Supporting Information

**Calix[4]pyrrolato Stannate(II): A Tetraamido Tin(II) Dianion and Strong Metal-Centered σ-Donor**

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## Supporting Information

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1 Experimental Details

All manipulations were carried out under a dry argon atmosphere by using standard Schlenk techniques to prevent oxidation and hydrolysis of the sensitive compounds. *meso*-Octamethylcalix[4]pyrrole as well as the deprotonated *tris*-(*thf*) *tetra*-lithium *meso*-octamethylcalix[4]pyrrole have been synthesized by literature known procedures.[1] The commercially available chemicals were used as received. All solvents and liquid chemicals were rigorously dried by applying standard procedures, freshly degassed and stored over activated molecular sieve (3 Å resp. 4 Å) prior to use. All glassware, syringes, magnetic stirring bars, and needles were thoroughly dried. All air sensitive compounds were stored in a glove box (MBraun LABmaster dp, MB-20-G, SylaTech Y05G) under N₂ atmosphere. Analytical data of literature known compounds were compared to data of the respective reference and were found to be consistent in all cases. Purity and identity of novel compounds were confirmed by high resolution multinuclear NMR-spectroscopy, mass spectrometry, elemental analysis and if possible, X-ray diffraction analysis.

¹H, ¹³C, ¹⁹F, ³¹P, ⁷⁷Se and ¹¹⁹Sn NMR spectra were collected with a Bruker (DPX) 200, a Bruker Advance II 400 or a Bruker 2 Advance III 600 NMR spectrometer and referenced to tetramethylsilane (¹H, ¹³C), tetramethylstannane (¹¹⁹Sn), or dimethyl selenide (⁷⁷Se). Chemical shifts are reported as dimensionless δ values in ppm, coupling constants J are given in hertz (Hz).

High-resolution electrospray ionization mass spectra (HRMS-ESI) were obtained with a Bruker ApexQe FTICR instrument.

Fourier-transform infrared (FTIR) spectra at 298 K were obtained with an Agilent Cary 630 FTIR spectrometer, which was operated with the MicroLab PC software, and processed with BioRad Merlin and OriginPro 2020 64Bit.

Cyclic voltammetry was done inside a dry nitrogen-filled glove box at room temperature with a EmStat3+blue device from PalmSens, which was operated with the PSTrace 5.7 software. A glassy carbon electrode (working area of 0.07 cm²) was used as a working electrode, a platinum wire as a counter electrode, and a silver wire as a quasi-reference electrode. The scan rate was set to 0.05 V s⁻¹. As solvent, 1,2-difluorobenzene (oDFB), as supporting electrolyte, [NnBu₄][PF₆] was used. The analyte concentration was approximately c = 10⁻³ mol L⁻¹, the supporting electrolyte concentration c_{supp} = 0.1 mol L⁻¹. The acquired data was externally referenced against the decamethyl-ferrocene/decamethylferrocenium (dmfc/dmfc⁺) redox couple and then transferred to the Ag/AgCl/KCl reference. Under the same conditions as described fc/fc⁺ has a redox potential of 532 mV and dmfc/dmfc⁺ a redox potential of 30 mV against the Ag/AgCl/KCl redox couple.[2] The dmfc/dmfc⁺ reference measurement was carried out under the same conditions as described.

Elemental analysis for the determination of the C-,H- and N-content was carried out by the microanalysis laboratory of the Institute of Inorganic Chemistry at Heidelberg University using a vario MICRO cube of Elementar Analysensysteme.

Suitable crystals of the compounds were taken directly out of the mother liquor, immersed in perfluorinated polyether oil, and fixed on top of a cryo loop. Measurements were made on Bruker D8 Venture CCD diffractometer with a low-temperature unit using (100 K) Mo-Kα radiation chromated by mirror optics. The data collected were processed using standard Bruker APEX3 software. Structures were solved by intrinsic phasing using the SHELXT program[3] and refined with the SHELXL.[4] Graphical handling
of the structural data during solution and refinement was performed with shelXL. Atomic coordinates and anisotropic thermal parameters of non-hydrogen atoms were refined by full-matrix least-squares calculations and displacement ellipsoids are displayed with 50 % probability. Hydrogen atoms were included using a riding model. Crystallographic data for the structures reported in this article are deposited within the Cambridge Crystallographic Data Centre as supplementary publication no. 2125915-2125920 and can be obtained free of charge. Crystal data and structure are summarized in the tables under the crystallographic figures.
2 Computational Details

All computations employing the Orca 4.2.1 software or the Amsterdam Modelling Suite AMS2021.102 were carried out with the computational resources available on the bwFor Cluster JUSTUS2 located at Ulm University within the Baden Württemberg High Performance Computing program.

All structures were optimized with the Orca 4.2.1 software at the B97M-D3(BJ)/def2-TZVP level of theory. Minima structures were obtained with the following ORCA input line:

! RKS B97M-D3BJ def2-TZVPP Grid5 NoFinalGrid Opt NumFreq TightSCF

All calculated geometries have been confirmed as energetic minima on the potential energy surface by numerical calculation of harmonic frequencies at the B97M-D3(BJ)/def2-TZVP level, revealing only positive values.

Subsequent single point calculations employing the Conductor-like Polarizable Continuum Model (C-PCM) were performed with the following ORCA input line:

! RKS B97M-D3BJ def2-TZVPP CPCM(THF) Grid5 NoFinalGrid SP NumFreq TightSCF

Natural Bond Orbital (NBO) calculations were conducted on the PBE0/def2-TZVPP level of theory including a C-PCM solvation model using NBO6.0.18a as included in Orca 4.2.1 via the following ORCA input line:

! RKS PBE0 def2-TZVPP CPCM(THF) NBO TightSCF Grid5 NoFinalGrid

Calculations employing the Extended Transition State (ETS) method for energy decomposition analysis (EDA) combined with the natural orbitals for chemical valence (NOCV) calculations were performed on the BP86-G3/TZ2P level of theory as implemented in the AMS2021.201 software.

Computational $^{77}$Se and $^{119}$Sn NMR absolute chemical shieldings ($\sigma$) were calculated with AMS2021.201 software at the PBE0/TZ2P level of theory, chemical shifts were obtained by referencing to the computed value of SeMe$_2$ and SnMe$_4$ respectively. NMR chemical shift computations were carried out without the frozen core approximation and with the scalar relativistic spin-orbit ZORA approximation to address correct treatment of heavy elements.

Isosurface plots were created using the IboView software v20150427.
3 Synthesis

3.1 Lithium tin(II) meso-octaethylcalix[4]pyrrolate [Li₂(thf)₅][2]

In a 200 mL Schlenk tube, tris-(thf) tetra-lithium meso-octamethylcalix[4]pyrrolate [Li₄(thf)₅][1] (1.0 eq, 2.82 mmol, 2.2 g) was dissolved in 55 mL THF. While stirring at room temperature tin(II) chloride (1.0 eq, 2.82 mmol, 545 mg) was added in portions. After turning slightly yellow for 5 minutes the clear, colorless solution was stirred at room temperature for 30 minutes before the solvent was evaporated at reduced pressure. The obtained crude was extracted with 200 mL Et₂O and the extract filtered over a low porosity frit to remove surplus lithium chloride. After evaporation of Et₂O the obtained crude was redissolved in 20 mL THF and the product precipitated by adding of 85 mL pentane. Isolation of the precipitant by filtration over a low porosity frit and drying at reduced pressure yielded [Li₂(thf)₅][2] as a colorless solid (2.237 g, 2.26 mmol (x=4.2), 80% yield). Cooling of a concentrated toluene solution of [Li₂(thf)₅][2] to −30 °C yielded single crystals suitable for X-ray diffraction.

¹H NMR [¹H, ²H, ³H-COSY] (600.13 MHz, THF-d₈, 295 K): δ [ppm] = 5.85 (s, ⁰¹⁷Sn-satellites ⁴Jₓₓₜₜ = 156.41 Hz, ¹¹⁹Sn-satellites ⁵Jₓₓₜₜ = 162.29 Hz, H₇, 8H), 3.62 (m, Hₓₓ₂, 16.8H), 1.88 (q, ³Jₓₓₜₜ = 7.3 Hz, H₉, 8H), 1.78 (m, Hₓₓ₃, 16.8H), 1.76 (q, ³Jₓₓₜₜ = 7.3 Hz, H₉, 8H, overlapped with thf), 0.79 (t, ³Jₓₓₜₜ = 7.3 Hz, H₉, 12H), 0.50 (t, ³Jₓₓₜₜ = 7.3 Hz, H₉, 12H).

³Li NMR (233.25 MHz, THF-d₈, 295 K): δ [ppm] = −2.12 (s).

²⁷Li NMR (233.25 MHz, C₆D₆, 295 K): δ [ppm] = −1.40 (s, broad), −3.01 (s), −4.30 (s, broad).

¹³C NMR [¹³C[¹⁴H], ¹³C-DEPT135, ¹⁴H, ¹³C-HSQC, ¹³H, ¹³C-HMBC ] (150.92 MHz, THF-d₈, 295 K): δ [ppm] = 144.05 (s, C₁), 106.56 (s, C₂H₂), 68.02 (s, C₆H₆), 46.33 (s, C₀), 45.94 (s, C₀), 45.94 (s, C₀), 39.47 (s, ¹¹⁷Sn-satellites ⁴Jₓₓₜₜ = 16 Hz, C₁H₂), 33.69 (s, C₀H₂), 26.15 (s, C₀H₂), 10.47 (s, C₀H₂), 10.22 (s, C₀H₂).

¹⁹F NMR [¹⁹F[¹⁷]C⁻⁷] (150.92 MHz, C₆D₆, 295 K): δ [ppm] = 143.92 (s, C₀), 105.14 (s, C₁H), 67.79 (s, C₁H), 46.63 (s, C₁H), 37.86 (s, C₂H₂), 36.50 (s, C₂H₂), 32.72 (s, C₂H₂), 25.06 (s, C₂H₂), 9.99 (s, C₂H₂), 9.76 (s, C₂H₂), 9.69 (s, C₂H₂).

¹¹⁹Sn NMR [¹¹⁷Sn,¹⁹H-HMBC] (223.81 MHz, THF-d₈, 295 K): δ [ppm] = −481.32.

¹¹⁹Sn NMR [¹¹⁷Sn,¹⁹H-HMBC] (223.81 MHz, C₆D₆, 295 K): δ [ppm] = −618.90.

HR-MS (ESI, negative, THF): calcd. for [C₃₅H₄₈Li₂N₄Sn+Cl]⁻ (Cl⁻ from ESI atmosphere) m/z = 705.2918, found m/z = 705.2929.

EA: Due to loss of THF upon isolation, a correct elemental analysis could not be obtained.
3.2 Tetrabutylammonium tin(II) meso-octaethylcalix[4]pyrrolate [(NBu₄)₂][2]

In a 50 mL Schlenk tube, [Li₂(thf)]₂[2] (1.0 eq, x = 4.2, 522 µmol, 500 mg) and tetrabutylammonium chloride (2.0 eq, 1.044 mmol, 522 mg) were dissolved in 30 mL 1,2-difluorobenzene (oDFB) and stirred at room temperature for 2 hours. The colorless suspension was filtered over a PTFE syringe filter (pore size 0.22 µm) and the filtrate evaporated at reduced pressure to obtain [(NBu₄)₂][2] as a colorless solid (550 mg, 482 µmol, 92% yield). Gas phase diffusion of pentane into a concentrated solution of [(NBu₄)₂][2] in oDFB at −30 °C yielded single crystals suitable for X-ray diffraction.

1H NMR [1H, 1H, 1H-COSY] (600.18 MHz, THF-d₈, 295 K): δ [ppm] = 5.68 (s, 119Sn-satellites ¹JSn,H = 12 Hz, H₇, 8H), 2.60 – 2.89 (m, H₈, 16), 2.08 (q, ¹JH,H = 8.0 Hz, H₉, 8H), 1.95 (q, ³JH,H = 9.0 Hz, H₅, 8H), 1.34 (m, H₉, 16H), 1.24 (q, ³JH,H = 4.0 Hz, H₁₀, 16H), 1.18 (t, ³JH,H = 7.3 Hz, H₁₀, 12H), 0.89 (t, ³JH,H = 9.0 Hz, H₁₁, 24H), 0.39 (t, ³JH,H = 6.0 Hz, H₁₂, 12H).

13C NMR [¹³C{¹H}, ¹³C-DEPT135, ¹³C-HSQC, ¹H, ¹³C-HMBC ] (150.92 MHz, THF-d₈, 295 K): δ [ppm] = 144.05 (s, C₁), 101.96 (s, C₂H), 59.15 (s, C₃H₂), 46.37 (s, C₄), 41.36 (s, C₅H₂), 29.40 (s, C₆H₂), 25.02 (s, C₇H₂), 21.00 (s, C₈H₂), 14.41 (s, C₁₀H₂), 12.02 (s, C₁₁H₃), 10.25 (s, C₁₂H₃).

119Sn NMR [¹¹⁹Sn, ¹H-HMBC] (223.81 MHz, THF-d₈, 295 K): δ [ppm] = −517.83 (s).

EA: calcd. for C₆₈H₁₂₀N₆Sn: C, 71.62; H, 10.61; N, 7.37. Found: C, 71.41; H, 10.91; N, 7.69.
3.3 Tetraphenylphosphonium tin(II) meso-octaethylcalix[4]pyrrolate ([PPh₄]₂(oDFB)₆₃)[2]

In a 50 mL Schlenk tube, [Li₂(thf)]₂[2] (x = 4.2, 1.0 eq, 514 µmol, 500 mg) was dissolved in 15 mL oDFB and tetraphenylphosphonium chloride (2.0 eq, 1.028 mmol, 386 mg) was added while stirring at room temperature. The clear colorless solution immediately turned orange and a colorless solid precipitated. After stirring for 30 minutes precipitation of an orange solid occurred which could be redissolved by adding 6 mL acetonitrile. Filtration of the reaction mixture over a PTFE syringe filter (pore size 0.22 µm) to remove the lithium chloride formed during the reaction yielded an orange clear solution. To remove residue lithium chloride, the solvent was evaporated at reduced pressure and the remaining was redissolved in 9 mL oDFB/MeCN (2:1) and kept at −30 °C over night. Filtration over a PTFE syringe filter and subsequent addition of three times the volume of pentane at −30 °C caused the slow precipitation of [(PPh₄)₂(oDFB)₆₃][2] as a dark red solid (372 mg, 267 µmol, 52% yield). Gas phase diffusion of pentane into a concentrated solution of [(PPh₄)₂(oDFB)₆₃][2] in oDFB and CH₃CN at −30 °C yielded single crystals suitable for X-ray diffraction.

¹H NMR [¹H, ¹H-1H-COSY] (399.89 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = 7.78 (m, H₁₃, 8H), 7.58 – 7.68 (m, H₉₋₁₀, 32H), 7.20 – 7.30 (m, H₀DFB, 1H), 7.10 – 7.17 (m, H₀DFB, 1H), 5.66 (s, H₁, 8H), 1.79 – 1.94 (m, H₃₋₅, overlayed with CD₃CN, 16H), 0.72 (t, 3J_H,H = 9.0 Hz, H₄, 12H), 0.58 (t, 3J_H,H = 9.0 Hz, H₄, 12H).

¹³C NMR [¹³C(¹H), ¹³C-DEPT135, ¹⁴H,¹³C-HSQC, ¹⁴H,¹³C-HMBC ] (100.55 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = 143.45 (s, C₁), 137.20 (d, 3J_C,C = 3.0 Hz, CH₁₁), 136.00 (d, 3J_C,C = 10.4 Hz, CH₅), 131.93 (d, 3J_C,C = 13.07 Hz, CH₁₀), 119.18 (d, 3J_C,C = 89.49 Hz, C₈), 102.92 (s, C₁H), 47.06 (s, C₁), 39.69 (s, C₁H₂), 35.75 (s, C₁H₂), 11.99 (s, C₁H₃), 11.46 (s, C₁H₃).

¹⁹F NMR (376.27 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = −140.36 – −140.29 (m, oDFB).

³¹P [³¹H] NMR (161.88 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = 22.82 (s, PPh₄⁺).

¹¹⁹Sn NMR [¹¹⁹Sn,¹⁴H-HMBC] (223.81 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = −485.98.

