	2.363490	0.667894
H	-1.605710	-1.402696	-3.333880	C	2.997794	3.963177	-0.766038
C	-2.246095	-3.430421	-3.001816	H	3.379955	4.685834	-0.040271
H	-2.039544	-3.732239	-4.032026	C	2.742995	4.358725	-2.083360
C	-2.743004	-4.358663	-2.083482	H	2.928316	5.390915	-2.391748
H	-2.928328	-5.390844	-2.391901	C	2.246081	3.430511	-3.001719
C	-2.997796	-3.963155	-0.766147	H	2.039525	3.732359	-4.031919

H	2.243207	-1.797455	2.371668	H	0.283248	2.341887	0.856700
H	-0.283245	-2.341913	0.856634	H	0.318673	2.479183	3.973370
H	-0.318662	-2.479298	3.973300	H	-2.243199	1.797386	2.371726
H	1.535848	-0.201599	4.952142	H	-1.535834	0.201456	4.952151
H	2.641148	1.151317	2.374552	H	-2.641141	-1.151387	2.374526



Zero-point correction= 0.516328 (Hartree/Particle)

Thermal correction to Energy= 0.549657

Thermal correction to Enthalpy= 0.550601

Thermal correction to Gibbs Free Energy= 0.447881

Sum of electronic and zero-point Energies= -1266.926845

Sum of electronic and thermal Energies= -1266.893515

Sum of electronic and thermal Enthalpies= -1266.892571

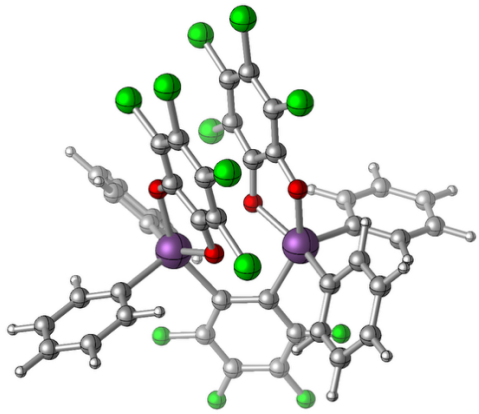
Sum of electronic and thermal Free Energies= -1266.995291

***o*-(C_6F_4)($SbPh_2$(diolate))$_2$**

E(scf) = -6002.45784725 a.u.

Cl	-5.552366	0.266790	-2.009720	Sb	0.985174	1.800902	-0.525219
Cl	-5.552366	-0.266790	2.009720	C	2.788934	-0.678872	0.170275
C	2.788934	0.678872	-0.170275	C	4.003270	-1.338944	0.334026
C	4.003271	1.338943	-0.334026	C	5.225216	-0.677371	0.167166
C	5.225216	0.677371	-0.167166	C	1.366054	-2.704503	2.398065
C	1.366054	2.704503	-2.398065	C	1.170488	3.321898	0.937745
C	1.170488	-3.321898	-0.937745	C	-1.734931	-1.145033	1.107201
C	-1.734931	1.145033	-1.107201	C	-3.126903	-1.217268	1.221835
C	-3.126903	1.217268	-1.221835	C	-3.819073	-0.228244	1.945672
C	-3.819073	0.228244	-1.945672	C	-3.103479	0.794928	2.596711
C	-3.103479	-0.794928	-2.596711	C	-1.700275	0.855763	2.485185
C	-1.700275	-0.855763	-2.485185	C	-1.026255	-0.070850	1.686466
C	-1.026255	0.070850	-1.686466	Cl	-3.948536	-2.508716	0.401618
Cl	-3.948536	2.508716	-0.401618	Cl	-3.946001	2.004340	3.515783
Cl	-3.946001	-2.004340	-3.515783	Cl	-0.773077	2.060739	3.323805
Cl	-0.773077	-2.060739	-3.323805	F	4.038619	-2.641133	0.646061
F	4.038619	2.641133	-0.646061	F	6.373023	-1.323068	0.325312
F	6.373023	1.323067	-0.325312	O	-1.025389	-2.034926	0.406422
O	-1.025389	2.034926	-0.406422	O	0.297201	0.002069	1.395334
O	0.297201	-0.002069	-1.395334	Sb	0.985174	-1.800902	0.525219

C	1.864663	3.899524	-4.877307	C	2.287021	-4.292433	-2.854834
H	2.057672	4.366763	-5.846421	H	3.081386	-4.255154	-3.604489
C	1.944567	4.660936	-3.706958	C	2.194703	-3.285090	-1.890633
H	2.201487	5.721989	-3.758021	H	2.909950	-2.459778	-1.912164
C	1.694904	4.066399	-2.466774	C	0.231253	-4.364837	-0.953420
H	1.761945	4.668283	-1.556409	H	-0.599969	-4.370385	-0.245903
C	1.289111	1.938730	-3.572371	C	0.333107	-5.373041	-1.915080
H	1.035037	0.877398	-3.523860	H	-0.402795	-6.180742	-1.930887
C	1.537942	2.541548	-4.809181	C	1.358090	-5.337315	-2.865676
H	1.473291	1.945781	-5.723193	H	1.428082	-6.121840	-3.623479
C	0.231253	4.364837	0.953420	C	1.289111	-1.938730	3.572371
H	-0.599969	4.370385	0.245903	H	1.035037	-0.877398	3.523860
C	2.194703	3.285090	1.890633	C	1.537942	-2.541548	4.809181
H	2.909950	2.459778	1.912164	H	1.473291	-1.945781	5.723193
C	2.287021	4.292433	2.854834	C	1.864663	-3.899524	4.877307
H	3.081386	4.255154	3.604489	H	2.057672	-4.366763	5.846421
C	1.358090	5.337315	2.865676	C	1.944567	-4.660936	3.706958
H	1.428082	6.121840	3.623479	H	2.201487	-5.721989	3.758021
C	0.333107	5.373041	1.915080	C	1.694904	-4.066399	2.466774
H	-0.402795	6.180742	1.930887	H	1.761944	-4.668283	1.556409



Zero-point correction= 0.509703 (Hartree/Particle)

Thermal correction to Energy= 0.565679

Thermal correction to Enthalpy= 0.566623

Thermal correction to Gibbs Free Energy= 0.414217

Sum of electronic and zero-point Energies= -6001.948144

Sum of electronic and thermal Energies= -6001.892169

Sum of electronic and thermal Enthalpies= -6001.891224

Sum of electronic and thermal Free Energies= -6002.043630

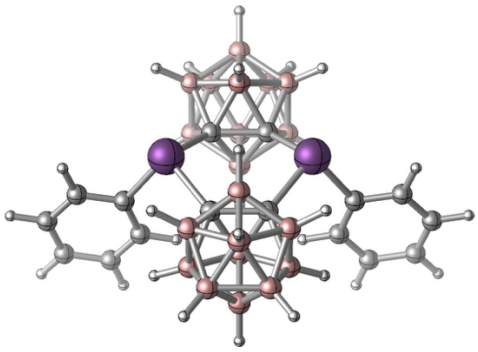
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$

E(scf) = -1135.14196085 a.u.

Sb	-2.128588	0.000045	-1.057140	B	-0.891131	-4.478759	-0.051695
C	-0.828985	-1.727407	-0.485126	B	-1.434960	-3.192659	-1.153203
C	-0.828918	1.727441	-0.485111	B	-1.438161	-2.913878	0.601675
C	-3.395215	0.000052	0.681296	B	-1.434838	3.192720	-1.153175

B	-1.438043	2.913926	0.601701	C	3.861915	-0.000065	3.065091
B	-0.000044	-1.940045	0.999981	H	3.499974	-0.000074	4.096274
B	-0.000079	-3.695606	1.294915	C	2.946123	-0.000068	2.011988
B	-0.000073	-4.159476	-1.574320	H	1.880782	-0.000079	2.238810
B	-0.000038	-2.402701	-1.834695	C	5.237187	-0.000049	2.803409
B	0.000038	1.940035	0.999994	H	5.951276	-0.000046	3.630794
Sb	2.128596	-0.000040	-1.057124	C	5.694711	-0.000037	1.484216
C	0.828922	-1.727440	-0.485118	H	6.766915	-0.000025	1.272708
C	0.828989	1.727408	-0.485108	C	4.776755	-0.000041	0.427431
B	0.890956	-4.478794	-0.051685	H	5.155396	-0.000031	-0.599983
B	1.434847	-3.192715	-1.153188	C	3.395209	-0.000055	0.681323
B	1.438040	-2.913934	0.601690	B	1.434969	3.192665	-1.153171
B	1.438157	2.913871	0.601705	B	0.000051	2.402711	-1.834678
C	-5.237211	0.000044	2.803367	B	0.000085	4.159485	-1.574290
H	-5.951307	0.000040	3.630746	B	0.891132	4.478757	-0.051657
C	-5.694724	0.000050	1.484170	B	0.000072	3.695594	1.294941
H	-6.766926	0.000051	1.272653	B	-0.890954	4.478792	-0.051659
C	-4.776759	0.000055	0.427393	H	0.000101	4.901158	-2.516916
H	-5.155392	0.000059	-0.600024	H	2.457010	3.129882	-1.778735
C	-2.946140	0.000046	2.011965	H	0.000041	1.790918	-2.864475
H	-1.880802	0.000043	2.238796	H	-0.000021	-1.790899	-2.864487
C	-3.861941	0.000042	3.065060	H	-0.000083	-4.901143	-2.516951
H	-3.500009	0.000037	4.096247	H	-2.456997	-3.129872	-1.778774

H	-1.552691	-5.466898	0.110142	H	-2.458483	2.681786	1.175515
H	-0.000093	-4.108963	2.421134	H	-2.456880	3.129978	-1.778743
H	1.552691	5.466894	0.110192	H	-2.458593	-2.681702	1.175487
H	2.458586	2.681691	1.175523	H	-0.000031	-1.065994	1.804929
H	-1.552476	5.466954	0.110187	H	2.458476	-2.681798	1.175513
H	0.000078	4.108942	2.421164	H	1.552476	-5.466958	0.110158
H	0.000020	1.065978	1.804936	H	2.456893	-3.129968	-1.778748



Zero-point correction= 0.488680 (Hartree/Particle)

Thermal correction to Energy= 0.519598

Thermal correction to Enthalpy= 0.520542

Thermal correction to Gibbs Free Energy= 0.427421

Sum of electronic and zero-point Energies= -1134.653280

Sum of electronic and thermal Energies= -1134.622363

Sum of electronic and thermal Enthalpies= -1134.621419

Sum of electronic and thermal Free Energies= -1134.714540

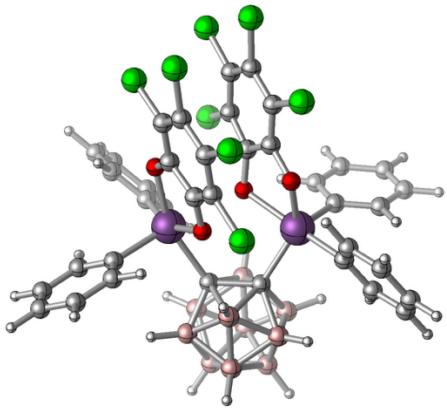
***o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$**

E(scf) = -5705.62910118 a.u.

Sb	0.557974	2.087580	-0.347523	Cl	-5.107516	-1.826569	1.793748
B	3.079878	0.435655	-1.902286	B	5.331779	1.988422	-0.964962
Cl	-4.442563	1.739984	0.095756	Cl	-3.073233	-3.355499	-0.134562
O	-1.475053	1.938010	-0.130778	B	5.204076	1.221331	0.649789
C	2.661766	1.355067	-0.482858	C	0.600768	3.479862	-1.940781
Sb	1.555707	-1.724805	0.315720	B	4.594502	-0.435697	0.398074
B	3.691136	2.091614	-1.654771	C	0.520988	3.341472	1.385175
Cl	-5.655789	-0.533531	-1.787100	B	5.736738	0.264994	-0.770109
O	0.130249	0.477863	-1.571026	C	-3.429996	0.804050	-0.960214
C	3.041098	-0.227180	-0.310812	C	-2.052903	1.042528	-0.933596
Cl	-3.715410	-2.202494	-3.651482	C	-3.950789	-0.205813	-1.796325
B	3.941983	2.350189	0.082861	C	-3.088424	-0.953919	-2.619629
O	0.469768	-0.040731	1.168825	C	-1.701525	-0.707811	-2.588237
O	-0.352879	-2.186439	-0.064605	C	-1.186075	0.261443	-1.728870
Cl	-0.579375	-1.587793	-3.585940	C	2.121657	-3.388023	-0.896196
B	3.497658	0.856525	0.939089	C	2.006456	-2.359137	2.289850
Cl	-0.976523	1.337908	3.475252	C	-0.787469	-0.463022	1.465298
B	4.344508	-0.681437	-1.344988	C	-1.622491	0.118837	2.423966
Cl	-4.024557	0.489571	3.652126	C	-2.962972	-0.302965	2.531116
B	4.792534	0.806005	-2.194972	C	-3.442327	-1.352643	1.723812

C	-2.564974	-2.019317	0.847712	H	1.006656	5.193413	-0.667042
C	-1.244693	-1.578540	0.737149	C	0.403343	3.038810	-3.258780
C	2.443165	-3.676215	2.504315	H	0.231159	1.981279	-3.467136
H	2.565627	-4.370191	1.670650	C	0.447497	3.955486	-4.312632
C	2.715330	-4.117451	3.802711	H	0.292552	3.608471	-5.337279
H	3.054630	-5.143565	3.963759	C	0.693932	5.308595	-4.058824
C	2.547388	-3.252013	4.887205	H	0.731686	6.021809	-4.886193
H	2.759586	-3.599522	5.901423	C	0.894327	5.748644	-2.747158
C	2.096082	-1.945815	4.675198	H	1.089902	6.804772	-2.545226
H	1.945942	-1.270749	5.521180	C	3.417244	-3.919129	-0.774155
C	1.821813	-1.494452	3.381842	H	4.151785	-3.467055	-0.104237
H	1.445602	-0.482279	3.233792	C	1.194840	-3.996501	-1.755397
C	1.492131	3.365293	2.392249	H	0.181381	-3.607852	-1.842568
H	2.350420	2.700934	2.363641	C	1.575065	-5.117900	-2.500291
C	1.351476	4.230999	3.480828	H	0.850813	-5.583004	-3.173607
H	2.112425	4.234954	4.265177	C	2.865080	-5.641690	-2.383547
C	0.243631	5.077544	3.569416	H	3.155264	-6.518862	-2.967447
H	0.133544	5.749269	4.424518	C	3.784381	-5.045838	-1.514260
C	-0.726565	5.057187	2.563844	H	4.793284	-5.453176	-1.413236
H	-1.601803	5.708239	2.628988	H	2.239693	0.129853	-2.682541
C	-0.594483	4.192380	1.474582	H	5.210488	0.775003	-3.318438
H	-1.381571	4.160366	0.720277	H	4.348448	-1.771541	-1.821555
C	0.846436	4.837185	-1.687797	H	4.748142	-1.368251	1.133999

H	6.850167	-0.172044	-0.867235	H	3.246121	2.965646	-2.331997
H	5.912942	1.490220	1.579341	H	3.661293	3.402990	0.572018
H	6.147214	2.834662	-1.206787	H	2.911379	0.800190	1.969726



Zero-point correction= 0.618116 (Hartree/Particle)

Thermal correction to Energy= 0.673835

Thermal correction to Enthalpy= 0.674779

Thermal correction to Gibbs Free Energy= 0.527780

Sum of electronic and zero-point Energies= -5705.010985

Sum of electronic and thermal Energies= -5704.955267

Sum of electronic and thermal Enthalpies= -5704.954322

Sum of electronic and thermal Free Energies= -5705.101321

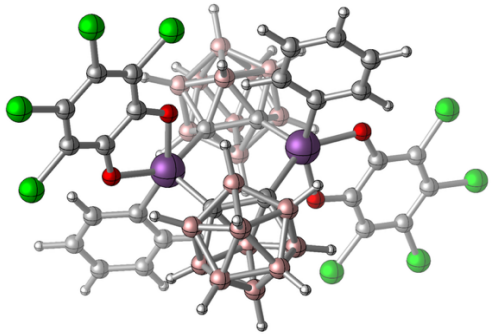
***o*-($C_2B_{10}H_{10}$)$_2$(SbPh(diolate))$_2$**

E(scf) = -5573.27371834 a.u.

