ASSOCIATED CONTENT

SUPPORTING INFORMATION

An Isolable Stannaimine and its Cycloaddition/Metathesis Reactions with Carbon Dioxide

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Contents

1. Syntheses and Spectra

General Considerations

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Pentane and diethyl ether were distilled over Na/K alloy (50:50), while hexane, toluene and THF were distilled over molten potassium. ^{1}H, ^{13}C{^{1}H}, ^{29}Si{^{1}H} and ^{119}Sn{^{1}H} NMR spectra were recorded on either Bruker DPX300, Bruker AvanceIII 600 or Bruker AvanceIII 400 spectrometers and were referenced to the resonances of the solvent used, $SiMe_4$ or $SnMe_4$. FTIR spectra were collected for solid samples or Nujol mulls on an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. LC/MS analyses were carried out at the Monash Analytical Platform (School of Chemistry, Monash University). HRMS analyses were conducted by direct injection on an Agilent 6546 LC / QTOF system (Santa Clara, CA, USA) using an APCI source. The instrument was operated in positive mode and data collected in the m/z range 100–1500. Microanalyses were carried out at by the Elemental Analysis Service at London Metropolitan University. Melting points were determined in sealed glass capillaries under dinitrogen and are uncorrected. 2,4,6–tricyclohexylphenyl bromide,[S1] NON^{Ad}–H_2,[S2] mesityl azide[S3] were prepared according to their literature procedures. Unless otherwise stated, chemicals were purchased from Sigma-Aldrich and used as received.

Preparation of 2,4,6-tricyclohexylphenyl magnesium bromide, TCHP-MgBr(THF)$_2$

Activated magnesium turnings (0.90 g, 37 mmol) were suspended in dry THF (20 ml) and a concentrated THF solution (50 ml) of 2,4,6-tricyclohexylphenyl bromide (5.00 g, 12.4 mmol) was added. The resultant grey/black mixture was heated at reflux overnight. Complete conversion to the corresponding Grignard reagent was determined by ^{1}H NMR spectroscopy. The mixture was filtered through celite and the volatiles removed *in vacuo*. The crude mass was dissolved in a toluene/THF mixture and stored at –30 ℃ to afford the title compound as colorless crystals. Yield 6.08 g, 86%.

m.p.: 267–269 ℃ (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 1.21 – 1.30 (m, 8H, THF), 1.31 – 1.56 (m, 4H, Cy–*H*), 1.61 – 2.01 (m, 6H, Cy–*H*), 2.05 – 2.21 (m, 20H, Cy–*H*), 2.55 – 2.70 (m, 1H, Cy–*H*), 2.83 – 2.97 (m, 2H, Cy–*H*), 3.69 – 3.78 (m, 8H, THF), 7.22 (s, 2H, Ar–*H*).

$^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ 25.2, 26.9, 27.1, 27.7, 27.9, 35.5 (Cy–*C*), 36.8 (THF), 46.0, 51.8 (Cy–*C*), 69.4 (THF), 120.5, 145.9, 158.4, 159.7 (Ar–*C*).

IR ν/cm^{-1} (solid): 738 (w), 786 (m), 857 (s), 921 (w), 958 (w), 1014 (s), 1252 (m), 1446 (m), 2848 (s), 2911 (s).

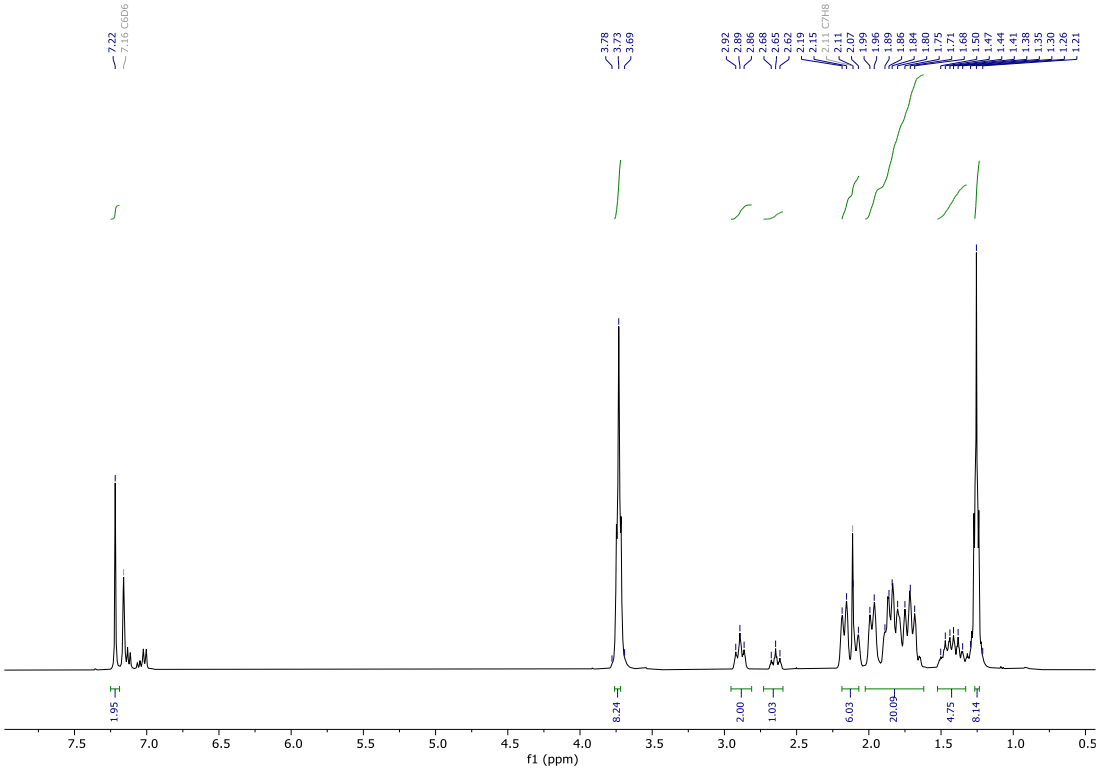


Figure S1: ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of TCHP-MgBr(THF)$_2$.

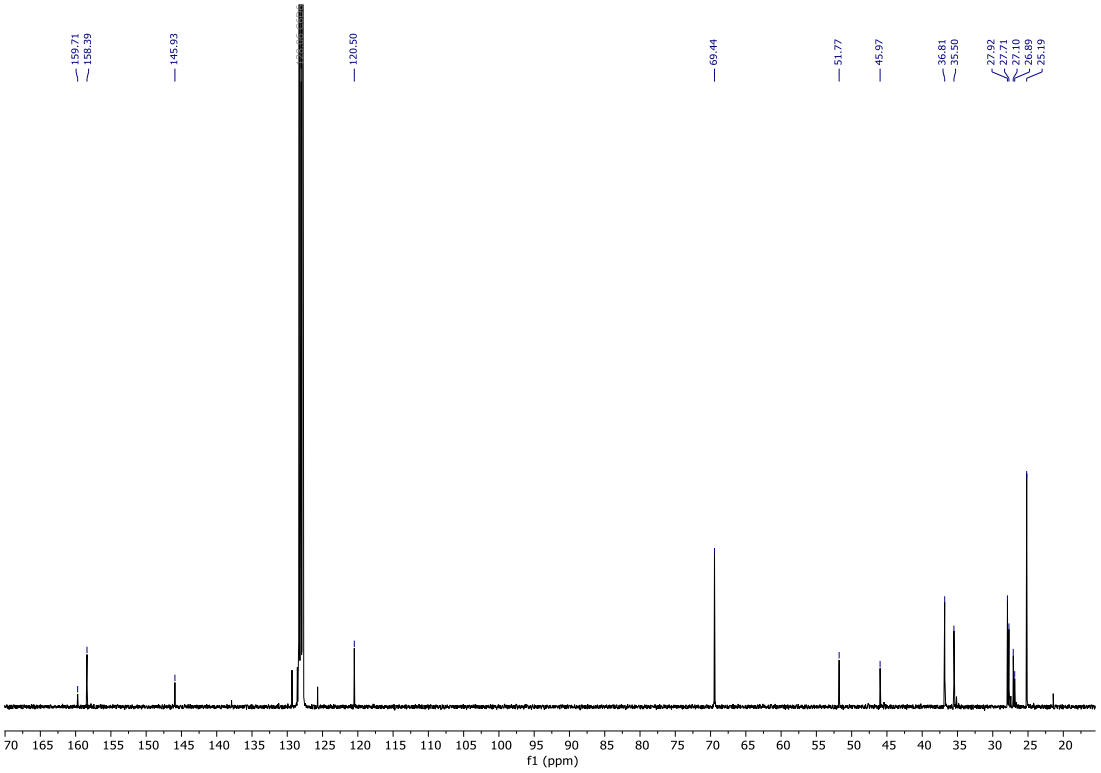


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of TCHP-MgBr(THF)$_2$.

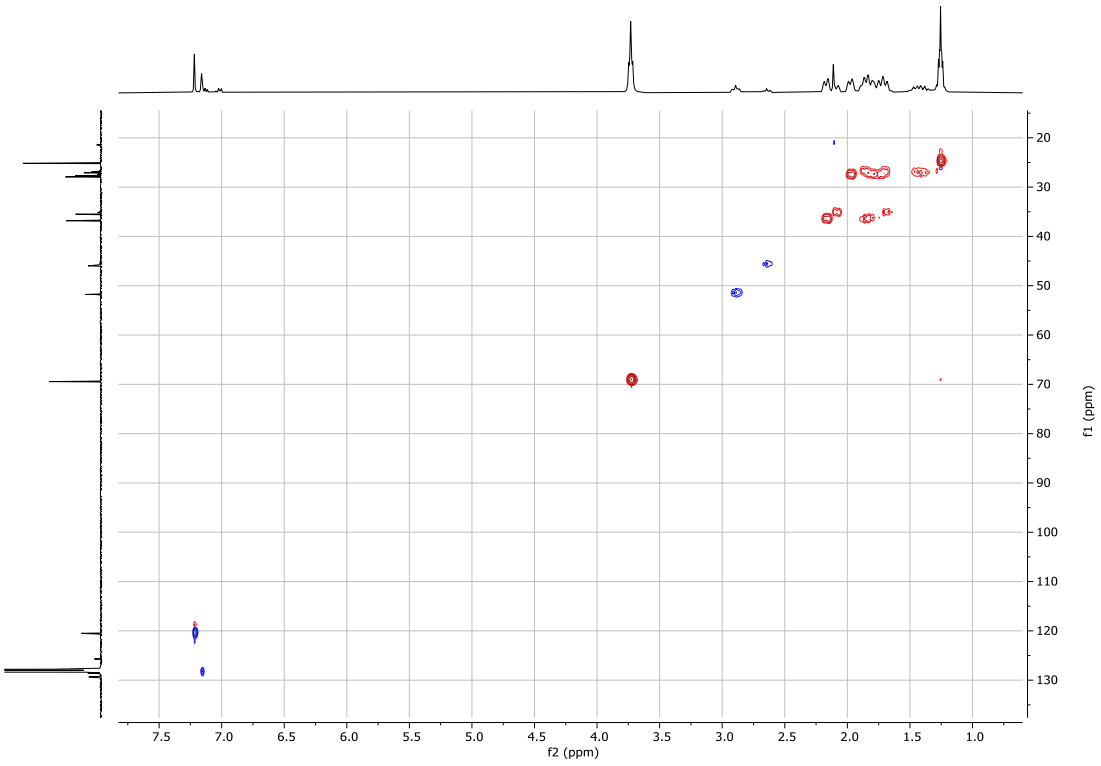


Figure S3: HSQC NMR spectrum (298 K, C_6D_6) of TCHP-MgBr(THF)$_2$.

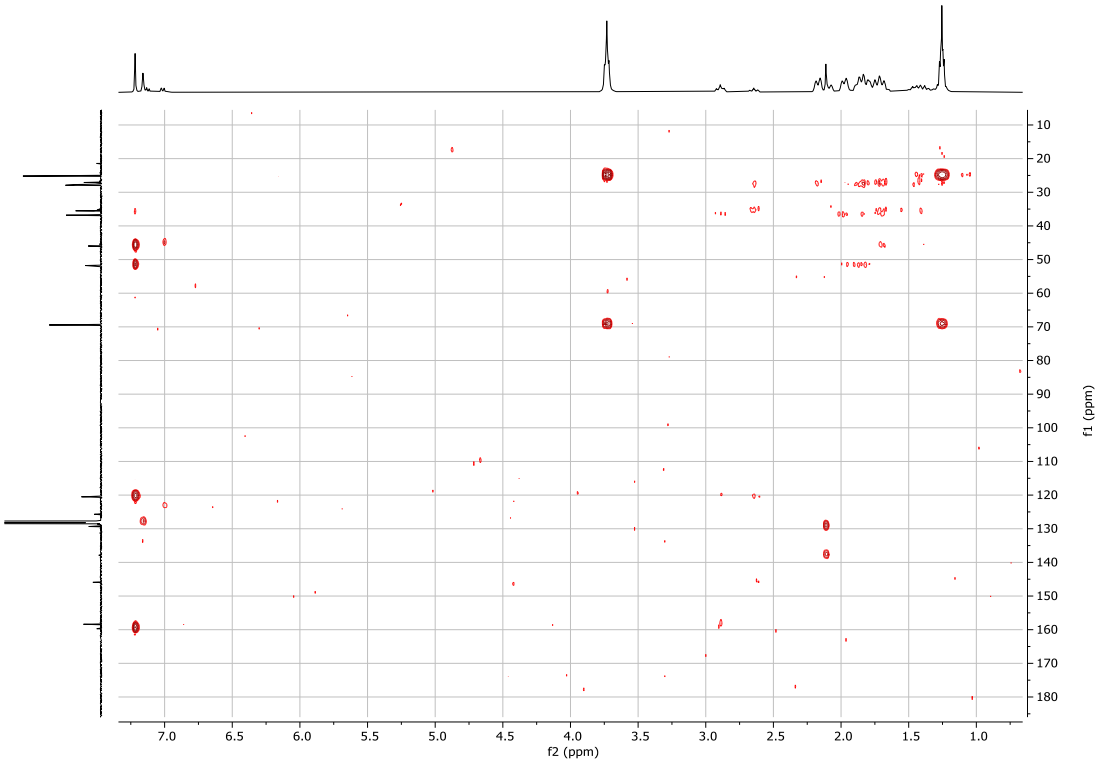


Figure S4: HMBC NMR spectrum (298 K, C_6D_6) of TCHP-MgBr(THF)$_2$.

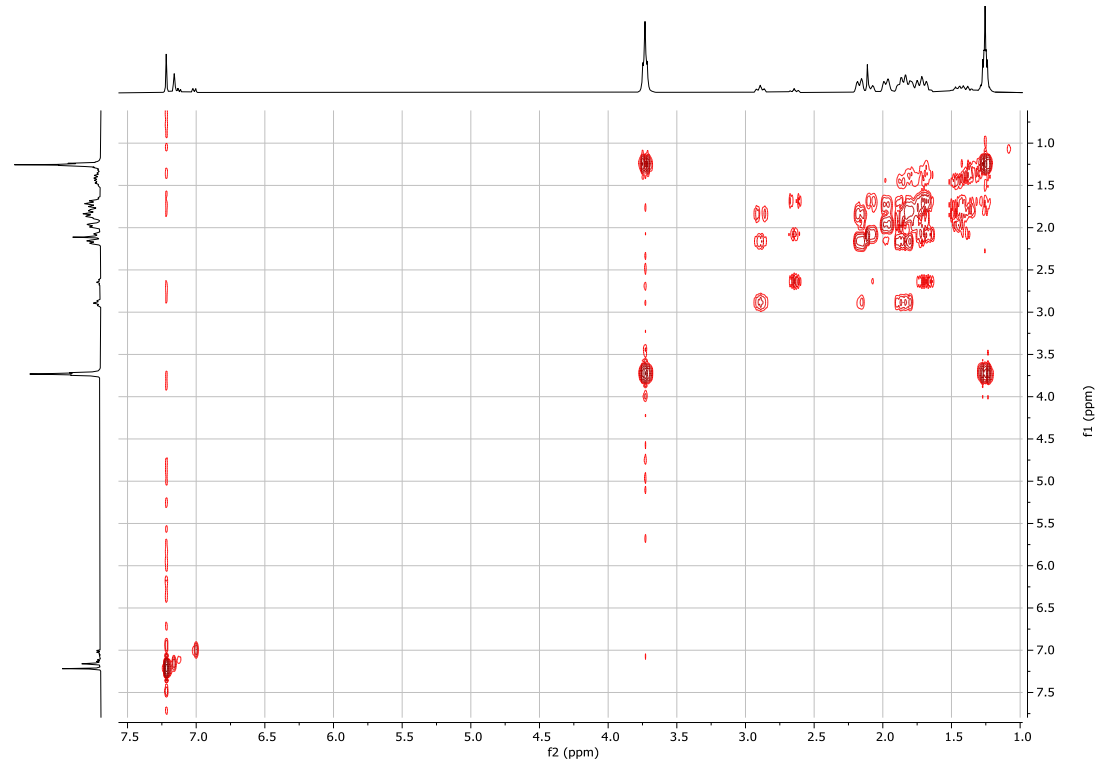


Figure S5: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of TCHP-MgBr(THF)$_2$.

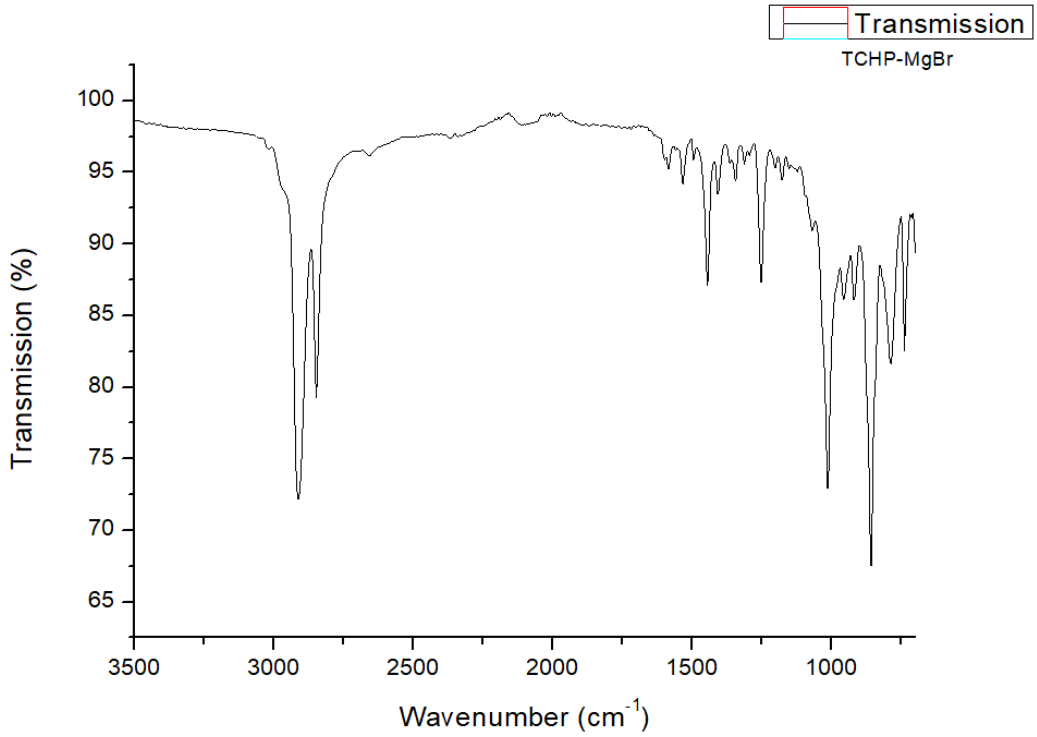


Figure S6: FT-IR spectrum of TCHP-MgBr(THF)$_2$.

Preparation of 2,4,6-tricyclohexylphenyl azide (TCHP-N$_3$)

Activated magnesium turnings (4.51 g, 185.6 mmol) were suspended in dry THF (20 ml) and a concentrated THF solution (150 ml) of 2,4,6-tricyclohexyl bromide (25.00 g, 62 mmol) was added. The resultant grey/black mixture was heated at reflux overnight. Complete conversion to the corresponding Grignard reagent was determined by ^{1}H NMR spectroscopy. The *in situ* prepared Grignard reagent was subsequently filtered onto a solution of tosyl azide (12.26 g, 62.2 mmol) in diethyl ether at 0 °C affording a tan precipitate. After stirring for 2 hours, the mixture was settled, the top solution decanted, and the solid suspended in diethyl ether. A solution of $Na_4P_2O_7$ (16.51 g, 62.1 mmol) in water was then added at 0 °C and the mixture allowed to stir overnight. The organic layer was then extracted and the aqueous phase washed with diethyl ether (2 x 200 ml). The combined organic layers were dried with $MgSO_4$ and the volatiles removed *in vacuo* to give a red oil/solid. The residue was purified by column chromatography over silica gel (hexane) to give the title compound as a pale yellow-white powder. Crystals suitable for single crystal X-ray diffraction were obtained by slow evaporation from a toluene solution. Yield 20.10 g, 89%.

m.p.: 101–103 °C (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 1.07 – 1.52 (m, 16H, Cy–*H*), 1.59 – 1.98 (m, 14H, Cy–*H*), 2.38 – 2.51 (m, 1H, Cy–*H*), 3.04 – 3.18 (m, 2H, Cy–*H*), 7.05 (s, 2H, Ar–*H*).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ 26.5, 26.6, 27.3, 27.3, 34.5, 35.0, 40.1, 45.1 (Cy–*C*), 123.4, 133.9, 142.3, 146.6 (Ar–*C*).

IR ν/cm^{-1} (solid): 786 (w), 809 (w), 846 (w), 861 (s), 950 (w), 999 (m), 1029 (w), 1073 (w), 1096 (m), 1271 (m), 1308 (s), 1349 (w), 1442 (s), 1599 (w), 2098 (s), 2128 (s), 2848 (s), 2922 (s).

HRMS was not obtained due to the explosive nature of azides towards thermal decomposition. Melting point obtained in a sealed capillary behind a blast shield.

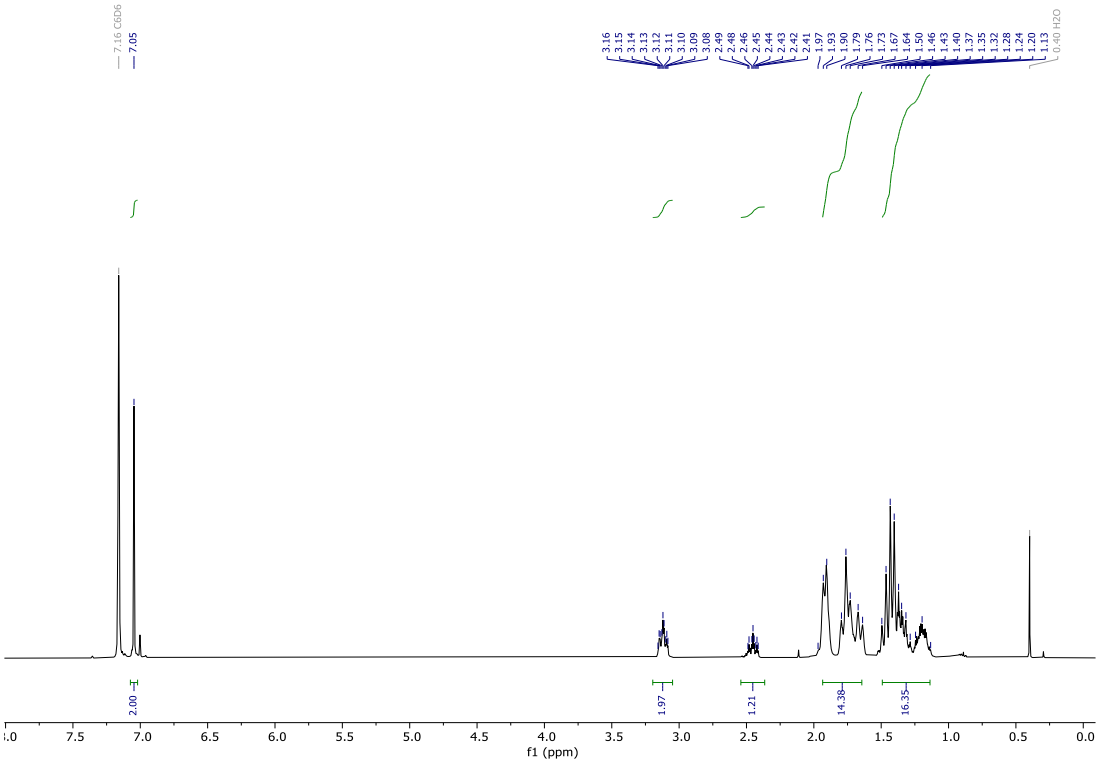


Figure S7: ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of 2,4,6-tricyclohexylphenyl azide.

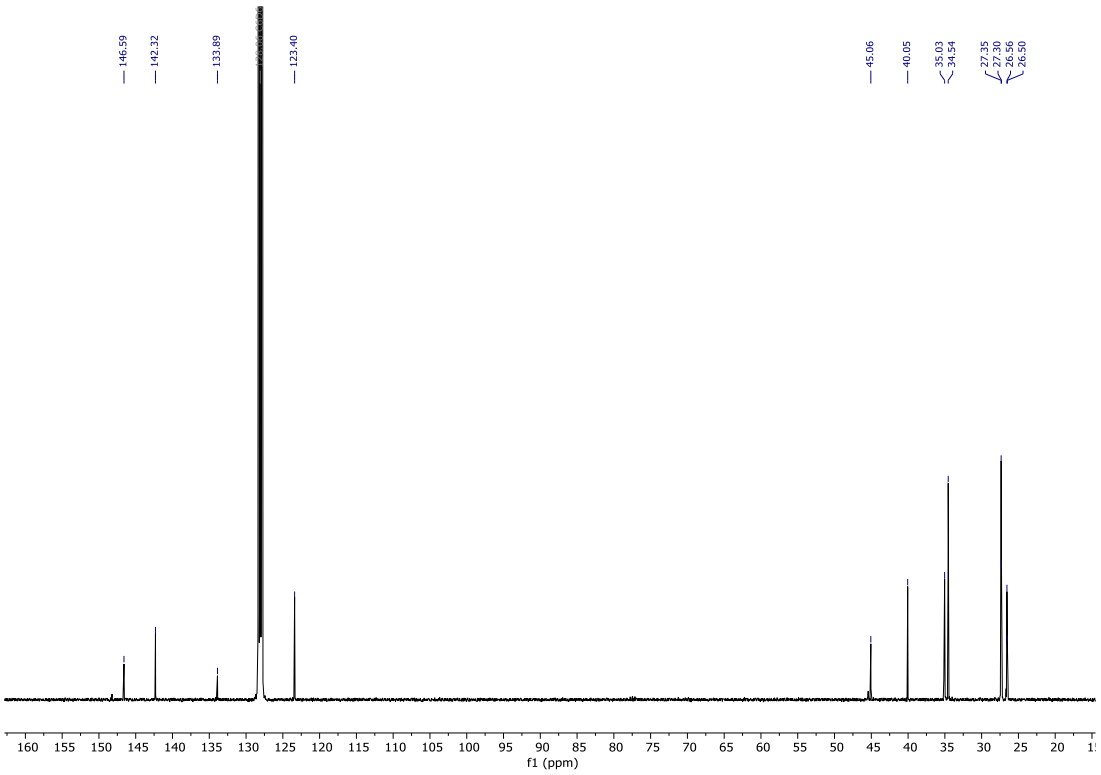


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of 2,4,6-tricyclohexylphenyl azide.