EA: calcd. for C₈₇H₉₀FN₄P₂Sn: C, 75.10; H, 6.52; N, 4.03. Found: C, 75.09; H, 6.57; N, 4.25.
0.5 mL THF-d₈ were added to [Li₂(thf)ₓ][2] (x = 4.2, 1.0 eq, 20.56 µmol, 20 mg) and selenium powder (3.0 eq, 61.67 µmol, 4.9 mg) in a Young NMR tube and mixed at room temperature for 30 minutes. The dark red reaction solution was filtered over a PTFE syringe filter (pore size 0.22 µm) to remove surplus selenium and the selenium adduct was characterized via NMR spectroscopy and HR-MS ESI(−) measurements. No yield was determined.

¹H NMR [¹H, ¹H- bastardy] (399.89 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = 5.88 (s, H₇, 8H), 3.69 – 3.59 (m, thf, 13H), 2.13 (q, 3J_H,H = 7.3 Hz, H₅, 6H), 2.02 – 1.91 (m, H₅, 2H), 1.85 (q, 3J_H,H = 7.1 Hz, H₃, 8H), 1.81 – 1.74 (m, thf, 13H), 0.69 (t, 3J_H,H = 7.4 Hz, H₆, 12H), 0.62 (t, 3J_H,H = 7.1 Hz, H₆, 12H).

¹³C NMR [¹³C{¹H}, ¹³C-DEPT135, ¹H,¹³C-HSQC, ¹H,¹³C-HMBC ] (100.55 MHz, THF-d₈, 295 K): δ [ppm] = 143.64 (s, C₁), 104.13 (s, C₁H), 67.39 (s, thf), 45.43 (s, C₂), 38.13 (s, C₃H₂), 36.01 (s, C₃H₂), 25.53 (s, thf), 9.74 (s, C₄H₃), 9.65 (s, C₅H₃).

⁷Li NMR (155.41 MHz, THF-d₈/CD₃CN, 295 K): δ [ppm] = -0.29 (s).

⁷⁷Se NMR [⁷⁷Se{¹H}, ¹H,⁷⁷Se-HMBC ] (114.46 MHz, THF-d₈, 295 K): δ [ppm] = -391.99 (s).

¹¹⁹Sn NMR [¹¹⁹Sn,¹H-HMBC ] (149.12 MHz, THF-d₈, 295 K): δ [ppm] = -560.18 (s).

HR-MS (ESI, negative, THF): calcd. for [C₃₆H₄₈N₄SnSe+H]⁻ (H⁺ from ESI atmosphere) m/z = 735.2225, found m/z =735.2225.
3.5 Tetraphenylphosphonium $^{1}\eta$-(tin(II) meso-octaethylcalix[4]pyrrolate) pentacarbonyl tungsten(0) [(PPh$_4$)$_2$][W($^{1}\eta$-2)(CO)$_5$]

Tungsten hexacarbonyl (3.0 eq, 107.7 µmol, 38 mg) was suspended in 1.0 mL THF in a quartz glass flask and irradiated with a Hg-lamp for 4 hours until gas evolution stopped and solid got dissolved into a clear yellow solution. [(PPh$_4$)$_2$(oDFB)$_{0.5}$][2] (1.0 eq, 35.9 µmol, 50 mg) was added to the solution and stirred for 36 hours at room temperature. The solvent was removed at reduced pressure. Crystallization from a concentrated solution in acetonitrile (MeCN) layered with pentane at −30 °C yielded [(PPh$_4$)$_2$][W($^{1}\eta$-2)(CO)$_5$] as a yellow-orange crystalline solid (35 mg, 21.9 µmol, 61% yield). Storing a concentrated solution of [(PPh$_4$)$_2$][W($^{1}\eta$-2)(CO)$_5$] in MeCN at room temperature yielded single crystals suitable for X-ray diffraction.

$^1$H NMR [$^1$H, $^1$H,$^1$H-COSY] (600.18 MHz, CD$_3$CN, 295 K): $\delta$ [ppm] = 7.92 – 7.87 (m, H$_{11}$, 8H), 7.74 – 7.70 (m, H$_{10}$, 16H), 7.68 – 7.63 (m, H$_9$, 8H), 5.77 (s, H$_7$, 8H), 1.92 (q, $^3$J$_{H,H}$ = 7.4 Hz, 8H), 1.86 (q, $^3$J$_{H,H}$ = 7.1 Hz, 8H), 0.65 (t, $^3$J$_{H,H}$ = 7.1 Hz, 12H), 0.50 (t, $^3$J$_{H,H}$ = 7.4 Hz, 12H).

$^{13}$C NMR [13C{[1H], 13C-DEPT135, [1H, 13C-HSQC, [1H, 13C-HMBC]} (150.92 MHz, CD$_3$CN, 295 K): $\delta$ [ppm] = 202.48 (s, CO), 143.90 (s, C$_1$), 136.39 (d, $^4$J$_{P,C}$ = 3.0 Hz, CH$_{11}$), 135.68 (d, $^4$J$_{P,C}$ = 10.5 Hz, CH$_9$), 131.31 (d, $^4$J$_{P,C}$ = 13.07 Hz, CH$_{10}$), 118.89 (d, $^1$J$_{P,C}$ = 90.6 Hz, C$_4$), 105.07 (s, C$_7$H), 46.28 (s, C$_2$), 42.25 (s, C$_3$H$_2$), 34.10 (s, C$_4$H$_3$), 10.90 (s, C$_5$H$_3$), 10.50 (s, C$_6$H$_3$).

$^{31}$P[$^1$H] NMR (161.88 MHz, CD$_3$CN, 295 K): $\delta$ [ppm] = 22.92 (s, PPh$_4^+$).

$^{119}$Sn NMR [119Sn,$^1$H-HMBC] (223.81 MHz, CD$_3$CN, 295 K): $\delta$ [ppm] = −482.78.

EA: calcd. for C$_{89}$H$_{88}$N$_4$O$_5$P$_2$SnW: C, 64.47; H, 5.35; N, 3.38; O, 4.82; P, 3.74; Sn, 7.16; W, 11.09. Found: C, 63.10; H, 5.38; N, 3.43. Low carbon content might be related to metal carbide formation during combustion.[19]
3.6 Tetrabutylammonium \( ^{\eta}(\text{tin(II)} \text{ meso-octaethylcalix[4]pyrrolate}) \) triscarbonyl nickel(0) \([\text{NBu}_4]_2[\text{Ni}(^{\eta}(\text{2})(\text{CO})_3)]\)

Bis(cyclooctadiene)nickel(0) (1.3 eq, 57.0 µmol, 15.7 mg) and \([\text{NBu}_4]_2[2]\) (1.0 eq, 43.85 µmol, 50 mg) were dissolved in 0.5 mL THF-\(d_8\) in a NMR pressure tube yielding a yellow clear solution. Addition of 3 atm CO gas and mixing at room temperature for 30 minutes caused the discoloration of the solution. Evaporation of the solvent at reduced pressure and washing of the crude with 5 mL pentane yielded \([\text{NBu}_4]\)\([\text{Ni}(^{\eta}(\text{2})(\text{CO})_3)]\) as an off-white crystalline solid (45 mg, 35.9 µmol, 82% yield).

\( ^1H\) NMR \([^1H, ^1H, ^1H-COSY] (600.18 MHz, THF-\(d_8\), 295 K): \( \delta [\text{ppm}] = 5.72 (s, H_7, 8H), 2.94 – 2.74 (m, H_8, 16H), 2.09 (q; \( ^3J_{H,H} = 6.3 \text{ Hz}, H_9, 8H), 2.05 (q; \( ^3J_{H,H} = 6.1 \text{ Hz}, H_5, 8H), 1.45 – 1.34 (m, H_5, 16H), 1.29 – 1.22 (m, H_10, 16H), 1.16 (t; \( ^3J_{H,H} = 7.2 \text{ Hz}, H_4, 12H), 0.92 (t; \( ^3J_{H,H} = 7.3 \text{ Hz}, H_{11}, 24H), 0.40 (t; \( ^3J_{H,H} = 7.3 \text{ Hz}, H_6, 12H).\)

\( ^{13}C\) NMR \([^{13}C[^1H], ^{13}C-\text{DEPT135}, ^{1H, ^1H-C-SQC, ^1H, ^1H-\text{HMBC}] (150.92 MHz, THF-\(d_8\), 295 K): \( \delta [\text{ppm}] = 198.46 (s, CO), 141.89 (s, C_1), 99.89 (s, C_7H), 56.14 (s, C_8H), 42.74 (s, C_2), 38.65 (s, C_3H), 26.37 (s, C_4H), 23.55 (s, C_5H), 20.38 (s, C_6H), 11.39 (s, C_11H), 9.02 (s, C_4H), 7.04 (s, C_6H).\)

\( ^{119}\text{Sn}\) NMR \([^{119}\text{Sn}, ^{1H-\text{HMBC}] (223.81 MHz, THF-\(d_8\), 295 K): \( \delta [\text{ppm}] = -335.24 (s).\)

EA: calcd. for \(C_{71}H_{120}N_6O_3NiSn\): C, 66.42; H, 9.43; N, 6.55; O, 3.74; Ni, 4.52; Sn, 9.35. Found: C, 66.01; H, 9.73; N, 6.44.
3.7 Ruthenium(II) $^5\eta$-(tin(II) meso-octaethylcalix[4]pyrrolate) para-cymene Ru($^5\eta$-2)(p-cymene)

$[\text{Li}_2(\text{thf})_2][2]$ ($x = 4.2, 1.0$ eq, $102.85$ µmol, $100$ mg) and $[(\text{Ru}(\text{Cl})(p-\text{cymene})),(\mu-\text{Cl})_2]$ ($0.5$ eq, $51.43$ µmol, $31.5$ mg) were dissolved in $4$ mL THF and stirred at room temperature for $1$ hour. The solvent was evaporated at reduced pressure and the remaining extracted with $6$ mL oDFB. Filtration of the extract over a PTFE syringe filter (pore size $0.22$ µm) to remove the lithium chloride formed during the reaction followed by the evaporation of the oDFB at reduced pressure yielded Ru($^5\eta$-2)(p-cymene) as an orange solid ($83.5$ mg, $93.58$ µmol, $91\%$ yield). Keeping a concentrated solution of Ru($^5\eta$-2)(p-cymene) in benzene for $12$ hours at room temperature yielded single crystals suitable for X-ray diffraction.

$^1$H NMR [$^1$H, $^1$H-$^1$H-COSY] (399.89 MHz, THF-$d_8$, 295 K): $\delta$ [ppm] = $5.99$ ($d$, $^3J_{HH} = 3.20$ Hz, $H_{9,10}$, 2H), $5.93$ ($d$, $^3J_{HH} = 3.20$ Hz, $H_{9,10}$, 2H), $5.91$ ($s$, $H_{1,18}$, 2H), $5.76$ ($s$, $H_{1,18}$, 2H), $5.46$ ($d$, $^3J_{HH} = 6.20$ Hz, $H_{22}$, 2H), $5.06$ ($d$, $^3J_{HH} = 6.10$ Hz, $H_{21}$, 2H), $2.71$ (hept, $^1J_{HH} = 6.90$ Hz, $H_{24}$, 1H), $2.21$ – $2.09$ ($m$, $H_{4,13,15}$, 10H), $2.08$ – $1.98$ ($m$, $H_{4,15}$, 2H), $1.87$ – $1.80$ ($m$, $H_{4,15}$, 4H), $1.23$ ($t$, $^3J_{HH} = 7.3$ Hz, $H_{9,14}$, 6H), $1.14$ ($d$, $^3J_{HH} = 6.9$ Hz, $H_{25}$, 6H), $1.09$ ($t$, $^3J_{HH} = 7.2$ Hz, $H_{9,14}$, 6H), $0.96$ ($s$, $H_{19}$, 3H), $0.56$ ($t$, $^3J_{HH} = 7.3$ Hz, $H_{6,16}$, 6H), $0.50$ ($t$, $^3J_{HH} = 7.3$ Hz, $H_{5,16}$, 6H).

$^{13}$C NMR [$^{13}$C($^1$H), $^{13}$C-DEPT135, $^1$H, $^{13}$C-HSQC, $^1$H, $^{13}$C-HMBC ] (150.92 MHz, C$_6$D$_{10}$, 295 K): $\delta$ [ppm] = $146.05$ ($s$, $C_{6,13}$), $142.32$ ($s$, $C_{2,17}$), $136.13$ ($s$, $C_{8,11}$), $134.27$ ($s$, $C_{2,17}$), $110.68$ ($s$, $C_{20}$), $110.53$ ($s$, $C_{23}$), $105.49$ ($s$, $C_{9,10,18}$H), $105.26$ ($s$, $C_{9,10,18}$), $105.00$ ($s$, $C_{9,10,18}$H), $103.57$ ($s$, $C_{11}$), $89.82$ ($s$, $C_{21,22}$H), $76.72$ ($s$, $C_{21,22}$H), $46.40$ ($s$, $C_{3,12}$), $43.42$ ($s$, $C_{3,12}$), $34.44$ ($s$, $C_{24}$H) $31.13$ ($s$, $C_{6,15}$H), $29.54$ ($s$, $C_{6,15}$H), $28.65$ ($s$, $C_{4,13}$H), $27.07$ ($s$, $C_{4,13}$H), $17.29$ ($s$, $C_{18}$H), $11.41$ ($s$, $C_{25}$H), $10.26$ ($s$, $C_{4,13}$H), $10.02$ ($s$, $C_{4,13}$H), $9.44$ ($s$, $C_{6,15}$H), $8.18$ ($s$, $C_{6,15}$H).

$^{119}$Sn NMR [$^{119}$Sn, $^1$H-HMBC] (149.12 MHz, THF-$d_8$, 295 K): $\delta$ [ppm] = $-424.83$ ($s$).

EA: calcd. for C$_{46}$H$_{62}$N$_4$RuSn: C, 61.86; H, 7.00; N, 6.28; Ru, 11.42; Sn, 13.44. Found: C, 61.78; H, 7.03; N, 6.24.
3.8 Reaction of [Li₂(thf)]₂ with Electrophiles

[Li₂(thf)]₂ (x = 4.2, 1.0 eq, 17.54 µmol, 17.0 mg) was dissolved in 0.45 mL toluene-d₈ and one equivalent of the respective electrophile was added in one portion at room temperature. The reaction conditions for each electrophile are summarized in Table S1 below. The reaction products were characterized by ¹H, ¹³C, ¹¹⁹Sn as well as 2D-NMR methods and HRMS ESI(−) measurements. For Entry 3 storing of the reaction solution at −30 °C after removal of the precipitated lithium chloride yielded single crystals suitable for X-ray diffraction.

Table S1: Reaction conditions for the reaction of [Li₂(thf)]₂ with electrophiles.

| Entry | Electrophile            | Reaction Conditions                        |
|-------|--------------------------|--------------------------------------------|
| 1     | Methylene chloride      | No reaction                                |
| 2     | Benzyl chloride         | Unselective reaction forming mixture of compounds |
| 3     | Benzoyl chloride        | Reaction completed at rt within minutes    |
| 4     | Benzaldehyde            | Reacted at rt over 20 hours, formation of side products |
| 5     | 4-CF₃-Benzaldehyde      | Reacted at rt over 20 hours, formation of side products |

3.8.1 Entry 3 (Benzoyl Chloride)

¹H NMR [¹H, ¹H, ¹H-COSY] (600.15 MHz, Toluene-d₈, 295 K): \( \delta \) [ppm] = 7.26 – 7.21 (m, H₁₁, 2H), 7.00 – 6.98 (m, H₁₁₂, 2H), 6.94 (d, \( 3J_{H,H} = 7.3 \) Hz, H₁₁₂, 1H), 6.29 (s, H₁₇, 8H), 2.04 (q, \( 3J_{H,H} = 7.2 \) Hz, H₃, 8H), 1.95 (q, \( 3J_{H,H} = 7.3 \) Hz, H₅, 8H), 0.91 (t, \( 3J_{H,H} = 7.2 \) Hz, H₄, 13H), 0.86 (t, \( 3J_{H,H} = 7.3 \) Hz, H₆, 13H).