Cl	7.652330	2.161432	-0.761629	B	0.201495	-0.721630	4.270784
Cl	6.191483	-2.950290	0.614593	B	-0.870829	0.491688	3.514036
Cl	8.468758	-0.751989	0.167101	B	0.110840	1.925800	3.126577
Sb	1.596323	-1.073131	-0.244393	B	1.793469	1.619157	3.609798
Cl	4.555851	2.840332	-1.242619	B	1.853432	-0.019728	4.333067
O	3.443890	-1.859107	0.078769	B	0.433927	1.018358	4.618026
O	2.800679	0.493173	-0.708822	Sb	-1.756317	1.357493	0.399039
C	1.060638	-0.241839	1.687878	Cl	-3.710505	-3.182197	1.351601
C	-0.249380	0.739700	1.937043	O	-3.721078	1.632738	-0.049421
C	-1.658350	3.479032	0.619125	O	-2.544408	-0.465162	0.843702
C	4.467560	-1.005272	-0.095134	C	-0.996115	0.868452	-1.573487
C	5.807964	-1.335208	0.109964	C	0.303993	-0.129206	-1.814613
C	6.799921	-0.351762	-0.097578	C	0.911553	-3.088178	-0.391495
C	6.437752	0.945710	-0.514602	C	-4.480693	0.529813	0.020658
C	5.081221	1.264788	-0.732751	C	-5.824651	0.483209	-0.354510
C	4.110272	0.286137	-0.522536	C	-6.537907	-0.727834	-0.224386
B	1.317986	1.451550	1.908562	C	-5.899145	-1.873918	0.290821
B	2.397301	0.242458	2.658994	C	-4.542038	-1.813916	0.670968
B	1.425165	-1.194173	3.065347	C	-3.838462	-0.619008	0.517926
B	-0.257770	-0.892919	2.572181	B	-1.282022	-0.730126	-2.142185

B	-2.187506	0.660735	-2.801052	H	0.467772	3.618814	0.160529
B	-1.102924	2.076378	-2.781077	C	-2.823156	4.190156	0.941306
B	0.477124	1.568530	-2.120321	H	-3.775135	3.674422	1.065318
B	0.266382	1.748240	-3.871702	C	-0.400243	5.543619	0.538658
B	1.162171	0.348407	-3.230268	H	0.544621	6.066056	0.372363
B	0.079156	-1.065358	-3.233725	C	-1.555132	6.257517	0.872471
B	-1.499175	-0.562606	-3.892553	H	-1.514700	7.344840	0.973017
B	-1.382580	1.182008	-4.297274	C	-2.761449	5.581209	1.071630
B	0.015882	0.113814	-4.569597	H	-3.668428	6.135617	1.324237
Cl	-6.553005	1.929033	-0.974799	H	-0.406346	2.995109	3.022334
Cl	-8.204815	-0.794954	-0.702084	H	1.649606	2.095020	0.967465
Cl	-6.771197	-3.364996	0.462028	H	2.519129	2.517244	3.930539
C	1.813590	-4.089521	-0.784844	H	3.495486	0.127418	2.208926
H	2.863572	-3.856249	-0.960655	H	2.640973	-0.313064	5.187934
C	1.357681	-5.403605	-0.922298	H	1.859680	-2.291041	2.869184
H	2.058422	-6.183530	-1.229804	H	-0.219914	-1.508572	5.070159
C	0.020290	-5.719007	-0.664571	H	0.169846	1.499666	5.684142
H	-0.329843	-6.748120	-0.776584	H	-2.054326	0.587643	3.668451
C	-0.867877	-4.720486	-0.256792	H	-0.937910	-1.723751	2.080243
H	-1.912779	-4.954043	-0.042524	H	1.114891	2.229198	-1.370227
C	-0.427988	-3.400964	-0.120045	H	0.831878	2.637118	-4.442611
H	-1.141872	-2.647982	0.209841	H	2.346144	0.203578	-3.249721
C	-0.444912	4.153093	0.416983	H	0.527099	-2.174860	-3.235955

H	0.416380	-0.183413	-5.660091	H	-2.020151	1.677496	-5.183549
H	-2.206312	-1.336633	-4.472992	H	-1.515576	3.148939	-2.451263
H	-3.334765	0.775498	-2.495495	H	-1.778998	-1.515499	-1.408114



Zero-point correction= 0.588815 (Hartree/Particle)

Thermal correction to Energy= 0.643137

Thermal correction to Enthalpy= 0.644081

Thermal correction to Gibbs Free Energy= 0.499990

Sum of electronic and zero-point Energies= -5572.684903

Sum of electronic and thermal Energies= -5572.630581

Sum of electronic and thermal Enthalpies= -5572.629637

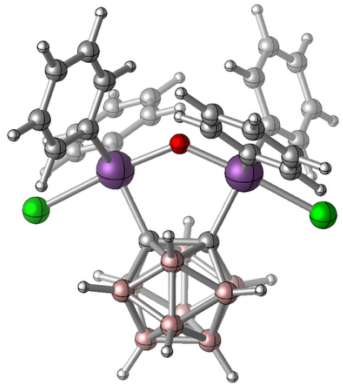
Sum of electronic and thermal Free Energies= -5572.773728

***o*-($C_2B_{10}H_{10}$)($SbPh_2Cl)_2O$**

E(scf) = -2262.80282225 a.u.

C	2.576067	-4.309539	-1.621953	C	2.011396	-1.987565	-1.256941
H	2.960985	-5.258734	-1.241065	C	2.521362	-3.197758	-0.774344
C	2.150452	-4.205689	-2.949513	H	2.889934	-3.274094	0.250003
H	2.205038	-5.074501	-3.610463	C	1.576840	-1.879992	-2.586668
C	1.660694	-2.988027	-3.434490	H	1.157789	-0.941786	-2.955787
H	1.334238	-2.900537	-4.473869	C	-2.011278	1.987511	-1.256462
C	-3.391738	-4.145682	-1.516178	C	-1.577752	1.879659	-2.586497
H	-3.726720	-5.133487	-1.843209	H	-1.159522	0.941203	-2.955921
C	-4.246219	-3.330718	-0.766899	C	-1.661594	2.987723	-3.434285
H	-5.249101	-3.678372	-0.506775	H	-1.335950	2.900025	-4.473902
C	-3.825221	-2.067377	-0.340043	C	-2.150303	4.205674	-2.948976
H	-4.494025	-1.436273	0.246509	H	-2.204874	5.074504	-3.609905
Sb	1.798374	-0.265538	-0.022706	C	-2.574905	4.309793	-1.621113
Sb	-1.798291	0.265463	-0.022277	H	-2.959014	5.259213	-1.239969
Cl	3.924132	-0.886184	1.129743	C	-2.520222	3.197996	-0.773523
Cl	-3.923593	0.886702	1.130696	H	-2.888026	3.274557	0.251085
O	-0.000087	-0.000273	-0.791826	C	-2.537123	-1.622005	-0.668524
C	0.815389	-0.163673	1.940494	C	-1.679121	-2.435909	-1.421365
C	1.678495	2.435333	-1.422661	H	-0.678077	-2.091403	-1.668837
H	0.677824	2.090139	-1.670692	C	-2.109127	-3.696483	-1.843922

H	-1.430686	-4.324908	-2.426489	H	2.119796	-1.951804	3.110885
B	0.277959	1.415364	2.360421	B	-0.277324	-1.415647	2.360267
H	0.455616	2.304439	1.580715	H	-0.455140	-2.304601	1.580462
C	-0.814842	0.163452	1.940690	B	-1.242166	1.157064	3.261280
C	2.536513	1.622157	-0.669054	H	-2.118984	1.951419	3.111662
C	3.824105	2.068428	-0.339814	B	0.284548	1.426521	4.135534
H	4.492950	1.437865	0.247274	H	0.488140	2.450975	4.725562
C	4.244558	3.331961	-0.766641	B	0.874364	-0.173260	4.696291
H	5.247033	3.680330	-0.505907	H	1.515497	-0.300667	5.702536
C	3.390052	4.146205	-1.516675	B	-0.283536	-1.427084	4.135373
H	3.724607	5.134162	-1.843682	H	-0.487003	-2.451629	4.725284
C	2.107964	3.696091	-1.845210	B	-1.589841	-0.593629	3.257349
H	1.429503	4.323947	-2.428368	H	-2.704384	-0.991191	3.100148
B	1.590663	0.593212	3.257107	B	-0.873231	0.172612	4.696503
H	2.705167	0.990809	3.099747	H	-1.514150	0.299867	5.702904
B	1.242999	-1.157483	3.260833				



Zero-point correction= 0.524022 (Hartree/Particle)

Thermal correction to Energy= 0.561129

Thermal correction to Enthalpy= 0.562073

Thermal correction to Gibbs Free Energy= 0.452863

Sum of electronic and zero-point Energies= -2262.278800

Sum of electronic and thermal Energies= -2262.241694

Sum of electronic and thermal Enthalpies= -2262.240749

Sum of electronic and thermal Free Energies= -2262.349959

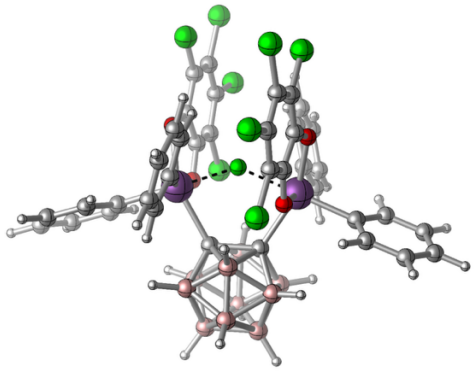
***o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$_FIA**

E(scf) = -5805.56517262 a.u.

H	-4.150060	-6.525964	-2.614818	H	-4.171299	4.409605	1.118353
Cl	-5.960247	2.023027	2.131271	C	-2.834592	4.087511	-0.552739
Cl	-4.977384	1.223446	-0.806239	H	-3.442980	4.659003	-1.258413
C	-3.238460	3.955025	0.777727	Cl	-4.424125	0.858455	4.642657

Cl	4.426294	-0.742220	4.661447	C	-2.910866	-0.546334	2.848195
C	-3.367614	-3.286261	-1.863705	C	-3.979448	0.359422	3.029747
C	-4.113512	-4.383796	-2.302992	C	-4.648046	0.891908	1.916183
H	-5.131167	-4.230842	-2.672639	C	-4.223547	0.555532	0.614303
C	-3.564376	-5.669406	-2.269296	C	-3.147050	-0.315052	0.435858
C	-2.266978	-5.856227	-1.785366	C	-2.057169	-3.465363	-1.389720
H	-1.833044	-6.859157	-1.745206	H	-3.804386	-2.286818	-1.882224
C	-1.517563	-4.759480	-1.345364	C	0.888300	-2.708865	-0.039785
H	-0.510628	-4.927833	-0.958110	C	1.661200	-3.491921	-0.909532
Sb	-0.932904	-1.782870	-0.672547	H	1.368371	-3.624303	-1.952987
Sb	0.932387	1.765270	-0.716570	C	2.834494	-4.099870	-0.452305
Cl	-2.031331	-1.213170	4.195251	H	3.442775	-4.688583	-1.143772
Cl	4.977285	-1.242879	-0.776883	C	3.238857	-3.934167	0.874284
Cl	5.961398	-1.968960	2.179185	H	4.171983	-4.379824	1.225747
Cl	2.032989	1.317239	4.163587	C	2.469049	-3.157139	1.743803
F	-0.000138	0.000569	0.069214	H	2.796060	-3.003422	2.774626
O	-1.549520	-1.784988	1.295734	C	1.299961	-2.538560	1.291414
O	-2.641327	-0.622460	-0.750560	H	0.708490	-1.927014	1.973600
O	2.640820	0.603329	-0.766266	C	3.147054	0.325652	0.427243
O	1.549528	1.816186	1.250891	C	4.223837	-0.539968	0.626879
C	-0.406655	-0.766963	-2.596926	C	4.648939	-0.843730	1.936555
C	0.406022	0.702045	-2.615115	C	3.980742	-0.283738	3.036786
C	-2.521402	-0.920013	1.558332	C	2.911900	0.617011	2.833170

C	2.521720	0.958238	1.534558	H	4.148709	6.458969	-2.776621
C	2.056262	3.429547	-1.475593	C	2.265812	5.809870	-1.930505
C	3.366653	3.238850	-1.945184	H	1.831794	6.813450	-1.915187
H	3.803503	2.239292	-1.938920	C	1.516565	4.724325	-1.463283
C	4.112396	4.325199	-2.411695	H	0.509691	4.902170	-1.080149
H	5.130013	4.163199	-2.777572	C	-0.888620	2.706663	-0.106454
C	3.563151	5.611204	-2.409852	C	-1.299857	2.569573	1.228703



Zero-point correction= 0.619466 (Hartree/Particle)

Thermal correction to Energy= 0.676519

Thermal correction to Enthalpy= 0.677463

Thermal correction to Gibbs Free Energy= 0.527656

Sum of electronic and zero-point Energies= -5804.945706

Sum of electronic and thermal Energies= -5804.888654

Sum of electronic and thermal Enthalpies= -5804.887710

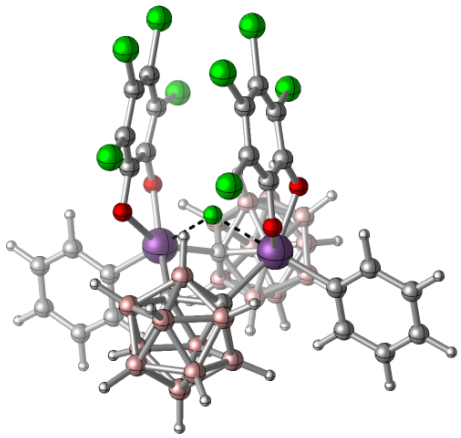
Sum of electronic and thermal Free Energies= -5805.037516

***o*-($C_2B_{10}H_{10}$)$_2$(SbPh(diolate))$_2$_FIA**

E(scf) = -5673.22371084 a.u.

H	-4.096449	7.007281	1.341018	Cl	5.463845	-1.307798	-1.346572
H	-5.417382	4.907034	1.079909	Cl	5.231368	-2.291289	1.655659
C	-3.583961	6.056348	1.172104	Cl	2.338735	-2.907748	2.870945
C	-4.326138	4.880305	1.026326	F	-0.131861	-0.000005	0.000002
H	-5.410806	0.480074	-3.563534	O	0.181843	2.712048	-0.795524
C	-4.325869	-4.880497	-1.026351	O	0.375465	2.039338	1.659585
C	-3.583632	-6.056501	-1.172133	O	0.181987	-2.712016	0.795537
H	-4.096072	-7.007459	-1.341054	O	0.375591	-2.039307	-1.659578
C	-2.187725	-6.018305	-1.098961	C	-2.046671	0.478689	1.972186
H	-1.605577	-6.936887	-1.209076	C	-2.169466	-1.113368	1.559361
C	-1.530192	-4.804151	-0.879791	C	-2.046623	-0.478774	-1.972194
H	-0.440918	-4.775752	-0.809434	C	1.423897	2.468131	-0.371506
H	-5.417112	-4.907280	-1.079938	C	1.530027	2.082810	0.986194
Sb	-1.222799	1.819009	0.394982	C	2.762819	1.669128	1.496998
Sb	-1.222687	-1.819044	-0.394981	C	3.914805	1.742510	0.682955
Cl	2.816856	1.033898	3.114258	C	3.810921	2.161050	-0.656745
Cl	5.463742	1.307991	1.346586	C	2.549848	2.489379	-1.196462
Cl	5.231239	2.291477	-1.655645	C	1.424032	-2.468054	0.371519
Cl	2.338590	2.907862	-2.870930	C	1.530152	-2.082734	-0.986182
Cl	2.816949	-1.033779	-3.114244	C	2.762931	-1.669013	-1.496984

C	3.914919	-1.742359	-0.682941	B	-3.517555	-1.828351	2.355687
C	3.811047	-2.160900	0.656760	H	-4.132109	-2.684591	1.790885
C	2.549983	-2.489264	1.196477	B	-3.140747	-1.740992	4.098422
C	-2.274421	-3.625186	-0.739593	H	-3.543985	-2.583862	4.855468
C	-3.673313	-3.663251	-0.811122	B	-2.984745	-0.021972	4.547571
B	-1.611921	-0.667484	-3.638289	H	-3.281798	0.407760	5.630753
H	-0.906199	-1.579611	-3.944522	B	-1.611993	0.667425	3.638284
B	-0.906229	0.634876	-2.655028	H	-0.906325	1.579593	3.944521
H	0.218453	0.616983	-2.298134	B	-1.861402	-2.121250	2.924027
H	-0.739106	1.296643	-5.132937	H	-1.341295	-3.178357	2.744796
B	-0.906220	-0.634896	2.655030	C	-2.274626	3.625097	0.739581
H	0.218465	-0.616940	2.298146	C	-1.530456	4.804100	0.879774
B	-1.517490	-1.000956	4.268326	H	-0.441181	4.775756	0.809418
H	-0.739079	-1.296650	5.132941	C	-2.188052	6.018222	1.098935



Zero-point correction= 0.591120 (Hartree/Particle)

Thermal correction to Energy= 0.646240

Thermal correction to Enthalpy= 0.647185

Thermal correction to Gibbs Free Energy= 0.504123

Sum of electronic and zero-point Energies= -5672.632591

Sum of electronic and thermal Energies= -5672.577470

Sum of electronic and thermal Enthalpies= -5672.576526

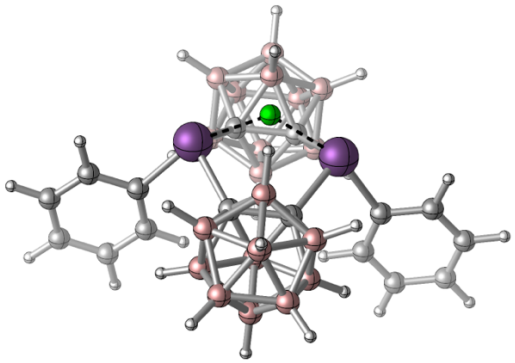
Sum of electronic and thermal Free Energies= -5672.719587

1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$ _FIA

E(scf) = - 1235.02608123 a.u.