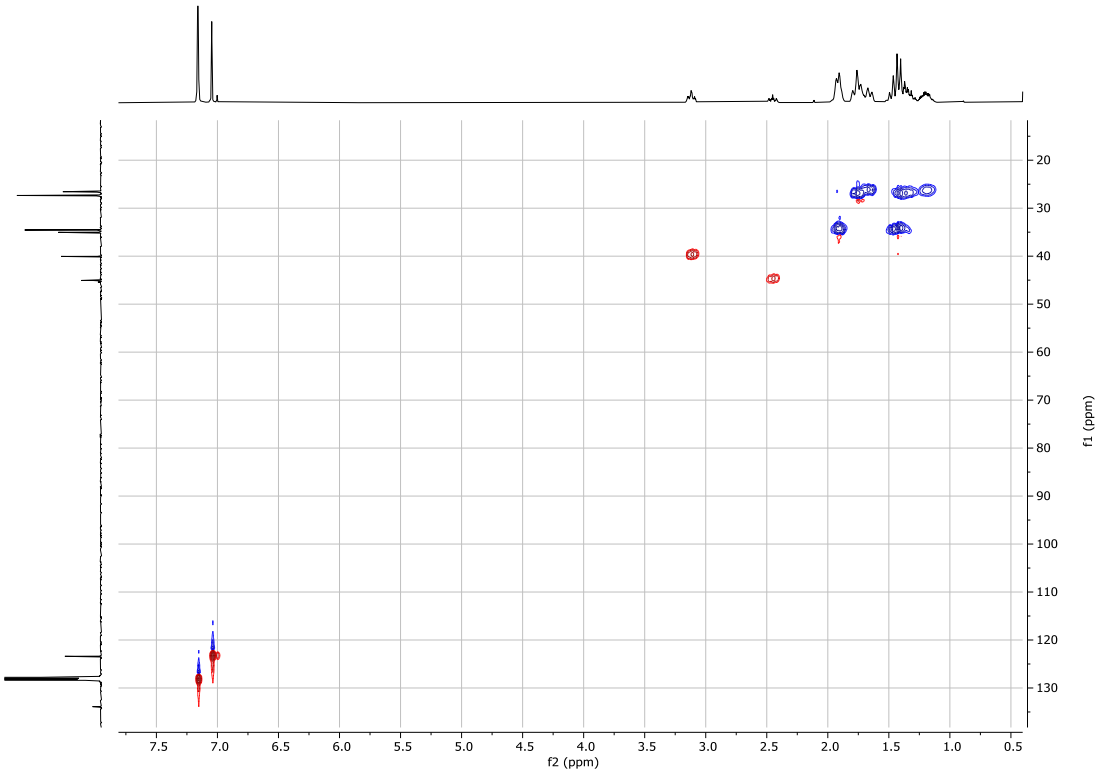


Figure S9: HSQC NMR spectrum (298 K, C_6D_6) of 2,4,6-tricyclohexylphenyl azide.

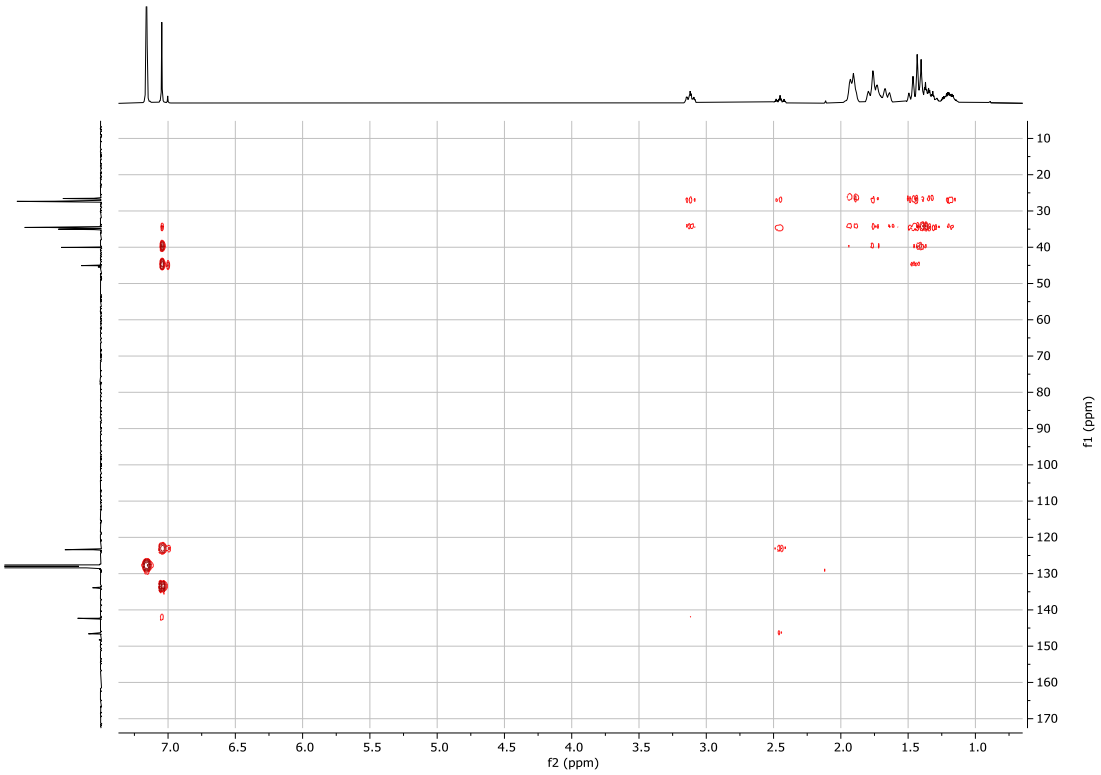


Figure S10: HMBC NMR spectrum (298 K, C_6D_6) of 2,4,6-tricyclohexylphenyl azide.

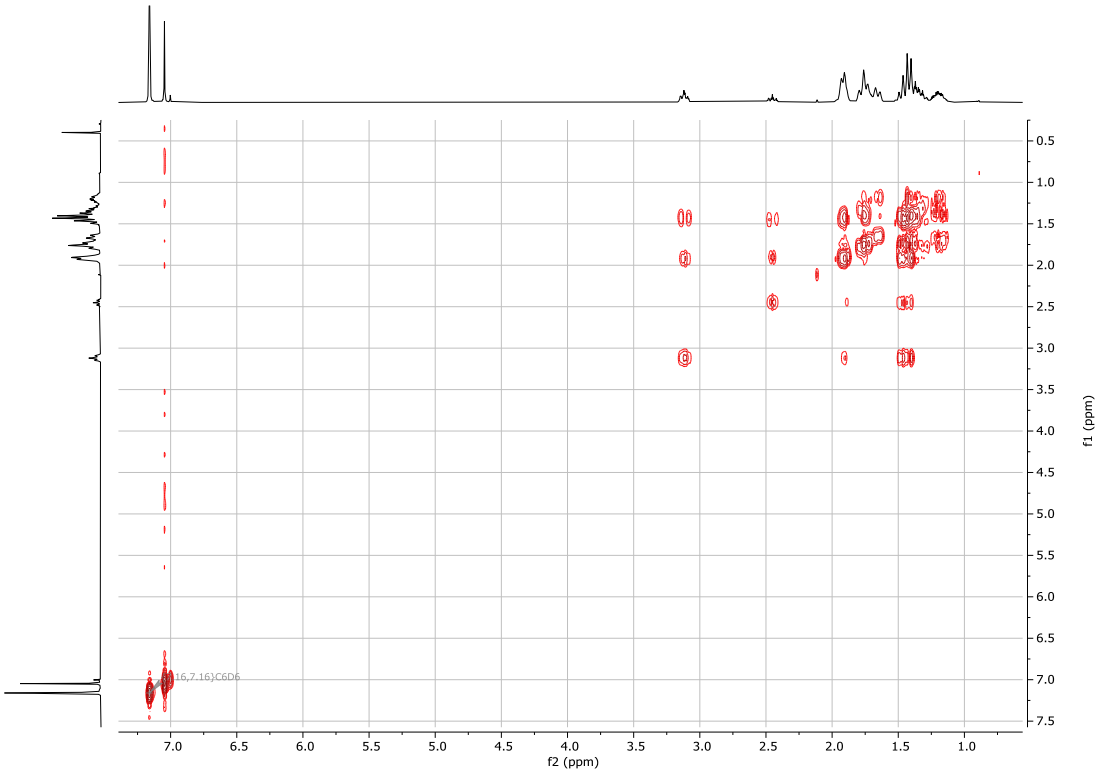


Figure S11: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of 2,4,6-tricyclohexylphenyl azide.

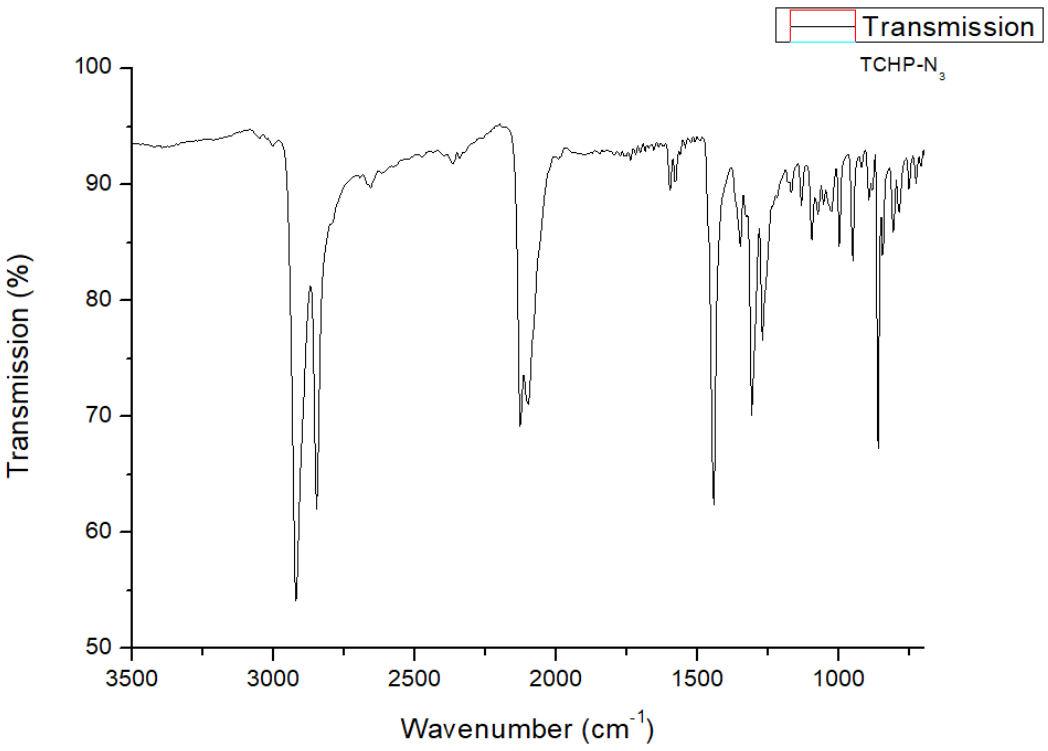


Figure S12: FT-IR spectrum of 2,4,6-tricyclohexylphenyl azide.

Preparation of :Sn(NON^{Ad}) (1)

A flame-dried Schlenk was charged with NON^{Ad}–H_2 (5.00 g, 11.6 mmol) and dissolved in diethyl ether (*ca.* 30 mL). A solution of ^{n}BuLi (1.6 M in hexanes, 23.2 mmol, 14.5 mL) was added dropwise to the reaction mixture and allowed to stir for 1 hour at room temperature. Solid $SnCl_2$ (2.19 g, 11.6 mmol) was added directly to the reaction mixture using a solid-addition Schlenk and stirred for an additional 18 hours. The volatiles were removed *in vacuo* and the product extracted in hexane (*ca.* 3 x 10 mL). Concentration of the mother liquor and storage at –30 °C afforded green-yellow dichroic crystals. The supernatant was decanted and the crystals were dried *in vacuo*. Yield 3.40 g, 54%. NOTE: Crystallisation at –30 °C provides the distannene [Sn(NON^{Ad})]$_2$ ([**1**]$_2$). Crystallisation from boiling hexane gives the stannylene :Sn(NON^{Ad}) (**1**). Crystallisation from minimum hexane at room temperature (25 °C) gives a mixture of the distannene ([**1**]$_2$)/stannylene (**1**).

m.p.: 161–163 °C (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 0.45 (s, 12H, Si*Me*$_2$), 1.53 – 1.64 (m, 12H, Ad–*H*), 1.96 – 2.05 (m, 6H, Ad–*H*), 2.05 – 2.10 (m, 12H, Ad–*H*).

$^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ 7.6 (Si*Me*$_2$), 31.2, 36.7, 51.6 (Ad–*C*).

$^{29}Si\{^1H\}$ NMR (80 MHz, C_6D_6): δ -11.8 (*Si*Me$_2$).

$^{119}Sn\{^1H\}$ NMR (149 MHz, C_6D_6): δ 832.3 (*Sn*).

IR ν/cm^{-1} (solid): 712 (m), 779 (s), 816 (w), 839 (s), 939 (w), 962 (w), 1003 (m), 1025 (w), 1070 (w), 1092 (w), 1114 (w), 1152 (m), 1249 (s), 1301 (w), 1342 (w), 1353 (m), 1401 (m), 1450 (m), 2844 (s), 2900 (s).

E.A.: Anal. Calcd. for $C_{24}H_{42}N_2OSi_2Sn$ (549.49): C, 52.46; H, 7.70; N, 5.10 %. Found: C, 52.25; H, 7.87; N, 4.62 %.

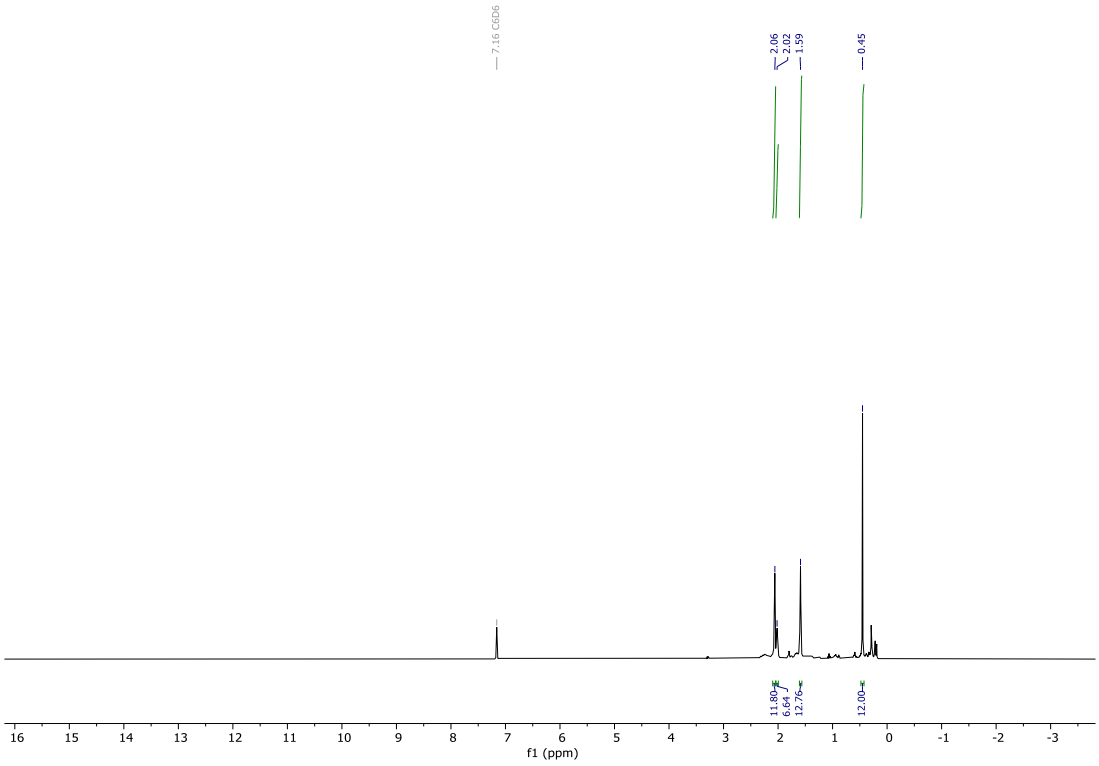


Figure S13: ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of **1**.

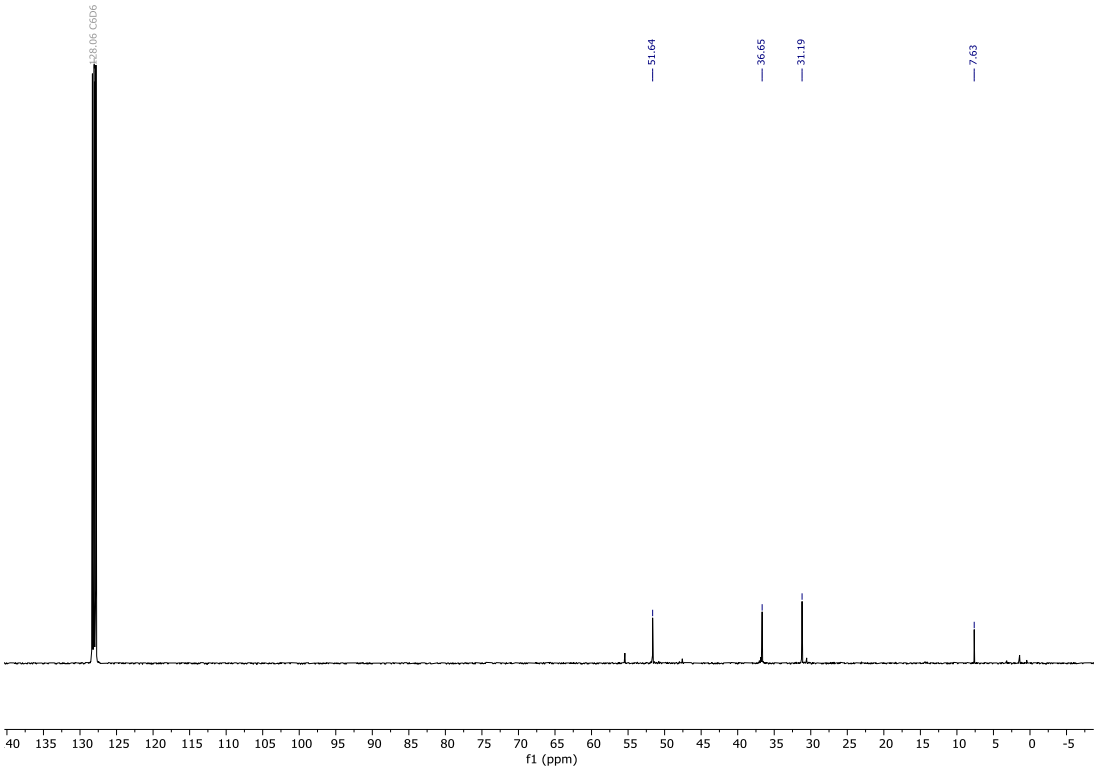


Figure S14: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **1**.

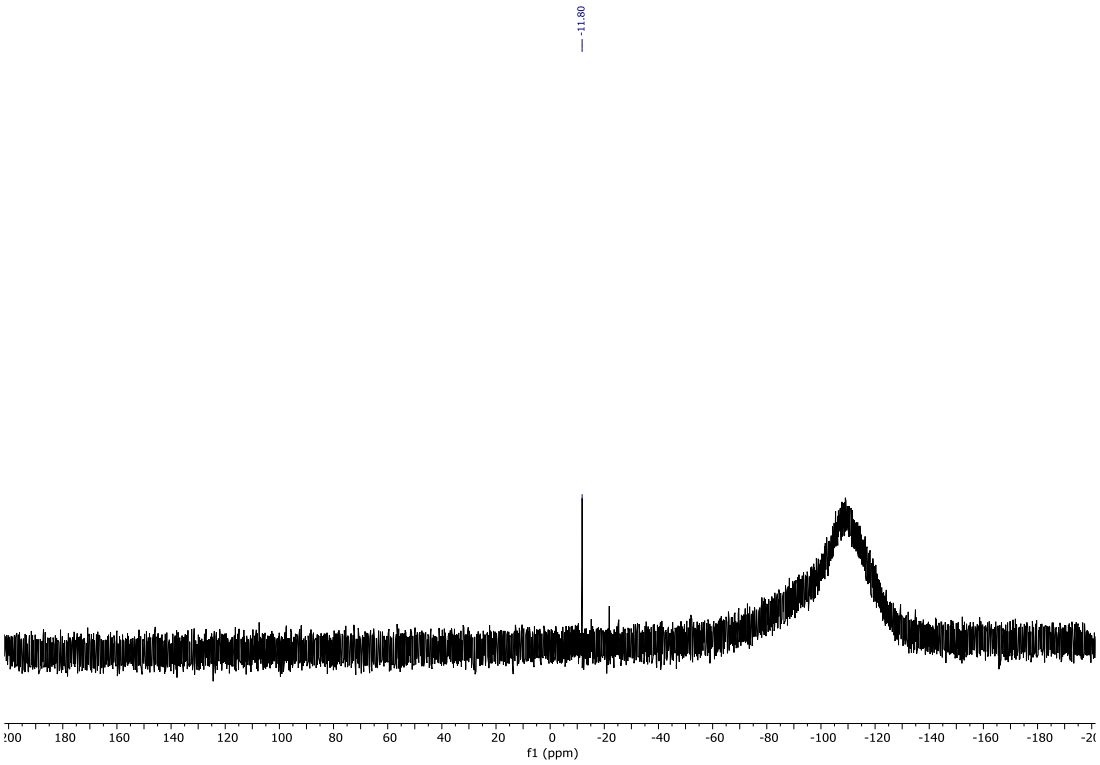


Figure S15: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of **1**.

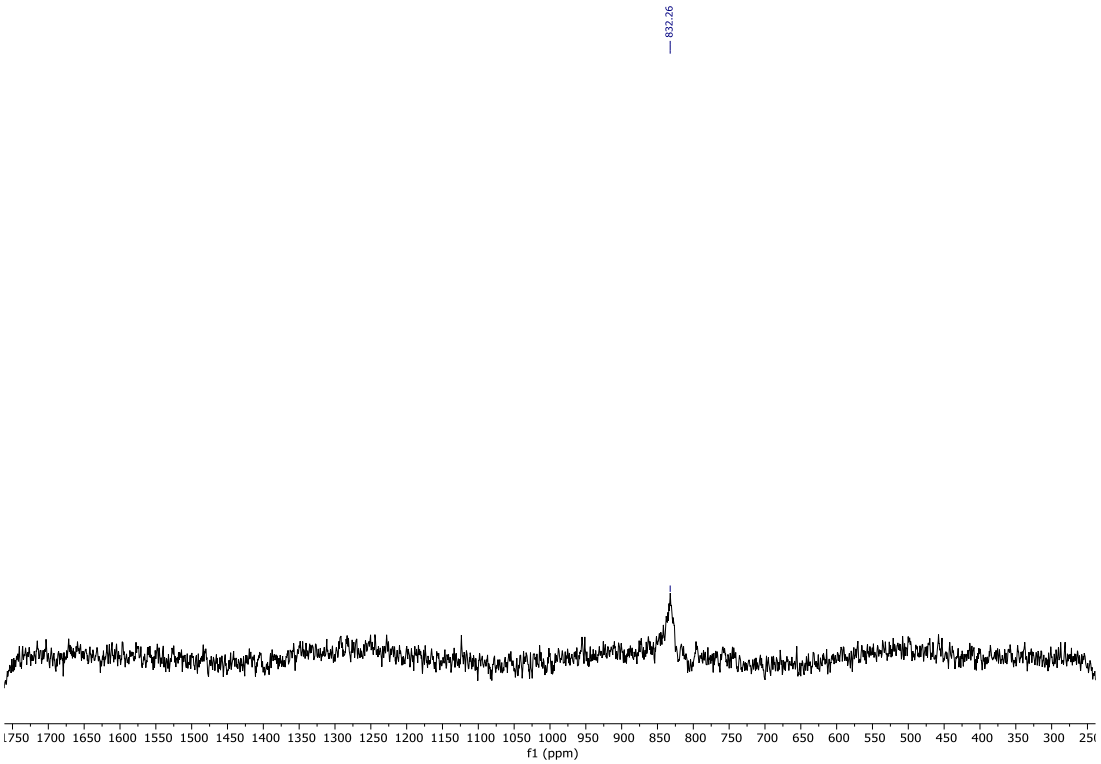


Figure S16: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, C_6D_6) of **1**.