¹³C NMR [¹³C{¹H}, ¹³C-DEPT135, ¹H,¹³C-HSQC, ¹H,¹³C-HMBC] (150.92 MHz, Toluene.-d₈, 295 K): \( \delta \) [ppm] = 143.93 (s, C₁), 134.91 (s, C₁₂H), 131.40 (s, C₁₀), 129.15 (s, C₁₀H), 128.22 (s, C₁₁H), 125.38 (s, C₈), 106.57 (s, 117/119Sn-satellites \( 3J_{Sn,C} = 30 \) Hz, C₇H), 67.86 (s, C₁₃H₂), 45.60 (s, 117/119Sn-satellites \( 3J_{Sn,C} = 7.5 \) Hz, C₂), 40.42 (C₅H₂), 34.89 (s, C₆H₃), 25.67 (s, C₇H₂), 10.14 (s, C₆H₃), 10.02 (s, C₆H₃).

¹¹⁹Sn NMR [¹¹⁹Sn,¹H-HMBC] (149.12 MHz, Toluene-d₈, 295 K): \( \delta \) [ppm] = −487.99.

HR-MS (ESI, negative, THF): calcd. for C₄₃H₅₃N₄O₄Sn⁻ m/z = 761.3267, found m/z = 761.3283.

3.8.2 Entry 4 (Benzaldehyde)

HR-MS (ESI, negative, THF): calcd. for C₄₃H₅₃N₄O₄Sn⁻ m/z = 761.3267, found m/z = 761.3243.
3.8.3 Entry 5 (4-CF₃-Benzaldehyde)

$^1$H NMR [$^1$H, $^1$H, $^1$H-COSY] (399.89 MHz, Toluene-$d_8$, 295 K): $\delta$ [ppm] = 7.41 ($d, J_{H,H} = 7.8$ Hz, $H_{10}, 2H$), 6.98 ($d, J_{H,H} = 7.8$ Hz, $H_{11}, 2H$), 6.34 (s, $H_7$, 8H), 1.94 ($q, J_{H,H} = 7.3$ Hz, $H_2$, 8H), 1.75 ($q, J_{H,H} = 7.3$ Hz, $H_5$, 8H), 0.76 ($t, J_{H,H} = 7.1$ Hz, $H_3$, 12H), 0.73 ($t, J_{H,H} = 7.1$ Hz, $H_6$, 12H).

$^{13}$C NMR [$^{13}$C, $^{13}$C-DEPT135, $^{1}$H, $^{13}$C-HSQC, $^{1}$H, $^{13}$C-HMBC] (100.55 MHz, Toluene-$d_8$, 295 K): $\delta$ [ppm] = 145.40 (s, $C_1$), 136.11 (s, $C_{12}$), 129.16 (s, $C_9$), 127.82 (s, $C_{10}$), 126.35 (s, $C_{11}$), 126.31 (s, $C_8$), 106.64 (m, $CF_3$), 105.45 (s, $C_7$), 47.20 (s, $C_2$), 35.61 ($C_3H_2$), 35.04 (s, $C_3H_2$), 10.02 (s, $C_4H_3$), 9.71 (s, $C_6H_3$).

$^{19}$F NMR (149.12 MHz, THF-$d_8$, 295 K): $\delta$ [ppm] = −62.36.

$^{119}$Sn NMR [$^{119}$Sn, $^1$H-HMBC] (149.12 MHz, THF-$d_8$, 295 K): $\delta$ [ppm] = −750.37.

HR-MS (ESI, negative, THF): calcd. for C$_{44}$H$_{52}$N$_4$OF$_3$Sn$^-$ m/z = −829.3141, found m/z = −829.3159.

3.9 Reaction of [(NBu$_4$)$_2$][2] with Electrophiles

[(NBu$_4$)$_2$][2] (1.0 eq, 17.54 µmol, 20.0 mg) was dissolved in 0.45 mL THF-$d_8$ and one equivalent of the respective electrophile was added in one portion at room temperature. The reaction conditions for each electrophile are summarized in Table S2 below. The products were characterized by $^1$H, $^{13}$C, $^{119}$Sn as well as 2D-NMR methods and HRMS ESI(−) measurements.

**Table S2**: Reaction conditions for the reaction of [(NBu$_4$)$_2$][2] with electrophiles. The yield was determined by NMR spectroscopy.

| Entry | Electrophile               | Reaction Conditions                      |
|-------|----------------------------|-----------------------------------------|
| 1     | Methylene chloride        | Near quantitative yield after mixed at rt for 24h |
| 2     | Benzyl chloride           | Near quantitative yield at rt within minutes |
| 3     | Benzyol chloride          | Near quantitative yield at rt within minutes |
| 4     | Benzaldehyde              | No reaction                             |
| 5     | 4-CF₃-Benzaldehyde        | No reaction                             |
| 6     | Iodobenzene               | Quantitative reduction of iodobenzene to benzene at rt, 48h |
3.9.1 Entry 1 (Methylene Chloride)

$^1$H NMR [$^1$H, $^1$H,$^2$H-COSY] (399.89 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = 5.90 (s, $^{117/119}$Sn-satellites $^4$J$_{Sn,H} = 8.0$ Hz, H$_2$, 8H), 3.56 – 3.35 (m, H$_{13}$, 16H), 2.67 (s, $^{117/119}$Sn-satellites $^3$J$_{Sn,H} = 36.0$ Hz, H$_{6}$, 2H), 1.90 (q, $^3$J$_{H,H} = 7.2$ Hz, H$_{6}$, 8H), 1.86 (q, $^3$J$_{H,H} = 7.2$ Hz, H$_{6}$, 8H), 1.78 – 1.68 (m, H$_{14}$ 16H, overlaid with THF-d$_8$), 1.46 – 1.35 (m, H$_{15}$, 16H), 0.99 (t, $^3$J$_{H,H} = 7.4$ Hz, H$_{16}$, 24H), 0.75 (t, $^3$J$_{H,H} = 7.2$ Hz, H$_{6}$, 12H), 0.62 (t, $^3$J$_{H,H} = 7.3$ Hz, H$_{6}$, 12H).

$^{13}$C NMR [$^{13}$C($^1$H), $^{13}$C-DEPT135, $^1$H,$^{13}$C-HSQC, $^1$H,$^{13}$C-HMBC ] (100.55 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = 143.56 (s, $^{117/119}$Sn-satellites $^3$J$_{Sn,C} = 8.0$ Hz, C$_7$), 106.22 (s, $^{117/119}$Sn-satellites $^3$J$_{Sn,C} = 23.1$ Hz, C$_7$H), 59.64 (s, C$_9$H$_2$), 46.49 (s, C$_2$), 40.26 (s, C$_{3,3}$H$_2$), 38.74 (s, C$_8$H$_2$), 36.05 (s, C$_{3,5}$H$_2$), 25.15 (s, C$_{10}$H$_2$), 20.90 (s, C$_{11}$H$_2$), 14.28 (s, C$_{12}$H$_3$), 10.92 (s, C$_{4,6}$H), 10.52 (s, C$_{4,6}$H).

$^{119}$Sn NMR [$^{119}$Sn n($^1$H), $^{119}$Sn,$^1$H-HMBC] (149.12 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = -477.52.

HR-MS (ESI, negative, THF): calcd. for C$_{37}$H$_{56}$N$_4$Sn$^-$ m/z = 747.3448, found m/z = 747.3456.

3.9.2 Entry 2 (Benzyl chloride)

$^1$H NMR [$^1$H, $^1$H,$^2$H-COSY] (399.89 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = 6.78 – 6.69 (m, H$_{11}$, 2H), 6.67 – 6.60 (m, H$_{12}$, 1H), 6.33 – 6.25 (m, H$_{10}$, 2H), 5.95 (s, $^{117/119}$Sn-satellites $^4$J$_{Sn,H} = 8.0$ Hz, H$_7$, 8H), 3.55 – 3.42 (m, H$_{13}$, 16H), 2.20 (s, $^{119}$Sn-satellites $^2$J$_{Sn,H} = 116.6$ Hz, $^{117}$Sn-satellites $^2$J$_{Sn,H} = 111.2$ Hz, H$_{9}$, 2H), 1.83 – 1.68 (m, H$_{3,5,14}$, 32H), 1.46 – 1.35 (m, H$_{15}$, 16H), 0.99 (t, $^3$J$_{H,H} = 7.4$ Hz, H$_{16}$, 24H), 0.60 (t, $^3$J$_{H,H} = 7.1$ Hz, H$_{4,6}$, 24H).

$^{13}$C NMR [$^{13}$C($^1$H), $^{13}$C-DEPT135, $^1$H,$^{13}$C-HSQC, $^1$H,$^{13}$C-HMBC ] (100.55 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = 143.91 (s, $^{117/119}$Sn-satellites $^3$J$_{Sn,C} = 8.0$ Hz, C$_7$), 141.46 (s, C$_9$), 130.74 (s, C$_{10}$H), 128.02 (s, C$_{11}$H), 123.69 (s, C$_{12}$H), 106.90 (s, $^{117/119}$Sn-satellites $^3$J$_{Sn,C} = 23.1$ Hz, C$_7$H), 59.64 (s, C$_{3,3}$H$_2$), 46.65 (s, C$_2$), 39.41 (s, C$_{5,5}$H$_2$), 39.37 (s, C$_{3,3}$H$_2$), 31.76 (s, C$_8$H$_2$), 25.14 (s, C$_{4,6}$H$_2$), 20.89 (s, C$_{13,15}$H$_2$), 14.27 (s, C$_{16}$H$_2$), 10.68 (s, C$_{4,6}$H$_2$), 10.62 (s, C$_{4,6}$H$_2$).

$^{119}$Sn NMR [$^{119}$Sn n($^1$H), $^{119}$Sn,$^1$H-HMBC] (149.12 MHz, THF-d$_8$, 295 K): $\delta$ [ppm] = -409.19 (s).

HR-MS (ESI, negative, THF): calcd. for C$_{43}$H$_{58}$N$_4$Sn$^-$ m/z = 747.3448, found m/z = 747.3456.
3.9.3 Entry 3 (Benzoyl chloride)

**1H NMR** [1H, 1H, 1H-COSY] (399.89 MHz, THF-δ6, 295 K): δ [ppm] = 7.20 – 7.13 (m, H12, 1H), 7.11 – 7.00 (m, H10, 11, 4H), 5.89 (s, 117/119Sn-satellites J_{Sn,H} = 12.0 Hz, H8, 8H), 3.54 – 3.44 (m, H13, 16H), 1.83 – 1.68 (m, H8,5,14 overlayed, 32H), 1.35 – 1.46 (m, H15, 16H), 0.99 (t, J_{H,H} = 7.4 Hz, H16, 24H), 0.66 (t, J_{H,H} = 7.1 Hz, H4,6, 12H), 0.64 (t, J_{H,H} = 7.1 Hz, H4,6, 12H).

**13C NMR** [13C(1H), 13C-DEPT135, 1H, 13C-HSQC, 1H, 13C-HMBC ] (100.55 MHz, THF-δ6, 295 K): δ [ppm] = 135.44 (s, C8), 143.23 (s, 117/119Sn-satellites J_{Sn,C} = 9.0 Hz, C1), 143.07 (s, C9), 135.49, 132.20 (s, C12H2), 131.37, 129.98, 129.39 (s, C10,11H), 128.93 (s, C10,11H), 128.03, 106.03 (s, 117/119Sn-satellites J_{Sn,C} = 26.1 Hz, C8), 59.63 (s, C13H1), 45.96 (s, C2), 39.07 (s, C3,5H2), 37.60 (s, C3,5H2), 25.15 (s, C16H2), 20.89 (s, C15H2), 14.30 (s, C16H2), 10.82 (s, C4,6H2), 10.54 (s, C4,6H2).

**119Sn NMR** [119Sn(1H), 119Sn, 1H-HMBC] (149.12 MHz, THF-δ6, 295 K): δ [ppm] = -542.67.

**HR-MS** (ESI, negative, THF): calcd. for C43H53N4OSn m/z = 761.3267, found m/z = 761.3256.

3.9.4 Entry 6 (Iodobenzene)

**1H NMR** [1H, 1H, 1H-COSY] (399.89 MHz, THF-δ6, 295 K): δ [ppm] = 7.30 (s, H6, 5H), 6.11 (s, 117/119Sn-satellites J_{Sn,H} = 16.0 Hz, H5, 8H), 3.47 – 3.37 (m, H8, 16H), 1.84 (q, J_{H,H} = 7.3 Hz, H9, 16H), 1.79 – 1.68 (m, H9 overlayed, 21H), 1.50 – 1.37 (m, H6 overlayed, 25H), 1.36 – 1.25 (m, H8 overlayed, 9H), 1.00 (t, J_{H,H} = 7.3 Hz, H10 overlayed, 28H), 0.65 (t, J_{H,H} = 7.3 Hz, H4, 24H).

**13C NMR** [13C(1H), 13C-DEPT135, 1H, 13C-HSQC, 1H, 13C-HMBC ] (100.55 MHz, THF-δ6, 295 K): δ [ppm] = 143.14 (s, 117/119Sn-satellites J_{Sn,C} = 7.0 Hz, C1), 129.20 (s, C9), 109.26 (s, 117/119Sn-satellites J_{Sn,C} = 42.2 Hz, C8H2), 59.76 (s, C13H2), 46.78 (s, C2), 30.93 (s, C3H2), 25.29 (s, C16H2), 20.83 (s, C15H2), 14.33 (s, C10aH2), 10.22 (s, C4H2).

**119Sn NMR** [119Sn(1H), 119Sn, 1H-HMBC] (149.12 MHz, THF-δ6, 295 K): δ [ppm] = -560.83.
4  NMR Spectra

4.1  [Li₂(thf)₅][2]

Figure S1. ¹H NMR spectrum of [Li₂(thf)₅][2] (600.18 MHz, THF-d₈, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S2. ¹H NMR spectrum of [Li₂(thf)₅][2] (600.18 MHz, C₆D₆, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S3. $^7$Li NMR spectrum of $[\text{Li}_2(\text{thf})_x][2]$ (233.24 MHz, THF-$d_8$, 295 K).

Figure S4. $^7$Li NMR spectrum of $[\text{Li}_2(\text{thf})_x][2]$ (233.24 MHz, $\text{C}_6\text{D}_{10}$, 295 K).
Figure S5. $^{13}$C NMR spectrum of $[\text{Li}_2(\text{thf})_x][\text{2}]$ (150.92 MHz, THF-$d_8$, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S6. $^{13}$C NMR spectrum of $[\text{Li}_2(\text{thf})_x][\text{2}]$ (150.92 MHz, $C_6D_{14}$, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S7. $\text{^{119}Sn}$--$\text{^{1}H}$ HMBC NMR spectrum of $[\text{Li}_2(\text{thf})_2][2]$ (THF-$d_8$, 295 K).

4.2 $[(\text{NBu}_4)_2][2]$

Figure S8. $\text{^{1}H}$ NMR spectrum of $[(\text{NBu}_4)_2][2]$ (600.18 MHz, THF-$d_8$, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S9. $^{13}$C NMR spectrum of $[(NBu_4)_2][2]$ (150.92 MHz, THF-$d_8$, 295 K). Solvent resonances are indicated by an asterisk (*).

4.3 $[(PPh_4)_2(oDFB)_{0.8}][2]$

Figure S10. $^1$H NMR spectrum of $[(PPh_4)_2(oDFB)_{0.8}][2]$ (399.89 MHz, THF-$d_8$/CD$_3$CN, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S11. $^{13}$C NMR spectrum of $\left[\left(\text{PPh}_4\right)_2\text{oDFB}\right]_{0.5}[2]$ (100.55 MHz, THF-$d_8$/CD$_3$CN, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S12. $^{19}$F NMR spectrum of $\left[\left(\text{PPh}_4\right)_2\text{oDFB}\right]_{0.5}[2]$ (376.27 MHz, THF-$d_8$/CD$_3$CN, 295 K).
Figure S13. $^{31}$P($^1$H) NMR spectrum of [(PPh$_4$)$_2$((oDFB)$_0.5$)][2] (161.88 MHz, THF-$_d$8/CD$_3$CN, 295 K).