Sb	1.966597	0.000023	-1.129944	B	-1.437774	-2.885098	0.826984
C	0.825570	1.824093	-0.386727	C	5.323950	0.000010	2.631396
C	0.825601	-1.824075	-0.386749	H	6.097414	0.000005	3.404987
C	3.314813	0.000020	0.635406	C	5.678496	0.000013	1.281185
B	0.891760	4.516176	0.367905	H	6.732869	0.000011	0.988527
B	1.436473	3.360670	-0.876717	C	4.678419	0.000018	0.299036
B	1.437855	2.885094	0.826878	H	4.980558	0.000020	-0.755594
B	1.436529	-3.360635	-0.876759	C	2.982293	0.000017	2.001284
B	1.437906	-2.885079	0.826843	H	1.937128	0.000018	2.310084
B	0.000039	1.886424	1.111914	C	3.969958	0.000012	2.988504
B	0.000045	3.588775	1.609665	H	3.682109	0.000009	4.043880
B	-0.000095	4.375665	-1.173706	C	-3.969701	-0.000046	2.988851
B	-0.000100	2.674053	-1.652462	H	-3.681759	-0.000055	4.044201
B	0.000073	-1.886436	1.111893	C	-2.982124	-0.000039	2.001543
Sb	-1.966698	-0.000010	-1.129751	H	-1.936931	-0.000042	2.310248
C	-0.825632	1.824077	-0.386649	C	-5.323725	-0.000042	2.631864
C	-0.825601	-1.824086	-0.386669	H	-6.097120	-0.000048	3.405524
B	-0.891807	4.516158	0.367989	C	-5.678392	-0.000031	1.281684
B	-1.436614	3.360641	-0.876582	H	-6.732792	-0.000028	0.989121
B	-1.437825	2.885065	0.827015	C	-4.678404	-0.000024	0.299445

H	-4.980636	-0.000015	-0.755158	H	0.000097	3.869397	2.779370
C	-3.314769	-0.000028	0.635695	H	-1.552373	-5.483771	0.644885
B	-1.436559	-3.360654	-0.876618	H	-2.458586	-2.605123	1.377555
B	-0.000058	-2.674034	-1.652492	H	1.552520	-5.483751	0.644732
B	-0.000023	-4.375651	-1.173756	H	0.000168	-3.869429	2.779325
B	-0.891729	-4.516177	0.367939	H	0.000100	-0.944225	1.830162
B	0.000109	-3.588793	1.609624	H	2.458767	-2.605089	1.377314
B	0.891837	-4.516165	0.367851	H	2.461410	-3.387595	-1.501768
H	-0.000060	-5.225242	-2.025757	H	2.458721	2.605115	1.377348
H	-2.461501	-3.387627	-1.501526	H	0.000079	0.944204	1.830173
H	-0.000116	-2.254689	-2.763401	H	-2.458633	2.605066	1.377580
H	-0.000150	2.254721	-2.763376	H	-1.552467	5.483739	0.644946
H	-0.000144	5.225266	-2.025697	H	-2.461556	3.387603	-1.501492
H	2.461355	3.387654	-1.501725	F	-0.000048	0.000014	-2.284046
H	1.552426	5.483770	0.644798				



Zero-point correction= 0.490102 (Hartree/Particle)

Thermal correction to Energy= 0.522212

Thermal correction to Enthalpy= 0.523157

Thermal correction to Gibbs Free Energy= 0.429874

Sum of electronic and zero-point Energies= -1234.535979

Sum of electronic and thermal Energies= -1234.503869

Sum of electronic and thermal Enthalpies= -1234.502925

Sum of electronic and thermal Free Energies= -1234.596207

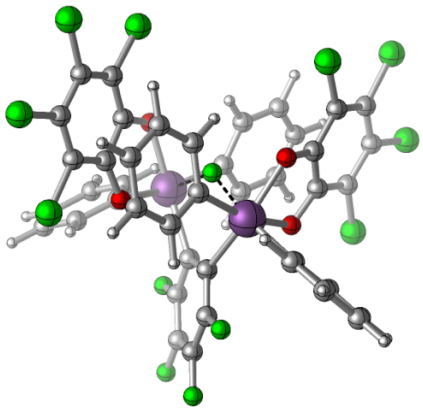
_o_-(C_6F_4)($SbPh_2$(diolate))$_2$_FIA

E(scf) = -6102.36741067 a.u.

Cl	4.986845	-0.549812	-4.381845	C	0.038577	0.692491	4.764815
Cl	-4.986763	0.552254	-4.381589	C	1.779868	3.464180	1.298589
C	0.087243	0.701770	2.322475	C	1.055731	-2.642920	-0.233212
C	0.102097	1.368846	3.539858	C	2.604183	1.009989	-1.514884

C	3.185250	0.710978	-2.751485	C	-3.096966	-0.372174	-0.340278
C	4.310841	-0.139494	-2.823912	Cl	-2.472016	-1.407782	-4.180805
C	4.854234	-0.685093	-1.651760	Cl	-6.261311	1.718403	-1.725250
C	4.242408	-0.424866	-0.407904	Cl	-4.866755	1.082662	1.081733
C	3.096948	0.372344	-0.340064	F	-0.185490	-2.712808	3.598694
Cl	2.472075	1.410088	-4.180027	F	-0.071142	-1.365938	5.916990
Cl	6.261358	-1.717411	-1.726125	O	-1.575560	-1.833660	-1.364300
Cl	4.866726	-1.083250	1.081180	O	-2.423108	-0.590798	0.780270
F	0.185445	2.710847	3.600166	Sb	-0.728565	-1.767906	0.518088
F	0.071100	1.362721	5.917729	C	3.191248	5.683101	2.282894
O	1.575542	1.834378	-1.363305	H	3.740724	6.547125	2.667447
O	2.423060	0.590327	0.780589	C	2.014266	5.869334	1.552227
Sb	0.728541	1.767606	0.519046	H	1.640203	6.879024	1.360324
C	-0.087285	-0.703038	2.322096	C	1.311041	4.763465	1.061716
C	-0.102141	-1.370775	3.539117	H	0.391859	4.922924	0.491516
C	-0.038619	-0.695084	4.764439	C	2.968079	3.282426	2.023073
C	-1.779867	-3.464929	1.296691	H	3.349748	2.272474	2.190225
C	-1.055736	2.643062	-0.231781	C	3.667211	4.388470	2.515373
C	-2.604185	-1.009172	-1.515442	H	4.591643	4.237263	3.079999
C	-3.185218	-0.709463	-2.751890	C	-1.398043	2.495362	-1.584342
C	-4.310795	0.141065	-2.823870	H	-0.733829	1.948458	-2.256042
C	-4.854205	0.686022	-1.651427	C	-1.912757	3.329400	0.637642
C	-4.242410	0.425095	-0.407701	H	-1.665469	3.427561	1.699494

C	-3.102028	3.883504	0.152974	C	1.912744	-3.329754	0.635826
H	-3.778721	4.401844	0.836878	H	1.665446	-3.428521	1.697619
C	-3.440968	3.740856	-1.194530	C	1.398049	-2.494450	-1.585686
H	-4.389648	4.135423	-1.564479	H	0.733845	-1.947160	-2.257081
C	-2.592475	3.042938	-2.060115	C	2.592484	-3.041757	-2.061762
H	-2.878893	2.895737	-3.104493	H	2.878910	-2.893964	-3.106054
C	3.102018	-3.883584	0.150852	C	3.440969	-3.740170	-1.196569
H	3.778705	-4.402314	0.834466				



Zero-point correction= 0.510745 (Hartree/Particle)

Thermal correction to Energy= 0.568066

Thermal correction to Enthalpy= 0.569010

Thermal correction to Gibbs Free Energy= 0.414261

Sum of electronic and zero-point Energies= -6101.856666

Sum of electronic and thermal Energies= -6101.799345

Sum of electronic and thermal Enthalpies= -6101.798401

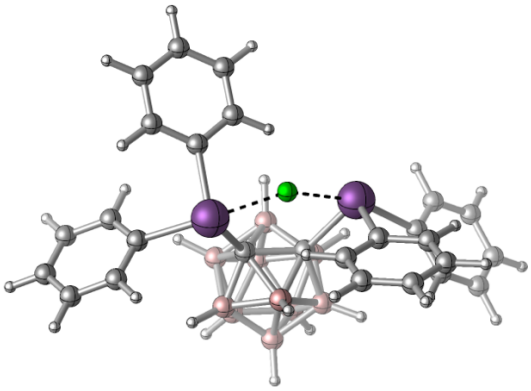
Sum of electronic and thermal Free Energies= -6101.953150

1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$ _FIA

E(scf) = -1367.31079639 a.u.

Sb	2.021820	-0.759512	0.678051	C	4.388618	0.609256	2.168767
Sb	-2.021801	-0.759530	-0.678013	H	3.794207	0.235161	3.011232
C	0.844003	1.128422	0.176911	C	5.585153	1.284824	2.440801
C	-0.843991	1.128418	-0.176908	H	5.908784	1.431018	3.476162
C	3.932706	0.407985	0.854737	C	6.362117	1.773559	1.387217
C	-3.932679	0.407973	-0.854790	H	7.297401	2.303895	1.590376
B	1.216902	2.468504	1.163694	C	5.933821	1.577971	0.069251
B	-1.216892	2.468492	-1.163702	H	6.534602	1.957554	-0.763275
B	1.588859	2.474447	-0.566721	C	-1.720898	-1.805144	2.302589
B	-1.588850	2.474447	0.566713	H	-0.670795	-1.552160	2.168090
B	0.302506	1.555818	-1.380940	C	-2.140849	-2.390768	3.501545
B	-0.302494	1.555829	1.380939	H	-1.414611	-2.554697	4.303327
B	0.302927	3.347172	-1.416664	C	-3.474706	-2.772762	3.674221
B	-0.302920	3.347183	1.416649	H	-3.801264	-3.234336	4.610905
C	2.628712	-1.564002	-1.257992	C	-4.385225	-2.566520	2.633924
C	-2.628746	-1.563948	1.258044	H	-5.430676	-2.868712	2.749281
B	0.868273	3.916157	0.186330	C	-3.964966	-1.964301	1.442523
B	-0.868267	3.916153	-0.186350	H	-4.701896	-1.802252	0.651260
C	4.734951	0.904723	-0.187701	C	-4.734947	0.904760	0.187606
H	4.424660	0.763150	-1.226155	H	-4.424684	0.763229	1.226075

C	-5.933805	1.578006	-0.069404	H	3.801142	-3.234515	-4.610822
H	-6.534605	1.957629	0.763090	C	2.140762	-2.390881	-3.501460
C	-6.362067	1.773542	-1.387390	H	1.414507	-2.554820	-4.303225
H	-7.297342	2.303876	-1.590595	H	2.077112	2.340223	1.986126
C	-5.585080	1.284755	-2.440933	H	-0.493426	0.821763	2.304364
H	-5.908684	1.430907	-3.476309	H	-0.521675	3.935292	2.444024
C	-4.388557	0.609190	-2.168840	H	1.513559	4.923446	0.327000
H	-3.794128	0.235055	-3.011274	H	2.705067	2.362502	-0.970959
C	1.720842	-1.805212	-2.302515	H	0.493442	0.821744	-2.304358
H	0.670746	-1.552203	-2.168009	H	0.521681	3.935273	-2.444044
C	3.964920	-1.964387	-1.442482	H	-2.077101	2.340204	-1.986134
H	4.701867	-1.802326	-0.651236	H	-1.513556	4.923440	-0.327029
C	4.385148	-2.566650	-2.633871	H	-2.705057	2.362501	0.970953
H	5.430592	-2.868865	-2.749236	F	-0.000009	-1.527588	0.000056
C	3.474608	-2.772906	-3.674147				



Zero-point correction= 0.516862 (Hartree/Particle)

Thermal correction to Energy= 0.551394

Thermal correction to Enthalpy= 0.552338

Thermal correction to Gibbs Free Energy= 0.448977

Sum of electronic and zero-point Energies= -1366.793935

Sum of electronic and thermal Energies= -1366.759402

Sum of electronic and thermal Enthalpies= -1366.758458

Sum of electronic and thermal Free Energies= -1366.861819

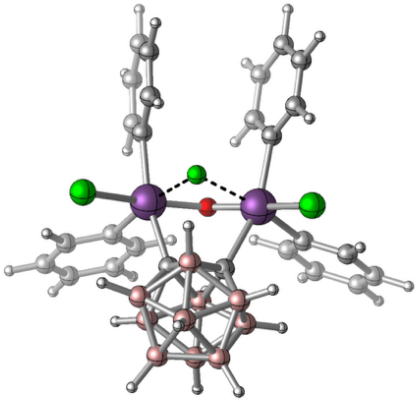
***o*-($C_2B_{10}H_{10}$)($SbPh_2Cl$)$_2$O_FIA**

E(scf) = -2362.69506766 a.u.

C	2.044539	4.319943	-1.198998	H	3.305722	4.371548	1.971471
H	1.796289	4.989953	-2.026833	C	-1.744499	5.175665	-0.139931
C	2.585558	4.836894	-0.016956	H	-1.728917	6.269199	-0.112112
H	2.769211	5.910961	0.079459	C	-2.480510	4.507964	-1.122904
C	2.883409	3.976084	1.042856	H	-3.046864	5.076422	-1.866579

C	-2.493379	3.108740	-1.168016	H	-6.029634	-1.199933	2.386662
H	-3.068304	2.593268	-1.938707	C	-4.222515	-0.619925	1.353457
Sb	1.607733	-0.007347	-0.350874	H	-4.705274	-0.574279	0.374625
Sb	-1.649312	0.211736	-0.214335	C	-1.764168	2.369706	-0.230783
Cl	3.195556	-0.292035	-2.222243	C	-1.026417	3.041204	0.755685
Cl	-3.464435	0.051573	-1.920118	H	-0.424477	2.468998	1.462199
O	0.031067	0.263987	0.825896	C	-1.019670	4.438299	0.800439
C	0.633433	-1.969871	-0.898130	H	-0.422864	4.947952	1.561303
C	2.349128	-0.823734	2.515224	B	-0.196920	-2.652448	0.450759
H	1.331647	-0.473132	2.699956	H	-0.134624	-2.132113	1.515409
C	2.093435	2.084866	-0.260772	C	-0.992353	-1.853825	-0.854806
C	1.799245	2.949981	-1.321971	C	2.861487	-0.774120	1.209507
H	1.348617	2.552531	-2.232372	C	4.163366	-1.229323	0.962182
C	2.637958	2.602608	0.920415	H	4.562172	-1.197675	-0.054746
H	2.869111	1.940359	1.759595	C	4.944757	-1.730687	2.008742
C	-2.855653	-0.332940	1.467672	H	5.957840	-2.089638	1.805628
C	-2.238113	-0.401494	2.726234	C	4.430619	-1.779950	3.308410
H	-1.171135	-0.185089	2.807536	H	5.040980	-2.176403	4.125097
C	-2.982423	-0.754500	3.856411	C	3.132467	-1.324648	3.560409
H	-2.492499	-0.810372	4.832833	H	2.724232	-1.364248	4.574473
C	-4.345929	-1.041585	3.738240	B	1.169267	-3.487792	-0.305428
H	-4.926272	-1.322281	4.622046	H	2.204597	-3.537254	0.293730
C	-4.964364	-0.972463	2.485990	B	1.147273	-3.135251	-2.044802

H	2.168519	-2.958397	-2.637438	B	0.502713	-4.686019	-1.442829
B	-0.232430	-2.063367	-2.387784	H	1.080966	-5.719589	-1.661501
H	-0.189089	-1.163410	-3.160630	B	-0.362868	-3.795867	-2.729220
B	-1.708086	-3.281660	-0.229667	H	-0.420713	-4.173459	-3.870108
H	-2.707204	-3.184095	0.423101	B	-1.727804	-2.933963	-1.970518
B	-0.330053	-4.373969	0.107364	H	-2.743333	-2.620537	-2.512247
H	-0.362268	-5.159107	1.018777				



Zero-point correction= 0.525097 (Hartree/Particle)

Thermal correction to Energy= 0.563453

Thermal correction to Enthalpy= 0.564397

Thermal correction to Gibbs Free Energy= 0.454047

Sum of electronic and zero-point Energies= -2362.169970

Sum of electronic and thermal Energies= -2362.131615

Sum of electronic and thermal Enthalpies= -2362.130670

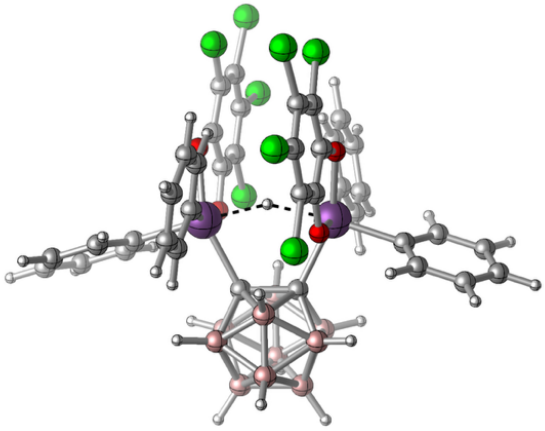
Sum of electronic and thermal Free Energies= -2362.241021

***o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$_HIA**

E(scf) = -5706.33010826 a.u.