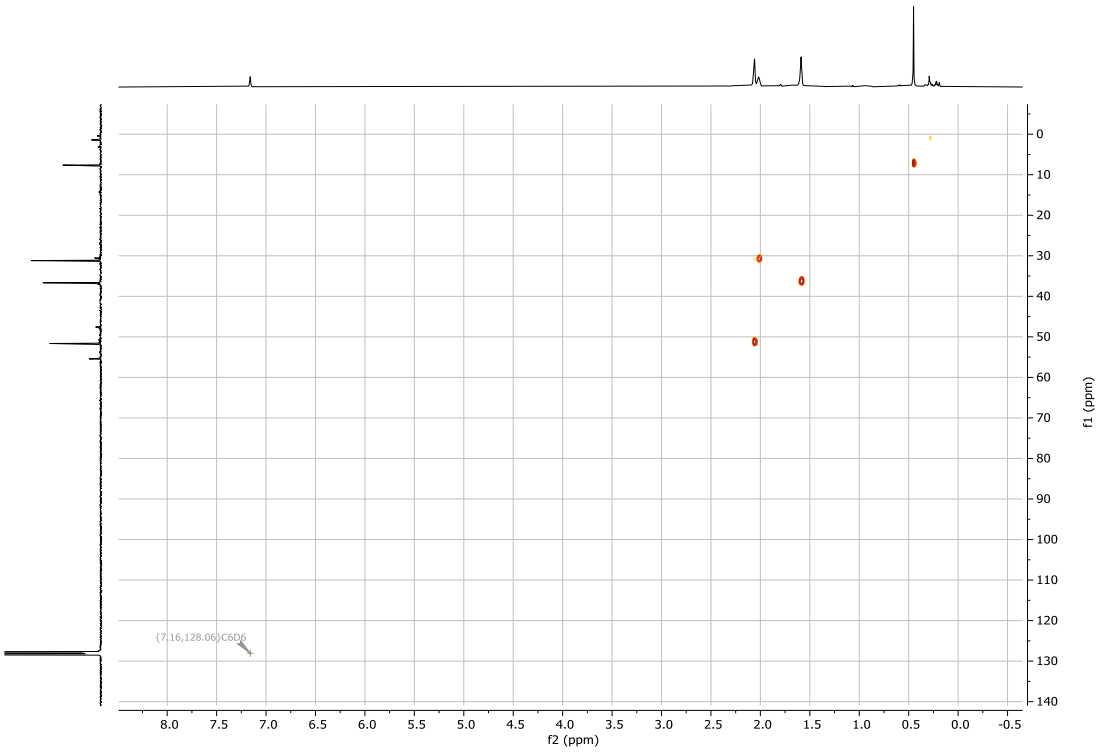


Figure S17: HSQC NMR spectrum (298 K, C_6D_6) of **1**.

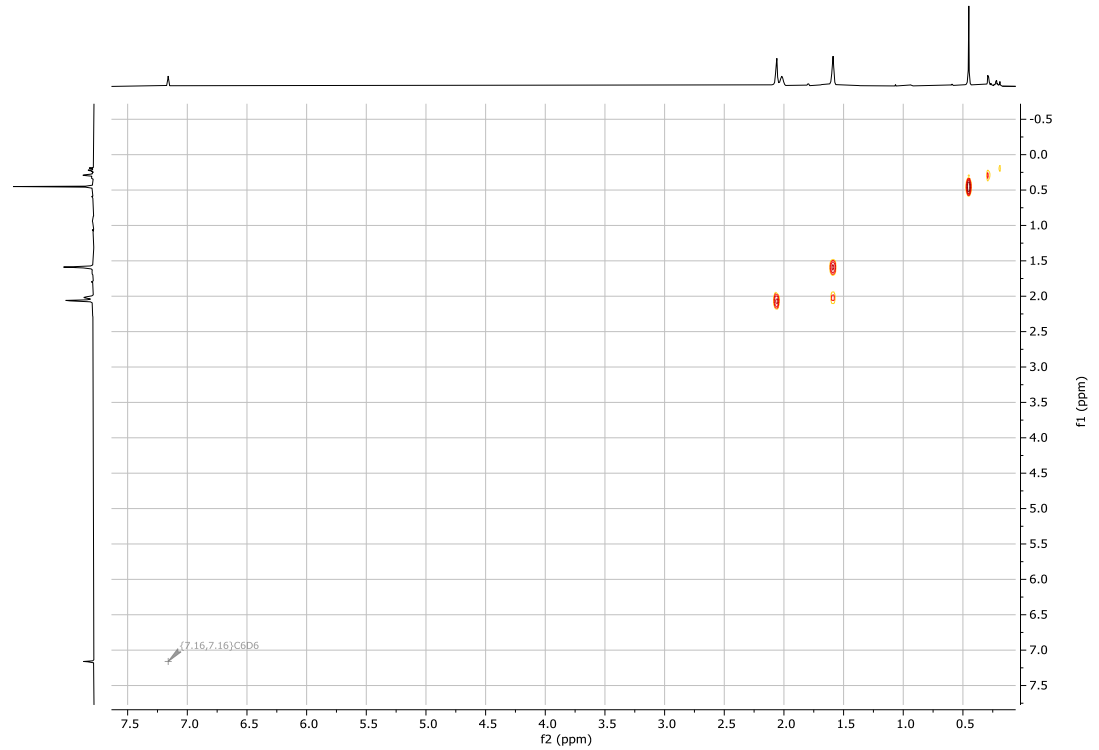


Figure S18: HMBC NMR spectrum (298 K, C_6D_6) of **1**.

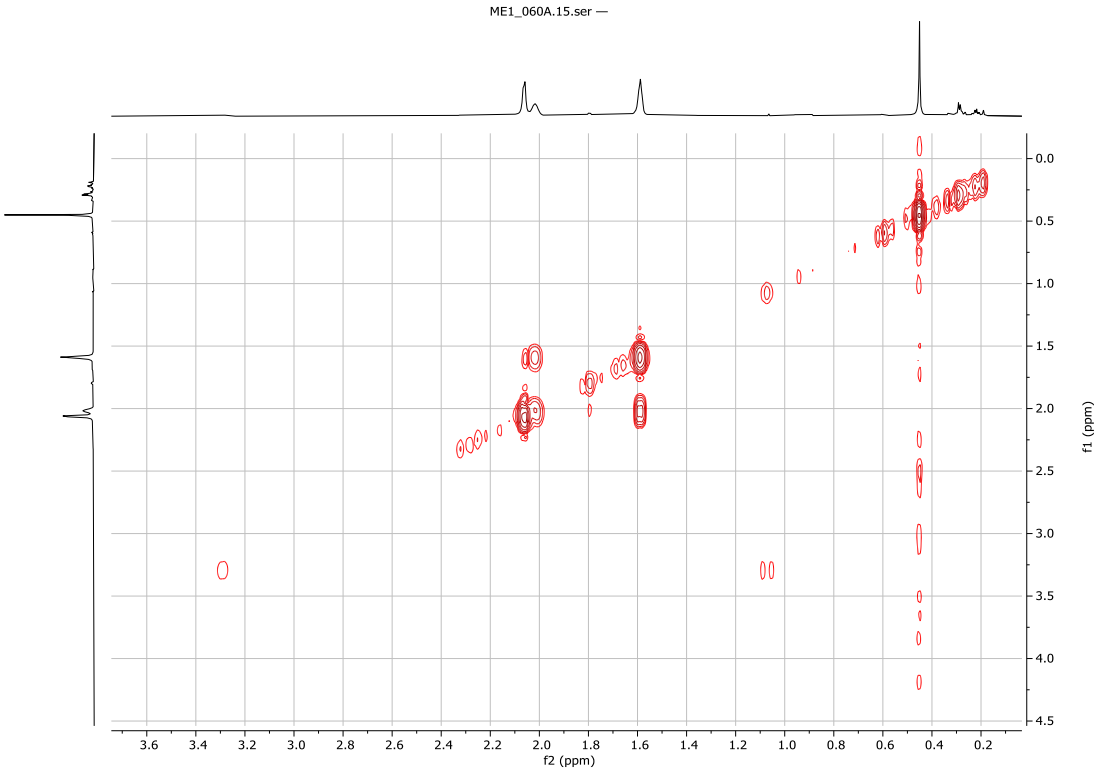


Figure S19: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of **1**.

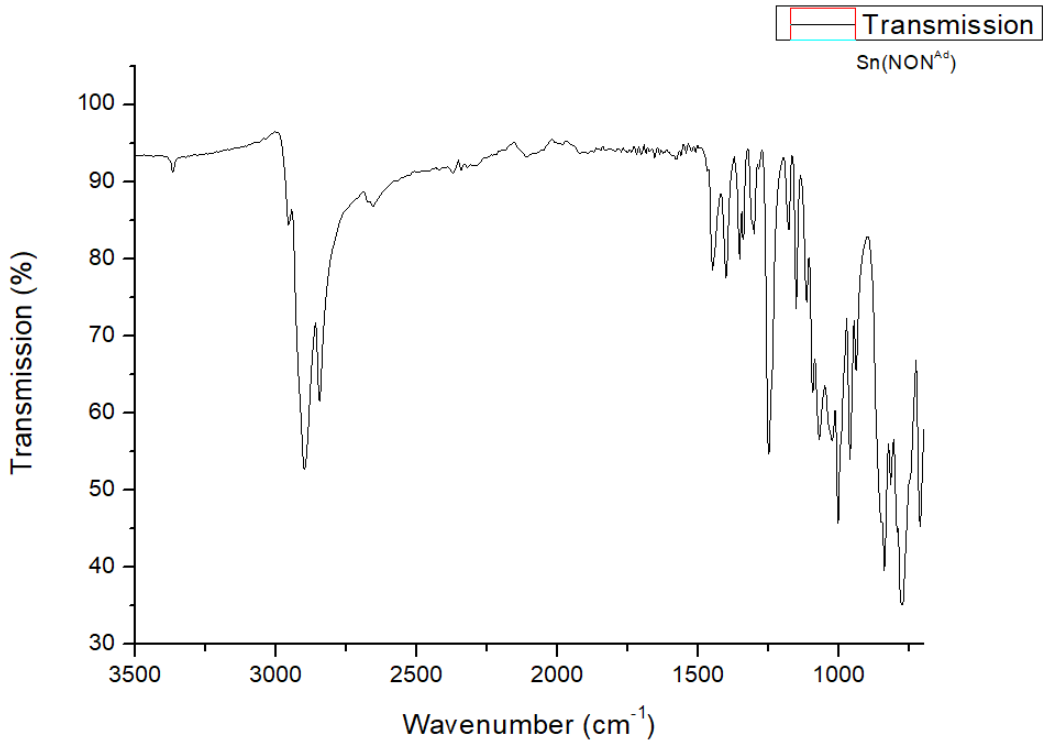


Figure S20: FT-IR spectrum of **1**.

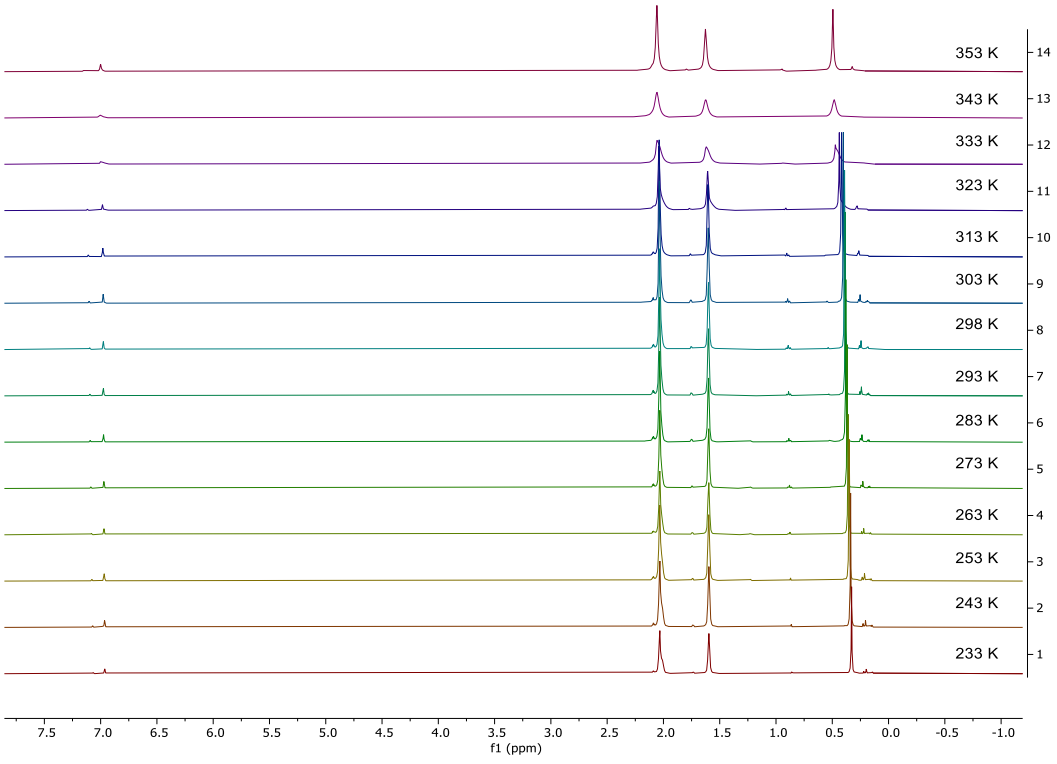


Figure S21: VT-^{1}H NMR spectrum (400 MHz, C_7D_8) of **1**.

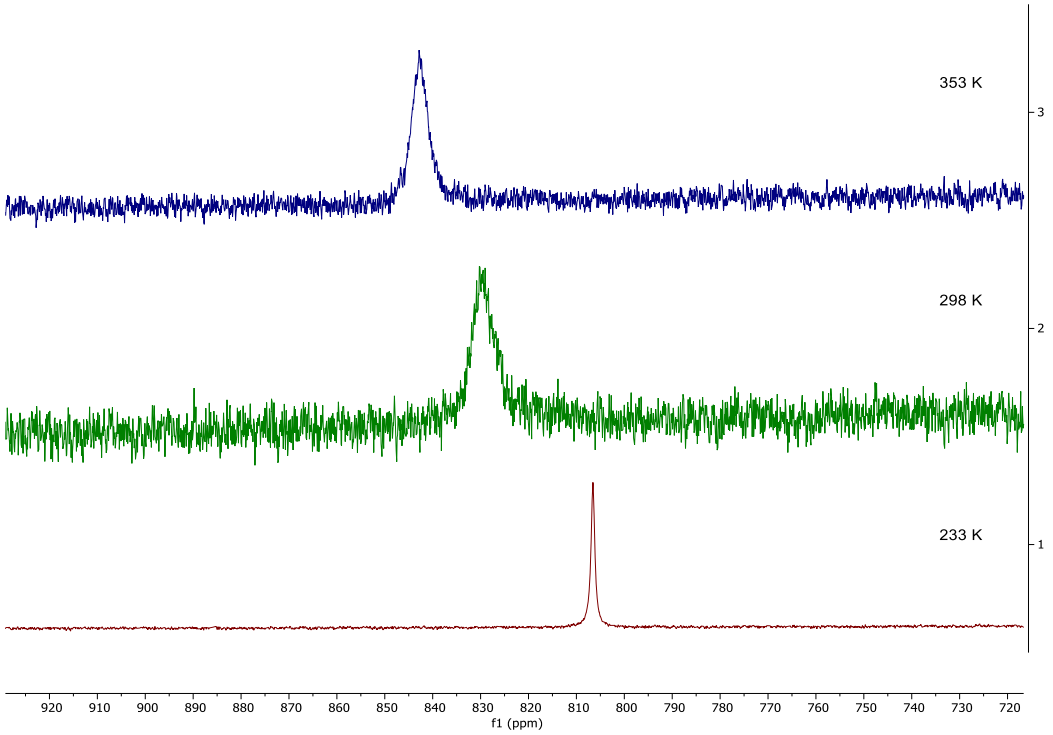


Figure S22: VT-^{119}Sn{^{1}H} NMR spectrum (149 MHz, C_7D_8) of **1**.

Preparation of Sn(NON^{Ad})(Mes$_2$N$_4$) (2)

1 (100 mg, 0.18 mmol) was charged to a flame-dried Schlenk flask and hexane (~5 mL) was added. The mixture was cooled to –78 °C and mesityl azide (58 mg, 0.36 mmol) was added dropwise. The solution was allowed to warm to room temperature and stirred for 2 hours to give a pale orange-yellow solution. Crystals were obtained from a saturated hexane solution stored at –30 °C and washed with cold hexane. Yield 75 mg, 49%.

m.p.: 142–144 °C (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 0.30 (s, 12H, Si*Me*$_2$), 1.28 – 1.34 (m, 12H, Ad–*H*), 1.72 – 1.78 (m, 6H, Ad–*H*), 1.80 – 1.85 (m, 12H, Ad–*H*), 2.17 (s, 6H, *p*-C*H*$_3$), 2.81 (s, 12H, *o*-C*H*$_3$), 6.90 (s, 4H, $_{Mes}$Ar–*H*).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ 6.6 (Si*Me*$_2$), 20.6 (*p*-*C*H$_3$), 23.8 (*o*-*C*H$_3$), 30.8, 35.8, 46.9, 56.2 (Ad–*C*), 130.2, 131.3, 132.0, 143.1 ($_{Mes}$Ar–*C*).

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): δ -3.7 (*Si*Me$_2$).

^{119}Sn{^{1}H} NMR (149 MHz, C_6D_6): δ -253 (*Sn*).

IR v/cm^{-1} (solid): 723 (w), 783 (s), 850 (s), 921 (m), 962 (m), 995 (s), 1040 (m), 1066 (s), 1085 (w), 1252 (s), 1301 (w), 1401 (w), 1424 (w), 1450 (w), 1476 (m), 2117 (w), 2848 (s), 2904 (s).

E.A.: Anal. Calcd. for $C_{42}H_{64}N_6OSi_2Sn$ (843.89): C, 59.78; H, 7.64; N, 9.96 %. Found: C, 58.45; H, 7.73; N, 8.92 %.

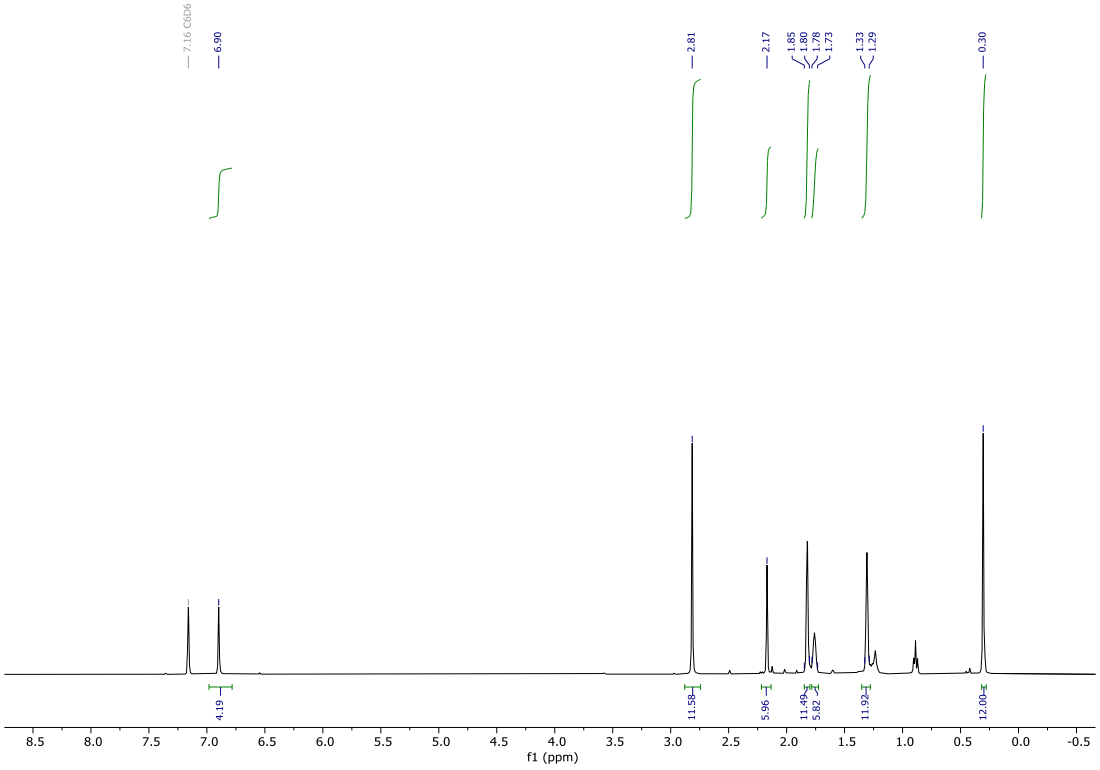


Figure S23: ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **2**.

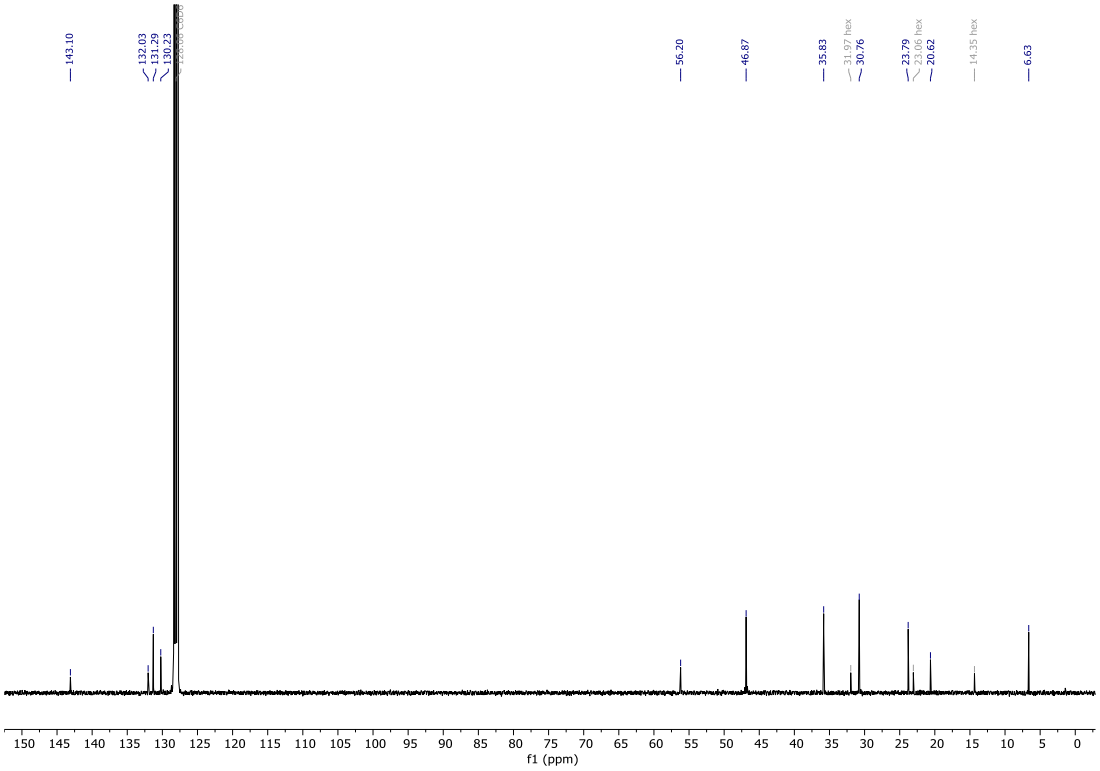


Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **2**.

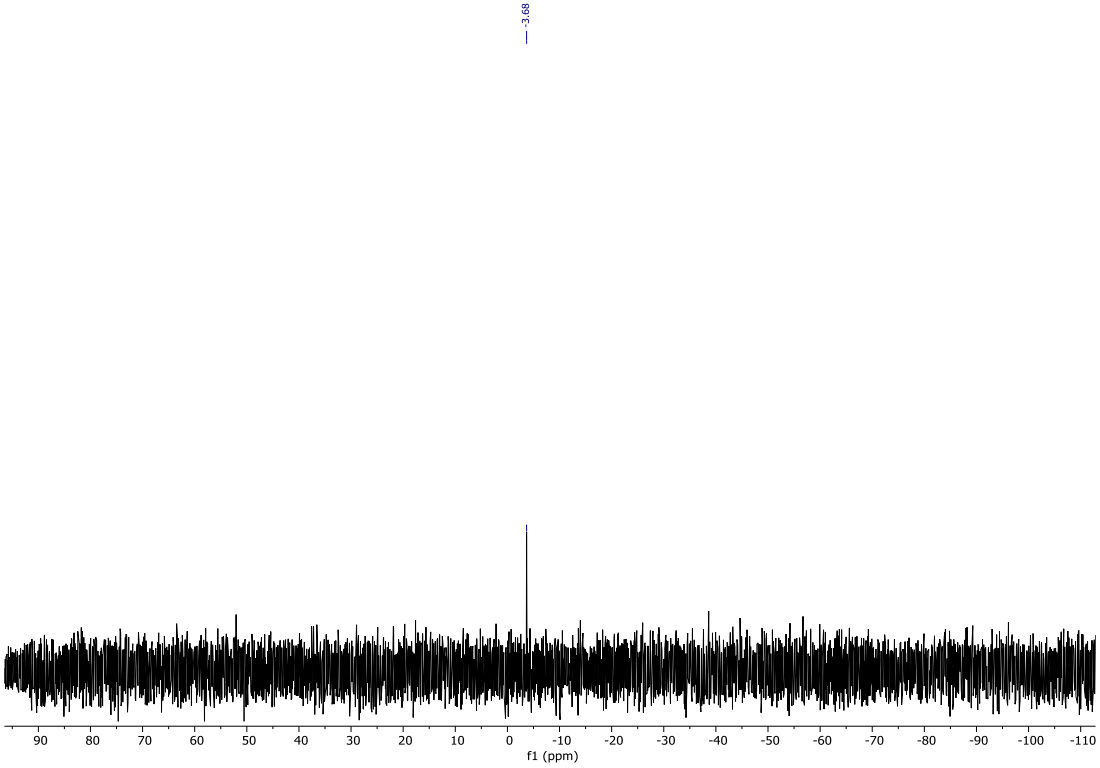


Figure S25: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of **2**.