4.4 [Li$_2$(thf)$_x$][2-Se]

Figure S14. $^1$H NMR spectrum of [Li$_2$(thf)$_x$][2-Se] (399.89 MHz, THF-$_d$8, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S15. $^{13}$C NMR spectrum of $\text{[Li}_2\text{(thf)}_x\text{]}\text{[2-Se]}$ (100.55 MHz, THF-$d_8$, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S16. $^{77}$Se-$^1$H HMBC NMR spectrum of $\text{[Li}_2\text{(thf)}_x\text{]}\text{[2]}$ (THF-$d_8$, 295 K).
4.5 \([(\text{PPh}_4)_2]\text{[W(}\text{η-2})(\text{CO})_5]\]

Figure S17. $^1$H NMR spectrum of \([(\text{PPh}_4)_2]\text{[W(}\text{η-2})(\text{CO})_5]\] (600.15 MHz, MeCN-$d_3$, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S18. $^{13}$C NMR spectrum of \([(\text{PPh}_4)_2]\text{[W(}\text{η-2})(\text{CO})_5]\] (150.92 MHz, MeCN-$d_3$, 295 K). Solvent resonances are indicated by an asterisk (*).
Figure S19. $^{119}$Sn-$^1$H HMBC NMR spectrum of [(PPh$_4$)$_2$][W(1η-2)(CO)$_5$] (MeCN-$d_3$, 295 K).

4.6 [(NBu$_4$)$_2$][Ni(1η-2)(CO)$_3$]

Figure S20. $^1$H NMR spectrum of [(NBu$_4$)$_2$][Ni(1η-2)(CO)$_3$] (600.15 MHz, THF-$d_8$, 295 K). Solvent resonances and resonances of residue pentane are indicated by an asterisk (*).
Figure S21. $^{13}$C NMR spectrum of $\text{[NBu}_4\text{]}_2\text{[Ni(}^{1}\eta^{-2}\text{)(CO)}_3\text{]}$ (150.92 MHz, THF-$d_8$, 295 K). Solvent resonances and resonances of residue pentane are indicated by an asterisk (*).

Figure S22. $^{119}$Sn-$^1$H HMBC NMR spectrum of $\text{[NBu}_4\text{]}_2\text{[Ni(}^{1}\eta^{-2}\text{)(CO)}_3\text{]}$ (THF-$d_8$, 295 K). Traces of free stannate(II) dianion formed by decomposition are indicated by an asterisk (*).
4.7 Ru($^5\eta$-2)(cymene)

Figure S23. $^1$H NMR spectrum of Ru($^5\eta$-2)(cymene) (400 MHz, THF-$d_8$, 295 K). Solvent resonances and resonances of residue pentane are indicated by an asterisk (*).

Figure S24. $^{13}$C NMR spectrum of Ru($^5\eta$-2)(cymene) (150.29 MHz, C$_6$D$_6$, 295 K). Solvent resonances and resonances of residue pentane are indicated by an asterisk (*).
Figure S25. $^{119}\text{Sn}^{-1}\text{H}$ HMBC NMR spectrum of Ru($^{6}\eta$-2)(cymene) (THF-$d_8$, 295 K).

4.8 Reaction of [Li$_2$(thf)$_x$][2] with Benzoyl chloride

Figure S26. $^1\text{H}$ NMR spectrum of the reaction of [Li$_2$(thf)$_x$][2] with benzoyl chloride (600.15 MHz, Toluene-$d_8$, 295 K). Solvent resonances and resonances of THF from starting material are indicated by an asterisk (*).
Figure S27. $^{13}$C NMR spectrum of the reaction of $[\text{Li}_2(\text{thf})_x][2]$ with benzoyl chloride (155.29 MHz, Toluene-d$_8$, 295 K). Solvent resonances and resonances are indicated by an asterisk (*).

Figure S28. $^{129}$Sn-$^1$H HMBC spectrum of the reaction of $[\text{Li}_2(\text{thf})_x][2]$ with benzoyl chloride (399.89 MHz, Toluene-$d_8$, 295 K).
4.9 Reaction of \([\text{Li}_2(\text{thf})_x]_2\) with 4-CF\(_3\)-Benzaldehyde

**Figure S29.** \(^1\)H NMR spectrum of the reaction of \([\text{Li}_2(\text{thf})_x]_2\) with 4-CF\(_3\)-benzaldehyde (399.89 MHz, Toluene-\(d_8\), 295 K). Solvent resonances and resonances of THF from starting material are indicated by an asterisk (*).

**Figure S30.** \(^{13}\)C NMR spectrum of the reaction of \([\text{Li}_2(\text{thf})_x]_2\) with 4-CF\(_3\)-benzaldehyde (100.55 MHz, Toluene-\(d_8\), 295 K). Solvent resonances and resonances of THF from starting material are indicated by an asterisk (*).
Figure S31. $^{195}$Sn-$^1$H HMBC spectrum of the reaction of $[\text{Li}_2(\text{thf})_x][2]$ with 4-(CF$_3$)-benzaldehyde (Toluene-d$_8$, 295 K).

4.10 Reaction of $[(\text{NBu}_4)_2][2]$ with Methylene Chloride

Figure S32. $^1$H NMR spectrum of the reaction of $[(\text{NBu}_4)_2][2]$ with methylene chloride (399.89 MHz, THF-d$_8$, 295 K). Solvent and residual methylene chloride resonances are indicated by an asterisk (*).
Figure S33. $^{13}$C NMR spectrum of the reaction of [(NBu$_4$)$_2$][2] with methylene chloride (100.55 MHz, THF-d$_8$, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S34. $^{119}$Sn-$^1$H HMBC spectrum of the reaction of [(NBu$_4$)$_2$][2] with methylene chloride (THF-d8, 295 K).
4.11 Reaction of [(NBu₄)₂][2] with Benzyl Chloride

Figure S35. $^1$H NMR spectrum of the reaction of [(NBu₄)₂][2] with benzyl chloride (399.89 MHz, THF-d₈, 295 K). Solvent resonances are indicated by an asterisk (*).

Figure S36. $^{13}$C NMR spectrum of the reaction of [(NBu₄)₂][2] with benzyl chloride (100.55 MHz, THF-d₈, 295 K). Solvent resonances are indicated by an asterisk (*).
4.12 Reaction of [(NBu₄)₂][2] with Benzoyl Chloride

Figure S37. $^{119}\text{Sn}^{-1}\text{H}$ HMBC spectrum of the reaction of [(NBu₄)₂][2] with benzyl chloride (THF-d₈, 295 K).

Figure S38. $^1\text{H}$ NMR spectrum of the reaction of [(NBu₄)₂][2] with benzoyl chloride (399.89 MHz, THF-d₈, 295 K). Solvent and residue benzoyl chloride (slight excess) resonances are indicated by an asterisk (*).
Figure S39. $^{13}$C NMR spectrum of the reaction of [(NBu$_4$)$_2$][2] with benzoyl chloride (100.55 MHz, THF-d$_8$, 295 K). Solvent and residue benzoyl chloride (slight excess) resonances are indicated by an asterisk (*).

Figure S40. $^{119}$Sn-$^1$H HMBC spectrum of the reaction of [(NBu$_4$)$_2$][2] with benzoyl chloride (THF-d$_8$, 295 K).
4.13 Reaction of \([\text{NBu}_4]_2[2]\) with Iodobenzene

**Figure S41.** $^1$H NMR spectrum of the reaction of \([\text{NBu}_4]_2[2]\) with iodobenzene (399.89 MHz, THF-d8, 295 K). Solvent resonances are indicated by an asterisk (*).

**Figure S42.** $^{13}$C NMR spectrum of the reaction of \([\text{NBu}_4]_2[2]\) with iodobenzene (100.55 MHz, THF-d8, 295 K). Solvent resonances are indicated by an asterisk (*).
5 Crystallographic Data
5.1 [Li₂(thf)₅][2]

**Figure S43:** Solid state molecular structure of [Li₂(thf)₅][2] (left) and the isolated [Li(thf)][2]⁻ anion (left, *meso*-ethyl residues and solvated lithium counter cation are omitted for clarity). Ellipsoids are drawn with a probability of 50%. Hydrogen atoms are omitted for clarity.

**Table S3:** Crystal data for [Li₂(thf)₅][2].

| Property                        | Value                          |
|---------------------------------|--------------------------------|
| CCDC number                     | 2125920                        |
| Identification code             | mo_hr283_0ma                   |
| Empirical formula               | C₅₆H₈₈Li₂N₄O₅Sn                |
| Formula weight                  | 1029.87                        |
| Temperature/K                   | 100                            |
| Crystal system                  | monoclinic                     |
| Space group                     | P2₁/c                          |
| a/Å                             | 17.0606(16)                    |
| b/Å                             | 16.1225(14)                    |
| c/Å                             | 19.5523(18)                    |
| α/°                             | 90                             |
| β/°                             | 90.037(4)                      |
| γ/°                             | 90                             |
| Volume/Å³                       | 5378.0(8)                      |
| Z                               | 4                              |
| ρ_calcd/g cm⁻³                  | 1.272                          |
| μ/mm⁻¹                          | 0.525                          |
| F(000)                          | 2192.0                         |
| Crystal size/mm³                | 0.221 × 0.164 × 0.044          |
| Radiation                       | MoKα (λ = 0.71073)             |
| 2Θ range for data collection/°  | 4.052 to 52                    |
| Index ranges                    | -21 ≤ h ≤ 21, -19 ≤ k ≤ 19, -24 ≤ l ≤ 24 |
| Reflections collected           | 236904                         |
| Independent reflections         | 10548 [R(int) = 0.0979, R(sigma) = 0.0272 ] |
| Data/restraints/parameters      | 10548/0/650                    |
| Goodness-of-fit in F²           | 1.081                          |
| Final R indexes [I>=2σ(I)]      | R₁ = 0.0293, wR₂ = 0.0591      |
| Final R indexes [all data]      | R₁ = 0.0415, wR₂ = 0.0632      |
| Largest diff. peak/hole/eÅ⁻³    | 0.47/-0.50                    |
5.2 [(NBu₄)₂][2]

Figure S44: Solid state molecular structure of [(NBu₄)₂][2]. Ellipsoids are drawn with a probability of 50%. Hydrogen atoms are omitted for clarity.

Table S4: Crystal data for [(NBu₄)₂][2].

| Property                      | Value                          |
|-------------------------------|--------------------------------|
| CCDC number                   | 2125918                        |
| Identification code           | mo_hr342_2_0ma                  |
| Empirical formula             | C₆₈H₁₂₀N₆Sn                    |
| Formula weight                | 1140.38                        |
| Temperature/K                 | 100.0                          |
| Crystal system                | orthorhombic                   |
| Space group                   | Pbcₐ (61)                      |
| a/Å                           | 18.9095(7)                     |
| b/Å                           | 18.6657(5)                     |
| c/Å                           | 35.9481(10)                    |
| α/°                           | 90                             |
| β/°                           | 90                             |
| γ/°                           | 90                             |
| Volume/Å³                     | 12688.2(7)                     |
| Z                             | 8                              |
| ρ calc/g cm⁻³                 | 1.194                          |
| μ/mm⁻¹                        | 0.447                          |
| F(000)                        | 4960                           |
| Crystal size/mm³              | 0.349×0.342×0.263              |
| Radiation                     | MoKα (λ=0.71073 Å)             |
| 2Θ range for data collection/°| 4.31 to 51.00 (0.83 Å)         |
| Index ranges                  | -22 ≤ h ≤ 22, -22 ≤ k ≤ 22, -43 ≤ l ≤ 43 |
| Reflections collected         | 83712                          |
| Independent reflections       | 11805 [Rint = 0.0486, Rsigma = 0.0294] |
| Data/restraints/parameters    | 11805/0/731                    |
| Goodness-of-fit in F²         | 1.045                          |
| Final R indexes [I>=2σ(I)]    | R₁ = 0.0298, wR₂ = 0.0658      |
| Final R indexes [all data]    | R₁ = 0.0354, wR₂ = 0.0685      |
| Largest diff. peak/hole/eÅ⁻³  | 0.32/-0.53                    |
### 5.3 [(PPh₄)₂(oDFB)₀.₅][2]

**Figure S45:** Solid state molecular structure of [(PPh₄)₂(oDFB)₀.₅][2]. Ellipsoids are drawn with a probability of 50%. Hydrogen atoms are omitted for clarity.

**Table S5:** Crystal data for [(PPh₄)₂(oDFB)₀.₅][2].

| Property                  | Value                          |
|---------------------------|--------------------------------|
| CCDC number              | 2125916                        |
| Identification code      | mo_hr308_0ma                   |
| Empirical formula        | C₈₇H₉₀FN₄P₂Sn                  |
| Formula weight           | 1391.25                        |
| Temperature/K            | 100(2)                         |
| Crystal system           | triclinic                      |
| Space group              | P̅₁ (2)                         |
| a/Å                      | 12.227(4)                      |
| b/Å                      | 12.276(5)                      |
| c/Å                      | 23.438(10)                     |
| α/°                      | 87.397(10)                     |
| β/°                      | 84.496(11)                     |
| γ/°                      | 80.754(10)                     |
| Volume/Å³                | 3455(2)                        |
| Z                         | 2                              |
| ρcalc/g cm⁻³             | 1.337                          |
| μ/mm⁻¹                   | 0.470                          |
| F(000)                   | 1458                           |
| Crystal size/mm³         | 0.169×0.084×0.030              |
| Radiation                | MoKα (λ=0.71073 Å)             |
| 2Θ range for data collection/° | 3.95 to 50.00 (0.84 Å)        |
| Index ranges             | -14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -27 ≤ l ≤ 27 |
| Reflections collected    | 75371                          |
| Independent reflections  | 12169 [Rint = 0.1052, Rsigma = 0.0634] |
| Data/restraints/parameters | 12169/1209/935               |
| Goodness-of-fit in F²    | 1.041                          |
| Final R indexes [l>=2σ(l)] | R₁ = 0.0440, wR₂ = 0.0853  |
| Final R indexes [all data] | R₁ = 0.0672, wR₂ = 0.0929  |
| Largest diff. peak/hole/eÅ⁻³ | 0.50/-0.54               |
5.4 \([(\text{PPh}_4)_2][\text{W}(\eta^2-2)(\text{CO})_5]\]

Figure S46: Solid state molecular structure of \([(\text{PPh}_4)_2][\text{2-W(CO)}_5]\]. Ellipsoids are drawn with a probability of 50%. Hydrogen atoms are omitted for clarity.

Table S6: Crystal data for \([(\text{PPh}_4)_2][\text{2-W(CO)}_5]\).

| Property                                | Value                                      |
|-----------------------------------------|--------------------------------------------|
| CCDC number                             | 2125915                                    |
| Identification code                     | mo_hr313_2_2                               |
| Empirical formula                       | C_{93}H_{94}N_{6}O_{5}P_{2}SnW             |
| Formula weight                          | 1740.22                                    |
| Temperature/K                           | 100(2)                                     |
| Crystal system                          | triclinic                                  |
| Space group                             | \(P\overline{1}\) (2)                     |
| a/\(\text{Å}\)                           | 13.510(2)                                  |
| b/\(\text{Å}\)                           | 13.587(2)                                  |
| c/\(\text{Å}\)                           | 25.095(4)                                  |
| \(\alpha/^{\circ}\)                     | 81.048(6)                                  |
| \(\beta/^{\circ}\)                      | 84.270(7)                                  |
| \(\gamma/^{\circ}\)                     | 60.976(5)                                  |
| Volume/\(\text{Å}^3\)                   | 3977.3(12)                                 |
| \(Z\)                                   | 2                                          |
| \(\rho_{\text{calc}}/\text{g cm}^{-3}\) | 1.453                                      |
| \(\mu/\text{mm}^{-1}\)                  | 1.857                                      |
| \(F(000)\)                              | 1776                                       |
| Crystal size/\(\text{mm}^3\)            | 0.107×0.103×0.044                          |
| Radiation                               | MoK\(\alpha\) (\(\lambda=0.71073\ \text{Å}\)) |
| 2\(\Theta\) range for data collection/\(^{\circ}\) | 3.78 to 56.02 (0.76 Å)                     |
| Index ranges                            | -17 \leq h \leq 17, -17 \leq k \leq 17, -33 \leq l \leq 33 |
| Reflections collected                   | 193114                                     |
| Independent reflections                 | 19158 \([R_{\text{int}} = 0.1119, R_{\text{sigma}} = 0.0560]\) |
| Data/restraints/parameters              | 19158/2225/1011                            |
| Goodness-of-fit in \(F^2\)              | 1.017                                      |
| Final R indexes \([I>2\sigma(I)]\)      | \(R_1 = 0.0316, wR_2 = 0.0665\)            |
| Final R indexes \([\text{all data}]\)   | \(R_1 = 0.0430, wR_2 = 0.0720\)            |
| Largest diff. peak/hole/e\(\text{Å}^{-3}\) | 1.00/-1.01                               |
5.5 Ru(η-2)(cymene)

Figure S47: Solid state molecular structure of Ru(η-2)(cymene). Ellipsoids are drawn with a probability of 50%. Hydrogen atoms are omitted for clarity.