H	3.239892	-2.499560	-6.895916	Cl	-5.137521	-0.781470	-0.540344
Cl	6.146800	2.165576	1.278691	Cl	-6.147651	2.157836	-1.288284
Cl	5.138200	-0.777480	0.543569	Cl	-1.624051	4.185083	1.073670
C	3.747376	0.779107	3.586226	O	1.155813	1.297692	-1.718499
H	4.712955	1.114448	3.971369	O	2.508402	-0.754711	-0.846902
C	3.382436	-0.566388	3.674598	O	-2.507541	-0.751303	0.849521
H	4.055123	-1.289749	4.142591	O	-1.155849	1.305538	1.712048
Cl	4.337034	4.651584	0.527648	C	0.282831	-2.722044	-0.763465
Cl	-4.339102	4.648027	-0.548167	C	-0.282002	-2.718487	0.775987
C	2.864409	-1.826375	-3.567235	C	2.260390	1.559754	-1.029907
C	3.468783	-2.237169	-4.758873	C	2.664996	2.850031	-0.672319
H	4.497987	-2.606134	-4.741527	C	3.872953	3.042826	0.032650
C	2.764536	-2.176560	-5.965389	C	4.664577	1.938595	0.385890
C	1.452898	-1.695545	-5.977689	C	4.231314	0.633924	0.074691
H	0.896733	-1.635566	-6.917332	C	3.020390	0.438833	-0.595442
C	0.844631	-1.284503	-4.786298	C	1.541472	-1.352712	-3.570814
H	-0.177521	-0.902403	-4.819006	H	3.422464	-1.865407	-2.631092
Sb	0.614959	-0.706149	-1.740786	C	-1.303415	-0.100094	-2.513530
Sb	-0.614438	-0.698066	1.743681	C	-2.161261	-1.014241	-3.142946
Cl	1.622384	4.180222	-1.092409	H	-1.893323	-2.069287	-3.223635

C	-3.382084	-0.583967	-3.671833	C	-2.864126	-1.809900	3.575053
H	-4.054586	-1.309533	-4.136668	H	-3.422056	-1.853364	2.639029
C	-3.747381	0.761805	-3.589305	C	-3.468655	-2.215161	4.768509
H	-4.713051	1.095212	-3.975899	H	-4.497842	-2.584245	4.752738
C	-2.890347	1.677142	-2.973454	C	-2.764574	-2.148911	5.974824
H	-3.181190	2.726321	-2.885121	H	-3.240043	-2.467593	6.906782
C	-1.674835	1.250956	-2.428505	C	-1.452951	-1.667806	5.985058
H	-1.020095	1.972384	-1.937714	H	-0.896910	-1.603450	6.924486
C	-3.020204	0.440888	0.593065	C	-0.844538	-1.262284	4.791850
C	-4.231331	0.632438	-0.077700	H	0.177606	-0.880022	4.822916
C	-4.665275	1.935519	-0.394557	C	1.303646	-0.088111	2.514181
C	-3.874165	3.041670	-0.046216	C	1.674702	1.262658	2.423302
C	-2.666038	2.852561	0.659465	H	1.019771	1.981770	1.929369
C	-2.260685	1.564054	1.022545	C	2.890095	1.691532	2.966410
C	-1.541214	-1.336159	3.576603				



Zero-point correction= 0.624163 (Hartree/Particle)

Thermal correction to Energy= 0.680277

Thermal correction to Enthalpy= 0.681221

Thermal correction to Gibbs Free Energy= 0.533311

Sum of electronic and zero-point Energies= -5705.705945

Sum of electronic and thermal Energies= -5705.649831

Sum of electronic and thermal Enthalpies= -5705.648887

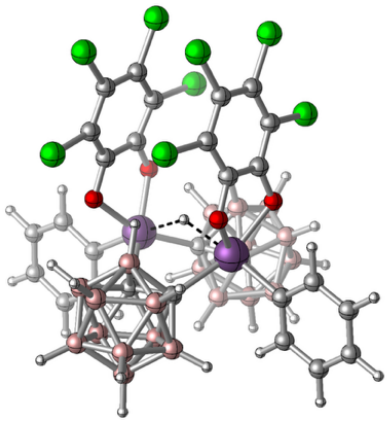
Sum of electronic and thermal Free Energies= -5705.796797

***o*-($C_2B_{10}H_{10}$)$_2$(SbPh(diolate))$_2$_HIA**

E(scf) = -5574.00123613 a.u.

H	4.027915	6.873135	1.688566	Cl	-5.237016	-2.348561	1.618067
H	5.375397	4.827079	1.217383	Cl	-5.489616	-1.245541	-1.341340
C	3.526572	5.928987	1.459007	Cl	-2.848628	-0.814636	-3.081986
C	4.283622	4.783369	1.195466	O	-0.392167	1.864755	1.685427
H	5.447744	-0.690926	3.635861	O	-0.188285	2.676204	-0.733059
C	4.284067	-4.783064	-1.195398	O	-0.391964	-1.864854	-1.685456
C	3.527115	-5.928736	-1.458989	O	-0.188058	-2.676293	0.733020
H	4.028539	-6.872841	-1.688545	C	2.220531	1.184916	-1.585285
C	2.130290	-5.869192	-1.427046	C	2.136400	-0.380492	-2.003208
H	1.536710	-6.764260	-1.630433	C	2.220607	-1.184772	1.585318
C	1.486655	-4.664093	-1.130493	C	-1.538605	1.941518	1.007217
H	0.396216	-4.618835	-1.094943	C	-1.425942	2.402313	-0.329426
H	5.375846	-4.826691	-1.217274	C	-2.553952	2.477807	-1.152208
Sb	1.235281	1.715860	0.416278	C	-3.819593	2.143852	-0.628732
Sb	1.235455	-1.715800	-0.416273	C	-3.931420	1.662166	0.689708
Cl	-2.336285	2.988024	-2.799550	C	-2.780210	1.518839	1.494350
Cl	-5.237228	2.348290	-1.618107	C	-1.538402	-1.941662	-1.007254
Cl	-5.489790	1.245237	1.341291	C	-1.425724	-2.402448	0.329390
Cl	-2.848788	0.814424	3.081938	C	-2.553733	-2.477980	1.152172
Cl	-2.336048	-2.988173	2.799519	C	-3.819387	-2.144077	0.628693

C	-3.931230	-1.662405	-0.689751	B	3.022223	0.160749	-4.577074
C	-2.780024	-1.519037	-1.494392	H	3.319150	-0.249965	-5.667829
C	2.245919	-3.515838	-0.871423	B	3.127494	1.880470	-4.117275
C	3.645192	-3.574689	-0.902900	H	3.496217	2.741710	-4.871507
B	1.854737	-2.212895	2.923171	B	1.854616	2.213003	-2.923153
H	1.303893	-3.249841	2.717431	H	1.303667	3.249898	-2.717438
B	0.959733	-0.694246	2.651348	B	1.686072	-0.577954	-3.659437
H	-0.151796	-0.634090	2.244192	H	1.009396	-1.514464	-3.960600
H	0.727932	-1.369128	5.128729	C	2.245583	3.515982	0.871437
B	0.959749	0.694269	-2.651357	C	1.486221	4.664183	1.130457
H	-0.151790	0.634018	-2.244243	H	0.395786	4.618843	1.094865
B	1.524516	1.092759	-4.274318	C	2.129752	5.869336	1.427012
H	0.727981	1.369116	-5.128752	H	1.536096	6.764363	1.630360
B	3.363578	-0.814352	-3.130681	C	3.644850	3.574939	0.902965
H	3.830853	-1.912940	-3.082691				



Zero-point correction= 0.595117 (Hartree/Particle)

Thermal correction to Energy= 0.649400

Thermal correction to Enthalpy= 0.650344

Thermal correction to Gibbs Free Energy= 0.508143

Sum of electronic and zero-point Energies= -5573.406119

Sum of electronic and thermal Energies= -5573.351836

Sum of electronic and thermal Enthalpies= -5573.350892

Sum of electronic and thermal Free Energies= -5573.493093

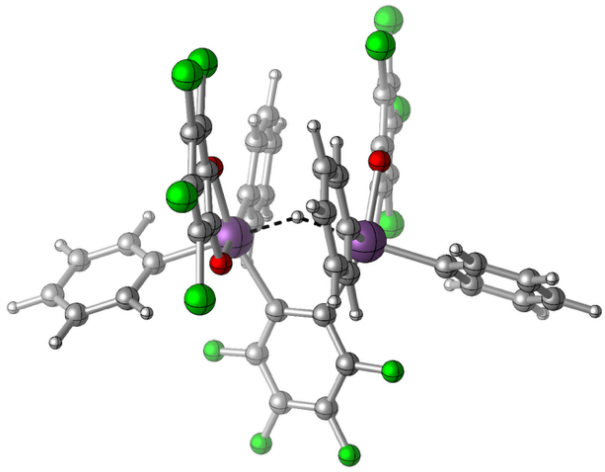
_o_-(C_6F_4)($SbPh_2$(diolate))$_2$_HIA

E(scf) = -6003.13675492 a.u.

Cl	-4.901694	-4.409763	-0.415917	C	-0.058610	2.440426	0.700170
Cl	4.901389	-4.410252	0.413405	C	-0.068949	3.649758	1.379948

C	-0.025445	4.871697	0.697507	C	3.010289	-2.776635	-0.703412
C	-1.508746	1.190333	3.495055	C	4.233926	-2.850221	-0.002700
C	-1.298361	-0.180246	-2.488241	C	4.879986	-1.673194	0.401986
C	-2.432223	-1.536136	0.989877	C	4.282139	-0.421672	0.149156
C	-3.010466	-2.776910	0.701801	C	3.043114	-0.345049	-0.495972
C	-4.234111	-2.850015	0.001052	Cl	2.158614	-4.210434	-1.211340
C	-4.880083	-1.672714	-0.402977	Cl	6.393353	-1.749606	1.270182
C	-4.282145	-0.421377	-0.149442	Cl	5.032710	1.072923	0.643840
C	-3.043115	-0.345205	0.495730	F	0.117562	3.702669	-2.720038
Cl	-2.158881	-4.211056	1.208903	F	0.044386	6.028847	-1.359684
Cl	-6.393452	-1.748528	-1.271224	O	1.302775	-1.397199	-1.675434
Cl	-5.032596	1.073547	-0.643311	O	2.386396	0.787787	-0.678900
F	-0.117197	3.701046	2.722272	Sb	0.550378	0.539299	-1.688933
F	-0.043819	6.028036	1.363312	C	-2.772773	2.028907	5.859170
O	-1.302827	-1.398153	1.674557	H	-3.264935	2.356338	6.779484
O	-2.386319	0.787485	0.679286	C	-1.563143	1.331543	5.920737
Sb	-0.550340	0.538308	1.689220	H	-1.105466	1.108569	6.888761
C	0.058789	2.440835	-0.698698	C	-0.933183	0.914395	4.742803
C	0.069263	3.650577	-1.377747	H	0.012660	0.370084	4.805658
C	0.025882	4.872111	-0.694572	C	-2.728770	1.882203	3.438936
C	1.508752	1.192387	-3.494400	H	-3.192991	2.079621	2.470174
C	1.298339	-0.181807	2.488152	C	-3.354515	2.301426	4.616574
C	2.432143	-1.535657	-0.990798	H	-4.304615	2.840507	4.562174

C	1.623251	-1.544813	2.413922	C	-3.416861	0.264175	-3.581391
H	0.929034	-2.247542	1.947940	H	-4.127589	0.974554	-4.010939
C	2.199833	0.720784	3.067310	C	-2.199813	0.722728	-3.066871
H	1.963135	1.788364	3.115458	H	-1.963057	1.790323	-3.114416
C	3.416840	0.261865	3.581605	C	-1.623361	-1.543271	-2.414766
H	4.127603	0.971957	4.011569	H	-0.929182	-2.246308	-1.949192
C	3.736901	-1.096284	3.513471	C	-2.842841	-1.995316	-2.927860
H	4.704064	-1.449395	3.877888	H	-3.110470	-3.051060	-2.838242
C	2.842686	-1.997224	2.926798	C	-3.737012	-1.093991	-3.514005
H	3.110248	-3.052936	2.836602				



Zero-point correction= 0.515781 (Hartree/Particle)

Thermal correction to Energy= 0.572287

Thermal correction to Enthalpy= 0.573232

Thermal correction to Gibbs Free Energy= 0.419605

Sum of electronic and zero-point Energies= -6002.620974

Sum of electronic and thermal Energies= -6002.564467

Sum of electronic and thermal Enthalpies= -6002.563523

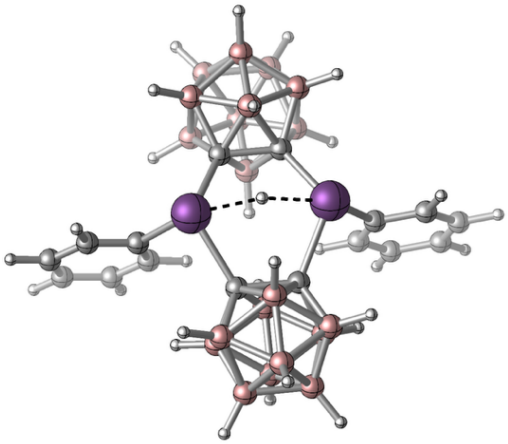
Sum of electronic and thermal Free Energies= -6002.717150

1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$_HIA

E(scf) = -1135.79509706 a.u.