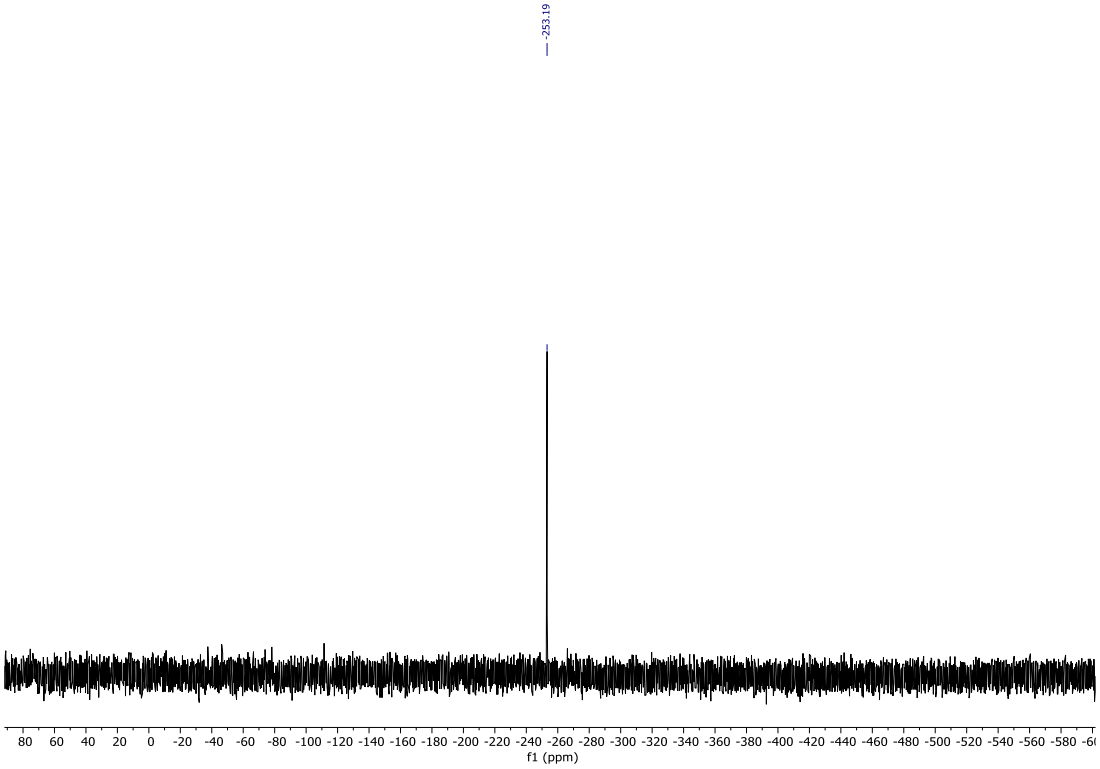


Figure S26: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, C_6D_6) of **2**.

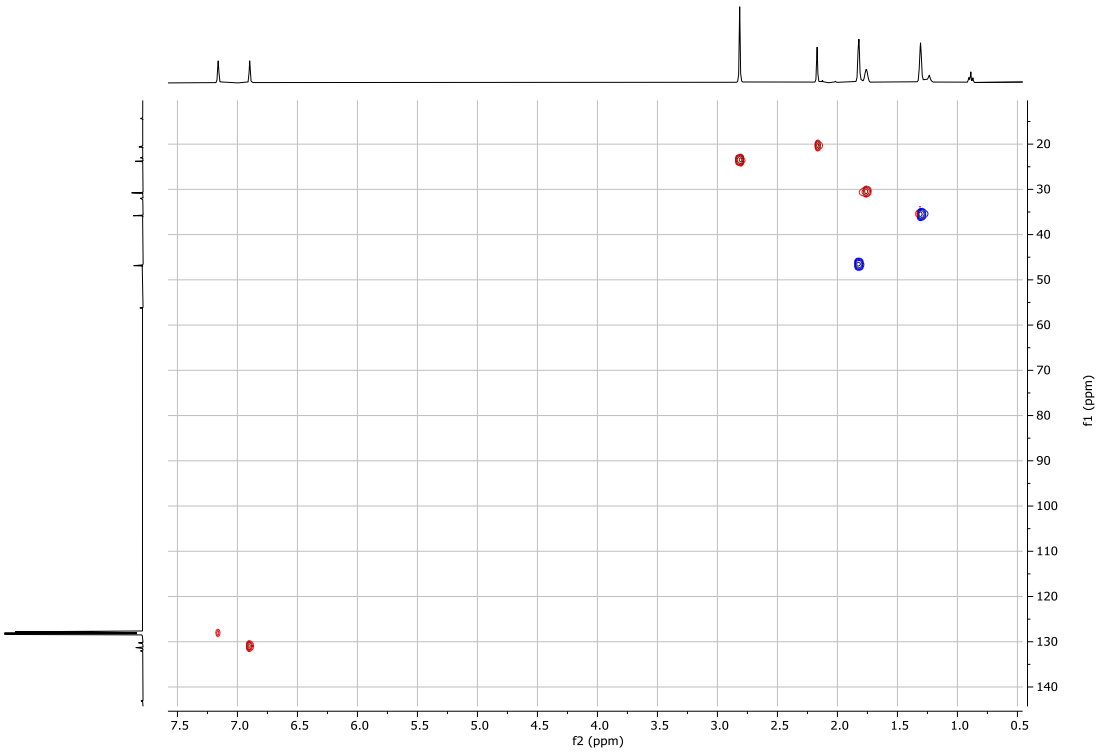


Figure S27: HSQC NMR spectrum (298 K, C_6D_6) of **2**.

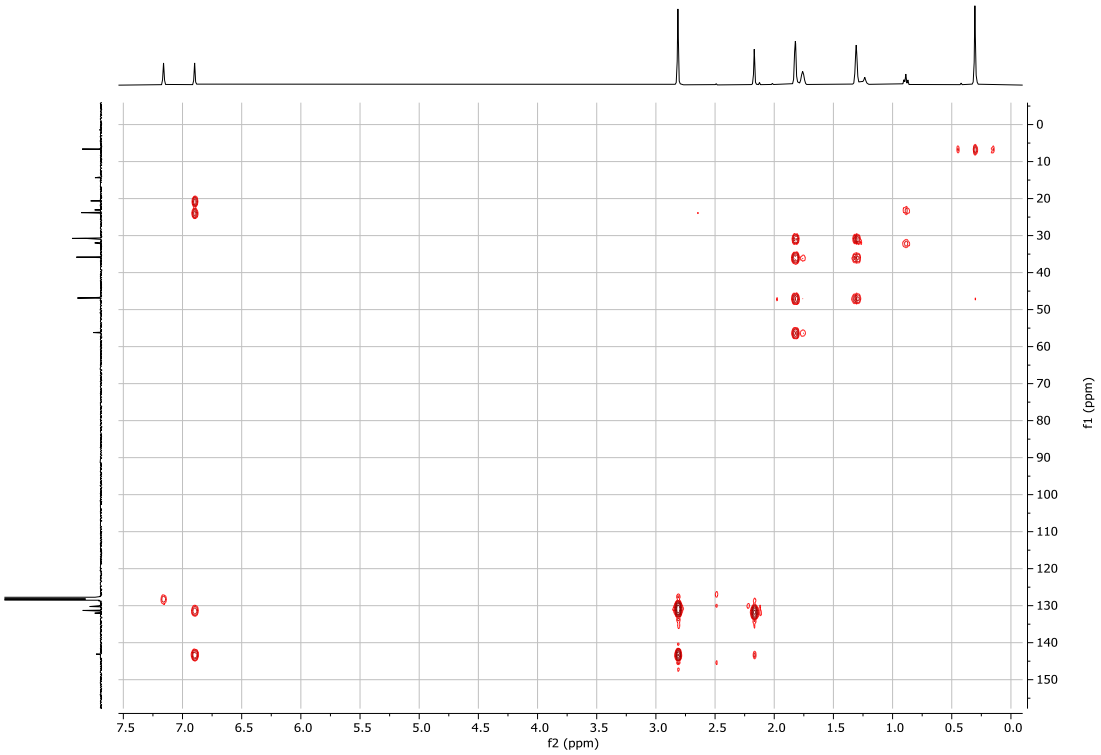


Figure S28: HMBC NMR spectrum (298 K, C_6D_6) of **2**.

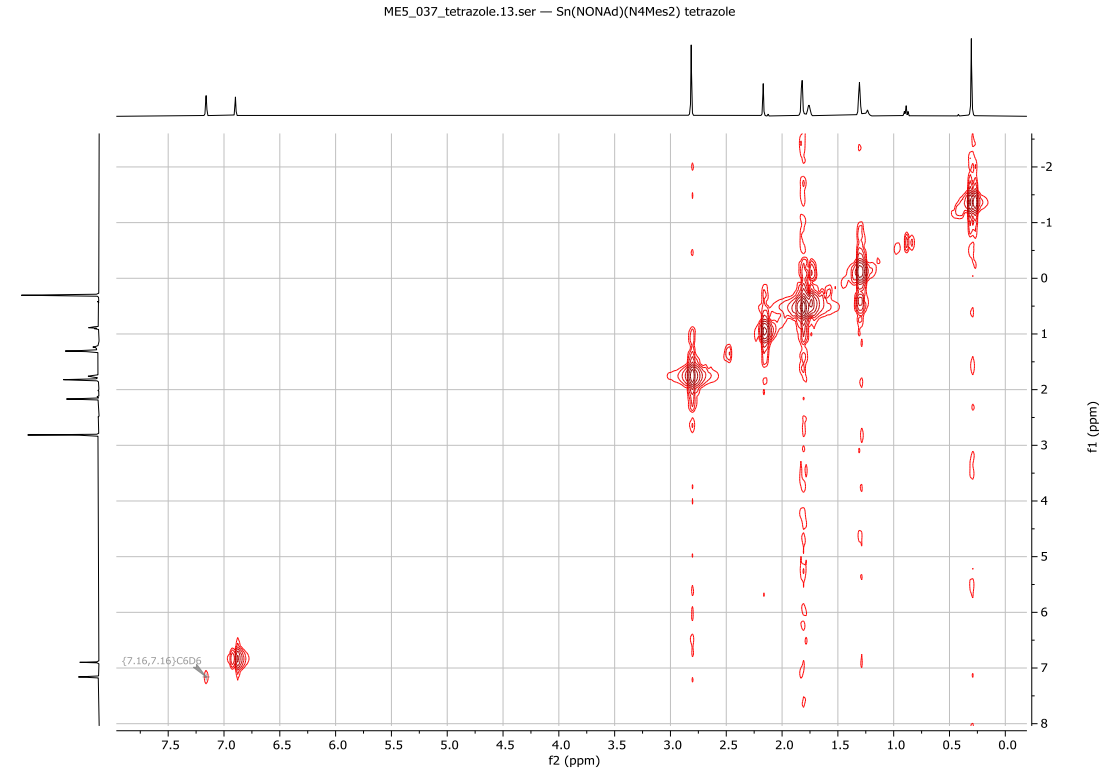


Figure S29: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of **2**.

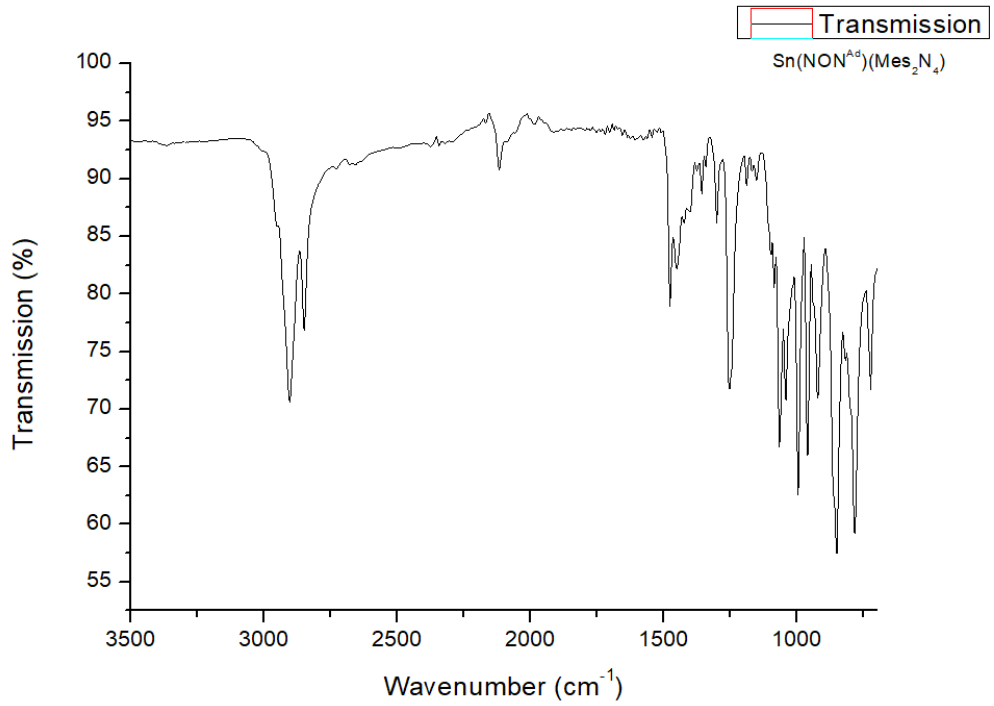


Figure S30: FT-IR spectrum of **2**.

Preparation of (NON^{Ad})Sn=N(TCHP) (3)

1 (250 mg, 0.45 mmol) was charged to a flame-dried Schlenk flask and hexane (~3 mL) was added. The mixture was cooled to 0 °C and 2,4,6-tricyclohexylphenyl azide (166 mg, 0.45 mmol) in hexane (~2 mL) was added in one portion. The solution was allowed to stir at room temperature for 5 minutes to give a dark red solution accompanied by vigorous gas evolution. The solvent was reduced (~1-2 mL) *in vacuo* and stored at –30 °C to give dark red crystals. The supernatant was decanted and the crystals were dried *in vacuo*. Yield 180 mg, 45%.

m.p.: 138–140 °C (dec).

^{1}H NMR (400 MHz, C_7D_8, 233 K): δ 0.33 (s, 12H, Si*Me*$_2$), 1.18 – 1.49 (m, 14H, Cy–*H*), 1.50 – 1.68 (m, 8H, Cy–*H*), 1.67 – 1.79 (m, 12H, Ad–*H*), 1.80 – 2.02 (m, 18H, Ad–*H*), 2.15 – 2.36 (m, 6H, Cy–*H*), 2.48 – 2.65 (m, 2H), 2.95 – 3.12 (m, 2H, Cy–*H*), 3.34 – 3.52 (m, 1H, Cy–*H*), 7.14 (s, 2H, Ar–*H*).

^{13}C{^{1}H} NMR (101 MHz, C_7D_8, 233 K): δ 5.8 (Si*Me*$_2$), 27.1, 27.5, 28.3, 30.2 (Cy–*C*), 30.8 (Ad–*C*), 33.3, 34.1 (Cy–*C*), 35.6 (Ad–*C*), 36.5, 38.5, 42.4, 45.6, 46.6, 47.1 (Cy–*C*), 47.8, 53.0 (Ad–*C*), 121.4, 125.6, 138.6, 152.6 (Ar–*C*).

^{29}Si{^{1}H} NMR (80 MHz, C_7D_8, 233 K): δ -2.9 (*Si*Me_2).

^{119}Sn{^{1}H} NMR (149 MHz, C_7D_8, 233 K): δ 46.5 (*Sn*).

IR ν/cm^{-1} (solid): 723 (s), 779 (s), 801 (w), 820 (w), 865 (s), 939 (w), 962 (m), 1003 (m), 1036 (w), 1070 (w), 1092 (w), 1118 (w), 1252 (s), 1301 (w), 1353 (m), 1446 (s), 2848 (s), 2904 (s).

E.A.: Anal. Calcd. for $C_{48}H_{77}N_3OSi_2Sn$ (887.04): C, 64.99; H, 8.75; N, 4.74 %. Found: C, 62.97; H, 8.48; N, 4.10 %.

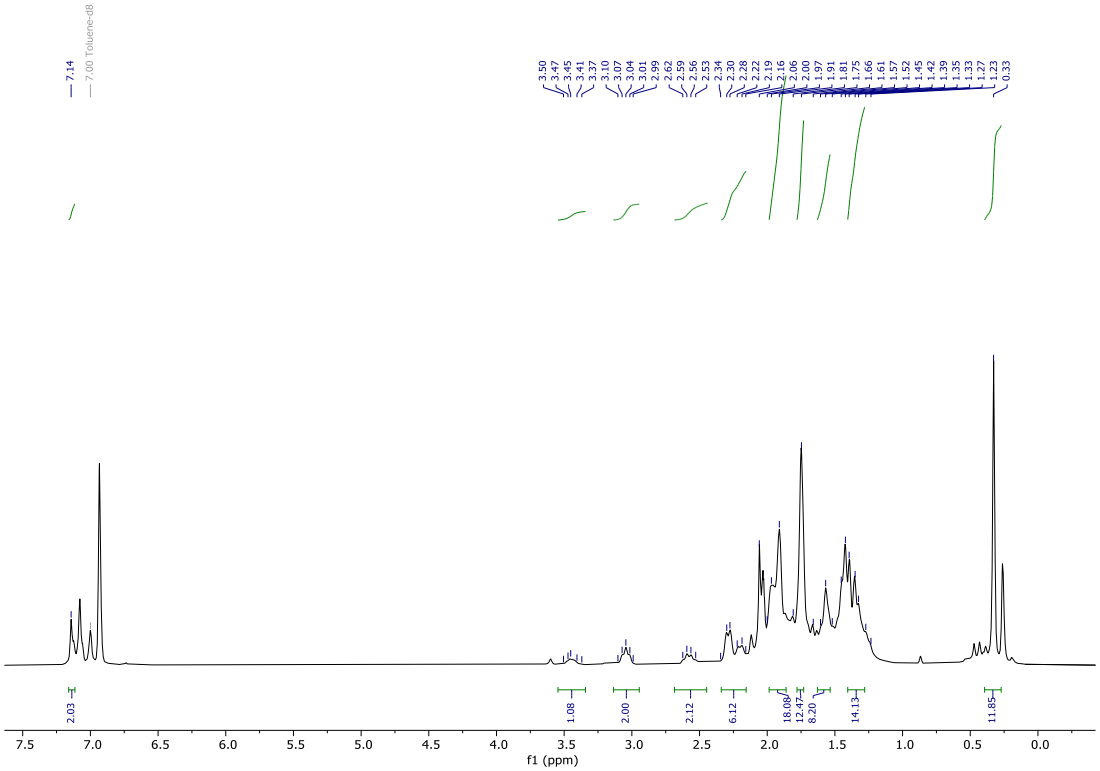


Figure S31: ^{1}H NMR spectrum (400 MHz, 233 K, C_6D_6) of **3**.

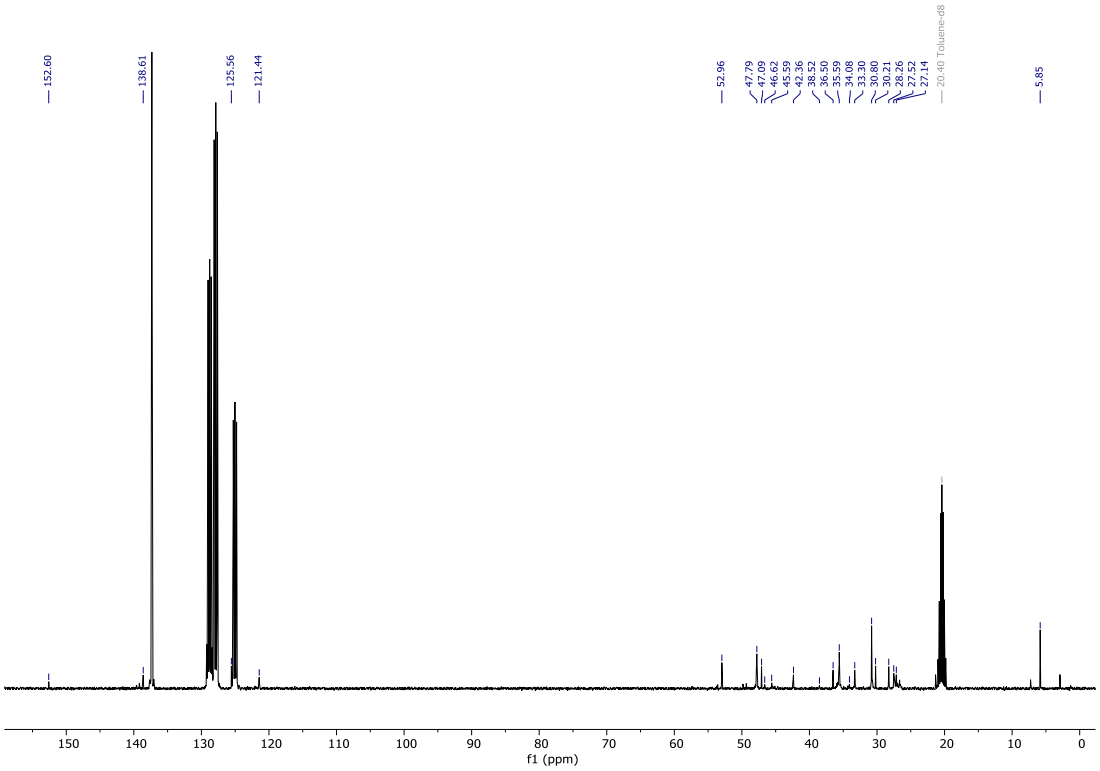


Figure S32: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 233 K, C_6D_6) of **3**.

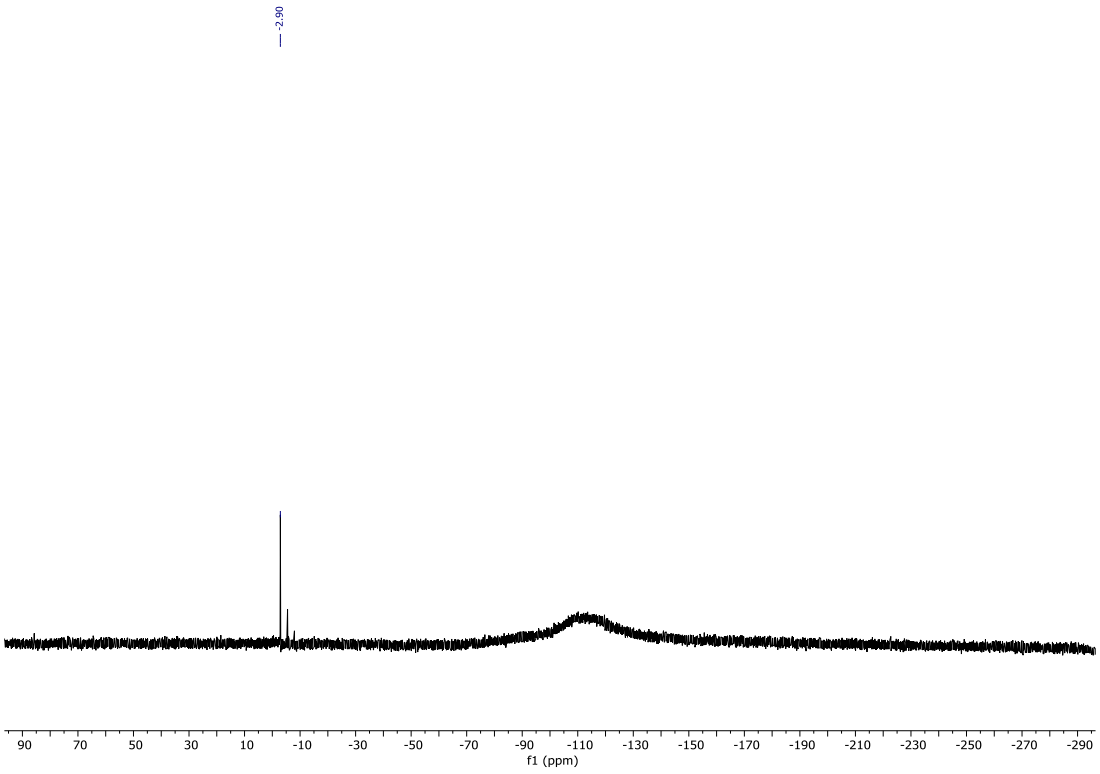


Figure S33: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 233 K, C_6D_6) of **3**.

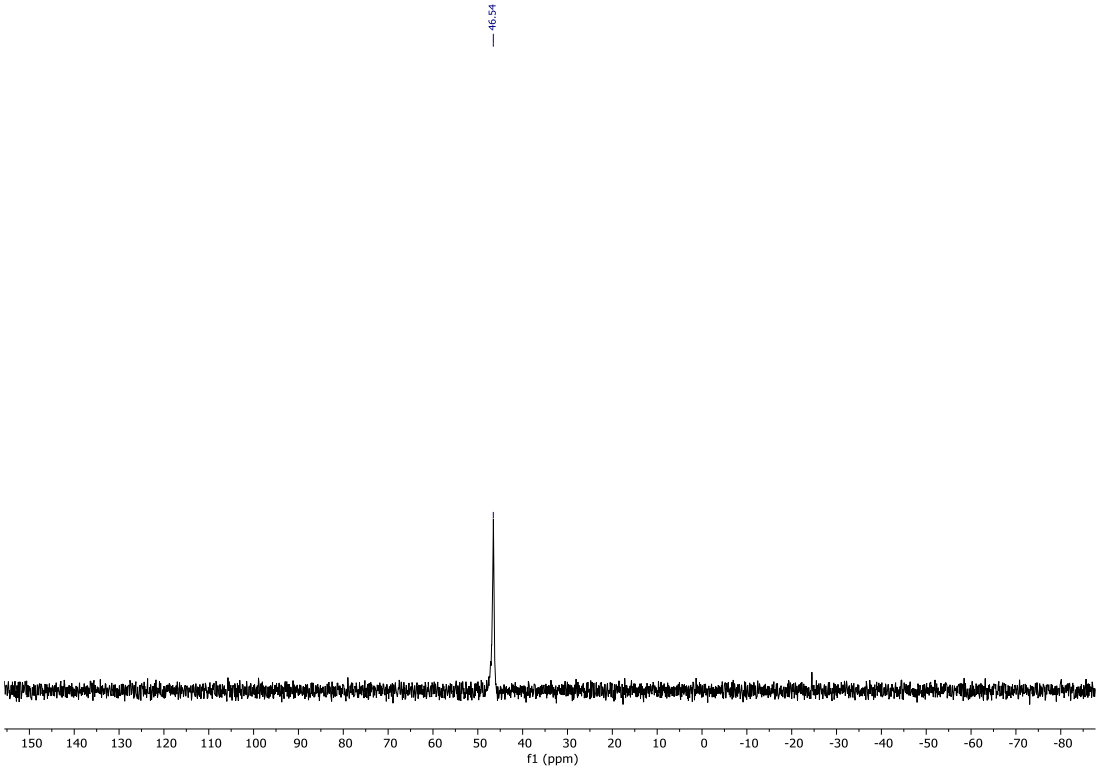


Figure S34: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 233 K, C_6D_6) of **3**.