Table S7: Crystal data for Ru(η-2)(cymene).

| Property                        | Value                          |
|---------------------------------|--------------------------------|
| CCDC number                     | 2125917                        |
| Identification code             | mo_hr372_0ma                   |
| Empirical formula               | C₅₈H₇₄N₄RuSn                   |
| Formula weight                  | 1046.97                        |
| Temperature/K                   | 100(2)                         |
| Crystal system                  | triclinic                      |
| Space group                     | P̅1 (2)                        |
| a/Å                             | 11.465(3)                      |
| b/Å                             | 12.8505(17)                    |
| c/Å                             | 19.451(4)                      |
| α/°                             | 97.710(8)                      |
| β/°                             | 101.873(10)                    |
| γ/°                             | 114.506(5)                     |
| Volume/Å³                       | 2473.0(9)                      |
| Z                               | 2                              |
| ρ_calc/g cm⁻³                   | 1.406                          |
| μ/mm⁻¹                          | 0.853                          |
| F(000)                          | 1088                           |
| Crystal size/mm³                | 0.123×0.106×0.074              |
| Radiation                       | MoKα (λ=0.71073 Å)             |
| 2Θ range for data collection/° | 4.02 to 57.46 (0.74 Å)        |
| Index ranges                    | -15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -26 ≤ l ≤ 26 |
| Reflecteds collected            | 155733                         |
| Independent reflections         | 12835 [R_int = 0.0390, R_sigma = 0.0165] |
| Data/restraints/parameters      | 12835/282/588                  |
| Goodness-of-fit in F²           | 1.089                          |
| Final R indexes [I>=2σ(I)]      | R₁ = 0.0180, wR₂ = 0.0476      |
| Final R indexes [all data]      | R₁ = 0.0207, wR₂ = 0.0485      |
| Largest diff. peak/hole/eÅ⁻³    | 0.46/-0.57                    |
5.6  [Li(thf)$_2$][3-COPh]

Figure S48: Solid state molecular structure of [Li(thf)$_2$][3-COPh]. Displacement ellipsoids are drawn at 50% probability level. Hydrogens and toluene solvent molecules are omitted for clarity.

Table S8: Crystal data for [Li(thf)$_2$][3-COPh].

| Property                              | Value                           |
|---------------------------------------|---------------------------------|
| CCDC number                          | 2125919                         |
| Identification code                  | mo_hr389c_0m_a                  |
| Empirical formula                    | C$_{58}$H$_{77}$LiN$_4$O$_3$Sn  |
| Formula weight                       | 1003.86                         |
| Temperature/K                        | 101(2)                          |
| Crystal system                       | triclinic                       |
| Space group                          | P$\bar{1}$ (2)                  |
| a/Å                                   | 10.618(3)                       |
| b/Å                                   | 11.653(3)                       |
| c/Å                                   | 21.103(5)                       |
| $\alpha$/°                            | 99.542(11)                      |
| $\beta$/°                            | 93.042(8)                       |
| $\gamma$/°                           | 92.079(12)                      |
| Volume/Å$^3$                         | 2568.7(12)                      |
| Z                                      | 2                               |
| $\rho$ calc/g cm$^{-3}$              | 1.298                           |
| $\mu$/mm$^{-1}$                      | 0.545                           |
| F(000)                                | 1060                            |
| Crystal size/mm$^3$                   | 0.339×0.313×0.207               |
| Radiation                             | MoK$_\alpha$ (\(\lambda = 0.71073\) Å) |
| 2$\Theta$ range for data collection/* | 3.92 to 61.11 (0.70 Å)          |
| Index ranges                          | -15 $\leq$ h $\leq$ 15, -16 $\leq$ k $\leq$ 16, -30 $\leq$ l $\leq$ 30 |
| Reflections collected                 | 101029                          |
| Independent reflections              | 15729 [R$_{int}$ = 0.0476, R$_{sigma}$ = 0.0311] |
| Data/restraints/parameters            | 15729/831/734                   |
| Goodness-of-fit in F$^2$              | 1.037                           |
| Final R indexes [I>2$\sigma$(I)]     | $R_1$ = 0.0242, $wR_2$ = 0.0560 |
| Final R indexes [all data]           | $R_1$ = 0.0263, $wR_2$ = 0.0572 |
| Largest diff. peak/hole/eÅ$^3$       | 0.49/-0.56                     |
6 Infrared Spectroscopy

Figure S49: FTIR spectrum of \([(\text{NBu}_4)_2\text{Ni}(\eta^2-2)(\text{CO})_3]\) in THF-\(d_8\).

7 Comparative TEP Scale

Figure S50. Comparison between TEP values of \([2]^{2-}\) and other literature known carbene and phosphine ligands.

Table S9. TEP values of \([2]^{2-}\) and other literature known carbene and phosphine ligands.

| Compound          | TEP [cm\(^{-1}\)] | Solvent | Reference |
|-------------------|-------------------|---------|-----------|
| \([2]^{2-}\)      | 2032.3            | THF     | This work |
| P(NIMes)\(_2\)iPr | 2038.6            | DCM     | [20]      |
| B                 | 2046              | DCM     | [21]      |
| IMes              | 2050.7            | DCM     | [22]      |
| IPr (A)           | 2051.5            | DCM     | [20]      |
| P\(_3\)Bu\(_3\)   | 2056.1            | DCM     | [20]      |
| [PPh\(_3\)(CH\(_2\)BF\(_3\))]\(^-\) | 2061      | DCM     | [23]      |
| PPh\(_3\)         | 2068.9            | DCM     | [20]      |
8 DFT Calculations

![Diagram showing structures and HOMO energies](image)

**Figure S51.** HOMO energy levels, s-character of the lone pair (lp), and NBO atomic charges $\delta_{\text{NBO}}$ of the central atom for the NHC A, the CAAC B, the NHSn C, ADSn D, the anionic stannate(II) $[\text{E}]^-$, the dianionic stannates(II) $[\text{F}]^{2-}$, and $[\text{G}]^{2-}$, the boryl H, the aluminum anion $[\text{J}]^-$, and $[\text{2}]^{2-}$. HOMO energies were calculated at the B97M-D3(BJ)/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TZVPP and NBO analysis at the PBE0/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TZVPP level of theory. For C and $[\text{2}]^{2-}$ the HOMO and HOMO-1 are mainly ligand-centered and the energies of their HOMO-2 containing a mayor contribution of their tin-centered lone pairs are given as well.
Figure S52. Frontier molecular orbital energies for the hypothetical pyrrolato stannanes $K$, $[M]^-$, and $[L]^-$, and $[2]^{2-}$ at the B97M-D3(BJ)/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TZVPP level of theory and s-character of the lone pair and NBO atomic charges at the central atom calculated on the PBE0/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TZVPP level of theory. Isosurfaces sampled at a value of 0.03.
Figure S53. Free reaction enthalpy for the σ-hole adduction formation between [2]^2− and iodobenzene and frontier molecular orbitals calculated on the B97M-D3(BJ)/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TZVPP level of theory. Isosurfaces sampled at a value of 0.03.
9 Cyclic Voltammetry

Figure S54: Cyclic voltammogram of [(NBu$_4$)$_2$][2] and [NBu$_4$][PF$_6$] in oDFB.

10 ETS-NOCV Results

Table S11: Bonding energy decomposition terms calculated on the BP86-D3/TZ2P COSMO(THF)//B97M-D3(BJ)/def2-TVZPP level of theory.

| Compound | Total Pauli Repulsion ($\Delta E_{Pauli}$) [Eh] | Total Electrostatic Interaction ($\Delta V_{ele}$) [Eh] | Total Orbital Interaction ($\Delta E_{oi,tot}$) [Eh] | Total Dispersion Energy ($E_{disp}$) [Eh] | Solvation Energy ($E_{solv}$) [Eh] | Residue [Eh] | Total Bonding Energy ($\Delta E$) [Eh] |
|----------|-----------------------------------------------|------------------------------------------------|------------------------------------------------|---------------------------------|---------------------------------|-------------|---------------------------------|
| [2]$^{2-}$ | 0.477164845 | -1.340814347 | -0.573479385 | -0.010706268 | -0.173999447 | 0.004544433 | -0.169455015 |
| [Sn(pyr)]$^{2-}$ | 0.463414466 | -1.446258898 | -0.535590216 | -0.006556682 | -0.20239567 | 0.00298029 | -0.19941538 |
| [2-Se]$^{2-}$ | 0.350999376 | -0.236227689 | -0.294142204 | -0.012874307 | -0.189065305 | 0.004530776 | -0.184534529 |
| [2$^{2-}$-Se]$^{2-}$ | 0.331996112 | -0.228345683 | -0.292003221 | -0.009634874 | -0.216411735 | 0.003181708 | -0.213230027 |
Figure S55. ETS-NOCV bond analysis of [2]²⁻ on the BP86-D3/TZ2P COSMO(THF)//B97M-D3(BJ)/def2-TZVPP level of theory. Isosurfaces sampled at a value of 0.03.
Figure S56. ETS-NOCV bond analysis of [2-Se]^{2-} and the meso-unsubstituted derivative [2^H-Se]^{2-} on the BP86-D3/TZ2P COSMO(THF)//B97M-D3(BJ)/def2-TZVPP level of theory. The Se fragment was considered in its closed shell \(^1\)D excited state with doubly occupied \(p_x\) and \(p_y\) orbitals and an empty \(p_z\) orbital directed towards the Sn(II) lone pair of a singlet tin(II) calix[4]pyrrolato fragment. NOCV deformation densities sampled at a value of 0.003. The color code of the charge flow is red to blue.
11 NBO Results

Table S12: NBO analysis results calculated on PBE0/def2-TZVPP CPCM(THF)//B97M-D3(BJ)/def2-TVZPP level of theory. NBO and second order perturbation theory stabilization energies $\Delta E^{(2)}$ for selected bonding interactions are given in kJ mol$^{-1}$. Additionally, Lewis density parameters $%\rho_L$ and single point energies are given for each system.

| System | Single Point Energy (Eh) | $%\rho_L$ | Natural Charge | Character of lp(1) | $\Delta E^{(2)}$ lp(2) $\rightarrow \pi^*$ | $\Delta E^{(2)}$ lp(3) $\rightarrow \sigma^*$ |
|--------|-------------------------|----------|----------------|-------------------|-----------------------------|-----------------------------|
| NHC (A) | -1159.062799534277 | 97.91     | 0.073          | 49.60%            | -925.49                   | 21.88                        |
| CAAC (B) | -874.060935133861 | 98.32     | 0.127          | 41.18%            | 6.31                       | 6.26                         |
| NHB Li THF Adduct (H) | -1617.970242201778 | 99.32     | 1.040          | 0.600             | 14.83                      | 14.78                        |
| NHSn (C) | -1335.373499564167 | 98.13     | 1.200          | 88.99%            | 14.30                      | 14.30                        |
| ADSn (D) | -1913.919385348876 | 99.98     | 0.600          | 87.09             | 21.09                      | 21.67                        |
| Bis dithiolato stannate(II) [G]$^{2-}$  | -2268.592659566669 | 98.23     | 0.600          | 87.09             | 21.09                      | 21.67                        |
| Stanna dodecaborate [F]$^{2-}$  | -494.486522724303 | 98.31     | 0.741          | 75.85%            | 14.30                      | 14.30                        |
| Gade’s stannate (II) ([E]$^{-}$) | -2627.689403573425 | 98.29     | 1.232          | 80.54%            | 21.09                      | 21.67                        |
| Aldridge’s Aluminyl Anion ([J]$^{-}$) | -2293.177232006270 | 97.85     | 1.129          | 79.30%            | 21.09                      | 21.67                        |
| [2]$^{2-}$  | -1832.964212044182 | 98.14     | 1.129          | 79.30%            | 21.09                      | 21.67                        |
| [2-Se]$^{2-}$  | -4234.292224 | 98.40     | 1.129          | 79.30%            | 21.09                      | 21.67                        |
| Reaction                     | ΔE(2) |  |  |
|-----------------------------|--------|---|---|
| $\Delta E^{(2)}$ | $\text{lp(3)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}1-\text{Sn}33}$ | 9.29 |  |
| $\Delta E^{(2)}$ | $\text{lp(3)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}13-\text{Sn}33}$ | 8.74 |  |
| $\Delta E^{(2)}$ | $\text{lp(3)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}19-\text{Sn}33}$ | 8.74 |  |
| $\Delta E^{(2)}$ | $\text{lp(3)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}29-\text{Sn}33}$ | 9.29 |  |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}1-\text{Sn}33}$ | 9.25 |  |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}13-\text{Sn}33}$ | 9.25 |  |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}19-\text{Sn}33}$ | 9.25 |  |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \pi^*_{\text{N}29-\text{Sn}33}$ | 9.25 |  |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \sigma^*_{\text{C}32-\text{H}40}$ | 4.14 | (C(sp$^3$)H-Se interaction) |
| $\Delta E^{(2)}$ | $\text{lp(2)}_{\text{Se}34} \rightarrow \sigma^*_{\text{C}8-\text{H}36}$ | 4.06 | (C(sp$^3$)H-Se interaction) |

**[2H-Se]^{2-}** (single point energy = $-3605.895922$ Eh, $\%\rho_l = 98.06$)

| Reaction                     | ΔE(2) |  |  |
|-----------------------------|--------|---|---|
| NBO111 $\sigma_{\text{Sn}33-\text{Se}34}$ (occupation = 1.94806) | $-953.08$ |  |  |

$\Delta E^{(2)}$
12 \textit{\textsuperscript{77}Se and \textsuperscript{119}Sn NMR Shift Calculation Results}

\textbf{Table S13:} \textsuperscript{77}Se and \textsuperscript{119}Sn NMR shifts calculated on the PBE0/SO-ZORA-TZ2P COSMO(THF)//B97M-D3(BJ)/def2-TZVPP level of theory and referenced against SeMe\textsubscript{2} and SnMe\textsubscript{4}, respectively.

| Compound       | Total \textsuperscript{119}Sn NMR isotropic shielding tensor [ppm] | \textsuperscript{119}Sn NMR chemical shift against SnMe\textsubscript{4} [ppm] | Total \textsuperscript{77}Se NMR isotropic shielding tensor [ppm] | \textsuperscript{77}Se NMR chemical shift against SeMe\textsubscript{2} [ppm] |
|-----------------|---------------------------------------------------------------------|--------------------------------------------------------------------------------|---------------------------------------------------------------------|--------------------------------------------------------------------------------|
| SnMe\textsubscript{4} | 3004.14                                                             | 0.00                                                                           | -                                                                   | -                                                                              |
| SeMe\textsubscript{4} | -                                                                  | -                                                                              | 1978.08                                                             | 0.00                                                                           |
| [2\textsuperscript{2−}]  | 3513.52                                                             | -509.38                                                                       | -                                                                   | -                                                                              |
| [2-Se]\textsuperscript{2−} | 3575.747                                                            | -571.606                                                                      | 2427.45                                                             | -449.37                                                                       |
| [2\textsuperscript{2−}]  | 3562.074                                                             | -557.933                                                                      | 2616.62                                                             | -638.54                                                                       |

Ahmet et al. \textit{J. Inorg. Chem.} 2018, 2018, 1670-1678.

\(\delta^{\textsuperscript{77}}\text{Se, }^\text{C}_6\text{D}_6 = -476.01 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, }^\text{C}_6\text{D}_6 = -566.30 \text{ ppm}\)

Park et al. \textit{Inorg. Chem.} 2020, 59, 3513-3517.

\(\delta^{\textsuperscript{77}}\text{Se, }^\text{C}_6\text{D}_6 = -218.13 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, }^\text{C}_6\text{D}_6 = -264.50 \text{ ppm}\)

Leung et al. \textit{Organometallics} 2000, 19, 296-303.