Sb	1.852186	0.000649	-1.174507	C	-0.827898	1.920159	-0.416959
C	0.826539	1.920773	-0.416758	C	-0.826567	-1.920725	-0.416946
C	0.827871	-1.920212	-0.416822	B	-0.892865	4.614809	0.264123
C	3.216821	0.000984	0.581730	B	-1.442062	3.431203	-0.948688
B	0.889218	4.615504	0.264319	B	-1.441471	2.995945	0.768287
B	1.439613	3.432320	-0.948359	B	-1.439343	-2.996946	0.768317
B	1.438984	2.997058	0.768618	C	5.223144	0.001255	2.576572
B	1.441957	-3.431331	-0.948469	H	5.996400	0.001355	3.350306
B	1.441112	-2.996091	0.768512	C	5.577881	0.001211	1.226188
B	-0.000893	1.996529	1.071317	H	6.632336	0.001277	0.933767
B	-0.001614	3.717041	1.532348	C	4.579340	0.001080	0.242989
B	-0.001597	4.431605	-1.281252	H	4.881369	0.001044	-0.811112
B	-0.000900	2.706223	-1.691272	C	2.880835	0.001036	1.945651
B	0.000570	-1.996550	1.071292	H	1.836399	0.000968	2.253492
Sb	-1.851715	-0.000642	-1.174864	C	3.869585	0.001171	2.932803

H	3.580775	0.001205	3.987901	H	0.000753	-2.203679	-2.778972
C	-3.870081	-0.001189	2.931902	H	-0.000669	2.203706	-2.778942
H	-3.581535	-0.001239	3.987071	H	-0.001840	5.261927	-2.152274
C	-2.881080	-0.001055	1.945000	H	2.463866	3.444799	-1.574502
H	-1.836721	-0.001003	2.253097	H	1.544105	5.594394	0.514637
C	-5.223548	-0.001252	2.575329	H	-0.001865	4.036457	2.692205
H	-5.996998	-0.001351	3.348869	H	-1.544681	-5.594260	0.514291
C	-5.577949	-0.001187	1.224856	H	-2.461144	-2.721027	1.322790
H	-6.632329	-0.001236	0.932171	H	1.547995	-5.593353	0.514495
C	-4.579164	-0.001057	0.241906	H	0.001062	-4.036498	2.692154
H	-4.880927	-0.001005	-0.812269	H	0.000270	-1.056119	1.799530
C	-3.216732	-0.000982	0.580999	H	2.462674	-2.719575	1.323121
B	-1.439719	-3.432183	-0.948665	H	2.466188	-3.443099	-1.574661
B	0.000914	-2.706210	-1.691307	H	2.460712	2.721240	1.323268
B	0.001417	-4.431597	-1.281308	H	-0.000611	1.056090	1.799544
B	-0.889654	-4.615429	0.264106	H	-2.463105	2.719314	1.322713
B	0.001042	-3.717067	1.532301	H	-1.548570	5.593190	0.514291
B	0.892429	-4.614906	0.264220	H	-2.466182	3.442873	-1.575065
H	0.001697	-5.261908	-2.152341	H	0.000773	0.000011	-1.799485
H	-2.463861	-3.444549	-1.574994				



Zero-point correction= 0.493953 (Hartree/Particle)

Thermal correction to Energy= 0.524180

Thermal correction to Enthalpy= 0.525124

Thermal correction to Gibbs Free Energy= 0.435919

Sum of electronic and zero-point Energies= -1135.301144

Sum of electronic and thermal Energies= -1135.270917

Sum of electronic and thermal Enthalpies= -1135.269973

Sum of electronic and thermal Free Energies= -1135.359178

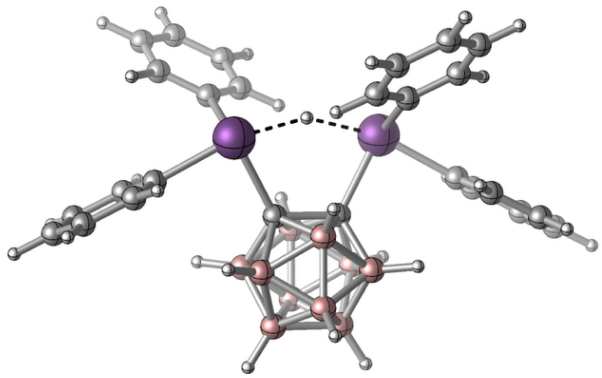
1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$_HIA

E(scf) = -1268.06959382 a.u.

Sb	1.833507	0.706779	-0.723199	C	3.819309	-0.382066	-0.785944
Sb	-1.833504	0.706889	0.723182	C	-3.819356	-0.381848	0.785992
C	0.812439	-1.285115	-0.213182	B	1.159616	-2.621921	-1.224062
C	-0.812488	-1.285060	0.213368	B	-1.159723	-2.621760	1.224380

B	1.617457	-2.626083	0.486668	H	-1.470054	2.674798	-4.244996
B	-1.617563	-2.626059	-0.486349	C	-3.375411	3.189051	-3.355983
B	0.373138	-1.720517	1.373790	H	-3.722198	3.759257	-4.222905
B	-0.373204	-1.720631	-1.373556	C	-4.189091	3.059321	-2.225265
B	0.373283	-3.505116	1.401514	H	-5.177045	3.529437	-2.202274
B	-0.373425	-3.505233	-1.401109	C	-3.745735	2.321157	-1.123480
C	2.479526	1.706317	1.117069	H	-4.409559	2.214234	-0.260274
C	-2.479408	1.706130	-1.117252	C	-4.624650	-0.701732	-0.320339
B	0.858996	-4.068217	-0.230309	H	-4.279754	-0.462701	-1.330257
B	-0.859163	-4.068158	0.230766	C	-5.866135	-1.326863	-0.162544
C	4.624622	-0.701882	0.320395	H	-6.470596	-1.569018	-1.042578
H	4.279764	-0.462736	1.330298	C	-6.331846	-1.651741	1.116808
C	4.308794	-0.711758	-2.059765	H	-7.300730	-2.144507	1.242561
H	3.711204	-0.477234	-2.949051	C	-5.548200	-1.342064	2.231691
C	5.548064	-1.342511	-2.231599	H	-5.900763	-1.592792	3.237321
H	5.900584	-1.593357	-3.237215	C	-4.308896	-0.711387	2.059832
C	6.331729	-1.652113	-1.116709	H	-3.711322	-0.476804	2.949113
H	7.300587	-2.144936	-1.242442	C	1.672055	1.855947	2.255629
C	5.866072	-1.327085	0.162625	H	0.678139	1.408063	2.285403
H	6.470549	-1.569182	1.042665	C	3.745939	2.321170	1.123216
C	-1.671976	1.855357	-2.255863	H	4.409788	2.213946	0.260068
H	-0.678125	1.407331	-2.285547	C	4.189346	3.059546	2.224841
C	-2.116559	2.583075	-3.367152	H	5.177366	3.529518	2.201778

C	3.375634	3.189673	3.355489	H	2.757546	-2.509497	0.817717
H	3.722465	3.760045	4.222285	H	0.614445	-0.981567	2.283741
C	2.116696	2.583879	3.366755	H	0.644017	-4.096562	2.414747
H	1.470169	2.675909	4.244551	H	-1.988812	-2.485440	2.078286
H	1.988713	-2.485705	-2.077979	H	-1.495806	-5.076545	0.400949
H	-0.614486	-0.981771	-2.283585	H	-2.757646	-2.509449	-0.817413
H	-0.644185	-4.096764	-2.414285	H	0.000102	1.177656	0.000126
H	1.495595	-5.076648	-0.400397				



Zero-point correction= 0.520427 (Hartree/Particle)

Thermal correction to Energy= 0.554034

Thermal correction to Enthalpy= 0.554978

Thermal correction to Gibbs Free Energy= 0.453138

Sum of electronic and zero-point Energies= -1267.549167

Sum of electronic and thermal Energies= -1267.515560

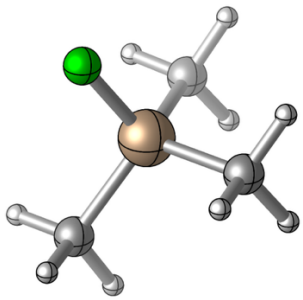
Sum of electronic and thermal Enthalpies= -1267.514616

Sum of electronic and thermal Free Energies= -1267.616456

$SiFMe_3$

E(scf) = -223.379169321 a.u.

C	-0.475717	1.727538	-0.536359	H	-2.268979	-1.032207	-0.170888
H	-1.476994	2.008073	-0.171357	C	1.733823	-0.451720	-0.536793
H	0.240239	2.481213	-0.170484	H	2.477451	0.275124	-0.171833
H	-0.491041	1.785232	-1.637759	H	2.028606	-1.448610	-0.171009
C	-1.258294	-1.275554	-0.536649	H	1.791369	-0.467246	-1.638199
H	-1.300491	-1.317671	-1.638053	Si	0.000007	-0.000002	0.026060
H	-1.000810	-2.282996	-0.171622	F	0.000187	-0.000274	1.692796



Zero-point correction= 0.113370 (Hartree/Particle)

Thermal correction to Energy= 0.121645

Thermal correction to Enthalpy= 0.122589

Thermal correction to Gibbs Free Energy= 0.081731

Sum of electronic and zero-point Energies= -223.265799

Sum of electronic and thermal Energies= -223.257525

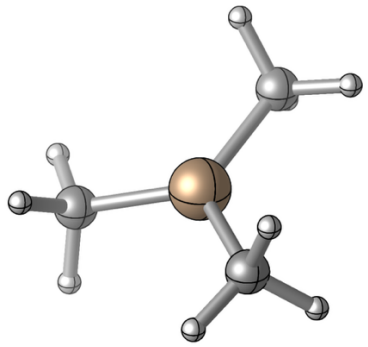
Sum of electronic and thermal Enthalpies= -223.256580

Sum of electronic and thermal Free Energies= -223.297439

$SiMe_3$

E(scf) = -123.268824221 a.u.

Si	-0.000089	-0.000075	-0.000052	H	1.176795	1.964702	-0.881031
C	-1.798809	-0.419056	0.000036	H	-0.307890	2.471456	-0.000864
H	-2.289776	0.035545	-0.881776	C	1.262442	-1.348024	0.000016
H	-1.986478	-1.502443	0.000460	H	1.114143	-2.000996	-0.881415
H	-2.289927	0.036357	0.881326	H	2.294397	-0.968514	-0.000086
C	0.536460	1.767161	0.000009	H	1.114166	-2.000677	0.881684
H	1.175259	1.965131	0.882070				



Zero-point correction= 0.108578 (Hartree/Particle)

Thermal correction to Energy= 0.116498

Thermal correction to Enthalpy= 0.117442

Thermal correction to Gibbs Free Energy= 0.075462

Sum of electronic and zero-point Energies= -123.160246

Sum of electronic and thermal Energies= -123.152326

Sum of electronic and thermal Enthalpies= -123.151382

Sum of electronic and thermal Free Energies= -123.193362

Fluoride

E(scf) = -99.6888339514 a.u.

F 0.000000 0.000000 0.000000

Zero-point correction= 0.000000 (Hartree/Particle)

Thermal correction to Energy= 0.001416

Thermal correction to Enthalpy= 0.002360

Thermal correction to Gibbs Free Energy= -0.014159

Sum of electronic and zero-point Energies= -99.688834

Sum of electronic and thermal Energies= -99.687418

Sum of electronic and thermal Enthalpies= -99.686473

Sum of electronic and thermal Free Energies= -99.702993

Hydride

E(scf) = -0.488729315372 a.u.

H 0.000000 0.000000 0.000000

Zero-point correction= 0.000000 (Hartree/Particle)

Thermal correction to Energy= 0.001416

Thermal correction to Enthalpy= 0.002360

Thermal correction to Gibbs Free Energy= -0.010000

Sum of electronic and zero-point Energies= -0.488729

Sum of electronic and thermal Energies= -0.487313

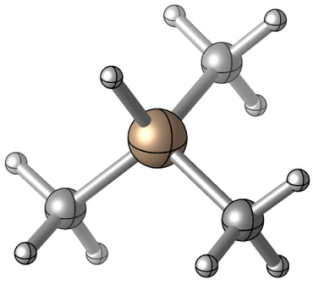
Sum of electronic and thermal Enthalpies= -0.486369

Sum of electronic and thermal Free Energies= -0.498729

$SiHMe_3$

E(scf) = -124.161825591 a.u.

C	1.557001	0.899365	0.226095
H	2.474390	0.401400	-0.128958
H	1.584612	1.942549	-0.129765
H	1.594436	0.921554	1.328195
C	0.000408	-1.798076	0.226077
H	0.000914	-1.841655	1.328177
H	-0.889497	-2.343629	-0.128995
H	0.890070	-2.343505	-0.129789
C	-1.557395	0.898670	0.226101
H	-1.584932	1.942165	-0.128857
H	-2.474581	0.400938	-0.129800
H	-1.595306	0.919864	1.328202
Si	-0.000014	0.000040	-0.386833
H	0.000010	0.000009	-1.862388



Zero-point correction= 0.118803 (Hartree/Particle)

Thermal correction to Energy= 0.126256

Thermal correction to Enthalpy= 0.127200

Thermal correction to Gibbs Free Energy= 0.088538

Sum of electronic and zero-point Energies= -124.043022

Sum of electronic and thermal Energies= -124.035570

Sum of electronic and thermal Enthalpies= -124.034626

Sum of electronic and thermal Free Energies= -124.073287

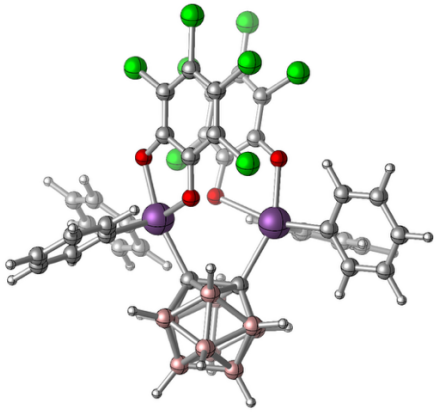
_o_-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$_anionic

E(scf) = -5705.72416999 a.u.

Sb	1.069985	1.771197	-0.412157	C	3.040044	0.637090	-0.310149
B	3.425071	-0.426378	-1.604462	Sb	1.038907	-2.011593	0.266390
Cl	-3.866215	2.750627	-0.495047	B	4.299825	1.110810	-1.400578
O	-0.923811	2.300773	-0.599527	Cl	-5.505024	0.463745	-1.997962

O	0.369193	0.320786	-1.733888	C	-3.069525	-0.611113	-2.621798
C	3.139041	-0.981647	-0.008603	C	-1.661877	-0.646472	-2.572068
Cl	-3.935625	-1.878781	-3.445189	C	-0.956397	0.349788	-1.893359
B	4.410559	1.443640	0.338082	C	1.189537	-4.024308	-0.526033
O	0.227652	0.244447	1.085874	C	1.266138	-2.497821	2.361521
O	-1.057408	-2.066673	0.231376	C	-1.086187	0.058273	1.354024
Cl	-0.745144	-1.928675	-3.314233	C	-1.841456	0.926518	2.165581
B	3.624947	0.098739	1.208491	C	-3.236518	0.788051	2.295058
Cl	-1.020041	2.170291	3.059999	C	-3.891189	-0.279898	1.663570
B	4.420360	-1.703026	-0.868193	C	-3.133673	-1.235002	0.968987
Cl	-4.149590	1.947858	3.223015	C	-1.735668	-1.110209	0.843925
B	5.202635	-0.376074	-1.748468	C	1.515989	-3.821302	2.760219
Cl	-5.624294	-0.425707	1.740404	H	1.603609	-4.616733	2.017641
B	5.815807	0.783962	-0.530466	C	1.651359	-4.148057	4.114128
Cl	-3.890552	-2.607479	0.208221	H	1.849174	-5.184434	4.402307
B	5.398245	0.166164	1.098065	C	1.528938	-3.156971	5.091123
C	1.656733	3.008273	-2.068551	H	1.631739	-3.411721	6.149777
B	4.541175	-1.382541	0.872141	C	1.266789	-1.839265	4.706155
C	1.260829	3.250418	1.133689	H	1.157572	-1.055957	5.461279
B	5.899000	-0.963437	-0.202298	C	1.135938	-1.509676	3.353719
C	-3.052573	1.454562	-1.324201	H	0.923998	-0.477478	3.075603
C	-1.653973	1.420076	-1.273437	C	2.038150	3.107135	2.287783
C	-3.763817	0.434872	-1.989996	H	2.605852	2.197244	2.467307

C	2.062813	4.120449	3.250854	H	3.277785	-4.358676	-0.019829
H	2.668752	3.991912	4.151771	C	0.048501	-4.578474	-1.130408
C	1.307368	5.282159	3.069890	H	-0.885343	-4.012698	-1.159208
H	1.321534	6.070205	3.828014	C	0.105537	-5.859401	-1.689604
C	0.525703	5.427597	1.920177	H	-0.788459	-6.283658	-2.155338
H	-0.080168	6.326254	1.775970	C	1.295864	-6.593282	-1.657174
C	0.500698	4.417025	0.955341	H	1.337151	-7.592481	-2.100072
H	-0.140899	4.526330	0.079110	C	2.433536	-6.045912	-1.055995
C	2.342294	4.213079	-1.853834	H	3.367359	-6.614369	-1.023275
H	2.586613	4.536905	-0.839566	H	2.615707	-0.636719	-2.453429
C	1.378267	2.612227	-3.385678	H	5.723013	-0.550494	-2.818134
H	0.869569	1.665585	-3.572862	H	4.290090	-2.817221	-1.282817
C	1.773321	3.410185	-4.464099	H	4.471783	-2.277064	1.668259
H	1.551131	3.086789	-5.484859	H	6.933475	-1.577145	-0.158288
C	2.454791	4.610231	-4.240837	H	6.056200	0.386423	2.080304
H	2.766963	5.230870	-5.085532	H	6.787638	1.466637	-0.724081
C	2.740166	5.009689	-2.932153	H	4.102827	1.993136	-2.176380
H	3.279401	5.942902	-2.746764	H	4.279699	2.561299	0.741898
C	2.381294	-4.765762	-0.493050	H	2.949132	0.229895	2.178269



Zero-point correction= 0.614531 (Hartree/Particle)

Thermal correction to Energy= 0.671034

Thermal correction to Enthalpy= 0.671978

Thermal correction to Gibbs Free Energy= 0.521879

Sum of electronic and zero-point Energies= -5705.109639

Sum of electronic and thermal Energies= -5705.053136

Sum of electronic and thermal Enthalpies= -5705.052192

Sum of electronic and thermal Free Energies= -5705.202291

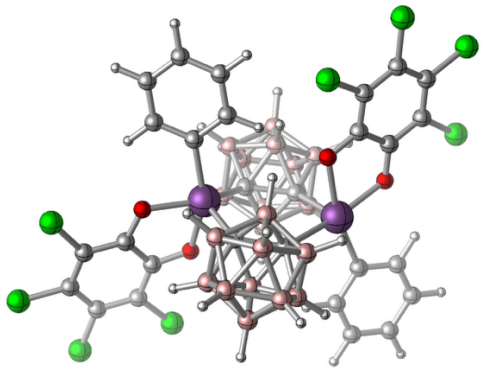
_o_-($C_2B_{10}H_{10}$)$_2$(SbPh(diolate))$_2$_anionic

E(scf) = -5573.39028536 a.u.