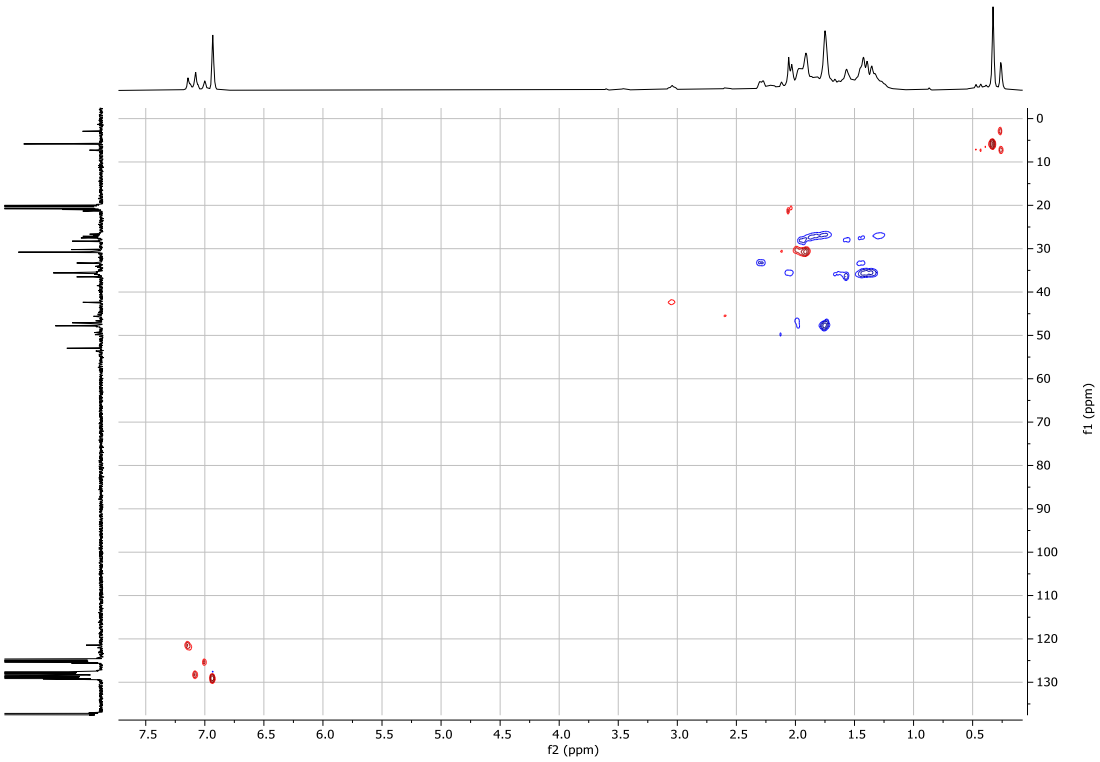


Figure S35: HSQC NMR spectrum (233 K, C_6D_6) of **3**.

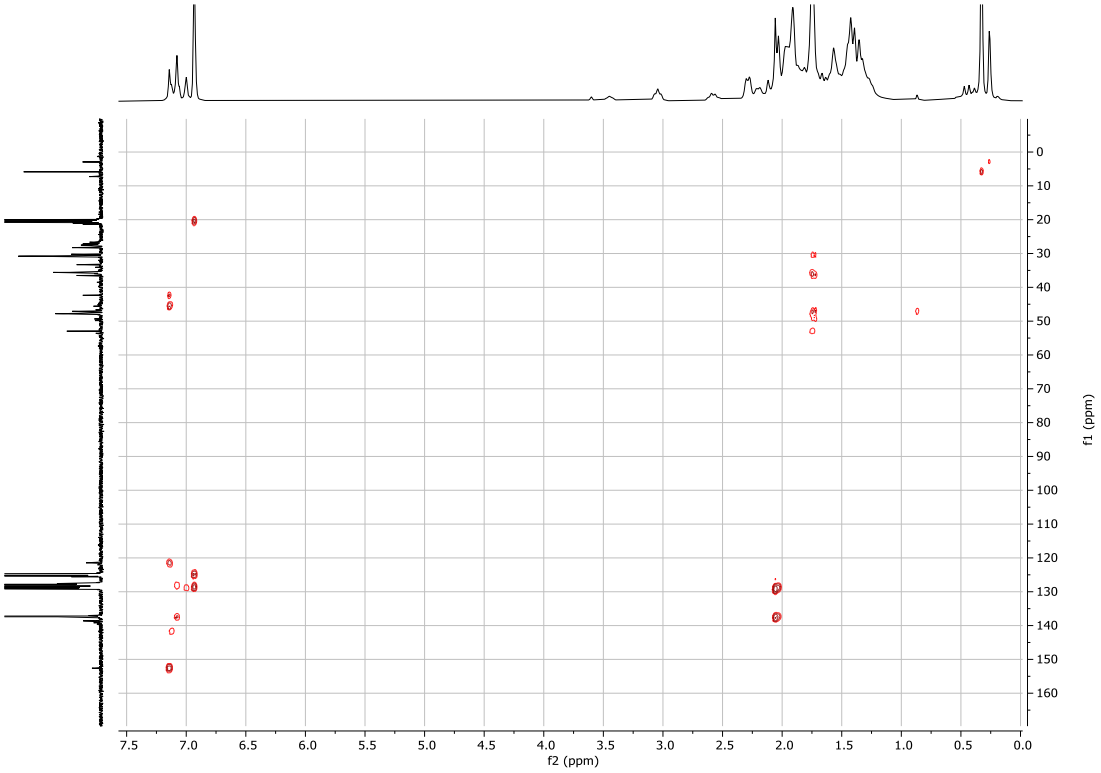


Figure S36: HMBC NMR spectrum (233 K, C_6D_6) of **3**.

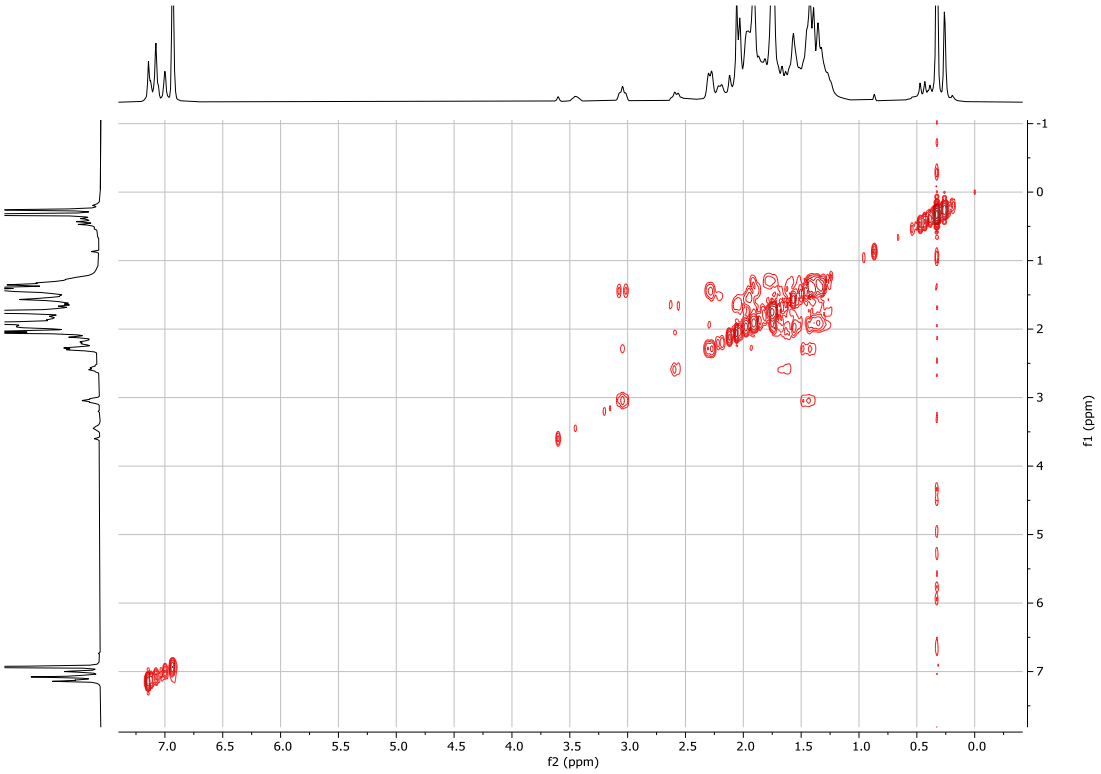


Figure S37: ^{1}H–^{1}H COSY NMR spectrum (233 K, C_6D_6) of **3**.

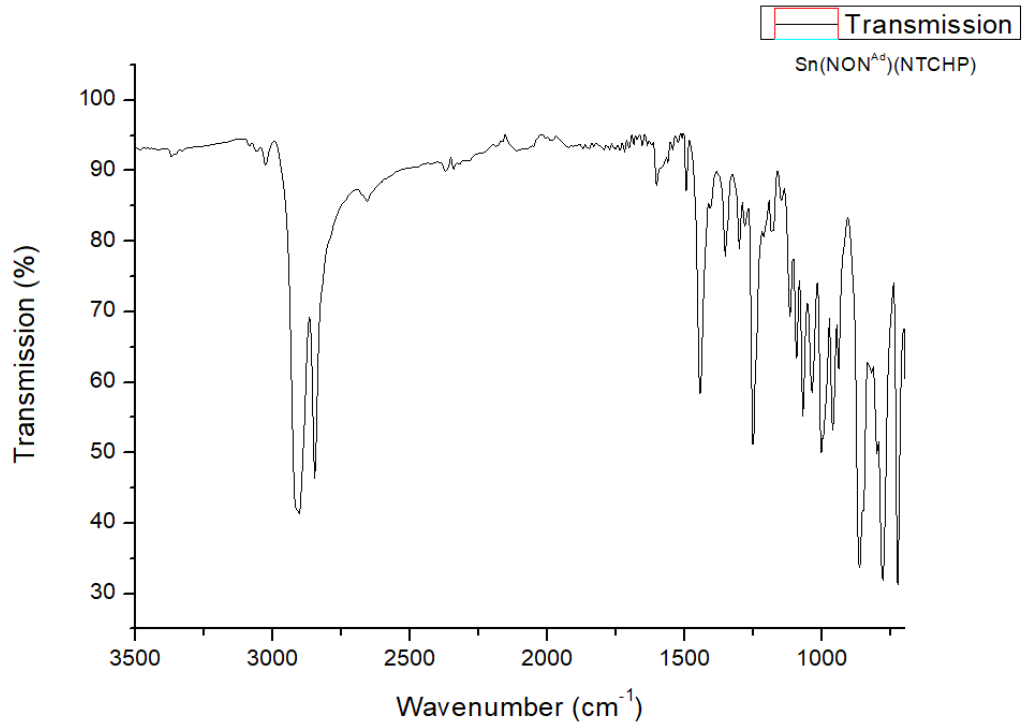


Figure S38: FT-IR spectrum of **3**.

Preparation of (NON^{Ad})Sn{NH(TCHP^{-H})} (4)

1 (100 mg, 0.18 mmol) was charged to a flame-dried Schlenk flask and hexane (~3 mL) was added. 2,4,6-Tricyclohexylphenyl azide (66 mg, 0.18 mmol) in hexane (~2 mL) was added in one portion. The solution was gently heated at 60 °C for 15 minutes to give a clear orange solution (through a dark red intermediate, see above). The solvent was reduced (~1-2 mL) *in vacuo* and stored at room temperature to give colourless crystals that were washed with cold hexane. Yield 97 mg, 45%.

m.p.: 184–186 °C (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 0.43 (s, 6H, Si*Me*$_2$), 0.46 (s, 6H, Si*Me*$_2$), 1.33 – 1.47 (m, 6H, Cy–*H*), 1.48 – 1.54 (m, 12H, Ad–*H*), 1.55 – 1.85 (m, 14H, Cy–*H*), 1.86 – 2.03 (m, 18H, Ad–*H*), 2.03 – 2.27 (m, 8H, Cy–*H*), 2.43 – 2.63 (m, 4H, Cy–*H*), 3.97 (s, 1H, N*H*), 7.01 (s, 1H, Ar–*H*), 7.13 (s, 1H, Ar–*H*).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ 6.5, 8.4 (Si*Me*$_2$), 26.5, 26.8, 26.9, 27.6, 27.8, 27.9 (Cy–*C*), 31.0 (Ad–*C*), 33.4, 35.8 (Cy–*C*), 36.5 (Ad–*C*), 37.8, 41.2, 45.2 (Cy–*C*), 48.1, 53.0 (Ad–*C*), 55.0 (Cy–*C*), 121.7, 122.0, 130.3, 135.3, 135.6, 144.7 (Ar–*C*).

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6): δ -3.9 (*Si*Me_2).

^{119}Sn{^{1}H} NMR (149 MHz, C_6D_6): δ -29.6 (*Sn*).

IR ν/cm^{-1} (solid): 723 (m), 786 (s), 816 (w), 865 (s), 939 (w), 962 (m), 988 (s), 1006 (m), 1096 (m), 1118 (m), 1249 (s), 1442 (s), 2844 (s), 2900 (s).

E.A.: Anal. Calcd. for $C_{48}H_{77}N_3OSi_2Sn$ (887.04): C, 64.99; H, 8.75; N, 4.74 %. Found: C, 64.86; H, 8.86; N, 4.15 %.

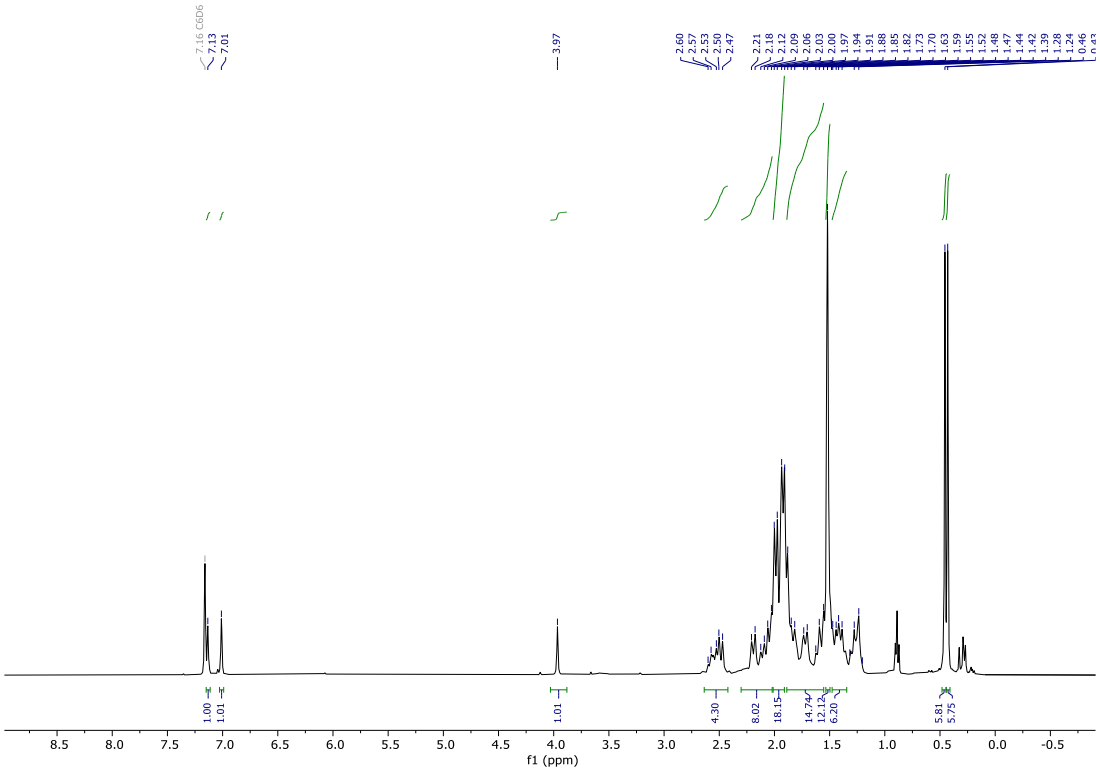


Figure S39: ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **4**.

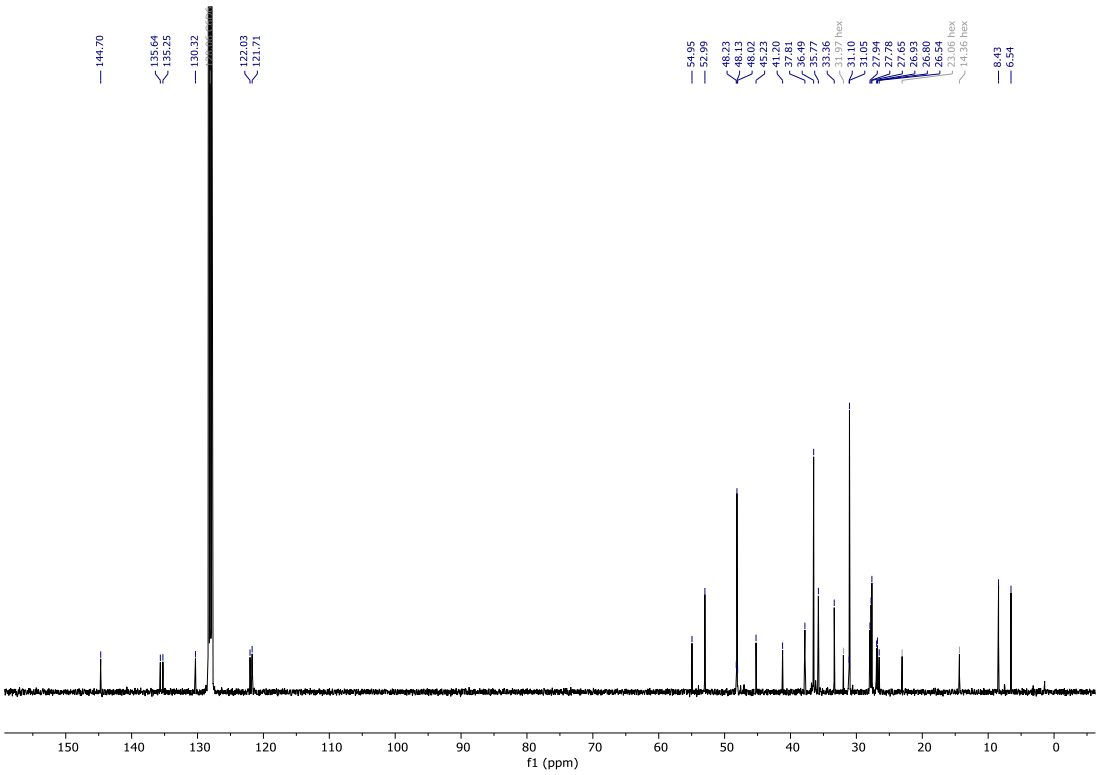


Figure S40: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **4**.

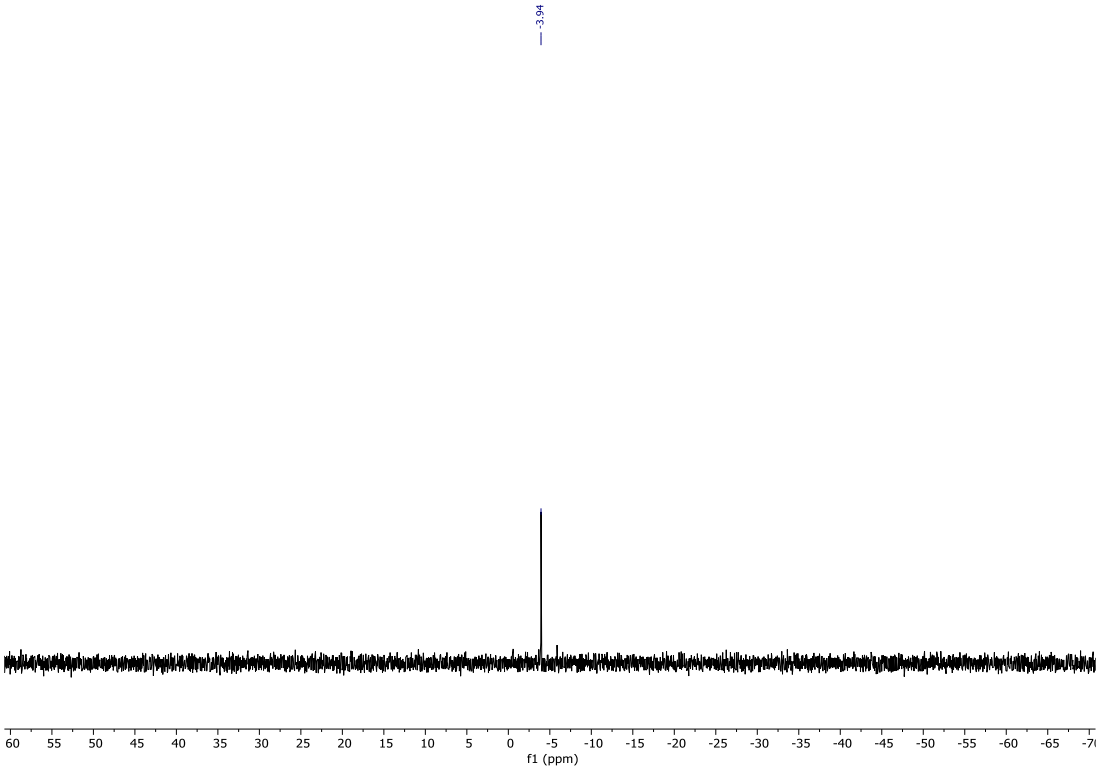


Figure S41: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of **4**.

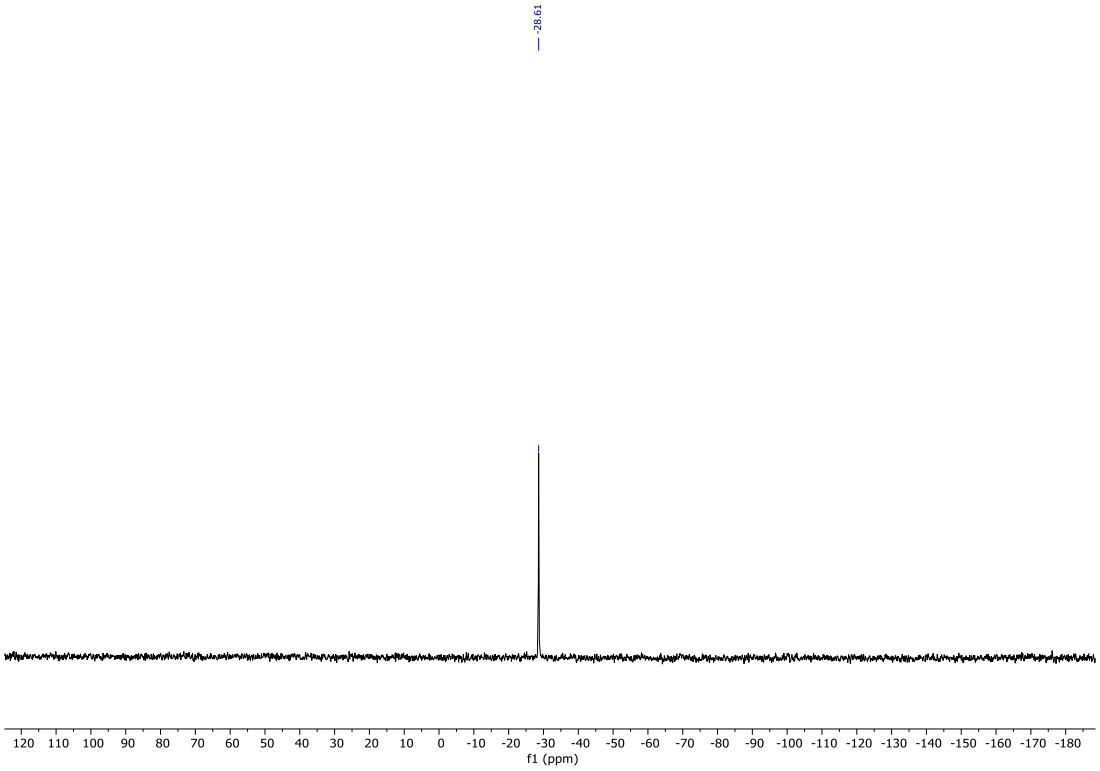


Figure S42: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, C_6D_6) of **4**.

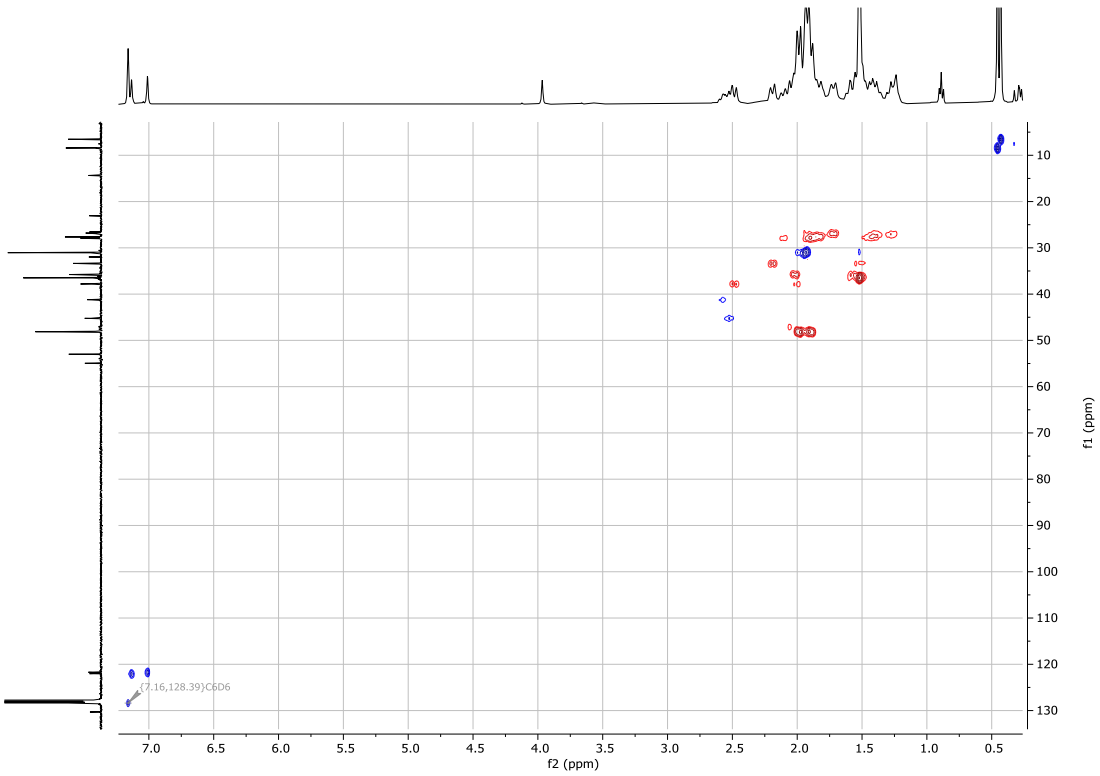


Figure S43: HSQC NMR spectrum (298 K, C_6D_6) of **4**.