\(\delta^{\textsuperscript{77}}\text{Se, THF/C}_6\text{D}_6 = -531.95 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, THF/C}_6\text{D}_6 = -179.18 \text{ ppm}\)

Leung et al. \textit{Organometallics} 2000, 19, 296-303.

\(\delta^{\textsuperscript{77}}\text{Se, THF/C}_6\text{D}_6 = -734.8 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, THF/C}_6\text{D}_6 = -111.55 \text{ ppm}\)

\(\delta^{\textsuperscript{77}}\text{Se, THF-d}_6 = -391.99 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, THF-d}_6 = -560.18 \text{ ppm}\)

Saito et al. \textit{J. Am. Chem. Soc.} 2004, 126, 15572-15582.

\(\delta^{\textsuperscript{77}}\text{Se, CDCl}_3 = 839 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, CDCl}_3 = 556 \text{ ppm}\)

Mairová et al. \textit{Organometallics} 2011, 30, 5904-5910.

\(\delta^{\textsuperscript{77}}\text{Se, CDCl}_3 = -570.90 \text{ ppm}\)
\(\delta^{\textsuperscript{119}}\text{Sn, CDCl}_3 = -4.70 \text{ ppm}\)

\textbf{Figure S57.} Experimental \textsuperscript{77}Se and \textsuperscript{119}Sn NMR data for [Li\textsubscript{2}(thf)]\textsubscript{2}[2-Se] and other literature-known, monomeric stanna(II) selenido complexes.

13 \textbf{Optimized Molecular Geometries}

\texttt{aldrdige_aluminyl_anion_B97M_D3_TZVPP_optfreq}

Total correction: 2823.8826 kJ/mol
Single point energy: -6032185.6891 kJ/mol

S53
Total enthalpy: -6029359.3278 kJ/mol
Final entropy term: 343.6942 kJ/mol
Total gibbs free enthalpy: -6029703.022 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -1, multiplicity: 1
C 0.561060 0.112350 0.399967
C 0.916841 -0.035129 3.089450
C 0.346933 -1.126870 0.988810
C 0.845545 1.279366 1.059714
C 1.042116 1.192620 2.433955
C 0.567449 -1.174009 2.375185
H 1.277005 2.078148 2.995806
H 0.416692 -2.111941 2.874651
C 0.861701 2.549502 0.214672
C 0.789340 3.797524 1.070399
H 1.645420 3.850361 1.734980
H -0.113815 3.817783 1.670766
H 0.806764 4.685072 0.446653
C 2.158465 2.584780 -0.604001
H 3.018769 2.618430 0.059136
H 2.173501 3.464888 -1.241176
H 2.244960 1.707188 -1.232328
C -0.326497 2.442259 -0.734196
C -2.599602 1.865423 -2.255763
C -1.241714 3.447182 -1.036875
C -0.558094 1.206001 -1.275472
C -1.722106 0.815326 -1.928653
C -2.359114 3.164342 -1.826754
H -1.094427 4.438921 -0.649754
H -3.497742 1.620601 -2.789335
O 0.295261 0.150420 0.963631
N -1.895535 -0.517053 -2.118486
N -0.100671 -2.117793 0.167679
Al -0.344549 -1.771904 -1.802808
C -0.121092 -3.428693 0.643364
C -0.308078 -6.097913 1.437613
C 1.035426 -4.113464 1.050111
C -1.330147 -4.122286 0.600890
C -1.446271 -5.446557 0.985165
C 0.905710 -5.434008 1.456146
H -2.198546 -3.587052 0.257772
H 1.788074 -5.971975 1.766777
H -0.358154 -7.128017 1.753806
C -3.061293 -0.904287 -2.805385
C -5.368831 -1.590132 -4.155772
C -3.081067 -0.858887 -4.205297
| C   | -4.190220  | -1.331622  | -2.076843 |
|-----|------------|------------|------------|
| C   | -5.363731  | -1.652311  | -2.768765  |
| C   | -4.246853  | -1.215205  | -4.861267  |
| H   | -4.282082  | -1.184498  | -5.939046  |
| H   | -6.277070  | -1.837428  | -4.684069  |
| C   | -1.882358  | -0.422156  | -5.004808  |
| H   | -1.082617  | -0.201765  | -4.307624  |
| C   | -4.078494  | -1.362063  | -0.568095  |
| H   | -3.014381  | -1.387676  | -0.361330  |
| C   | 2.407149   | -3.503271  | 0.926035   |
| H   | 2.291657   | -2.449400  | 0.710939   |
| C   | -2.771574  | -6.151498  | 0.900784   |
| H   | -3.503649  | -5.418979  | 0.566911   |
| C   | -1.394256  | -1.539879  | -5.913183  |
| H   | -0.514705  | -1.223022  | -6.468631  |
| H   | -2.158827  | -1.826151  | -6.632498  |
| H   | -1.126709  | -2.412403  | -5.327058  |
| C   | -2.178408  | 0.839172   | -5.803934  |
| H   | -1.293126  | 1.167367   | -6.342975  |
| H   | -2.495597  | 1.647531   | -5.152914  |
| H   | -2.965608  | 0.665880   | -6.534730  |
| C   | -4.602345  | -0.075150  | 0.058498   |
| H   | -5.664991  | 0.054061   | -0.135086  |
| H   | -4.081817  | 0.788659   | -0.337331  |
| H   | -4.460440  | -0.091251  | 1.136551   |
| C   | -4.680671  | -2.580177  | 0.121061   |
| H   | -4.496749  | -3.489989  | -0.442128  |
| H   | -5.749265  | -2.493194  | 0.276877   |
| H   | -4.224900  | -2.700893  | 1.099651   |
| C   | -2.730286  | -7.275011  | -0.124657  |
| H   | -2.012664  | -8.035795  | 0.171734   |
| H   | -2.432274  | -6.901488  | -1.098288  |
| H   | -3.702460  | -7.752945  | -0.221550  |
| C   | -3.220682  | -6.679385  | 2.254597   |
| H   | -3.274582  | -5.881535  | 2.988226   |
| H   | -2.523920  | -7.424774  | 2.628748   |
| H   | -4.199706  | -7.147531  | 2.184843   |
| C   | 3.228110   | -3.626897  | 2.198664   |
| H   | 2.719025   | -3.166745  | 3.039242   |
| H   | 4.190980   | -3.136672  | 2.080415   |
| H   | 3.420348   | -4.666624  | 2.451258   |
| C   | 3.137937   | -4.125500  | -0.257148  |
| H   | 4.117289   | -3.670202  | -0.388540  |
| H   | 2.569501   | -3.986198  | -1.171037  |
| H   | 3.279079   | -5.193371  | -0.105220  |
| C   | -6.647024  | -2.040552  | -2.097547  |
| H   | -6.626827  | -3.059145  | -1.721152  |
dipp_caac_B97M_D3_TZVPP_optfreq

Total correction: 1298.8758 kJ/mol
Single point energy: -2196405.6075 kJ/mol
Total enthalpy: -2195104.2527 kJ/mol
Final entropy term: 184.9048 kJ/mol
Total gibbs free enthalpy: -2195289.1576 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
C -0.712336 -0.492345 1.640589
C 0.569440 0.167547 2.086035
N 0.217252 1.188984 2.810161
C -1.266664 1.449481 3.024701
C -1.846254 0.485437 1.999896
H -2.146951 1.036216 1.113201
H -2.728181 -0.018459 2.381398
### dipp_cnc_sncl_B97M_D3_TZVPP_optfreq

**Total correction:** 1855.0072 kJ/mol  
**Single point energy:** -5032447.3356 kJ/mol  
**Total enthalpy:** -5030589.8495 kJ/mol  
**Final entropy term:** 263.0695 kJ/mol  
**Total gibbs free enthalpy:** -5030852.9191 kJ/mol  
**Method and Basis:** B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1

| Atom | X (Angstrom) | Y (Angstrom) | Z (Angstrom) |
|------|--------------|--------------|--------------|
| N    | 0.770739     | 1.251775     | 2.266860     |
| Sn   | 2.017439     | -0.540098    | 2.784476     |
| C    | -0.171313    | 1.027986     | 3.176781     |
| N    | 0.130326     | -0.055932    | 3.892699     |
| C    | -1.351615    | 1.948444     | 3.486895     |
| C    | -1.406844    | 3.187413     | 2.604593     |
| H    | -0.487684    | 3.757007     | 2.638084     |
| H    | -2.206073    | 3.821036     | 2.975675     |
| H    | -1.621113    | 2.957295     | 1.570154     |
| C    | -2.694726    | 1.232800     | 3.369524     |
| H    | -2.786294    | 0.410540     | 4.063025     |
| H    | -2.867982    | 0.863462     | 2.364789     |
| H    | -3.480592    | 1.947653     | 3.593738     |
| C    | -1.169563    | 2.422957     | 4.930016     |
| H    | -0.196775    | 2.882225     | 5.073094     |
| H    | -1.274240    | 1.610791     | 5.632839     |
| H    | -1.930578    | 3.163847     | 5.153414     |
| C    | -0.634860    | -0.765766    | 4.834823     |
| C    | -2.061164    | -2.285985    | 6.673837     |
| C    | -1.577176    | -1.707844    | 4.384980     |
| C    | -0.354956    | -0.646097    | 6.203271     |
| C    | -1.090882    | -1.404601    | 7.103142     |
| C    | -2.285569    | -2.445202    | 5.319773     |
| H    | -0.887427    | -1.310711    | 8.156187     |
| H    | -3.016450    | -3.160771    | 4.984629     |
| H    | -2.624525    | -2.863143    | 7.387301     |
| C    | 0.800825     | 2.082596     | 1.135002     |
| C    | 1.060265     | 3.575707     | -1.192563    |
| C    | 1.705283     | 3.149093     | 1.092200     |
| C    | 0.021290     | 1.763080     | 0.010356     |
| C    | 0.166454     | 2.522268     | -1.138779    |
| C    | 1.817500     | 3.881320     | -0.081348    |
| H    | -0.426871    | 2.288568     | -2.005724    |
| H    | 2.511271     | 4.704498     | -0.119479    |
| H    | 1.161737     | 4.153183     | -2.095679    |
| C    | -0.938872    | 0.604074     | 0.037804     |
| H    | -1.224694    | 0.439496     | 1.069168     |
C  -0.263516 -0.669111 -0.451839
H   0.051732 -0.555938 -1.485197
H  -0.941211 -1.516608 -0.393820
H   0.618895 -0.905492  0.135175
C   -2.220738  0.855611 -0.736427
H   -2.044785  0.905124 -1.806158
H  -2.693569  1.784488 -0.433722
H  -2.923532  0.045933 -0.564549
C    2.554031  3.516158  2.278713
H    2.267538  2.878485  3.106081
C    4.025119  3.259806  1.986295
H    4.630277  3.457415  2.865050
H    4.374389  3.890991  1.795040
H    4.196724  2.229084  1.696368
C    2.343585  4.962466  2.702645
H    2.926050  5.181825  3.592202
H    1.301062  5.168834  2.924093
H    2.657542  5.654028  1.926273
C    0.784277  0.200463  6.702527
H    1.103132  0.848868  5.895076
C    1.956432 -0.708116  7.053593
H    2.827115 -0.123838  7.332077
H    2.238268 -1.333360  6.213650
H    1.693700 -1.359263  7.883473
C    0.422895  1.065384  7.898961
H    1.261106  1.703199  8.161031
H    0.191669  0.463696  8.772683
H   -0.433017  1.700884  7.699188
C   -1.761284 -1.985870  2.916174
H   -1.407435 -1.123483  2.364565
C   -3.204136 -2.230614  2.509540
H   -3.857966 -1.432019  2.841810
H   -3.583104 -3.162656  2.916447
H   -3.278462 -2.301841  1.428404
C   -0.896324 -3.173987  2.511582
H    0.149932 -3.004871  2.747283
H   -0.973416 -3.367989  1.445572
H   -1.211111 -4.066993  3.044044
Cl   3.452451  0.671793  4.277701

**gaede_tol_sn_B97M_D3_TZVPP_optfreq**

| Property                                    | Value                |
|---------------------------------------------|----------------------|
| Total correction:                           | 1793.2969 kJ/mol     |
| Single point energy:                        | -6907356.5888 kJ/mol |
| Total enthalpy:                             | -6905560.8128 kJ/mol |
| Final entropy term:                         | 310.1679 kJ/mol      |
Total gibbs free enthalpy: -6905870.9808 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -1, multiplicity: 1

| C      | 1.438848 | 2.552618 | 0.497423 |
| C      | 1.343245 | 3.638034 | -0.387741 |
| H      | 1.372284 | 4.636327 | 0.018316 |
| C      | 1.245169 | 3.453600 | -1.753509 |
| H      | 1.177881 | 4.318649 | -2.397166 |
| C      | 1.250598 | 2.186658 | -2.320313 |
| C      | 1.355117 | 1.105039 | -1.454083 |
| H      | 1.358511 | 0.103567 | -1.860257 |
| C      | 1.437174 | 1.276673 | -0.086494 |
| H      | 1.482674 | 0.413954 | 0.557916 |
| C      | 1.112094 | 1.992328 | -3.795517 |
| H      | 0.071615 | 1.864467 | -4.094559 |
| H      | 1.648909 | 1.110486 | -4.134822 |
| H      | 1.496345 | 2.847020 | -4.345073 |
| C      | 1.652466 | 0.339370 | 3.662367 |
| H      | 0.755159 | 0.647900 | 4.188394 |
| H      | 2.305207 | -0.163397 | 4.373279 |
| H      | 1.363523 | -0.387260 | 2.905315 |
| C      | 4.022888 | 1.190882 | 1.987430 |
| H      | 3.788321 | 0.429054 | 1.250127 |
| H      | 4.728148 | 0.763763 | 2.697089 |
| H      | 4.521666 | 2.006941 | 1.472751 |
| C      | 4.796897 | 2.940452 | 5.389722 |
| H      | 5.611923 | 2.730228 | 4.703226 |
| H      | 4.654792 | 2.064791 | 6.016431 |
| H      | 5.104251 | 3.762121 | 6.030202 |
| C      | -1.133987 | 2.791569 | 4.947591 |
| C      | -1.790601 | 3.013431 | 6.166945 |
| H      | -1.356181 | 3.706158 | 6.869110 |
| C      | -2.989395 | 2.396235 | 6.468100 |
| H      | -3.462946 | 2.599974 | 7.417910 |
| C      | -3.614223 | 1.538849 | 5.571901 |
| C      | -2.980879 | 1.323627 | 4.354731 |
| H      | -3.437946 | 0.664560 | 3.630882 |
| C      | -1.773571 | 1.920376 | 4.050294 |
| H      | -1.293668 | 1.709663 | 3.108075 |
| C      | -4.901081 | 0.858031 | 5.909101 |
| H      | -4.748013 | -0.174198 | 6.223935 |
| H      | -5.575181 | 0.829760 | 5.056721 |
| H      | -5.414448 | 1.366130 | 6.720275 |
| C      | 1.327062 | 2.336825 | 7.066630 |
| H      | 0.484691 | 2.416785 | 7.747038 |
| H      | 2.239719 | 2.406493 | 7.654550 |
H    1.296016  1.348992  6.616265  
C    1.272180  5.324147  6.601039  
H    1.250399  6.130401  5.875452  
H    2.147868  5.461449  7.232400  
H    0.390235  5.417995  7.231894  
C    1.121195  6.992468  3.063088  
C    -0.089354  7.305912  3.699272  
C    -0.617913  6.520824  4.215685  
C    -0.601710  8.589920  3.691842  
H    -1.539459  8.784084  4.191640  
C    0.063998   9.636829  3.071558  
C    1.266623   9.338329  2.440298  
H    1.803959 10.125986  1.931247  
C    1.779091  8.057218  2.426474  
H    2.692375   7.853071  1.891726  
C    -0.474877 11.030562  3.093855  
H    0.058404  11.664932  3.801603  
H    -1.522290 11.041611  3.379660  
H    -0.392878 11.508974  2.120571  
C    4.161437  6.613479  4.223592  
C    4.260155   7.560401  3.701545  
H    5.160900  6.263034  4.471924  
C    3.633860  6.801951  5.154006  
C    4.184448   5.128475  1.591761  
H    3.698293   4.395563  0.956679  
H    5.208102   4.801296  1.763325  
H    4.224024   6.099665  1.047028  
N    1.505903   2.755440  1.857997  
N    0.051732   3.405381  4.610186  
N    1.596903   5.700140  3.046478  
Si   2.506749   1.824836  2.901499  
Si   1.328630   3.662924  5.733347  
Si   3.262330   5.305950  3.214681  
Si   3.208303   3.369801  4.448491  
Sn   0.085188   4.213961  2.599105