Cl	7.782147	2.030782	-0.823428	B	0.406483	-1.003512	4.372227
Cl	6.156544	-3.142542	0.059930	B	-0.639904	0.294767	3.737658
Cl	8.510677	-1.010733	-0.317495	B	0.358329	1.720798	3.427382
Sb	1.590555	-0.987354	-0.183424	B	2.046206	1.339596	3.857393
Cl	4.700552	2.901914	-0.950936	B	2.078221	-0.354895	4.449315
O	3.441503	-1.867254	-0.088884	B	0.695908	0.697896	4.848341
O	2.865521	0.587445	-0.525483	Sb	-1.919803	1.401783	0.786226
C	1.221450	-0.336070	1.831355	Cl	-3.867587	-3.364659	1.161516
C	-0.052957	0.643114	2.160519	O	-3.840434	1.546754	-0.039842
C	-1.692536	3.598200	0.603109	O	-2.630829	-0.692969	0.754637
C	4.485910	-1.046884	-0.244100	C	-1.050021	1.032807	-1.293262
C	5.818992	-1.456675	-0.205161	C	0.304369	0.100656	-1.628545
C	6.845436	-0.502763	-0.382639	C	0.862156	-2.984772	-0.472690
C	6.521983	0.847911	-0.609842	C	-4.548618	0.424962	-0.034604
C	5.171304	1.253771	-0.666097	C	-5.891584	0.383964	-0.431918
C	4.162343	0.306279	-0.481475	C	-6.620834	-0.822470	-0.385866
B	1.525139	1.319629	2.159884	C	-6.001916	-1.991468	0.088097
B	2.596822	0.025878	2.791665	C	-4.654607	-1.952756	0.500117
B	1.587032	-1.414190	3.106209	C	-3.901529	-0.769871	0.411209
B	-0.103204	-1.007291	2.670362	B	-1.242279	-0.509934	-2.045477

B	-2.171193	0.896122	-2.600946	H	0.431037	3.666182	1.065036
B	-1.141208	2.329133	-2.419245	C	-2.835993	4.360154	0.318698
B	0.421458	1.808089	-1.746910	H	-3.792514	3.865887	0.132611
B	0.267582	2.154934	-3.489684	C	-0.378769	5.632335	0.751141
B	1.188863	0.736298	-2.965740	H	0.584101	6.122403	0.919934
B	0.157644	-0.702396	-3.134447	C	-1.514280	6.391599	0.454199
B	-1.411647	-0.192287	-3.786040	H	-1.443686	7.481007	0.390159
B	-1.343011	1.579447	-4.020591	C	-2.741025	5.753803	0.241262
B	0.094877	0.591643	-4.353261	H	-3.632042	6.342990	0.005780
Cl	-6.615361	1.866301	-0.995237	H	-0.131550	2.813097	3.419229
Cl	-8.282876	-0.854898	-0.914830	H	1.861166	2.043160	1.278402
Cl	-6.893635	-3.489007	0.173218	H	2.805886	2.189029	4.236836
C	1.727767	-3.962751	-0.990215	H	3.684342	-0.095292	2.311444
H	2.774158	-3.729299	-1.182717	H	2.876928	-0.734102	5.263453
C	1.246437	-5.251352	-1.235206	H	1.995222	-2.502610	2.818129
H	1.923718	-6.008442	-1.639099	H	-0.016298	-1.839877	5.123211
C	-0.087684	-5.568625	-0.964933	H	0.476426	1.097044	5.960976
H	-0.462712	-6.576348	-1.163178	H	-1.816301	0.405685	3.937412
C	-0.941835	-4.597562	-0.438562	H	-0.831335	-1.769267	2.126204
H	-1.986087	-4.829117	-0.221904	H	1.029739	2.415277	-0.927948
C	-0.474704	-3.302364	-0.189573	H	0.818964	3.113968	-3.956633
H	-1.172480	-2.571513	0.221666	H	2.377335	0.632274	-2.973948
C	-0.467806	4.237929	0.832453	H	0.643981	-1.794149	-3.227358

H	0.540297	0.411440	-5.455277	H	-1.973177	2.139380	-4.877348
H	-2.075207	-0.931067	-4.461246	H	-1.591544	3.369780	-2.053564
H	-3.337765	0.940542	-2.371135	H	-1.722222	-1.402674	-1.437283



Zero-point correction= 0.586497 (Hartree/Particle)

Thermal correction to Energy= 0.641343

Thermal correction to Enthalpy= 0.642287

Thermal correction to Gibbs Free Energy= 0.496738

Sum of electronic and zero-point Energies= -5572.803788

Sum of electronic and thermal Energies= -5572.748942

Sum of electronic and thermal Enthalpies= -5572.747998

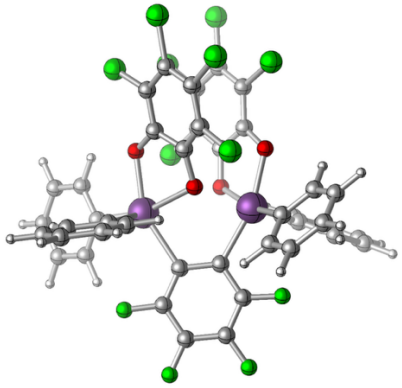
Sum of electronic and thermal Free Energies= -5572.893547

***o*-(C_6F_4)($SbPh_2$(diolate))$_2$_anionic**

E(scf) = -6002.53202530 a.u.

Cl	-5.602546	-0.202106	-2.069022	Sb	0.764531	2.049650	-0.129308
Cl	-5.561212	-1.071920	1.704859	C	2.913101	-0.276576	0.238080
C	2.835196	1.094765	-0.048869	C	4.176543	-0.867482	0.286683
C	3.993187	1.816813	-0.284335	C	5.347427	-0.133204	0.070712
C	5.258028	1.227695	-0.217679	C	1.892359	-2.674702	2.287654
C	0.983226	2.632624	-2.192436	C	0.698675	4.060165	0.737178
C	1.647416	-3.067848	-0.960350	C	-1.584485	-1.576512	1.258336
C	-1.887753	0.922103	-0.905858	C	-2.969414	-1.774578	1.216357
C	-3.278714	0.884692	-1.130145	C	-3.838439	-0.841457	1.817312
C	-3.871867	-0.150097	-1.870936	C	-3.313927	0.281703	2.479117
C	-3.059473	-1.137754	-2.446842	C	-1.920072	0.484733	2.518647
C	-1.669319	-1.115211	-2.221279	C	-1.056356	-0.423744	1.899744
C	-1.077908	-0.163891	-1.371339	Cl	-3.567710	-3.161391	0.350277
Cl	-4.240774	2.157448	-0.427006	Cl	-4.377073	1.439670	3.231365
Cl	-3.768409	-2.398752	-3.422321	Cl	-1.219512	1.878030	3.294554
Cl	-0.644746	-2.262621	-3.034842	F	4.330511	-2.184021	0.511867
F	3.943935	3.127852	-0.606051	F	6.543004	-0.725166	0.130950
F	6.369681	1.933615	-0.441203	O	-0.717644	-2.377539	0.647546
O	-1.357682	1.931323	-0.243268	O	0.263057	-0.232181	1.809713
O	0.222721	-0.196733	-1.013072	Sb	1.197393	-1.614182	0.542850

C	1.264264	3.390594	-4.890709	C	2.833323	-3.759502	-2.960683
H	1.371702	3.684536	-5.938881	H	3.543719	-3.535635	-3.761386
C	1.070170	4.362063	-3.904849	C	2.565757	-2.798884	-1.980785
H	1.026588	5.420663	-4.177246	H	3.060221	-1.825955	-2.038523
C	0.928759	3.984661	-2.564662	C	0.992749	-4.307474	-0.928157
H	0.777993	4.757410	-1.806241	H	0.240272	-4.506407	-0.162294
C	1.174275	1.662098	-3.191082	C	1.265234	-5.269870	-1.904353
H	1.195354	0.603535	-2.923634	H	0.743795	-6.230697	-1.878157
C	1.314164	2.040348	-4.529893	C	2.184521	-4.997458	-2.922501
H	1.454505	1.271579	-5.295189	H	2.389413	-5.747409	-3.691742
C	-0.571838	4.557564	1.079445	C	1.673281	-2.146024	3.570356
H	-1.466678	3.972124	0.854988	H	1.163205	-1.187025	3.677894
C	1.838984	4.815085	1.054693	C	2.106469	-2.836866	4.707573
H	2.835364	4.453158	0.796808	H	1.927322	-2.410746	5.698912
C	1.711156	6.054814	1.692901	C	2.761913	-4.064598	4.579366
H	2.607444	6.635411	1.931280	H	3.097587	-4.605265	5.469073
C	0.445653	6.550476	2.020784	C	2.988274	-4.596441	3.306279
H	0.347168	7.518922	2.519796	H	3.504381	-5.554385	3.194394
C	-0.693211	5.799500	1.711216	C	2.558428	-3.904345	2.169781
H	-1.686981	6.177868	1.967819	H	2.756821	-4.330032	1.183717



Zero-point correction= 0.506255 (Hartree/Particle)

Thermal correction to Energy= 0.562995

Thermal correction to Enthalpy= 0.563939

Thermal correction to Gibbs Free Energy= 0.409312

Sum of electronic and zero-point Energies= -6002.025770

Sum of electronic and thermal Energies= -6001.969030

Sum of electronic and thermal Enthalpies= -6001.968086

Sum of electronic and thermal Free Energies= -6002.122713

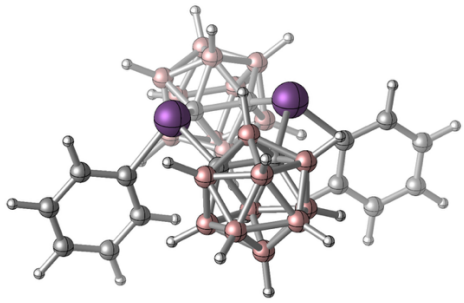
1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$_anionic

E(scf) = -1267.47867668 a.u.

Sb	1.697696	-0.278688	-0.869981	C	-3.612697	1.001244	-0.051407
Sb	-1.765556	0.368599	-1.017922	B	1.359699	-1.279542	2.491580
C	0.813716	-0.218118	1.260932	B	-1.277584	0.804208	2.728800
C	-0.813111	-0.032440	1.308114	B	1.574945	0.475481	2.625201
C	3.683372	-0.859604	-0.138307	B	-1.489978	-0.940171	2.587846

B	0.176026	1.249828	1.827816	H	-2.802370	-5.535086	-2.070770
B	-0.158211	-1.572097	1.604837	C	-3.122587	-3.891367	-0.692624
B	0.241412	1.130367	3.606085	H	-3.661302	-4.502032	0.038407
B	-0.109975	-1.745462	3.379920	C	-2.907141	-2.535231	-0.430331
C	2.086789	1.835722	-1.143629	H	-3.264418	-2.115914	0.511405
C	-2.212055	-1.718944	-1.345322	C	-4.817902	0.278031	-0.118944
B	0.966082	-0.456463	4.016933	H	-4.839783	-0.705763	-0.594454
B	-0.800596	-0.249890	4.084167	C	-6.004859	0.797881	0.408482
C	4.790652	0.002510	-0.063065	H	-6.925678	0.208750	0.351035
H	4.676903	1.064713	-0.289626	C	-6.019021	2.062077	1.007543
C	3.895645	-2.224889	0.132617	H	-6.946122	2.467389	1.423250
H	3.062911	-2.932645	0.067428	C	-4.833830	2.803174	1.066318
C	5.155605	-2.706721	0.497739	H	-4.828356	3.793241	1.532474
H	5.287581	-3.770364	0.717691	C	-3.649276	2.278538	0.541909
C	6.243155	-1.830944	0.585622	H	-2.735576	2.877266	0.609454
H	7.230628	-2.203886	0.872543	C	1.704552	2.410424	-2.370401
C	6.056035	-0.475991	0.297378	H	1.232723	1.791052	-3.140292
H	6.899855	0.218444	0.356656	C	2.665141	2.674463	-0.172211
C	-1.728713	-2.321809	-2.524905	H	2.945273	2.271080	0.802157
H	-1.174909	-1.722024	-3.255289	C	2.866535	4.034618	-0.425975
C	-1.934139	-3.679067	-2.784420	H	3.313383	4.666741	0.347078
H	-1.541866	-4.120930	-3.705712	C	2.487746	4.589164	-1.653234
C	-2.638427	-4.472474	-1.869800	H	2.641839	5.654258	-1.848541

C	1.901773	3.770868	-2.625370	H	2.671969	0.946871	2.505894
H	1.591431	4.194063	-3.585373	H	0.260087	2.238797	1.158689
H	2.303824	-1.984394	2.287430	H	0.381950	2.118201	4.282154
H	-0.267823	-2.439047	0.785775	H	-2.226175	1.532369	2.703569
H	-0.211895	-2.830960	3.893218	H	-1.422528	-0.254001	5.117192
H	1.649259	-0.618446	4.996968	H	-2.590813	-1.401197	2.466454



Zero-point correction= 0.512834 (Hartree/Particle)

Thermal correction to Energy= 0.546735

Thermal correction to Enthalpy= 0.547679

Thermal correction to Gibbs Free Energy= 0.441904

Sum of electronic and zero-point Energies= -1266.965843

Sum of electronic and thermal Energies= -1266.931942

Sum of electronic and thermal Enthalpies= -1266.930998

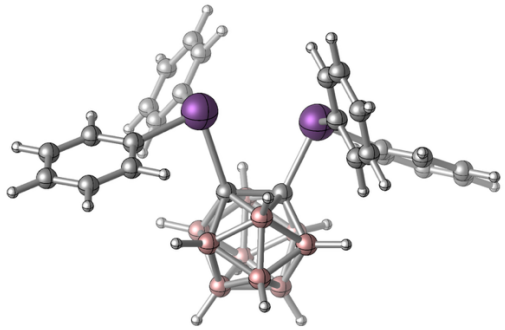
Sum of electronic and thermal Free Energies= -1267.036773

1,2-($SbPh_2$)$_2$-*ortho*-($C_2B_{10}H_{10}$)_anionic

E(scf) = -1267.47867668 a.u.