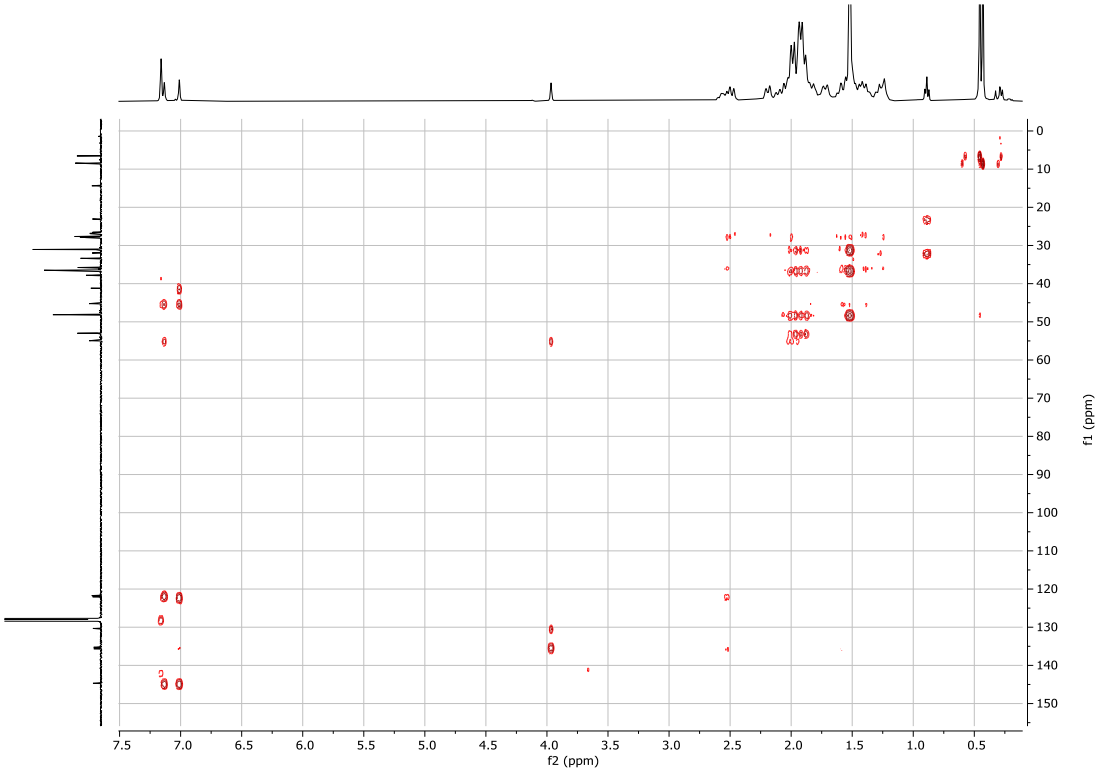


Figure S44: HMBC NMR spectrum (298 K, C_6D_6) of **4**.

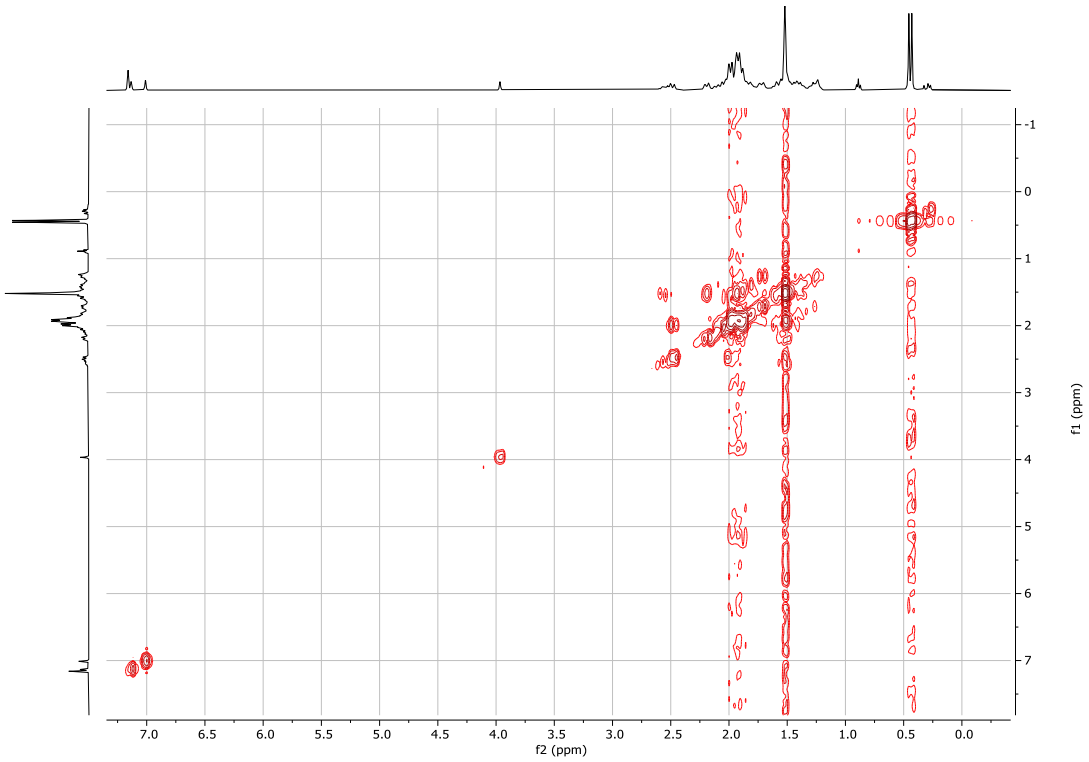


Figure S45: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of **4**.

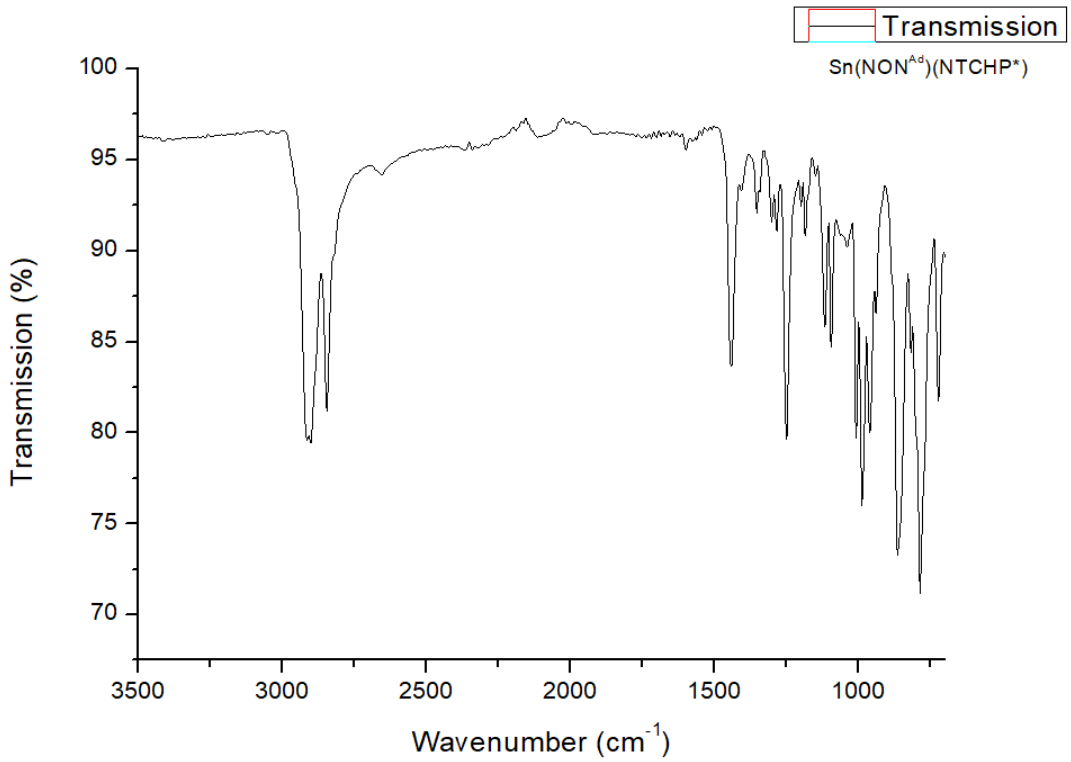


Figure S46: FT-IR spectrum of **4**.

Preparation of (NON^{Ad})Sn(OC(O)N(TCHP)) (5)

1 (200 mg, 0.36 mmol) was charged to a flame-dried Schlenk flask and hexane (~3 mL) was added. The mixture was cooled to 0 °C and 2,4,6-tricyclohexylphenyl azide (133 mg, 0.36 mmol) in hexane (~2 mL) was added in one portion. The solution was allowed to stir at room temperature for 5 minutes to give a dark red solution accompanied by vigorous gas evolution. The mixture was degassed and an atmosphere of CO_2 (pre-dried over P_2O_5) was added to give a colourless solution (instant reaction). The solvent was reduced *in vacuo* to give a colourless suspension which was dissolved in toluene (~2 mL). Crystals were obtained from a saturated solution stored at room temperature. The supernatant was decanted and the crystals were dried *in vacuo*. Yield 171 mg, 51%.

m.p.: 172–174 °C (dec).

^{1}H NMR (400 MHz, C_6D_6): δ 0.14 (s, 6H, Si*Me*$_2$), 0.21 (s, 6H), 1.14 – 1.43 (m, 8H, Cy–*H*), 1.45 – 1.60 (m, 16H, Cy–*H*, Ad–*H*), 1.62 – 1.89 (m, 10H), 1.86 – 2.19 (m, 27H, Cy–*H*, Ad–*H*), 2.49 – 2.60 (m, 1H, Cy–*H*), 2.77 – 2.87 (m, 2H, Cy–*H*), 3.60 – 3.73 (m, 2H, Cy–*H*), 7.30 (s, 2H, Ar–*H*).

$^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ 5.5, 5.9 (Si*Me*$_2$), 26.6, 26.9, 27.2, 27.2, 27.4 (Cy–*C*), 30.7 (Ad–*C*), 33.7, 35.0 (Cy–*C*), 35.9 (Ad–*C*), 37.2, 38.9, 45.1 (Cy–*C*), 49.2, 54.4 (Ad–*C*), 122.9, 135.2, 146.2, 147.0 (Ar–*C*), 160.8 (N*C*O$_2$).

$^{29}Si\{^1H\}$ NMR (80 MHz, C_6D_6): δ 4.6 (*Si*Me$_2$).

$^{1119}Sn\{^1H\}$ NMR (149 MHz, C_6D_6): δ -246.2 (*Sn*).

IR ν/cm^{-1} (solid): 723 (m), 775 (w), 805 (s), 842 (w), 861 (s), 924 (s), 965 (w), 980 (w), 1010 (w), 1066 (w), 1100 (w), 1148 (m), 1174 (w), 1252 (s), 1301 (m), 1446 (m), 1692 (s), 2848 (s), 2911 (s).

E.A.: Anal. Calcd. for $C_{49}H_{77}N_3O_3Si_2Sn\cdot(C_7H_8)$ (1023.19): C, 65.74; H, 8.37; N, 4.11 %. Found: C, 65.97; H, 8.54; N, 3.85 %.

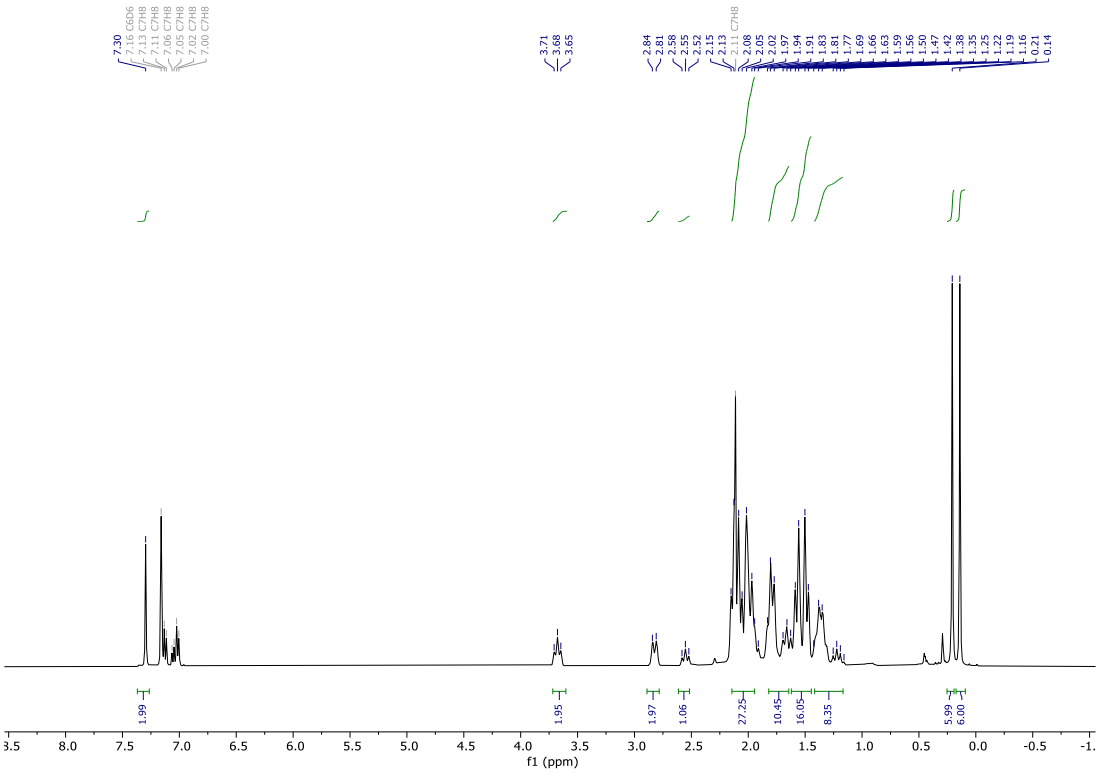


Figure S47: ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **5**.

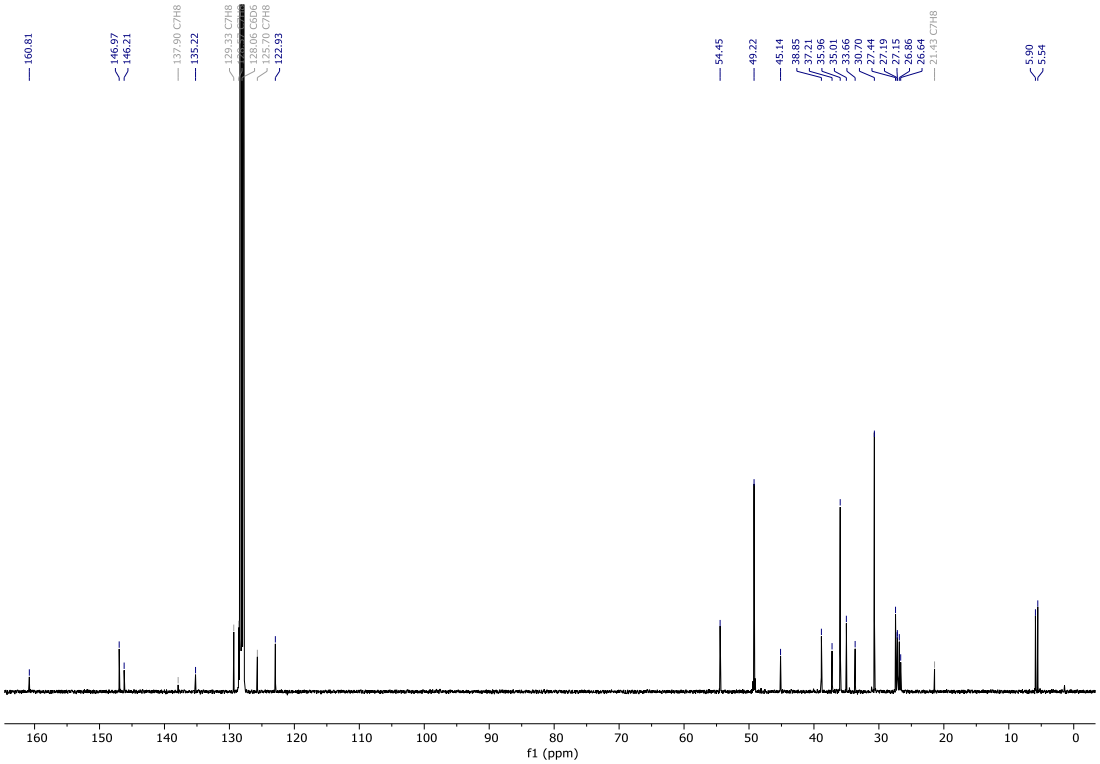


Figure S48: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **5**.

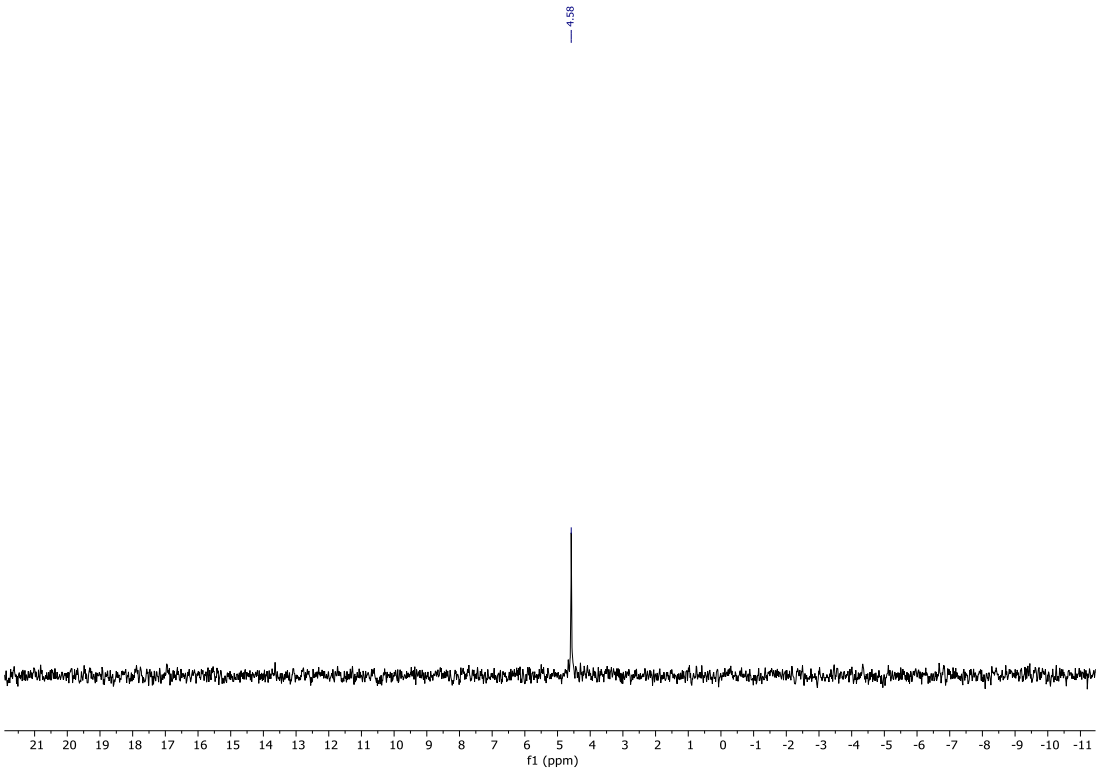


Figure S49: $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of **5**.

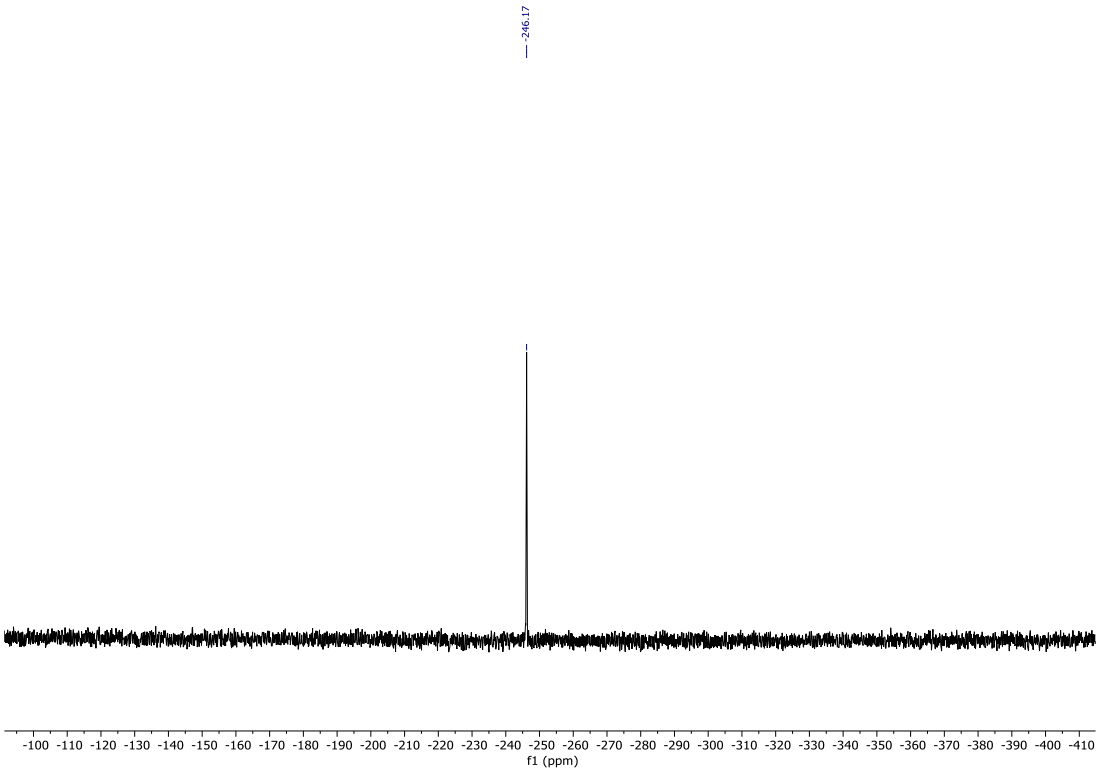


Figure S50: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, C_6D_6) of **5**.

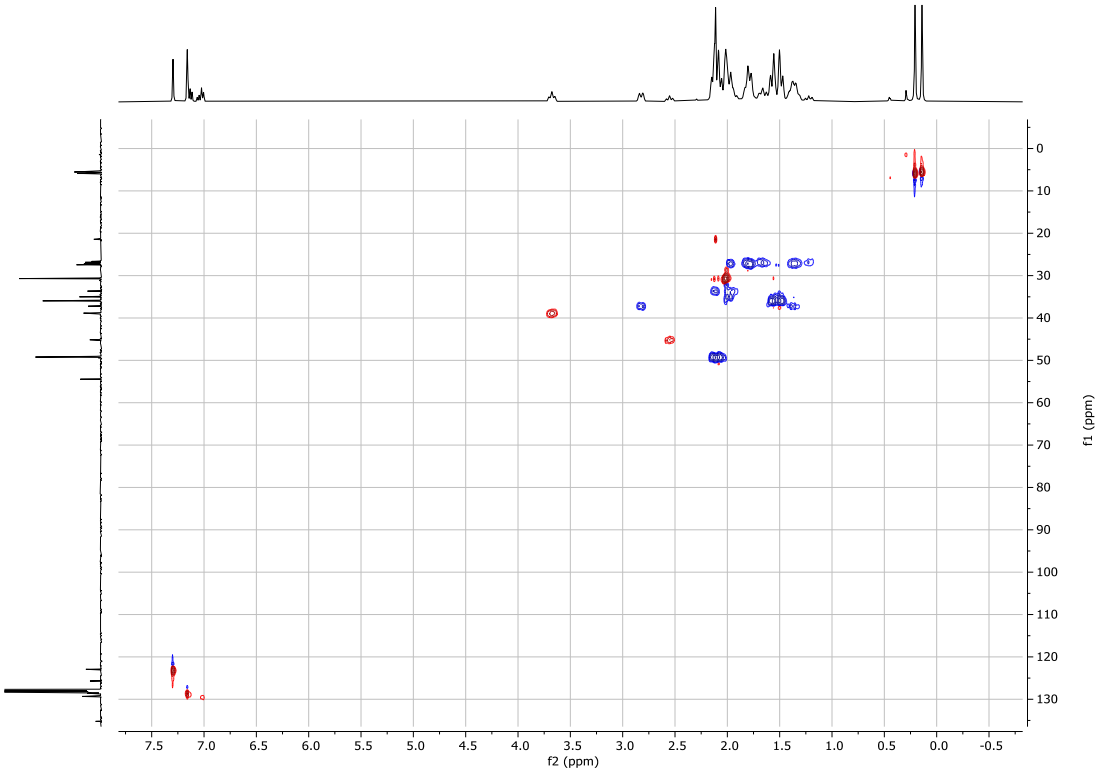


Figure S51: HSQC NMR spectrum (298 K, C_6D_6) of **5**.