iPr_NHC_B97M_D3_TZVPP_optfreq

Total correction:  1592.3559 kJ/mol  
Single point energy:  -3049451.8114 kJ/mol  
Total enthalpy:  -3047856.9764 kJ/mol  
Final entropy term:  222.8927 kJ/mol  
Total gibbs free enthalpy:  -3048079.869 kJ/mol  
Method and Basis:  B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
C  1.511139  4.576613  1.197914
H  2.495723  5.004997  1.366261
H  1.046822  5.112231  0.374250
H  1.640077  3.540567  0.908111
C  0.462680  6.150741  2.834904
H  1.407927  6.674923  2.937781
H  -0.082298  6.257608  3.767437
H  -0.097865  6.656362  2.055297
C  1.436395  0.197340  4.630578
H  0.570882  -0.026422  4.015575
H  1.145308  -0.297688  6.038172
H  0.309750  0.233319  6.482840
H  2.002965  -0.174778  6.692377
H  0.903144  -1.355889  6.019378
C  2.629154  -0.534704  4.030735
H  2.795495  -0.219287  3.007028
H  2.464810  -1.608202  4.038663
H  3.529195  -0.327177  4.603603

iPr_NHSn_B97M_D3_TZVPP_optfreq

Total correction: 1577.514 kJ/mol
Single point energy: -3512414.6779 kJ/mol
Total enthalpy: -3510834.6849 kJ/mol
Final entropy term: 239.2382 kJ/mol
Total gibbs free enthalpy: -3511073.9231 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
N  -0.304608  0.590122  0.755046
Sn  1.693699  0.896444  1.266522
N  0.660511  1.845190  2.809855
C  -0.699951  1.784512  2.705151
C  -1.204936  1.127469  1.630097
H  -1.311026  2.250824  3.458340
H  -2.258690  1.017631  1.441042
C  -0.773076  -0.064861  -0.408381
C  -1.552912  -1.361345  -2.724478
C  -0.975087  0.678329  -1.577030
C  -0.982453  -1.447876  -0.383798
C  -1.367491  -2.078475  -1.558803
C  -1.361090  0.006488  -2.728335
H  -1.520128  -3.144649  -1.561298
H  -1.508161  0.560895  -3.640004
H  -1.848625  -1.867372  -3.628035
C  1.242193  2.566401  3.879312
boryl_li_thf2_B97M_D3_TZVPP_optfreq

Total correction: 2260.2654 kJ/mol
Single point energy: -4256791.2991 kJ/mol
Total enthalpy: -4254528.5546 kJ/mol
Final entropy term: 296.8922 kJ/mol
Total gibbs free enthalpy: -4254825.4467 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
B  1.027853  1.956075  3.435961
N  1.088029  3.419834  3.517284
C  2.395416  3.880383  3.472468
H  2.632863  4.933140  3.511733
C  3.522467  2.834204  3.355835
H  4.292553  2.817909  3.291192
N  2.457819  1.673390  3.311364
Li -0.839844  0.753407  3.602372
C  0.013001  4.301311  3.737422
C  -0.161607  4.870195  5.005244
C  -1.226731  5.739075  5.202188
H  -1.377699  6.185593  6.169422
C  -2.105170  6.030301  4.176495
H  -2.926215  6.707340  4.344984
C  -1.932420  5.448130  2.935057
H  -2.624706  5.679389  2.144332
C  -0.879370  4.576936  2.692865
C  0.723338  4.459487  6.154780
H  1.705780  4.232252  5.755978
C  0.890612  5.533752  7.213504
H  1.212132  6.477000  6.783195
H  1.634083  5.223283  7.940916
H  -0.031684  5.712715  7.758970
C  0.180738  3.178230  6.778667
H  -0.809324  3.351734  7.195165
H  0.828116  2.836161  7.581793
H  0.110874  2.388160  6.037369
C  -0.665309  3.962856  1.334744
H  -0.278878  2.961591  1.504716
C  0.395066  4.739594  0.564421
H  0.068308  5.762716  0.393829
H  0.582021  4.280194  0.402535
H  1.330678  4.767996  1.110455
C  -1.935413  3.838763  0.515563
 sn2_cxet_C2_sym_B97M_D3_TZVPP_opt_freq

Total correction:  2137.4583 kJ/mol
Single point energy:  -4821002.9493 kJ/mol
Total enthalpy:  -4818863.0121 kJ/mol
Final entropy term:  282.2566 kJ/mol
Total gibbs free enthalpy:  -4819145.2687 kJ/mol
Method and Basis:  B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1
N  -0.124733  0.339902  0.321157
C   0.821571  -0.652542  0.286980
C   0.313432  -1.782488  0.901857
C  -0.988584  -1.459847  1.343478
C  -1.229801  -0.151528  0.964979
H   0.821783  -2.718132  1.049424
H  -1.636466  -2.094931  1.919190
C   2.165924  -0.497418  -0.379633
C   3.171917  -1.429218  0.321539
H   4.124010  -1.357686  -0.197193
H   2.828684  -2.452148  0.174928
C   3.387571  -1.176302  1.801180
C   3.729610  -0.162754  1.973068
H   4.133365  -1.861703  2.204322
H   2.465300  -1.313313  2.353331
C   2.030952  -0.997081  -1.846672
H   1.179158  -0.495159  -2.294938
H   1.770763  -2.055723  -1.804167
C   3.239330  -0.778991  -2.734545
C   3.481077   0.276247  -2.798548
H   3.043530  -1.147002  -3.740598
H   4.125001  -1.290903  -2.365561
C   2.693909   0.913328  -0.345603
C   4.006533  1.316688  -0.174640
| Atoms | X-Coordinates | Y-Coordinates | Z-Coordinates |
|-------|--------------|--------------|--------------|
| C     | 4.024090     | 2.722721     | -0.285580    |
| C     | 2.722564     | 3.122547     | -0.535831    |
| N     | 1.914542     | 2.020794     | -0.567235    |
| H     | 4.854877     | 0.684490     | 0.012527     |
| H     | 4.882424     | 3.358640     | -0.168243    |
| C     | 2.167188     | 4.520258     | -0.500934    |
| C     | 1.625470     | 4.719684     | 0.945219     |
| H     | 0.979009     | 3.872703     | 1.153556     |
| H     | 2.472369     | 4.640886     | 1.628622     |
| C     | 0.850964     | 5.998898     | 1.189192     |
| H     | 0.532159     | 6.056715     | 2.228531     |
| H     | -0.032498    | 6.036829     | 0.561654     |
| H     | 1.442232     | 6.887013     | 0.977492     |
| C     | 3.294010     | 5.529716     | -0.743070    |
| H     | 2.887231     | 6.530402     | -0.624220    |
| H     | 4.028875     | 5.404755     | 0.050747     |
| C     | 3.984277     | 5.427576     | -2.091632    |
| H     | 4.462209     | 4.462588     | -2.209745    |
| H     | 4.744597     | 6.201573     | -2.198415    |
| H     | 3.272360     | 5.539055     | -2.900735    |
| C     | -2.304969    | 0.777393     | 1.452588     |
| C     | -1.642916    | 1.728566     | 2.492570     |
| H     | -2.434779    | 2.333883     | 2.936375     |
| H     | -1.009974    | 2.409106     | 1.931358     |
| C     | -3.410093    | -0.018740    | 2.154260     |
| H     | -4.082313    | 0.693870     | 2.629756     |
| H     | -2.959285    | -0.592976    | 2.959205     |
| C     | -4.210320    | -0.951262    | 1.262392     |
| H     | -4.723607    | -0.397424    | 0.485584     |
| H     | -4.954306    | -1.498731    | 1.841470     |
| H     | -3.563979    | -1.671612    | 0.775244     |
| C     | -0.810237    | 1.056700     | 3.565466     |
| H     | 0.019199     | 0.515713     | 3.123702     |
| H     | -1.388235    | 0.347564     | 4.153911     |
| H     | -0.405113    | 1.798926     | 4.251147     |
| C     | -2.912433    | 1.677307     | 0.411156     |
| N     | -2.151199    | 2.335257     | -0.513633    |
| C     | -2.950060    | 3.251456     | -1.150353    |
| C     | -4.228259    | 3.171516     | -0.626347    |
| C     | -4.202848    | 2.177419     | 0.373980     |
| H     | -5.081490    | 3.755307     | -0.919008    |
| H     | -5.024406    | 1.888601     | 1.003677     |
| C     | 1.022918     | 4.790285     | -1.435914    |
| C     | 0.764452     | 5.934097     | -2.169341    |
| C     | -0.579625    | 5.854622     | -2.595464    |
| C     | -1.093063    | 4.674118     | -2.089746    |
| N     | -0.111088    | 4.022918     | -1.387442    |
se_me2_B97M_TZVPP_optfreq

Total correction: 210.9131 kJ/mol
Single point energy: -6514382.6723 kJ/mol
Total enthalpy: -6514169.2802 kJ/mol
Final entropy term: 90.8452 kJ/mol
Total gibbs free enthalpy: -6514260.1254 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
Se  0.212154  -0.948711  0.849987
C  1.765040  -0.005770  1.519983
H  2.610990  -0.161371  0.863089
H  1.992476  -0.410668  2.497021
H  1.551744  1.051257  1.612318
C  0.097787  -0.005328  -0.837178
H  0.999770  -0.159013  -1.415232
H  -0.062407  1.051409  -0.666828
H  -0.746382  -0.411804  -1.377963

sn2_py2_B97M_D3_TZVPP_optfreq

Total correction: 406.6968 kJ/mol
Single point energy: -1664672.2335 kJ/mol
Total enthalpy: -1664263.0576 kJ/mol
Final entropy term: 127.4968 kJ/mol
Total gibbs free enthalpy: -1664390.5544 kJ/mol
sn2_py3_B97M_D3_TZVPP_optfreq

Total correction: 606.1873 kJ/mol
Single point energy: -2215822.5461 kJ/mol
Total enthalpy: -2215213.8797 kJ/mol
Final entropy term: 156.8635 kJ/mol
Total gibbs free enthalpy: -2215370.7432 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -1, multiplicity: 1
Sn -0.512397 0.317129 0.827212
N  1.617228 0.011173 0.780088
C  2.312285 -0.309422 -0.352065
C  3.660348 -0.327656 -0.077265
C  3.794362 -0.004225 1.293896
C  2.523679 0.197067 1.784238
H  4.449454 -0.547060 -0.772377
H  4.708294 0.069221 1.853594
H  2.190300 0.463221 2.767868
N -0.445998 0.650399 2.951733
C -0.136636 1.799055 3.622199
C -0.112322 1.544544 4.975017
C -0.420315 0.173446 5.141854
C  -0.619370  -0.337712  3.880052
H   0.046613   2.705773  3.080179
H   0.097628   2.258078  5.750108
H  -0.489462  -0.368280  6.066924
H  -0.863182  -1.337444  3.571172
N  -0.244228   2.420182  0.457415
C   0.918450   3.135737  0.430421
C   0.628482   4.469561  0.250382
C  -0.779901   4.576901  0.163871
C  -1.276858   3.300383  0.292951
H   1.860567   2.637202  0.546345
H   1.342378   5.269584  0.185291
H  -1.354847   5.473383  0.023149
H  -2.293197   2.952029  0.289739
H   1.793998  -0.490837  -1.275555

\textbf{sn2\_py4\_B97M\_D3\_TZVPP\_optfreq}

Total correction: 801.6555 kJ/mol
Single point energy: -2766550.168 kJ/mol
Total enthalpy: -2765746.0335 kJ/mol
Final entropy term: 186.8122 kJ/mol
Total gibbs free enthalpy: -2765932.8457 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1
Sn  -0.403203  -0.069244  1.036870
N   1.760954   0.050065  0.714290
C   2.434020   1.106262  0.170182
C   3.758782   0.768320 -0.010827
C   3.900692  -0.566297  0.441490
C   2.655023  -0.970196  0.873580
H   4.527420   1.407833 -0.409560
H   4.800293  -1.157236  0.459225
H   2.339253  -1.903195  1.294506
N  -0.190572   0.613543  3.097949
C   0.959346   0.926161  3.750008
C   0.668529  1.307297  5.046099
C  -0.736858  1.220118  5.186742
C  -1.219616   0.790625  3.966229
H   1.900297   0.852387  3.240842
H   1.378975   1.609283  5.795599
H  -1.319728   1.442839  6.063469
H  -2.230371   0.598399  3.655669
N  -0.421796   2.262370  0.628996
C  -0.095724   3.342788  1.383363
\begin{verbatim}
C  -0.211205  4.503153  0.635917
C  -0.634213  4.103960 -0.654265
C  -0.750869  2.725283 -0.604660
H   0.201868  3.212240  2.407018
H  -0.021997  5.508206  0.975584
H  -0.831699  4.739074 -1.502123
H  -1.041554  2.035484 -1.378858
N   0.029986 -2.164093  2.052295
C   0.459719 -2.531500  3.286447
C   0.599312 -3.907913  3.356515
C   0.230688 -4.409524  2.085568
C  -0.112020 -3.303415  1.326840
H   0.641798 -1.784343  4.036182
H   0.918144 -4.478847  4.213076
H   0.214035 -5.439754  1.769939
H  -0.441902 -3.252567  0.302958
H   1.922153  2.025139 -0.033171