Sb	1.697696	-0.278688	-0.869981	C	3.895645	-2.224889	0.132617
Sb	-1.765556	0.368599	-1.017922	H	3.062911	-2.932645	0.067428
C	0.813716	-0.218118	1.260932	C	5.155605	-2.706721	0.497739
C	-0.813111	-0.032440	1.308114	H	5.287581	-3.770364	0.717691
C	3.683372	-0.859604	-0.138307	C	6.243155	-1.830944	0.585622
C	-3.612697	1.001244	-0.051407	H	7.230628	-2.203886	0.872543
B	1.359699	-1.279542	2.491580	C	6.056035	-0.475991	0.297378
B	-1.277584	0.804208	2.728800	H	6.899855	0.218444	0.356656
B	1.574945	0.475481	2.625201	C	-1.728713	-2.321809	-2.524905
B	-1.489978	-0.940171	2.587846	H	-1.174909	-1.722024	-3.255289
B	0.176026	1.249828	1.827816	C	-1.934139	-3.679067	-2.784420
B	-0.158211	-1.572097	1.604837	H	-1.541866	-4.120930	-3.705712
B	0.241412	1.130367	3.606085	C	-2.638427	-4.472474	-1.869800
B	-0.109975	-1.745462	3.379920	H	-2.802370	-5.535086	-2.070770
C	2.086789	1.835722	-1.143629	C	-3.122587	-3.891367	-0.692624
C	-2.212055	-1.718944	-1.345322	H	-3.661302	-4.502032	0.038407
B	0.966082	-0.456463	4.016933	C	-2.907141	-2.535231	-0.430331
B	-0.800596	-0.249890	4.084167	H	-3.264418	-2.115914	0.511405
C	4.790652	0.002510	-0.063065	C	-4.817902	0.278031	-0.118944
H	4.676903	1.064713	-0.289626	H	-4.839783	-0.705763	-0.594454

C	-6.004859	0.797881	0.408482	H	0.260087	2.238797	1.158689
H	-6.925678	0.208750	0.351035	H	0.381950	2.118201	4.282154
C	-6.019021	2.062077	1.007543	H	-2.226175	1.532369	2.703569
H	-6.946122	2.467389	1.423250	H	-1.422528	-0.254001	5.117192
C	-4.833830	2.803174	1.066318	H	-2.590813	-1.401197	2.466454
H	-4.828356	3.793241	1.532474				
C	-3.649276	2.278538	0.541909				
H	-2.735576	2.877266	0.609454				
C	1.704552	2.410424	-2.370401				
H	1.232723	1.791052	-3.140292				
C	2.665141	2.674463	-0.172211				
H	2.945273	2.271080	0.802157				
C	2.866535	4.034618	-0.425975				
H	3.313383	4.666741	0.347078				
C	2.487746	4.589164	-1.653234				
H	2.641839	5.654258	-1.848541				
C	1.901773	3.770868	-2.625370				
H	1.591431	4.194063	-3.585373				
H	2.303824	-1.984394	2.287430				
H	-0.267823	-2.439047	0.785775				
H	-0.211895	-2.830960	3.893218				
H	1.649259	-0.618446	4.996968				
H	2.671969	0.946871	2.505894				



Zero-point correction= 0.512834 (Hartree/Particle)

Thermal correction to Energy= 0.546735

Thermal correction to Enthalpy= 0.547679

Thermal correction to Gibbs Free Energy= 0.441904

Sum of electronic and zero-point Energies= -1266.965843

Sum of electronic and thermal Energies= -1266.931942

Sum of electronic and thermal Enthalpies= -1266.930998

Sum of electronic and thermal Free Energies= -1267.036773

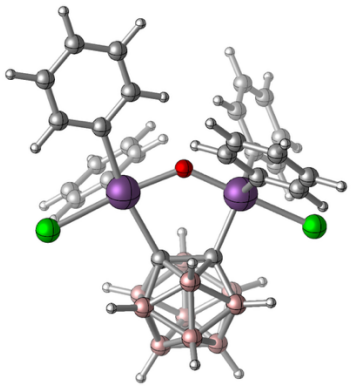
***o*-($C_2B_{10}H_{10}$)($SbPh_2Cl$)$_2$O_FIA**

E(scf) = -2262.87697761 a.u.

C	4.905847	-2.984829	1.003040	H	2.679184	-4.825543	-0.812978
H	5.900307	-3.055704	1.454971	C	-2.597643	-4.156383	2.925597
C	4.374049	-4.076756	0.308147	H	-2.755768	-4.976818	3.631458
H	4.948071	-5.003780	0.216534	C	-3.687289	-3.419341	2.451738
C	3.102766	-3.976533	-0.266728	H	-4.700474	-3.659284	2.786011

C	-3.491401	-2.367481	1.550741	H	-2.914301	0.413629	-5.314143
H	-4.341317	-1.792819	1.180317	C	-2.477687	0.001240	-3.240781
Sb	1.702947	0.189572	0.775738	H	-3.199408	0.728375	-2.865743
Sb	-1.768240	-0.435106	-0.229168	C	-2.195593	-2.049198	1.122538
Cl	3.530874	1.457018	2.179402	C	-1.100789	-2.786729	1.599533
Cl	-4.264790	0.046539	-0.499269	H	-0.093569	-2.532518	1.269543
O	0.143555	-0.745806	-0.137004	C	-1.305427	-3.838993	2.497210
C	-0.005424	1.919574	1.093146	H	-0.445337	-4.406605	2.862346
C	1.870362	0.602037	-2.274556	B	-0.659827	2.671177	-0.294262
H	1.168182	-0.230203	-2.259385	H	-0.282751	2.340677	-1.379213
C	2.899815	-1.691313	0.544658	C	-1.539877	1.561108	0.650498
C	4.171508	-1.798587	1.125065	C	2.373841	1.102341	-1.065272
H	4.588355	-0.947441	1.671710	C	3.264056	2.184307	-1.096934
C	2.369224	-2.789665	-0.147021	H	3.673207	2.572170	-0.161584
H	1.376816	-2.707616	-0.595016	C	3.632035	2.760864	-2.318518
C	-1.710324	-0.753195	-2.345661	H	4.321512	3.610377	-2.328117
C	-0.805690	-1.708419	-2.830465	C	3.120566	2.260586	-3.519900
H	-0.182220	-2.271411	-2.134674	H	3.406336	2.717120	-4.472380
C	-0.678669	-1.915433	-4.207175	C	2.239851	1.174501	-3.495241
H	0.024250	-2.666191	-4.578116	H	1.827516	0.772989	-4.425821
C	-1.432109	-1.150060	-5.103088	B	0.310555	3.575560	0.885172
H	-1.320568	-1.300541	-6.180532	H	1.411649	3.917965	0.565259
C	-2.326370	-0.190934	-4.618235	B	0.007166	2.890144	2.492020

H	0.908043	2.756667	3.268696
B	-1.148064	1.559435	2.306936
H	-1.078878	0.510902	2.884224
B	-2.390017	2.935990	0.094367
H	-3.197914	2.806152	-0.777091
B	-1.217826	4.264804	0.265155
H	-1.231615	5.203406	-0.487645
B	-0.806493	4.401049	2.006539
H	-0.515539	5.454162	2.512604
B	-1.715024	3.137132	2.899409
H	-2.085096	3.265414	4.037220
B	-2.694842	2.241453	1.712945



Zero-point correction= 0.520819 (Hartree/Particle)

Thermal correction to Energy= 0.558694

Thermal correction to Enthalpy= 0.559638

Thermal correction to Gibbs Free Energy= 0.447347

Sum of electronic and zero-point Energies= -2262.356158

Sum of electronic and thermal Energies= -2262.318284

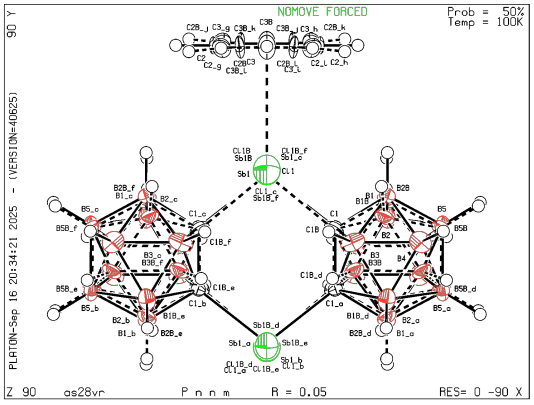
Sum of electronic and thermal Enthalpies= -2262.317340

Sum of electronic and thermal Free Energies= -2262.429630

VI. Crystallographic Structure Determination

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. CCDC entries listed below contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/ structures.

[1,2-$(SbCl)_2$-*ortho*-$(C_2B_{10}H_{10})_2$]



A colourless, plate-shaped crystal was mounted on the goniometer. Data for [1,2-$(SbCl)_2$-*ortho*-$(C_2B_{10}H_{10})_2$] was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[13,14] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic

displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. This report and the CIF file were generated using FinalCif.[17]

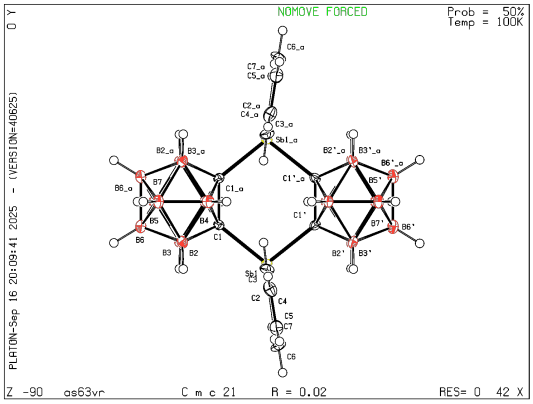
Table S7. Crystal data and structure refinement for [1,2-$(SbCl)_2$-*ortho*-$(C_2B_{10}H_{10})_2$]

CCDC number	2514934
Empirical formula	$C_{10}H_{26}B_{20}Cl_2Sb_2$
Formula weight	676.91
Temperature [K]	100(2)
Crystal system	orthorhombic
Space group (number)	$Pnnm$ (58)
a [Å]	6.8546(19)
b [Å]	10.786(3)
c [Å]	17.373(5)
α [°]	90
β [°]	90
γ [°]	90
Volume [$Å^3$]	1284.4(6)
Z	2

ρ_{calc} [gcm^{-3}]	1.750
μ [mm^{-1}]	2.314
F(000)	644
Crystal size [mm^3]	0.025×0.091×0.095
Crystal colour	colourless
Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.45 to 50.02 (0.84 Å)
Index ranges	−7 ≤ h ≤ 8 −12 ≤ k ≤ 12 −20 ≤ l ≤ 18
Reflections collected	7613
Independent reflections	1179 R_{int} = 0.0896 R_{sigma} = 0.0592
Completeness to θ = 25.012°	99.8 %
Data / Restraints / Parameters	1179 / 294 / 163
Absorption correction T_{min}/T_{max} (method)	0.6335 / 0.7452 (multi-scan)
Goodness-of-fit on F^2	1.087

Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0542 wR_2 = 0.1445
Final *R* indexes [all data]	R_1 = 0.0903 wR_2 = 0.1596
Largest peak/hole [eÅ^{-3}]	0.73/−0.87

1,2-(SbPh)$_2$-*ortho*-($C_2B_{10}H_{10}$)$_2$ [1a]



A colorless, rod-shaped crystal was mounted on the goniometer. Data for 1,2-(SbPh)$_2$-*ortho*-($C_2B_{10}H_{10}$)$_2$ was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[13,14] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic

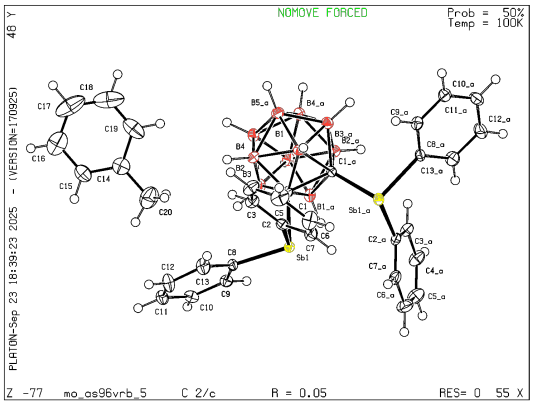
displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

Table S8. Crystal data and structure refinement for 1,2-$(SbPh)_2$-*ortho*-$(C_2B_{10}H_{10})_2$

CCDC number	2514935
Empirical formula	$C_{16}H_{30}B_{20}Sb_2$
Formula weight	682.10
Temperature [K]	100(2)
Crystal system	orthorhombic
Space group (number)	$Cmc2_1$ (36)
a [Å]	14.641(3)
b [Å]	19.230(4)
c [Å]	9.7810(19)
α [°]	90
β [°]	90
γ [°]	90
Volume [$Å^3$]	2753.7(9)
Z	4
ρ_{calc} [gcm^{-3}]	1.645

μ [mm^{-1}]	1.972
F(000)	1312
Crystal size [mm^3]	0.051×0.078×0.206
Crystal colour	colorless
Crystal shape	rod
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.24 to 56.67 (0.75 Å)
Index ranges	−19 ≤ h ≤ 19 −25 ≤ k ≤ 25 −13 ≤ l ≤ 13
Reflections collected	21445
Independent reflections	3562 R_{int} = 0.0318 R_{sigma} = 0.0218
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	3562 / 1 / 185
Absorption correction T_{min}/T_{max} (method)	0.6702 / 0.7457 (multi-scan)
Goodness-of-fit on F^2	1.067
Final R indexes [I≥2σ(I)]	R_1 = 0.0196 wR_2 = 0.0436
Final R indexes [all data]	R_1 = 0.0244 wR_2 = 0.0449
Largest peak/hole [eÅ^{-3}]	0.50/−0.29
Flack X parameter	0.05(3)

1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$ [2a]



A colorless, block-shaped crystal was mounted on the goniometer. Data for 1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$ was collected from a shock-cooled single crystal at 100(2)K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph graphite monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using TWINABS Bruker was applied.[13,14] The structure was solved by dual space methods with SHELXD and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic

displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

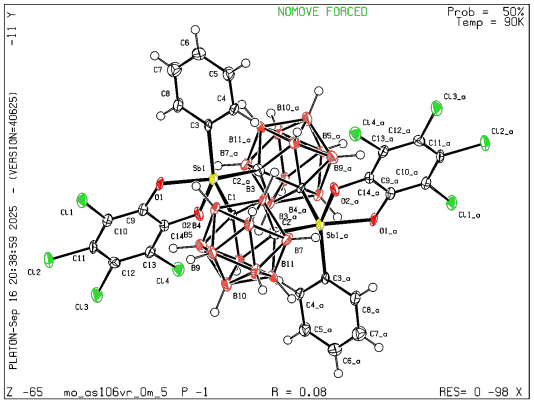
Table S9. Crystal data and structure refinement for 1,2-$(SbPh_2)_2$-*ortho*-$(C_2B_{10}H_{10})$

CCDC number	2514937
Empirical formula	$C_{40}H_{46}B_{10}Sb_2$
Formula weight	878.37
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	28.040(2)
b [Å]	9.8956(8)
c [Å]	19.6271(15)
α [°]	90
β [°]	133.3752(15)
γ [°]	90
Volume [$Å^3$]	3958.6(5)

Z	4
ρ_{calc} [gcm^{-3}]	1.474
μ [mm^{-1}]	1.394
F(000)	1752
Crystal size [mm^3]	0.120×0.235×0.250
Crystal colour	colorless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	4.00 to 50.04 (0.84 Å)
Index ranges	−33 ≤ h ≤ 24 0 ≤ k ≤ 11 0 ≤ l ≤ 23
Reflections collected	9412
Independent reflections	9412 R_{int} = 0.0574 R_{sigma} = 0.0250
Completeness to θ = 25.018°	99.9 %
Data / Restraints / Parameters	9412 / 0 / 237
Absorption correction T_{min}/T_{max} (method)	0.6812 / 0.7461 (multi-scan)
Goodness-of-fit on F^2	1.206
Final R indexes [I≥2σ(I)]	R_1 = 0.0455 wR_2 = 0.1042
Final R indexes [all data]	R_1 = 0.0520 wR_2 = 0.1085

Largest peak/hole [eÅ^{-3}]	1.60/−0.60

o-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$ [1b]



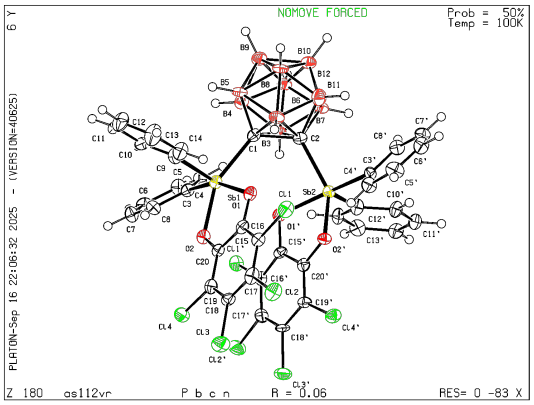
A yellow, block-shaped crystal was mounted on the goniometer. Data for *o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$ was collected from a shock-cooled single crystal at 90(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using TWINABS Bruker was applied.[13,14] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

Table S10. Crystal data and structure refinement for *o*-$(C_2B_{10}H_{10})_2(SbPh(diolate))_2$