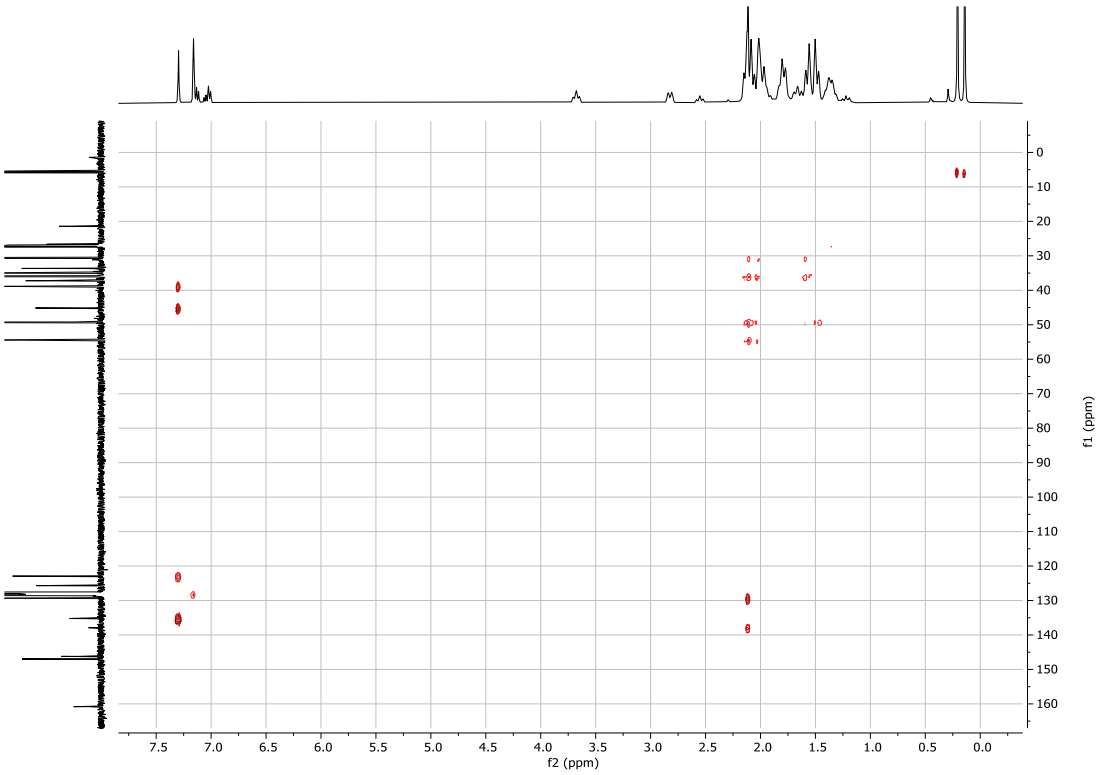


Figure S52: HMBC NMR spectrum (298 K, C_6D_6) of **5**.

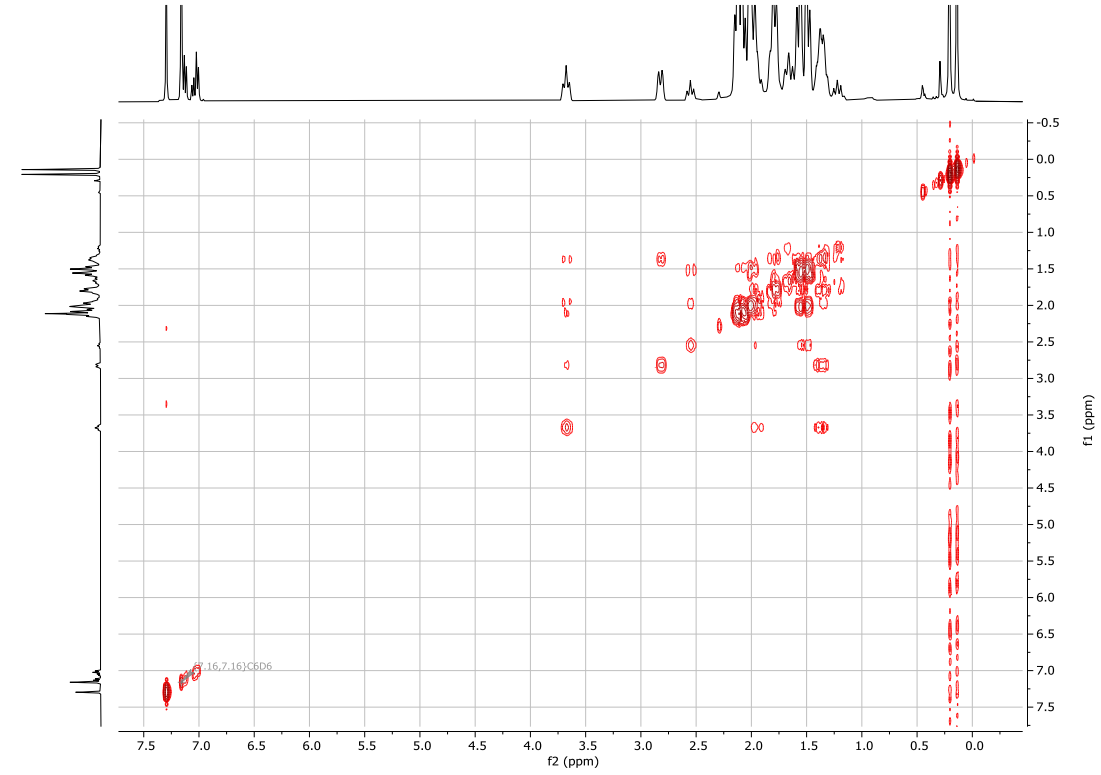


Figure S53: ^{1}H–^{1}H COSY NMR spectrum (298 K, C_6D_6) of **5**.

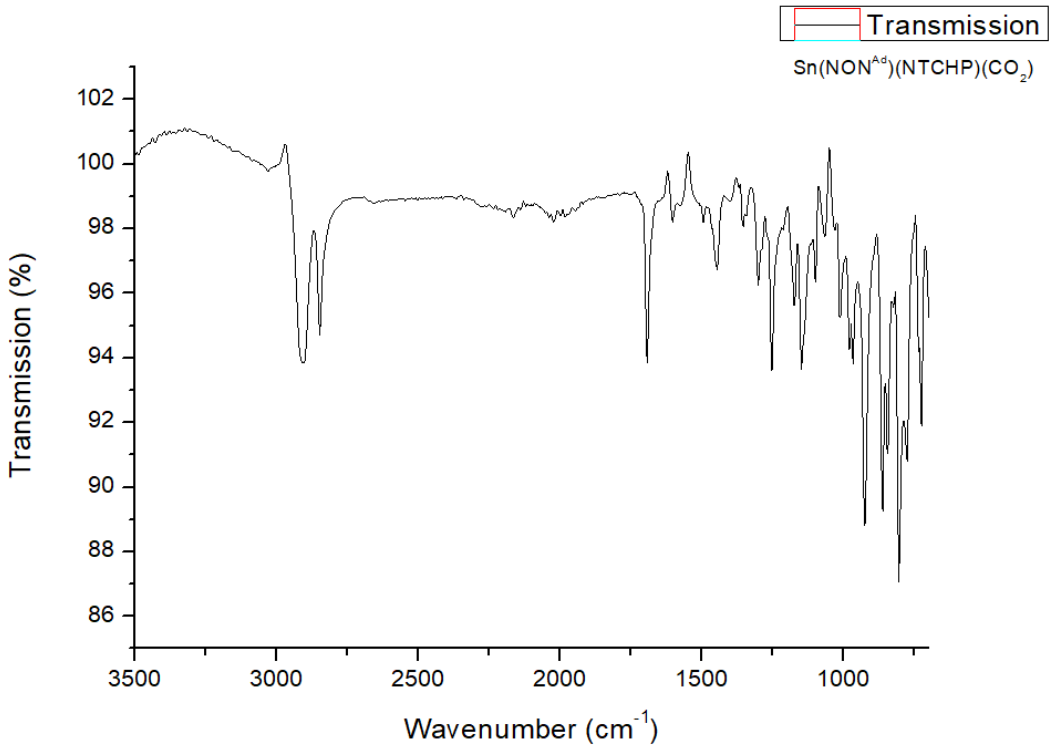


Figure S54: FT-IR spectrum of **5**.

Preparation of [Sn(NON^{Ad})(μ-O)]$_2$ (6)

A solution of **5** (30 mg, 0.03 mmol) was charged to a J Young fitted NMR tube and benzene-D_6 was added (~0.6 mL). The mixture was heated at 100 °C for 72 hours to give colourless crystals. The supernatant was decanted and the crystals were dried *in vacuo*. Yield 8 mg, 44%.

m.p.: >300 °C.

^{1}H NMR (400 MHz, CD_2Cl_2): δ 0.22 (s, 6H, Si*Me*$_2$), 0.32 (s, 6H, Si*Me*$_2$), 1.55 – 1.66 (m, 12H, Ad–*H*), 1.77 – 1.98 (m, 12H, Ad–*H*), 2.02 – 2.13 (m, 6H, Ad–*H*).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2): δ 5.9, 6.3 (Si*Me*$_2$), 31.0, 36.5, 49.7, 53.4 (Ad–*C*).

^{119}Sn{^{1}H} NMR (149 MHz, CD_2Cl_2): δ -157.4 (*Sn*).

IR ν/cm^{-1} (solid): 731 (s), 786 (s), 801 (m), 824 (w), 850 (s), 865 (s), 954 (s), 969 (s), 1014 (s), 1100 (m), 1129 (s), 1144 (s), 1245 (m), 2848 (m), 2904 (s).

E.A.: Anal. Calcd. for $C_{48}H_{84}N_4O_4Si_4Sn_2\cdot(C_6D_6)_2$ (1299.29): C, 55.47; H, 8.38; N, 4.31 %. Found: C, 56.28; H, 7.38; N, 3.96 %.

*Signals could not be detected in the $^{29}Si\{^{1}H\}$ NMR spectrum after 1000 scans (5 second relaxation delay).

The supernatant from the reaction mixture was assayed by HRMS and shown to contain 2,4,6-tricyclohexylphenyl isocyanate and 1-adamantyl-3-(2,4,6-tricyclohexylphenyl)urea. Slow evaporation of this solution yielded a small number of crystals of the unsymmetrical urea suitable for X-ray diffraction analysis.

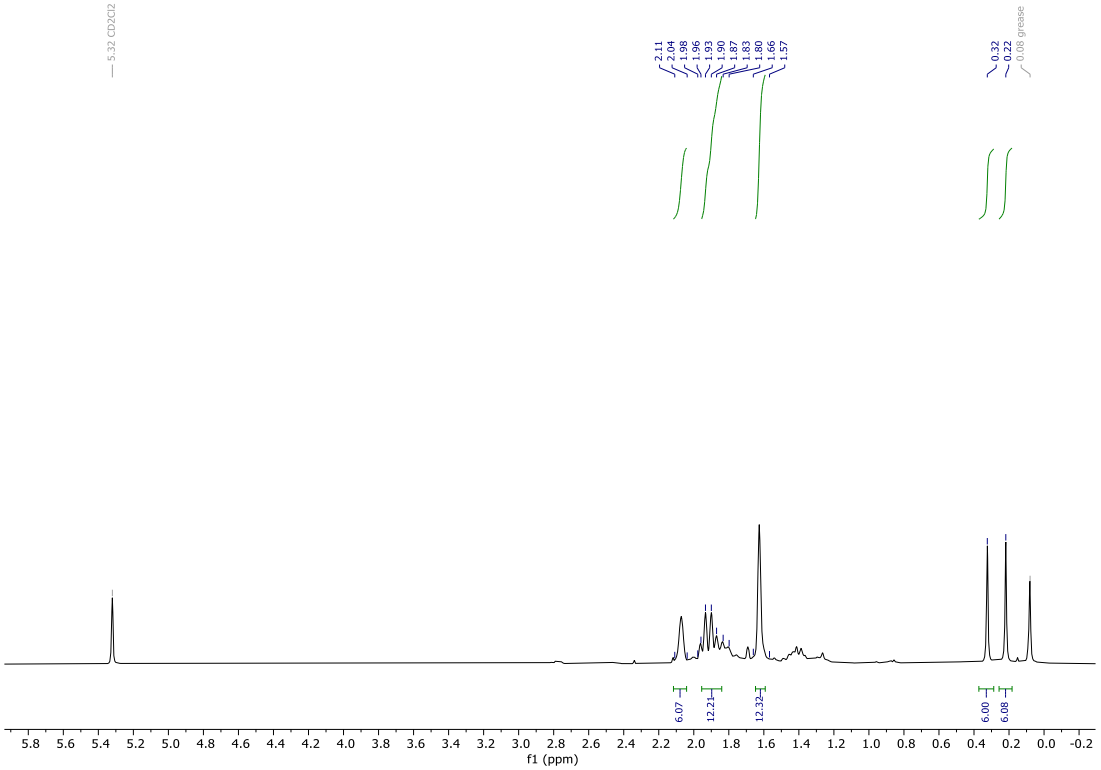


Figure S55: ^{1}H NMR spectrum (400 MHz, 298 K, CD_2Cl_2) of **6**.

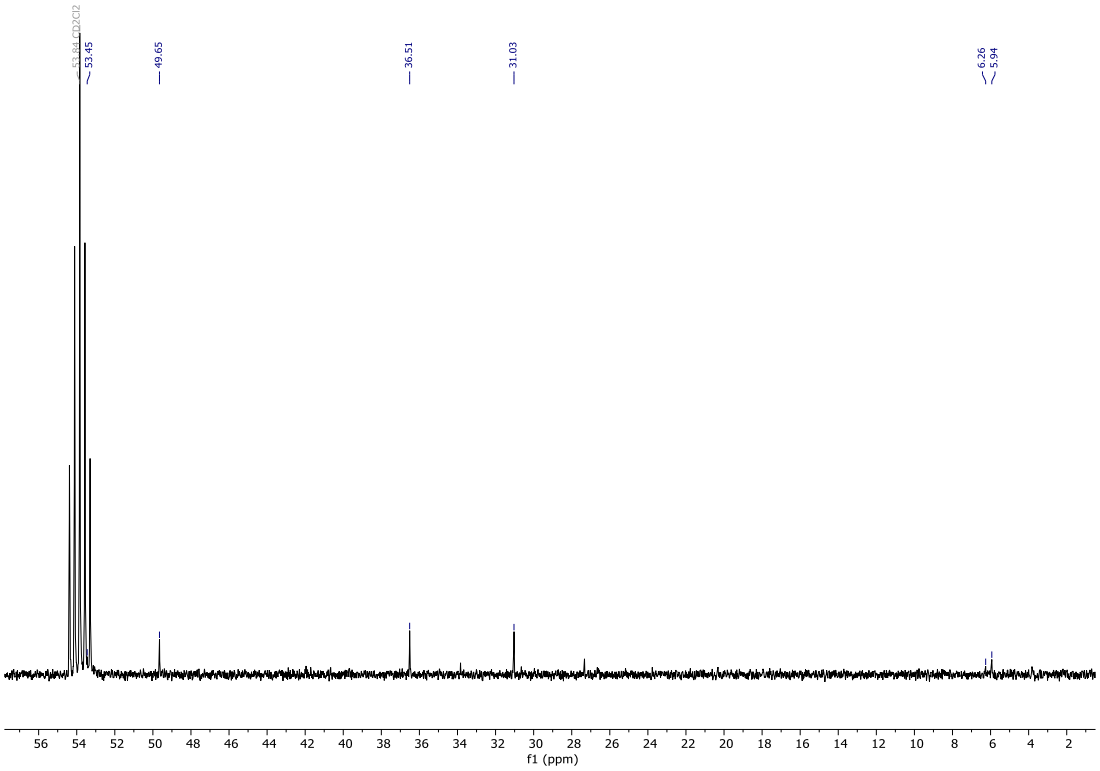


Figure S56: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, CD_2Cl_2) of **6**.

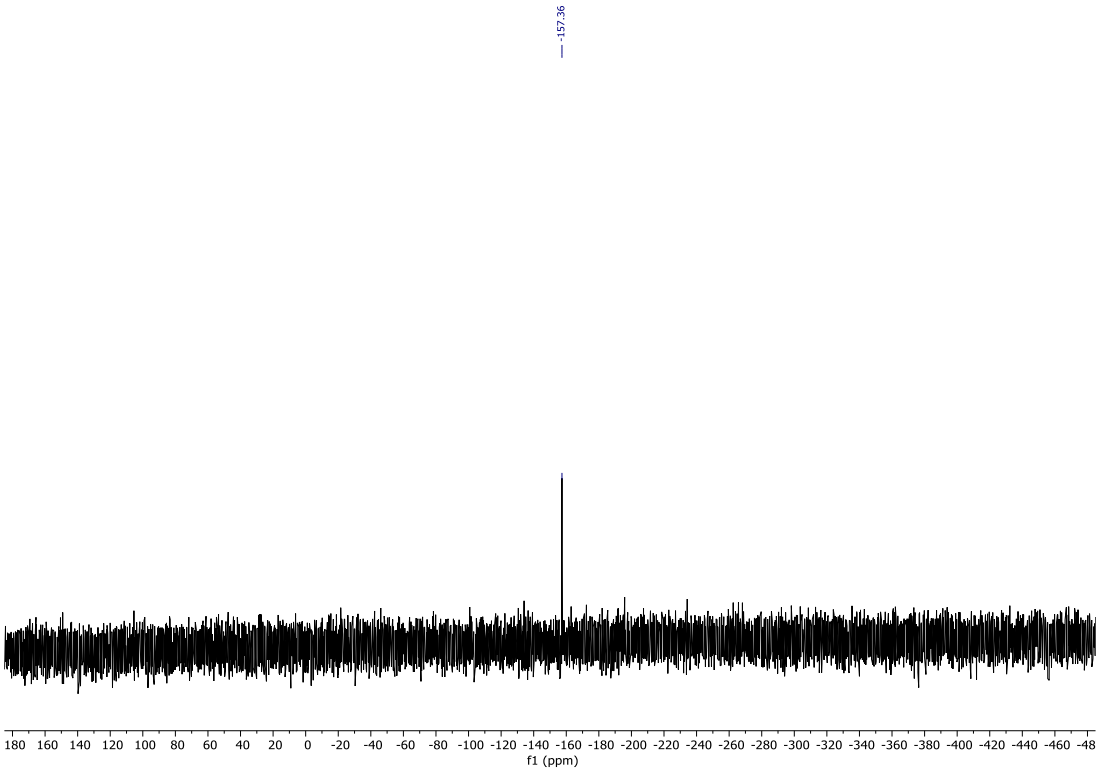


Figure S57: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, CD_2Cl_2) of **6**.

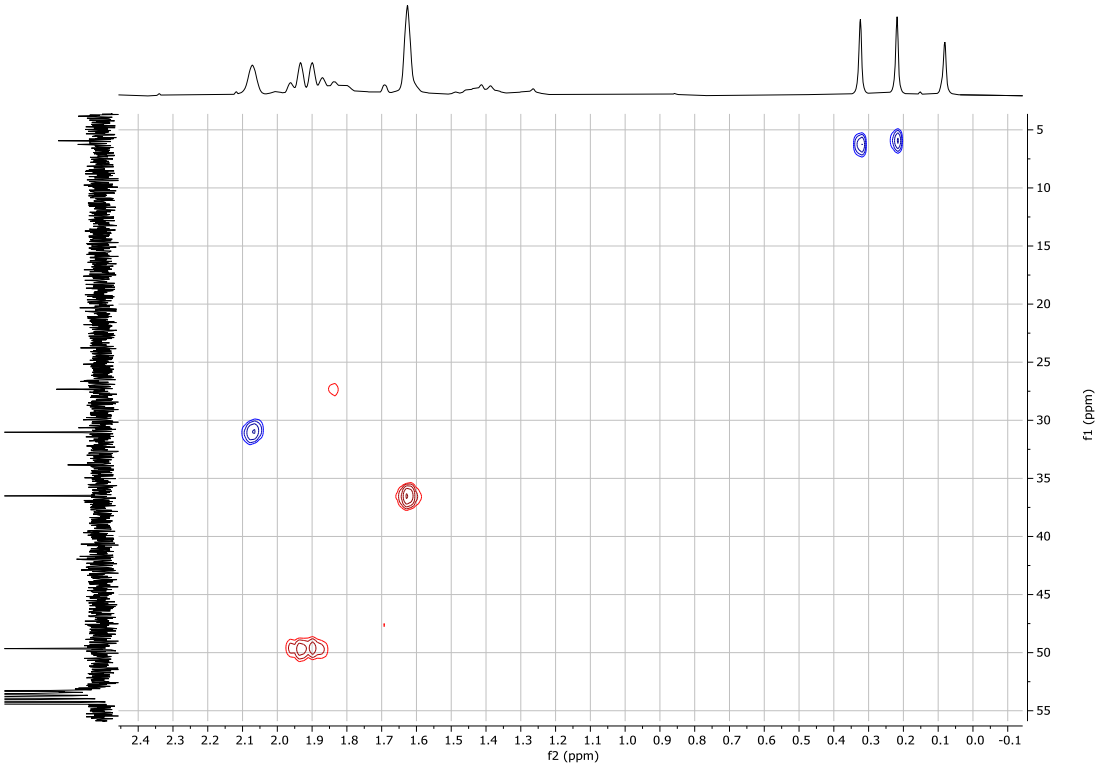


Figure S58: HSQC NMR spectrum (298 K, CD_2Cl_2) of **6**.

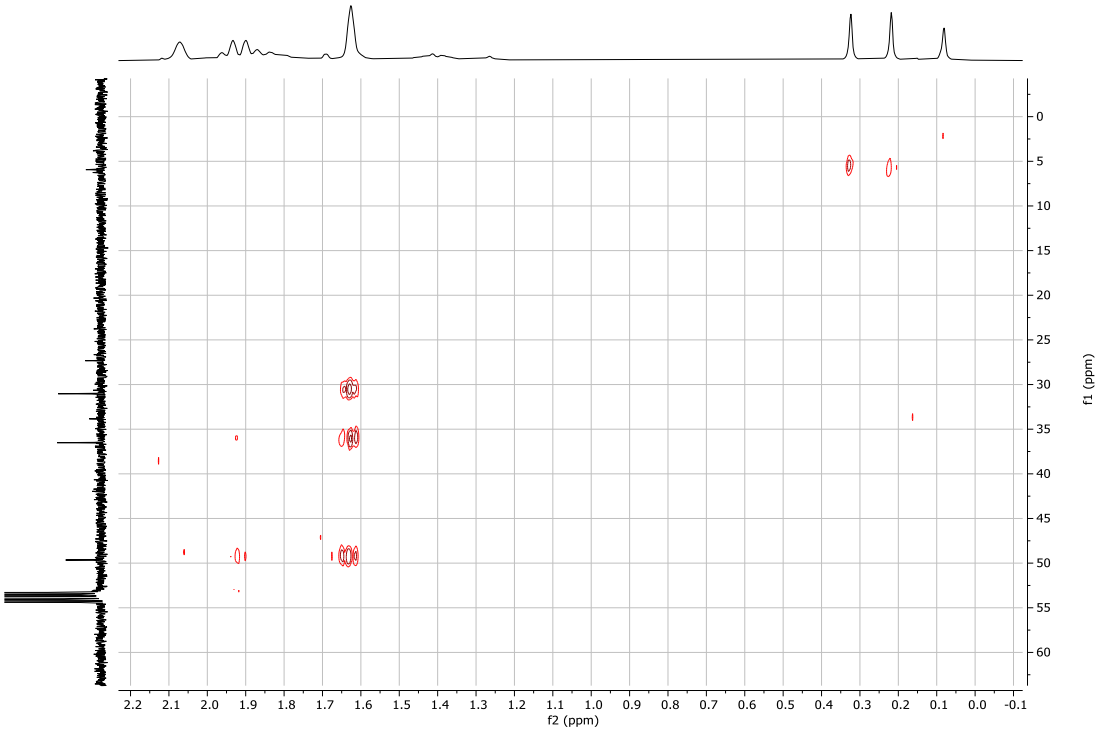


Figure S59: HMBC NMR spectrum (298 K, CD_2Cl_2) of **6**.

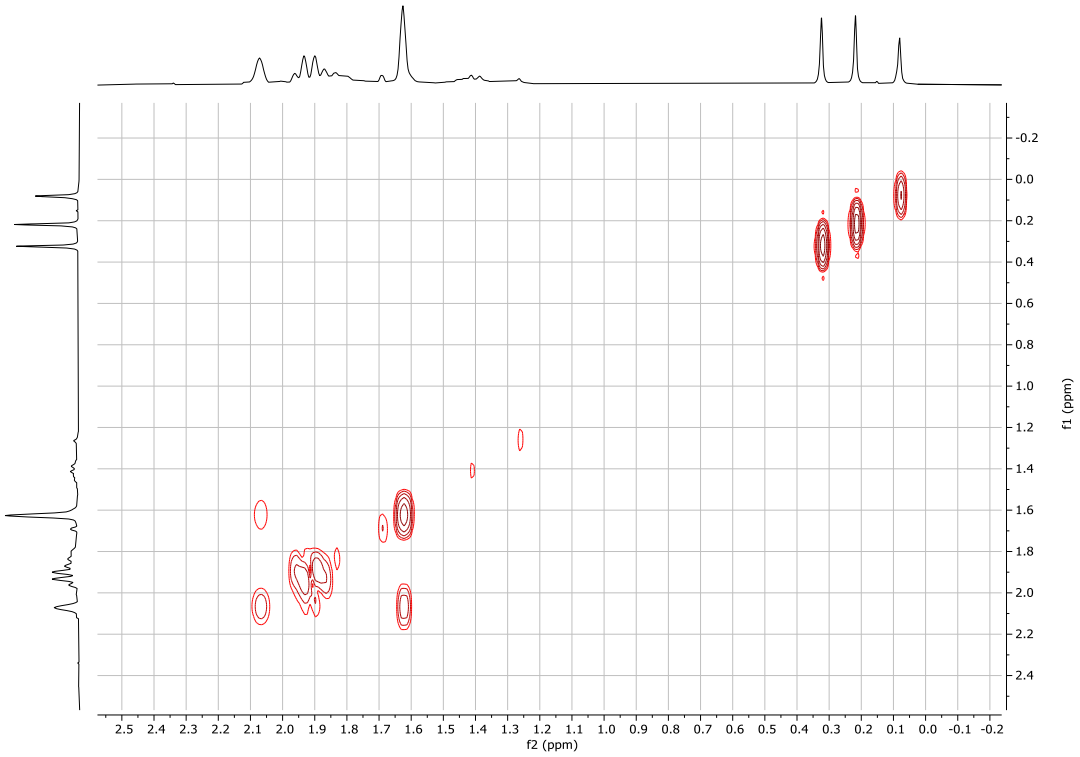


Figure S60: $^{1}H–^{1}H$ COSY NMR spectrum (298 K, CD_2Cl_2) of **6**.