\texttt{sn2\_se\_cxet\_B97M\_TZVPP\_optfreq}
\end{verbatim}

Total correction: 2150.8152 kJ/mol
Single point energy: -11125702.2397 kJ/mol
Total enthalpy: -11123548.9454 kJ/mol
Final entropy term: 291.002 kJ/mol
Total gibbs free enthalpy: -11123839.9473 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1
N  -0.125903  0.306799  0.262673
C   0.836076 -0.679961  0.257106
C   0.327174 -1.795188  0.886477
C  -0.981346 -1.479939  1.308298
C  -1.236054 -0.187296  0.908199
H   0.844054 -2.720743  1.056397
H  -1.629329 -2.109938  1.887314
C   2.210547 -0.540612 -0.338271
C   3.190352 -1.347627  0.544318
H   4.171366 -1.319330  0.078786
H   2.878178 -2.388339  0.505652
C   3.298341 -0.906990  1.990180
H   3.626969  0.123417  2.058745
H   4.010953 -1.528790  2.531654
H   2.337208 -0.985418  2.486343
C   2.205594 -1.216043 -1.736928
H   1.337891 -0.865594 -2.281981
H   2.061188 -2.284489 -1.568931
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| C       | 3.430088 | -0.972459 | -2.592436 |
| H       | 3.508352 | 0.077323  | -2.851233 |
| H       | 3.354675 | -1.538258 | -3.519056 |
| H       | 4.358233 | -1.260490 | -2.101596 |
| C       | 2.697171 | 0.881203  | -0.399991 |
| C       | 4.003364 | 1.301165  | -0.259223 |
| C       | 4.013402 | 2.703438  | -0.385636 |
| C       | 2.712760 | 3.098929  | -0.614065 |
| H       | 1.905374 | 1.989090  | -0.621846 |
| H       | 4.855610 | 0.675418  | -0.076308 |
| H       | 4.869200 | 3.344702  | -0.292843 |
| C       | 2.165627 | 4.493587  | -0.571186 |
| C       | 1.641679 | 4.700596  | 0.882004 |
| H       | 1.002532 | 3.852954  | 1.112352 |
| H       | 2.498983 | 4.629380  | 1.552455 |
| C       | 0.865876 | 5.978084  | 1.128612 |
| H       | 0.566023 | 6.043817  | 2.172754 |
| H       | -0.029022| 6.008327  | 0.517112 |
| H       | 1.449775 | 6.865709  | 0.898177 |
| C       | 3.292911 | 5.499905  | -0.826856 |
| H       | 2.889699 | 6.500488  | -0.698291 |
| H       | 4.036000 | 5.371462  | -0.041815 |
| C       | 3.965130 | 5.400649  | -2.184265 |
| H       | 4.439887 | 4.436132  | -2.314337 |
| H       | 4.724757 | 6.173903  | -2.295865 |
| H       | 3.245042 | 5.515236  | -2.985041 |
| C       | -2.315077| 0.731544  | 1.386929 |
| C       | -1.672314| 1.689283  | 2.435143 |
| H       | -2.476708| 2.279926  | 2.875130 |
| H       | -1.046834| 2.387025  | 1.885619 |
| C       | -3.420868| -0.072062 | 2.079835 |
| H       | -4.104938| 0.637105  | 2.542617 |
| H       | -2.972693| -0.633056 | 2.895088 |
| C       | -4.199548| -1.021257 | 1.187017 |
| H       | -4.719138| -0.482481 | 0.404487 |
| H       | -4.935559| -1.578408 | 1.766061 |
| H       | -3.539985| -1.731989 | 0.704512 |
| C       | -0.836202| 1.026695  | 3.510576 |
| H       | 0.008375 | 0.505087  | 3.074299 |
| H       | -1.405687| 0.302204  | 4.087428 |
| H       | -0.453108| 1.771710  | 4.205307 |
| C       | -2.915077| 1.617606  | 0.337813 |
| N       | -2.151125| 2.301731  | -0.574313 |
| C       | -2.963275| 3.214296  | -1.215426 |
| C       | -4.239164| 3.094657  | -0.705279 |
| C       | -4.208190| 2.091901  | 0.282556 |
| H       | -5.097299| 3.667978  | -0.998994 |
| Element | X   | Y   | Z    |
|---------|-----|-----|------|
| H       | -5.030679 | 1.778218 | 0.896806 |
| C       | 1.020089 | 4.760743 | -1.495430 |
| C       | 0.752125 | 5.908265 | -2.207655 |
| C       | -0.596138 | 5.838458 | -2.616047 |
| C       | -1.113443 | 4.658788 | -2.126449 |
| N       | -0.119708 | 3.991722 | -1.443437 |
| H       | 1.421019 | 6.731914 | -2.369539 |
| H       | -1.130163 | 6.583622 | -3.174863 |
| C       | -2.525434 | 4.167139 | -2.93692 |
| C       | -3.459438 | 5.398869 | -2.53855 |
| H       | -4.473402 | 5.065152 | -2.455370 |
| H       | -3.189619 | 6.036962 | -3.091654 |
| C       | -2.660863 | 3.546907 | -3.711638 |
| H       | -2.553975 | 4.366335 | -4.424226 |
| H       | -1.823177 | 2.880135 | -3.874267 |
| C       | -3.935773 | 2.775220 | -3.975168 |
| H       | -4.835159 | 3.359372 | -3.787660 |
| H       | -3.980869 | 1.893507 | -3.346133 |
| H       | -3.963249 | 2.445421 | -0.5012015 |
| C       | -3.431671 | 6.209286 | -0.973679 |
| H       | -3.711631 | 5.600215 | -0.122158 |
| H       | -4.122006 | 7.050451 | -1.032805 |
| H       | -2.436917 | 6.601331 | -0.791978 |
| Sn      | -0.155365 | 1.829301 | -1.282064 |
| Se      | -0.257363 | 0.833204 | -3.452635 |

**sn2_se_cxh_B97M_TZVPP_optfreq**

Total correction: 892.4403 kJ/mol
Single point energy: -9472035.7851 kJ/mol
Total enthalpy: -9471140.8659 kJ/mol
Final entropy term: 180.7943 kJ/mol
Total gibbs free enthalpy: -9471321.6601 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1

| Element | X   | Y   | Z    |
|---------|-----|-----|------|
| N       | -0.251770 | 0.338792 | 0.223980 |
| C       | 0.703399 | -0.642017 | 0.265509 |
| C       | 0.293814 | -1.630907 | 1.130210 |
| C       | -0.973680 | -1.235604 | 1.633497 |
| C       | -1.276602 | -0.021922 | 1.054909 |
| H       | 0.839159 | -2.529343 | 1.361665 |
| H       | -1.579387 | -1.752429 | 2.358209 |
| C       | 1.923452 | -0.534055 | -0.583397 |
| C       | 2.600006 | 0.790481 | -0.488086 |
| C       | 3.925715 | 1.112341 | -0.308386 |
| Element | x       | y       | z       |
|---------|---------|---------|---------|
| C       | 4.011623| 2.529059| -0.343575|
| C       | 2.733503| 3.005895| -0.540524|
| N       | 1.874960| 1.944458| -0.625186|
| H       | 4.730996| 0.410478| -0.177806|
| H       | 4.891697| 3.134028| -0.206748|
| C       | 2.251370| 4.410942| -0.457460|
| C       | -2.389693| 0.906378| 1.390530|
| C       | -2.930038| 1.771179| 0.307313|
| N       | -2.121128| 2.364965| -0.622219|
| C       | -2.875822| 3.243874| -1.353005|
| C       | -4.170352| 3.218674| -0.887195|
| C       | -4.205625| 2.275773| 0.173694|
| H       | -4.988648| 3.801700| -1.272697|
| H       | -5.048716| 2.018862| 0.792096|
| C       | 1.080800| 4.799733| -1.289297|
| C       | 0.780977| 6.037829| -1.815488|
| C       | -0.537522| 5.959459| -2.336509|
| C       | -0.979202| 4.676539| -2.107559|
| N       | 0.005489| 3.973141| -1.465860|
| H       | 1.424113| 6.900971| -1.791813|
| H       | -1.095436| 6.738536| -2.826352|
| C       | -2.258926| 4.006882| -2.474756|
| Sn      | -0.157518| 1.831923| -1.323413|
| Se      | -0.264344| 0.835084| -3.492476|
| H       | 3.079926| 5.077150| -0.691929|
| H       | 1.646945| -0.717177| -1.627494|
| H       | 2.625751| -1.313299| -0.297625|
| H       | -3.208341| 0.327176| 1.814362|
| H       | -2.050665| 1.560206| 2.207493|
| H       | -2.074147| 3.322636| -3.310092|
| H       | -2.964646| 4.755919| -2.825494|
| H       | 2.004839| 4.622235| 0.593455|

**sn_dodecaborate_B97M_D3_TZVPP_optfreq**

Total correction: 423.165 kJ/mol
Single point energy: -1300280.5692 kJ/mol
Total enthalpy: -1299854.9251 kJ/mol
Final entropy term: 112.0966 kJ/mol
Total gibbs free enthalpy: -1299967.0217 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1
B  0.917182 | 1.081397 | -0.867889
B  -0.566166| 0.409403 | -1.527349
B  0.857031 | -0.617081| -1.313820
### sn_me4_PBEh3c_optfreq

**Total correction:** 418.198 kJ/mol  
**Single point energy:** -980942.3411 kJ/mol  
**Total enthalpy:** -980521.6641 kJ/mol  
**Final entropy term:** 125.3206 kJ/mol  
**Total gibbs free enthalpy:** -980646.9847 kJ/mol  
**Method and Basis:** PBEh-3c / def2-mSVP

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**xyz, charge: 0, multiplicity: 1**

|   | X      | Y         | Z      |
|---|--------|------------|--------|
| Sn| 0.000012 | -0.000000  | 0.999958 |
| C | -1.018761 | -1.764587  | 1.720326 |
| H | -0.523849  | -2.669890  | 1.370424 |
| H | -2.050208  | -1.788687  | 1.370360 |
| H | -1.032696  | -1.788648  | 2.809440 |
| C | 2.037553   | -0.000004  | 1.720379 |
| H | 2.574141   | 0.881232   | 1.370467 |
| H | 2.574141   | -0.881235  | 1.370457 |
| H | 2.065323   | -0.000010  | 2.809492 |
| C | -1.018761  | 1.764579   | 1.720346 |
| H | -0.523850  | 2.669886   | 1.370453 |
| H | -1.032696  | 1.788628   | 2.809460 |
| H | -2.050209  | 1.788683   | 1.370380 |
| C | -0.000023  | 0.000012   | -1.161196 |
| H | 0.508741   | -0.881220  | -1.550463 |
H  0.508741  0.881249  -1.550454
H  -1.017596  0.000014  -1.550410

**sn_dithiolate_B97M_D3_TZVPP_optfreq**

| Total correction: | 468.1406 kJ/mol |
|--------------------|------------------|
| Single point energy: | -5959619.6617 kJ/mol |
| Total enthalpy: | -5959149.0422 kJ/mol |
| Final entropy term: | 168.4528 kJ/mol |
| Total gibbs free enthalpy: | -5959317.495 kJ/mol |
| Method and Basis: | B97M-D3BJ / def2-TZVPP |

xyz, charge: -2, multiplicity: 1

| Sn     | 5.190364 | -0.265657 | 4.791056 |
| S      | 6.712104 | 0.768042  | 6.787963 |
| S      | 7.191583 | 1.000637  | 3.921334 |
| S      | 3.790052 | 0.251249  | 2.528635 |
| S      | 3.381020 | 1.460964  | 5.148614 |
| C      | 7.835667 | 1.059616  | 5.531643 |
| C      | 9.190406 | 1.321073  | 5.756760 |
| C      | 9.840576 | 1.423202  | 7.028232 |
| H      | 9.339103 | 1.310469  | 7.971261 |
| C      | 11.174433| 1.678814  | 6.813467 |
| H      | 11.927972| 1.805753  | 7.574592 |
| C      | 11.398492| 1.746828  | 5.400370 |
| H      | 12.348071| 1.931415  | 4.923649 |
| C      | 10.199480| 1.532223  | 4.762289 |
| H      | 10.020056| 1.509745  | 3.703514 |
| C      | 2.731912 | 1.081906  | 3.585206 |
| C      | 1.424769 | 1.437410  | 3.239724 |
| C      | 0.784488 | 1.211951  | 1.979220 |
| H      | 1.257316 | 0.735599  | 1.140735 |
| C      | -0.498113| 1.702282  | 2.051042 |
| H      | -1.232108| 1.680391  | 1.261102 |
| C      | -0.698486| 2.250270  | 3.359136 |
| H      | -1.608652| 2.705497  | 3.716041 |
| C      | 0.463924 | 2.091391  | 4.076591 |
| H      | 0.647446 | 2.386164  | 5.093062 |

**phi_B97M_D3_TZVPP_opt_freq**

| Total correction: | 254.7123 kJ/mol |
|--------------------|------------------|
| Single point energy: | -1390798.861 kJ/mol |
| Total enthalpy: | -1390541.6697 kJ/mol |
| Final entropy term: | 100.8168 kJ/mol |

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Total gibbs free enthalpy: -1390642.4865 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: 0, multiplicity: 1
H  -0.000001 -0.005664 -0.005601
C  0.000003 -0.001131  1.069467
C  0.000002 -0.003106  3.842451
C  0.000005 -1.193260  1.772803
C  0.000002  1.194219  1.768733
C  0.000001  1.197165  3.152968
C  0.000004 -1.206350  3.156892
H  -0.000003  2.123510  1.224718
H  -0.000004  2.129041  3.691223
H  0.000000 -2.139651  3.690524
H  -0.000003 -0.009485  4.919231
I  -0.000007 -3.000151  0.729836

phi_sn2_czet_B97M_D3_TZVPP_TightOpt_opt_freq

Total correction: 2400.345 kJ/mol
Single point energy: -6211860.6354 kJ/mol
Total enthalpy: -6209457.8114 kJ/mol
Final entropy term: 328.8666 kJ/mol
Total gibbs free enthalpy: -6209786.678 kJ/mol
Method and Basis: B97M-D3BJ / def2-TZVPP

xyz, charge: -2, multiplicity: 1
N  -0.007564  0.522737  0.198932
C  1.014985 -0.396697  0.173938
C  0.584847 -1.562443  0.776036
C  -0.743097  1.345131  1.198593
C  -1.081401 -0.059369  0.826742
H  1.158839 -2.458988  0.918237
H  -1.349370  2.030975  1.759865
C  2.338646 -0.160722 -0.502889
C  3.399771  1.066145  0.151761
H  4.329378 -0.952066 -0.399698
H  3.088939 -2.096917 -0.004592
C  3.654558 -0.834726  1.628275
H  3.984272  0.180971  1.810742
H  4.422313 -1.514391  1.997335
H  2.751267 -0.998836  2.204230
C  2.192612  0.630972 -1.974956
H  1.261161 -0.241440 -2.361310
H  2.070213 -1.714312 -1.955941
C  3.307325 -0.235769 -2.918583
H  3.376398  0.843038  -3.000998
H  3.118312  -0.637586  -3.911837
H  4.278211  -0.598527  -2.588739
C  2.804991  1.267779  -0.426193
C  4.105893  1.713252  -0.298073
c  4.063764  3.122102  -0.275406
C  2.738477  3.489235  -0.407249
N  1.969703  2.357969  -0.499971
H  4.985849  1.103738  -0.213748
H  4.902130  3.779596  -0.141436
C  2.130897  4.840011  -0.159807
C  1.618084  4.800732  1.311510
H  1.023591  3.897802  1.412001
H  2.487207  4.670904  1.957905
c  0.786506  5.986503  1.755291
H  0.507135  5.881266  2.802001
H  -0.121867  6.060425  1.168034
H  1.319917  6.928330  1.650903
C  3.211517  5.920667  -0.267869
H  2.776921  6.870620  0.030863
H  3.978679  5.694711  0.470425
C  3.851536  6.072129  -1.636073
H  4.326682  5.149758  -1.947334
H  4.606419  6.857994  -1.625344
H  3.111512  6.324546  -2.385826
C  -2.230382  0.764935  1.323984
C  -1.676194  1.695109  2.444901
H  -2.527014  2.208000  2.895517
H  -1.082710  2.459367  1.952419
C  -3.303846  -0.143500  1.932101
H  -4.051404  0.495034  2.399161
H  -2.852111  -0.716316  2.737209
C  -3.980736  -1.093856  0.960960
H  -4.480662  -0.549537  0.169050
H  -4.720805  -1.708740  1.472533
H  -3.257722  -1.752363  0.494973
C  -0.827142  1.022883  3.504030
H  0.061968  0.585812  3.063620
H  -1.361001  0.227522  4.018784
H  -0.514394  1.747437  4.253646
C  -2.857398  1.683590  0.315197
N  -2.103073  2.506536  -0.480396
C  -2.946529  3.418134  -1.071293
C  -4.238255  3.162510  -0.655229
C  -4.181477  2.069124  0.232583
H  -5.121169  3.703283  -0.939698
H  -5.008811  1.644826  0.769764
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 0.960037| 5.194248| -1.025993|
| C       | 0.618711| 6.439113| -1.515538|
| C       | -0.722852| 6.361791| -1.944262|
| C       | -1.157374| 5.076590| -1.687579|
| N       | -0.124748| 4.358774| -1.130919|
| H       | 1.233067| 7.319751| -1.512879|
| H       | -2.497670| 4.484964| -2.032620|
| C       | -3.548437| 5.611830| -2.051024|
| H       | -4.491620| 5.189838| -2.388379|
| H       | -3.250664| 6.320887| -2.820448|
| C       | -2.402305| 3.936950| -3.482104|
| H       | -2.303608| 4.796749| -4.145491|
| H       | -1.473815| 3.391137| -3.575883|
| C       | -3.534734| 3.040882| -3.933605|
| H       | -4.504624| 3.526447| -3.853602|
| H       | -3.574447| 2.139871| -3.31974|
| H       | -3.390205| 2.746339| -4.970944|
| C       | -3.761289| 6.347657| -0.742632|
| H       | -4.080930| 5.667750| 0.037774|
| H       | -4.521727| 7.120125| -0.855104|
| H       | -2.843252| 6.821093| -0.414558|
| Sn      | -0.081312| 2.143830| -1.321338|
| I       | -0.135856| 1.074528| -4.381717|
| C       | -0.164523| 0.342539| -6.450274|
| C       | -0.195893| -0.588703| -9.080630|
| C       | 0.997275| -0.125283| -7.046350|
| C       | -1.342338| 0.339280| -7.182769|
| C       | -1.360125| -0.123752| -8.489277|
| C       | 0.984048| -0.587086| -8.353251|
| H       | 1.917209| -0.126971| -6.482390|
| H       | -2.250428| 0.701355| -6.726055|
| H       | -2.284091| -0.121093| -9.048559|
| H       | 1.896064| -0.947577| -8.805741|
| H       | -0.207952| -0.948517| -10.097335|
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