CCDC number	2514933
Empirical formula	$C_{28}H_{30}B_{20}Cl_8O_4Sb_2$
Formula weight	1173.82
Temperature [K]	90(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	9.619(8)
b [Å]	10.826(9)
c [Å]	12.050(10)
α [°]	106.922(8)
β [°]	105.428(8)
γ [°]	99.219(8)
Volume [Å^3]	1118.3(16)
Z	1
ρ_{calc} [gcm^{-3}]	1.743
μ [mm^{-1}]	1.723
F(000)	568
Crystal size [mm^3]	0.096×0.106×0.251
Crystal colour	yellow
Crystal shape	block

Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.74 to 50.23 (0.84 Å)
Index ranges	−11 ≤ h ≤ 10 −12 ≤ k ≤ 12 0 ≤ l ≤ 14
Reflections collected	8172
Independent reflections	8172 R_{int} = 0.1262 R_{sigma} = 0.0864
Completeness to θ = 25.114°	98.8 %
Data / Restraints / Parameters	8172 / 0 / 281
Absorption correction T_{min}/T_{max} (method)	0.2986 / 0.4900 (multi-scan)
Goodness-of-fit on F^2	0.999
Final R indexes [I≥2σ(I)]	R_1 = 0.0817 wR_2 = 0.2062
Final R indexes [all data]	R_1 = 0.1222 wR_2 = 0.2419
Largest peak/hole [eÅ^{-3}]	2.39/−2.26

o-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$ [2b]



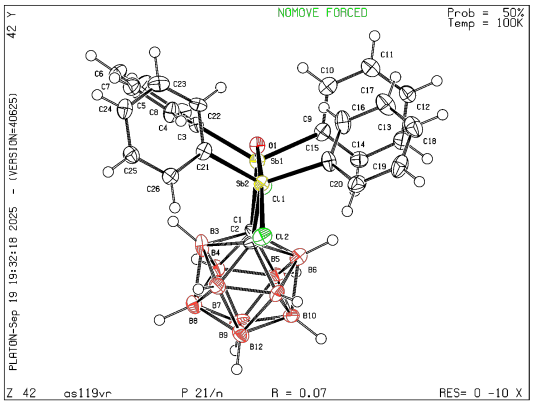
A colorless, block-shaped crystal was mounted on the goniometer. Data for *o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$ was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[13,14] The structure was solved by dual space methods with SHELXD and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

Table S11. Crystal data and structure refinement for *o*-($C_2B_{10}H_{10}$)($SbPh_2$(diolate))$_2$

CCDC number	2514941
Empirical formula	$C_{38}H_{30}B_{10}Cl_8O_4Sb_2$
Formula weight	1185.82
Temperature [K]	100(2)
Crystal system	orthorhombic
Space group (number)	$Pbcn$ (60)
a [Å]	34.498(5)
b [Å]	17.707(3)
c [Å]	14.599(2)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å^3]	8918(2)
Z	8
ρ_{calc} [gcm^{-3}]	1.766
μ [mm^{-1}]	1.733
F(000)	4624
Crystal size [mm^3]	0.144×0.222×0.336
Crystal colour	colorless
Crystal shape	block

Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.80 to 50.05 (0.84 Å)
Index ranges	−41 ≤ h ≤ 41 −21 ≤ k ≤ 21 −17 ≤ l ≤ 17
Reflections collected	75427
Independent reflections	7874 R_{int} = 0.0422 R_{sigma} = 0.0226
Completeness to θ = 25.025°	99.8 %
Data / Restraints / Parameters	7874 / 180 / 559
Absorption correction T_{min}/T_{max} (method)	0.1963 / 0.2602 (multi-scan)
Goodness-of-fit on F^2	1.354
Final R indexes [I≥2σ(I)]	R_1 = 0.0598 wR_2 = 0.1492
Final R indexes [all data]	R_1 = 0.0673 wR_2 = 0.1525
Largest peak/hole [eÅ^{-3}]	1.43/−1.07

o-($C_2B_{10}H_{10}$)($SbPh_2Cl$)$_2$O [1e]



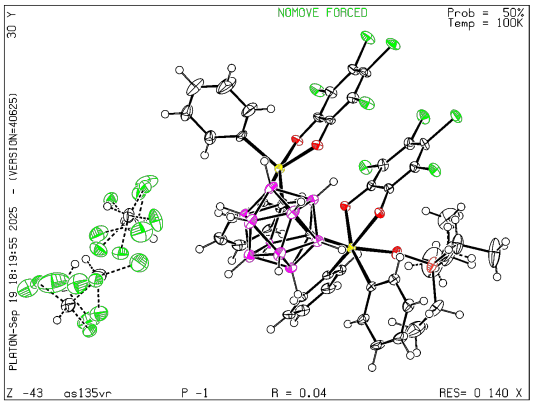
A colourless, plate-shaped crystal was mounted on the goniometer. Data for *o*-($C_2B_{10}H_{10}$)($SbPh_2Cl$)$_2$O was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using TWINABS Bruker was applied.[13,14] The structure was solved by direct methods with SHELXT and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

Table S12. Crystal data and structure refinement for *o*-$(C_2B_{10}H_{10})(SbPh_2Cl)_2O$

CCDC number	2514936
Empirical formula	$C_{26}H_{30}B_{10}Cl_2OSb_2$
Formula weight	781.00
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	12.465(3)
b [Å]	15.988(3)
c [Å]	15.958(3)
α [°]	90
β [°]	101.726(5)
γ [°]	90
Volume [Å^3]	3114.0(11)
Z	4
ρ_{calc} [gcm^{-3}]	1.666
μ [mm^{-1}]	1.928
F(000)	1520
Crystal size [mm^3]	0.046×0.082×0.121
Crystal colour	colourless

Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.64 to 52.78 (0.80 Å)
Index ranges	−15 ≤ h ≤ 15 0 ≤ k ≤ 19 0 ≤ l ≤ 19
Reflections collected	14192
Independent reflections	14192 R_{int} = 0.1336 R_{sigma} = 0.1613
Completeness to θ = 25.242°	100.0 %
Data / Restraints / Parameters	14192 / 0 / 372
Absorption correction T_{min}/T_{max} (method)	0.0192 / 0.0452 (multi-scan)
Goodness-of-fit on F^2	1.000
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0730 wR_2 = 0.1135
Final *R* indexes [all data]	R_1 = 0.1623 wR_2 = 0.1404
Largest peak/hole [eÅ^{-3}]	1.68/−1.19

[Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$(diolate))$_2$] [2c]



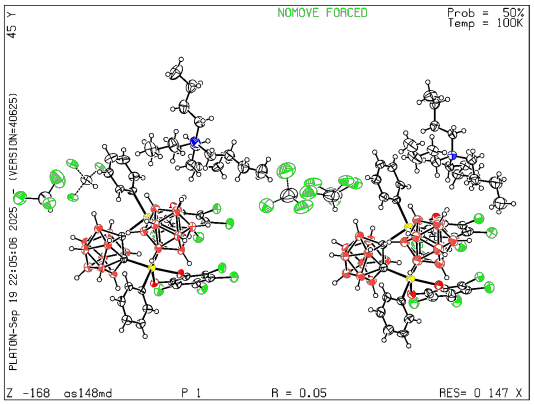
A colourless, prism-shaped crystal was mounted on the goniometer. Data for [Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$(diolate))$_2$] was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[13,14] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. This report and the CIF file were generated using FinalCif.[17]

Table S13. Crystal data and structure refinement for [Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$(diolate))$_2$]

CCDC number	2514938
Empirical formula	$C_{46}H_{47}B_{10}Cl_{14}O_5PSb_2$
Formula weight	1558.70
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	13.1762(14)
b [Å]	13.5391(14)
c [Å]	18.6724(19)
α [°]	71.828(2)
β [°]	74.388(2)
γ [°]	82.052(2)
Volume [Å^3]	3042.8(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.701
μ [mm^{-1}]	1.573
F(000)	1536
Crystal size [mm^3]	0.130×0.147×0.170
Crystal colour	colourless

Crystal shape	prism
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.37 to 56.66 (0.75 Å)
Index ranges	−17 ≤ h ≤ 17 −18 ≤ k ≤ 18 −23 ≤ l ≤ 24
Reflections collected	48340
Independent reflections	13847 R_{int} = 0.0540 R_{sigma} = 0.0637
Completeness to θ = 25.242°	99.9 %
Data / Restraints / Parameters	13847 / 1099 / 867
Absorption correction T_{min}/T_{max} (method)	0.6632 / 0.7457 (multi-scan)
Goodness-of-fit on F^2	1.070
Final R indexes [I≥2σ(I)]	R_1 = 0.0442 wR_2 = 0.0851
Final R indexes [all data]	R_1 = 0.0682 wR_2 = 0.0922
Largest peak/hole [eÅ^{-3}]	1.43/−0.91

[^{n}Bu$_4$N][μ^2-F$^-$][*o*-(C$_2$B$_{10}$H$_{10}$)$_2$(SbPh$_2$(diolate))$_2$] [1d]



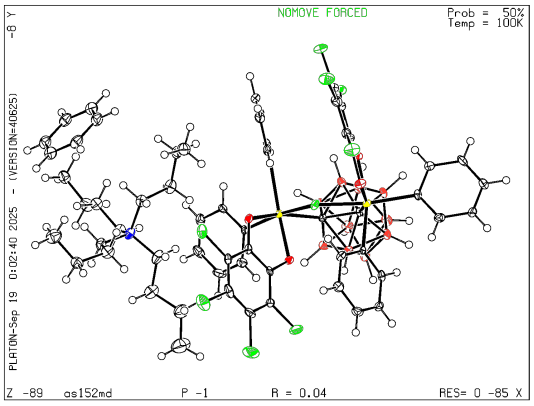
A yellow, prism-shaped crystal was mounted on the goniometer. Data for [^{n}Bu$_4$N][μ^2-F$^-$][*o*-(C$_2$B$_{10}$H$_{10}$)$_2$(SbPh$_2$(diolate))$_2$] was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[13,14] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. This report and the CIF file were generated using FinalCif.[17]

Table S14. Crystal data and structure refinement for $[^{n}Bu_4N][\mu^2\text{-}F^-][o\text{-}(C_2B_{10}H_{10})_2(SbPh_2(diolate))_2]$

CCDC number	2514942
Empirical formula	$C_{45}H_{67}B_{20}Cl_{11}FNO_4Sb_2$
Formula weight	1554.64
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P1$ (1)
a [Å]	11.9974(10)
b [Å]	12.9551(11)
c [Å]	25.121(2)
α [°]	91.423(2)
β [°]	102.023(2)
γ [°]	116.632(2)
Volume [$Å^3$]	3382.3(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.526
μ [mm^{-1}]	1.277
F(000)	1548
Crystal size [mm^3]	0.057×0.129×0.283
Crystal colour	yellow
Crystal shape	prism

Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	1.67 to 50.05 (0.84 Å)
Index ranges	−14 ≤ h ≤ 14 −15 ≤ k ≤ 15 −29 ≤ l ≤ 29
Reflections collected	83200
Independent reflections	23932 R_{int} = 0.0349 R_{sigma} = 0.0362
Completeness to θ = 25.026°	100.0 %
Data / Restraints / Parameters	23932 / 1945 / 1624
Absorption correction T_{min}/T_{max} (method)	0.0058 / 0.0183 (multi-scan)
Goodness-of-fit on F^2	1.145
Final R indexes [I≥2σ(I)]	R_1 = 0.0543 wR_2 = 0.1239
Final R indexes [all data]	R_1 = 0.0620 wR_2 = 0.1279
Largest peak/hole [eÅ^{-3}]	2.40/−1.37
Flack X parameter	-0.019(5)

[^{n}Bu$_4$N][μ^2-F$^-$][*o*-($C_2B_{10}H_{10}$)(SbPh$_4$(diolate))$_2$] [2d]



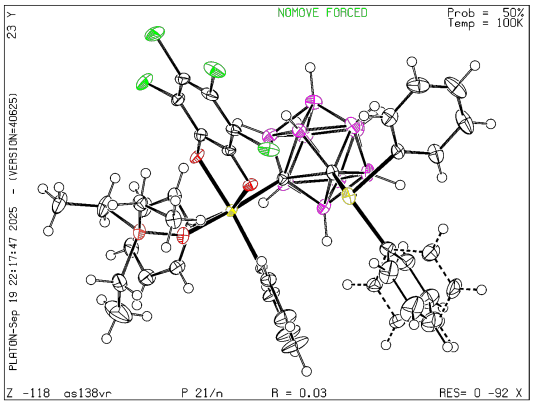
A yellow, block-shaped crystal was mounted on the goniometer. Data for [^{n}Bu$_4$N][μ^2-F$^-$][*o*-($C_2B_{10}H_{10}$)(SbPh$_4$(diolate))$_2$] was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using TWINABS Bruker was applied.[13,14] The structure was solved by dual space methods with SHELXD and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[15,16] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. This report and the CIF file were generated using FinalCif.[17]

Table S15. Crystal data and structure refinement for $[^{n}Bu_4N][\mu^2\text{-}F^-][o\text{-}(C_2B_{10}H_{10})(SbPh_4(diolate))_2]$

CCDC number	2514939
Empirical formula	$C_{57}H_{69}B_{10}Cl_8FNO_4Sb_2$
Formula weight	1486.33
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	14.6303(17)
b [Å]	15.9306(18)
c [Å]	16.1327(18)
α [°]	68.646(2)
β [°]	72.498(2)
γ [°]	68.897(2)
Volume [Å^3]	3204.2(6)
Z	2
ρ_{calc} [gcm^{-3}]	1.541
μ [mm^{-1}]	1.225
F(000)	1494
Crystal size [mm^3]	0.060×0.115×0.270
Crystal colour	yellow
Crystal shape	block

Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.51 to 52.86 (0.80 Å)
Index ranges	−18 ≤ h ≤ 18 −19 ≤ k ≤ 19 −20 ≤ l ≤ 20
Reflections collected	30395
Independent reflections	30395 R_{int} = 0.0505 R_{sigma} = 0.0605
Completeness to θ = 25.242°	98.6 %
Data / Restraints / Parameters	30395 / 0 / 753
Absorption correction T_{min}/T_{max} (method)	0.6646 / 0.7454 (multi-scan)
Goodness-of-fit on F^2	1.028
Final R indexes [I≥2σ(I)]	R_1 = 0.0386 wR_2 = 0.0627
Final R indexes [all data]	R_1 = 0.0610 wR_2 = 0.0685
Largest peak/hole [eÅ^{-3}]	0.82/−0.82

[Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$)$_2$(diolate)]



A colourless, prism-shaped crystal was mounted on the goniometer. Data for [Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$)$_2$(diolate)] was collected from a shock-cooled single crystal at 100(2) K on a Bruker Prospector three-circle diffractometer with a sealed X-ray tube using a Triumph monochromator and a Bruker Apex-II CCD detector. The diffractometer was equipped with an Oxford Cryostream 700 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All data were integrated with SAINT V8.41 and a multi-scan absorption correction using SADABS 2016/2 was applied.[14,15] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against F^2 using SHELXL-2019/2.[16,17] All non-hydrogen atoms were refined with anisotropic displacement parameters. All C-bound hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered moieties were refined using bond lengths restraints and displacement parameter restraints. This report and the CIF file were generated using FinalCif.[18]

Table S16. Crystal data and structure refinement for [Et_3PO][*o*-($C_2B_{10}H_{10}$)($SbPh_4$)$_2$(diolate)]

CCDC number	2514940
Empirical formula	$C_{38}H_{45}B_{10}Cl_4O_3PSb_2$
Formula weight	1074.11
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	14.4191(14)
b [Å]	19.0361(18)
c [Å]	16.3885(16)
α [°]	90
β [°]	100.573(2)
γ [°]	90
Volume [Å^3]	4422.0(7)
Z	4
ρ_{calc} [gcm^{-3}]	1.613
μ [mm^{-1}]	1.537
F(000)	2128
Crystal size [mm^3]	0.074×0.087×0.140
Crystal colour	colourless

Crystal shape	prism
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.31 to 50.21 (0.84 Å)
Index ranges	−17 ≤ h ≤ 17 −22 ≤ k ≤ 22 −19 ≤ l ≤ 19
Reflections collected	68396
Independent reflections	7861 R_{int} = 0.0573 R_{sigma} = 0.0318
Completeness to θ = 25.105°	99.6 %
Data / Restraints / Parameters	7861 / 598 / 572
Absorption correction T_{min}/T_{max} (method)	0.6875 / 0.7452 (multi-scan)
Goodness-of-fit on F^2	1.060
Final R indexes [I≥2σ(I)]	R_1 = 0.0296 wR_2 = 0.0608
Final R indexes [all data]	R_1 = 0.0441 wR_2 = 0.0653
Largest peak/hole [eÅ^{-3}]	0.73/−1.11

VII. References

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