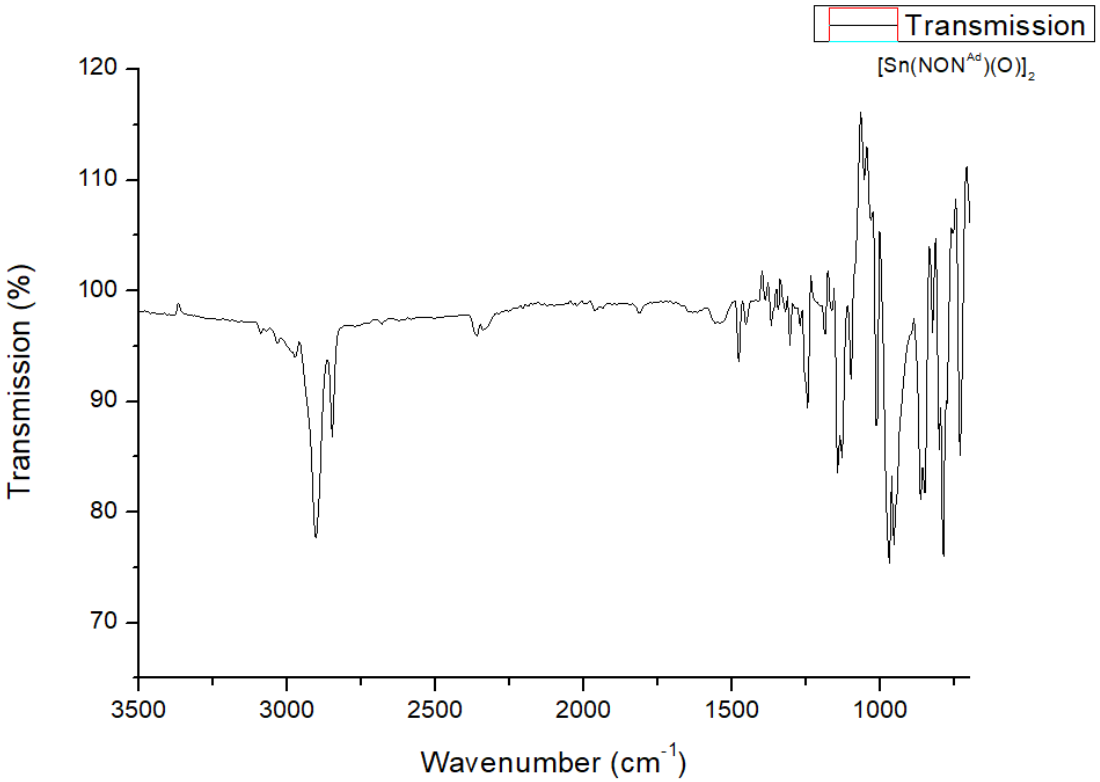


Figure S61: FT-IR spectrum of **6**.

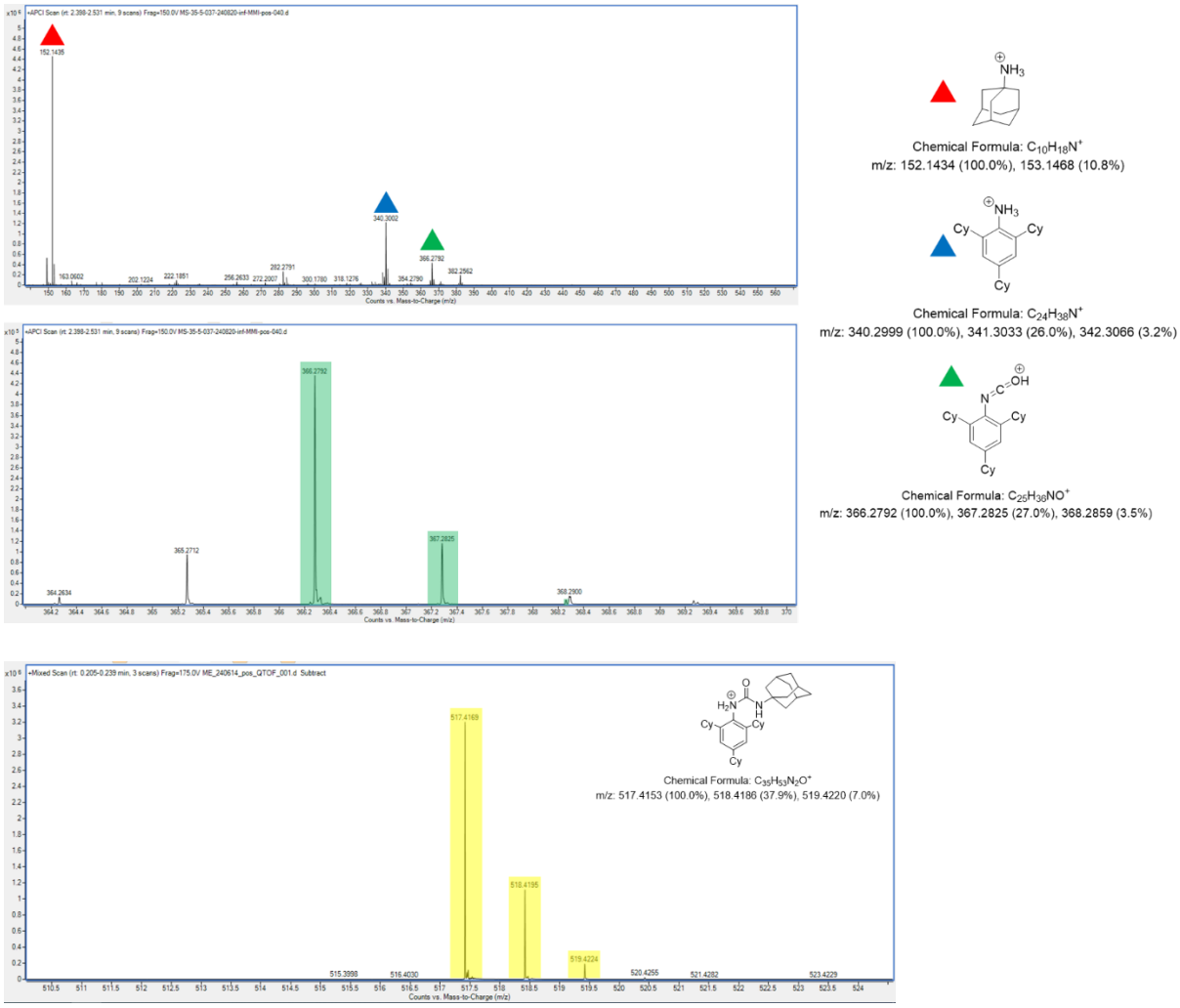


Figure S62: HRMS spectra of an aliquot of the supernatant of the reaction that gave **6**, showing formation of (TCHP)NCO after 24 hours heating (top), and onward formation of TCHP-NH-CO-NH-Ad after 72 hours heating (bottom).

Preparation of [Sn(NON^{Ad})(μ-S)]$_2$ (7)

1 (100 mg, 0.18 mmol) was charged to a flame-dried Schlenk flask and hexane (~3 mL) was added. The mixture was cooled to 0 °C and 2,4,6-tricyclohexylphenyl azide (66 mg, 0.18 mmol) in hexane (~2 mL) was added in one portion. The solution was allowed to stir at room temperature for 5 minutes to give a dark red solution accompanied by vigorous gas evolution. Carbon disulphide (0.05 mL, excess) was added to the reaction mixture and stirred for 15 minutes to give a pale orange/red solution. The solvent was reduced (~1-2 mL) *in vacuo* and stored at room temperature to give colourless crystals. The supernatant was decanted and the crystals were dried *in vacuo*. Yield 63 mg, 60%.

m.p.: >300 °C (dec).

^{1}H NMR (400 MHz, CD_2Cl_2): δ 0.27 (s, 12H, Si*Me*$_2$), 1.56 – 1.70 (m, 12H, Ad–*H*), 1.91 – 2.15 (m, 18H, Ad–*H*).

^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2): δ 5.6, 7.1 (Si*Me*$_2$), 31.2, 36.6, 48.9, 54.7 (Ad–*C*).

^{119}Sn{^{1}H} NMR (149 MHz, CD_2Cl_2): δ -122.2 (*Sn*).

IR ν/cm^{-1} (solid): 731 (m), 790 (s), 820 (w), 857 (s), 958 (s), 980 (s), 1010 (m), 1096 (m), 1129 (m), 1185 (w), 1252 (s), 1305 (w), 1450 (w), 2848 (m), 2896 (s).

E.A.: Anal. Calcd. for $C_{48}H_{84}N_4O_3Si_4Sn_2S\cdot(CS_2)$ (1239.24): C, 47.49; H, 6.83; N, 4.52 %. Found: C, 47.73; H, 6.66; N, 3.96 %.

*Signals could not be detected in the ^{29}Si{^{1}H} NMR spectrum after 1000 scans (5 second relaxation delay).

The supernatant from the reaction mixture was assayed by HRMS and shown to contain 2,4,6-tricyclohexylphenyl isothiocyanate.

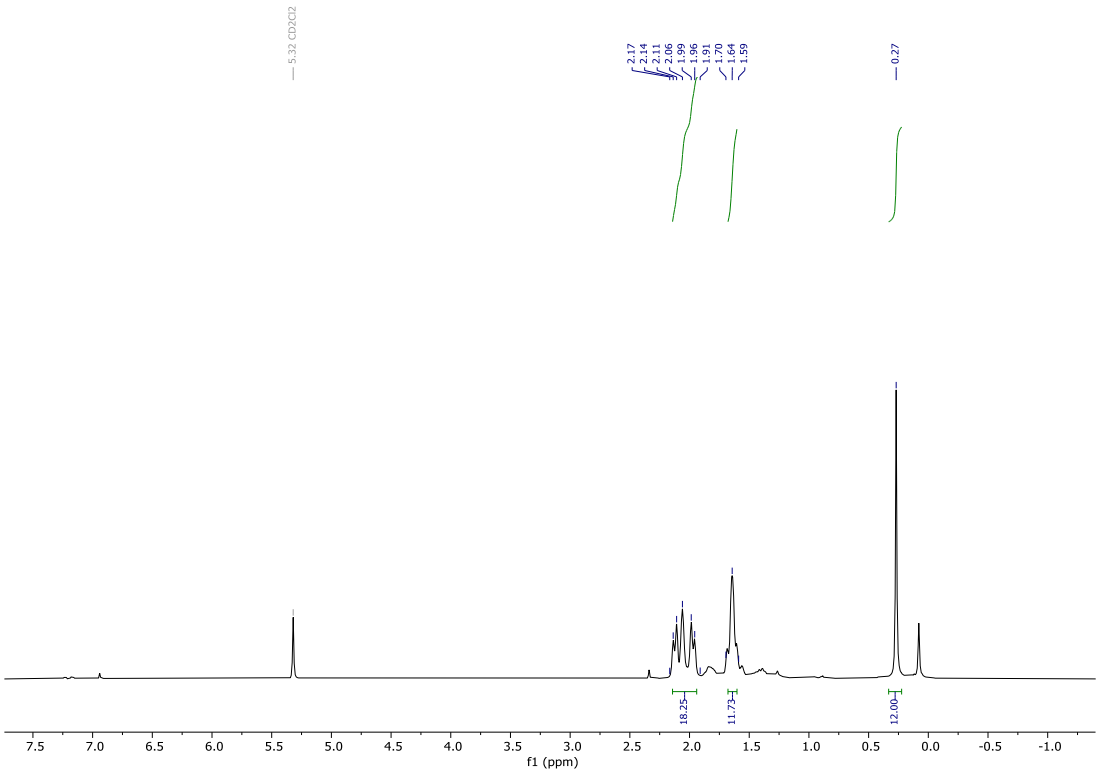


Figure S63: ^{1}H NMR spectrum (400 MHz, 298 K, CD_2Cl_2) of **7**.

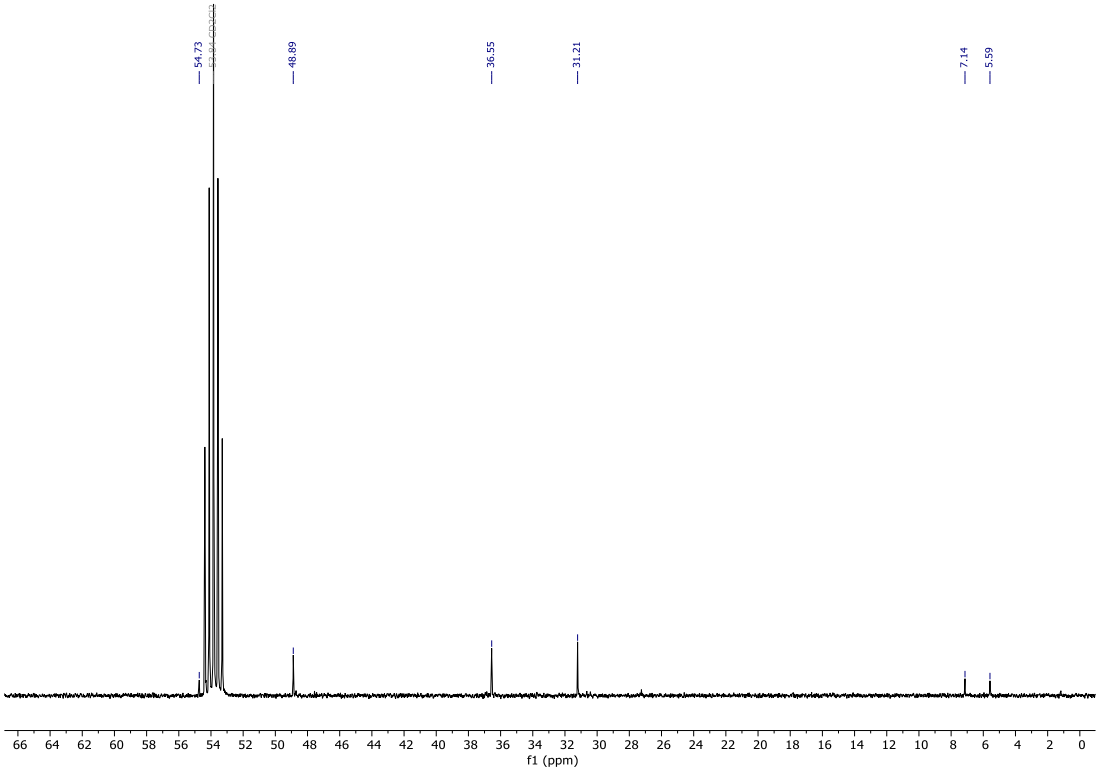


Figure S64: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, CD_2Cl_2) of **7**.

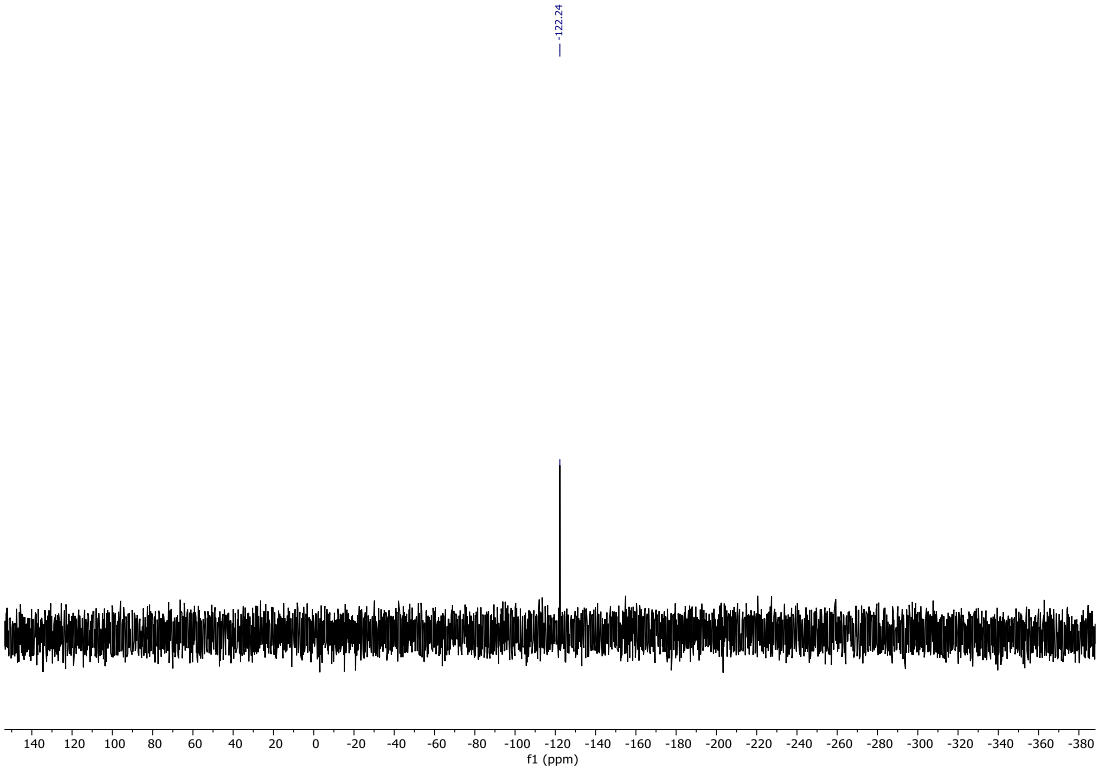


Figure S65: $^{119}Sn\{^{1}H\}$ NMR spectrum (149 MHz, 298 K, CD_2Cl_2) of **7**.

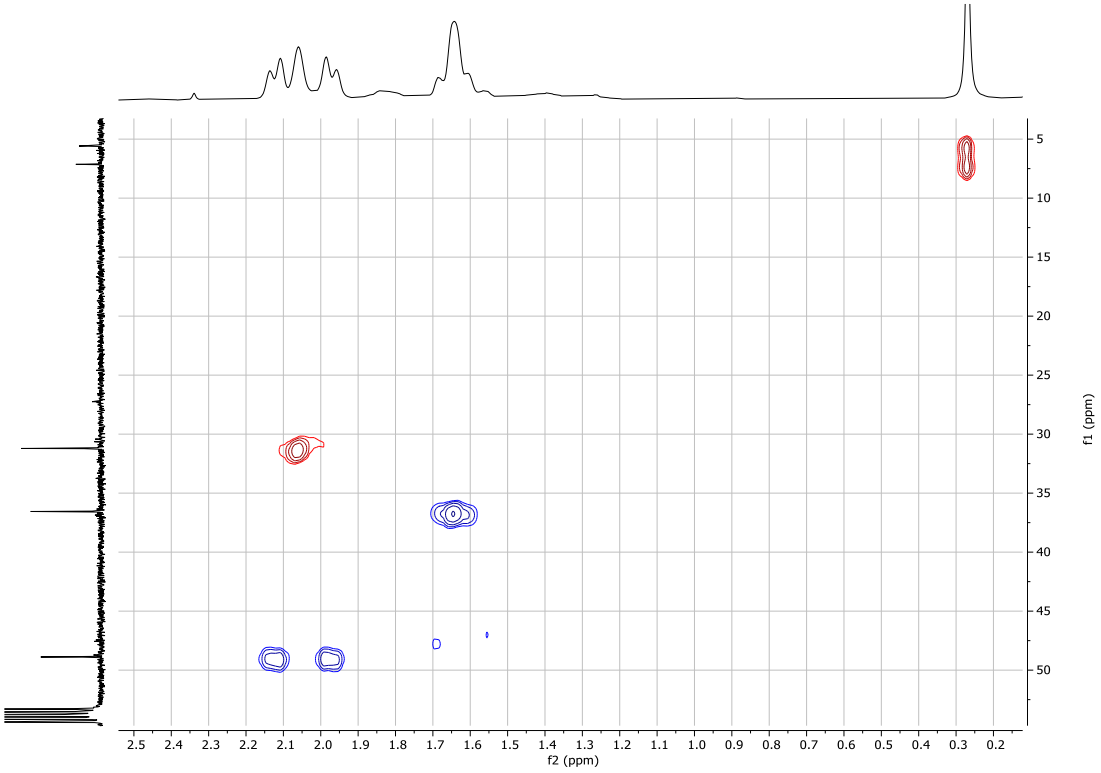


Figure S66: HSQC NMR spectrum (298 K, CD_2Cl_2) of **7**.

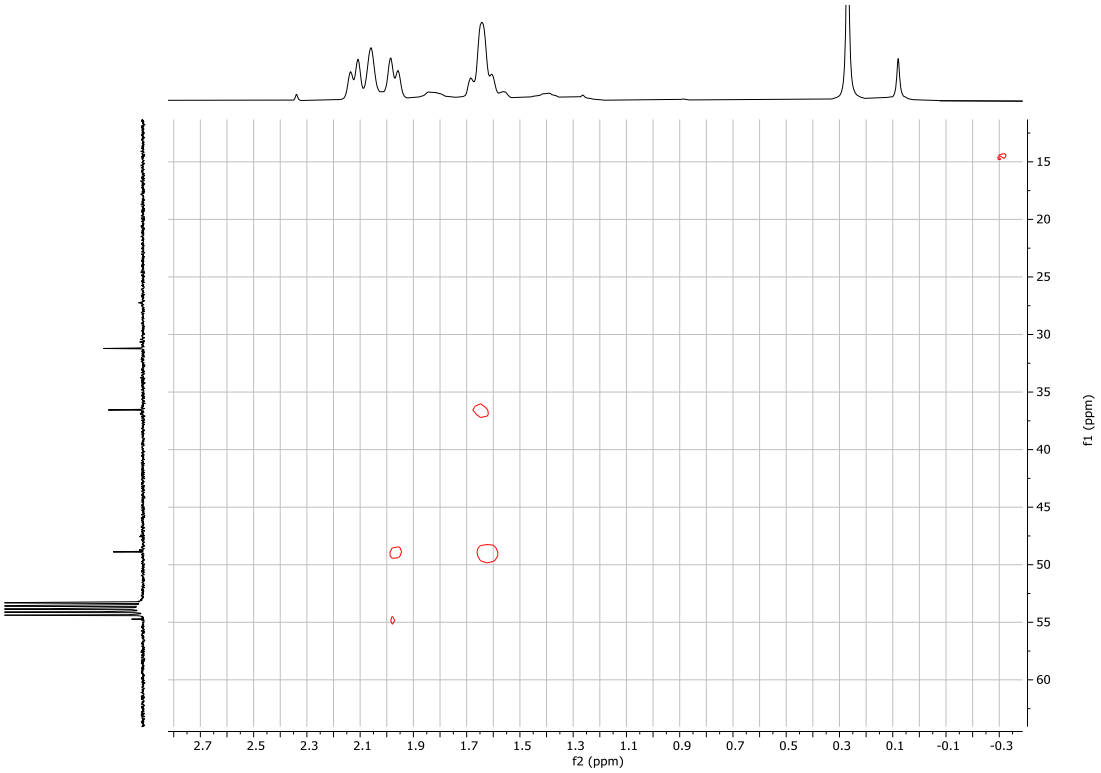


Figure S67: HMBC NMR spectrum (298 K, CD_2Cl_2) of **7**.

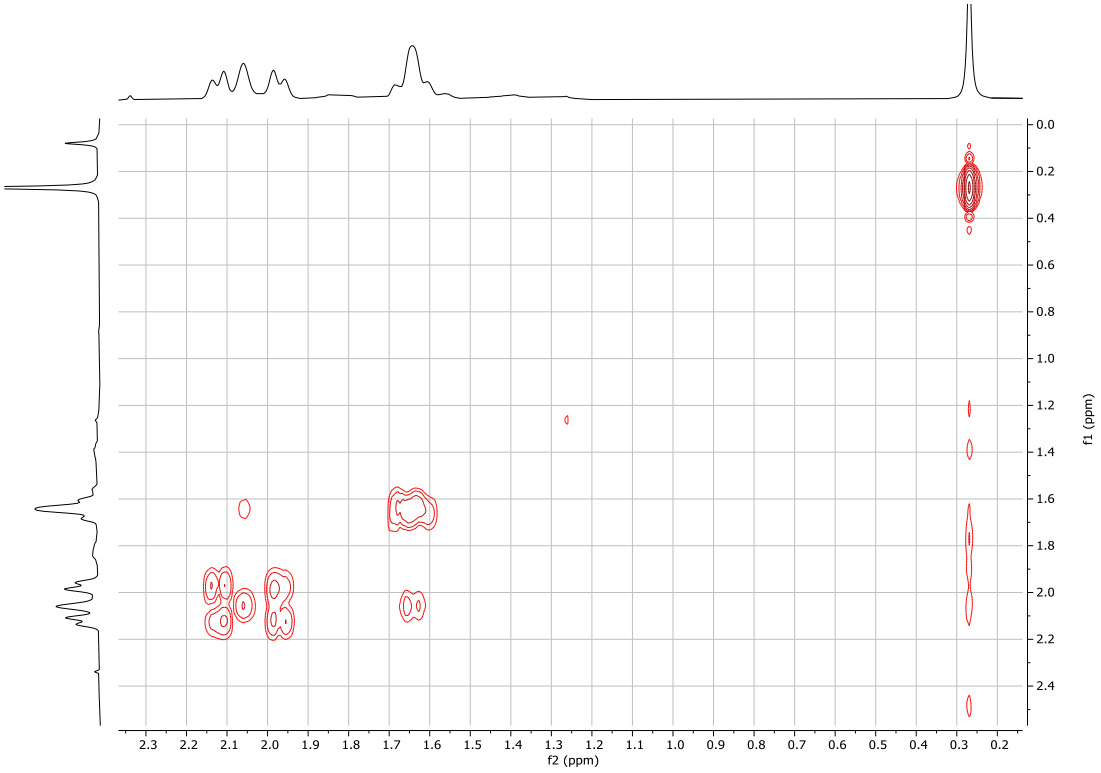


Figure S68: $^{1}H–^{1}H$ COSY NMR spectrum (298 K, CD_2Cl_2) of **7**.

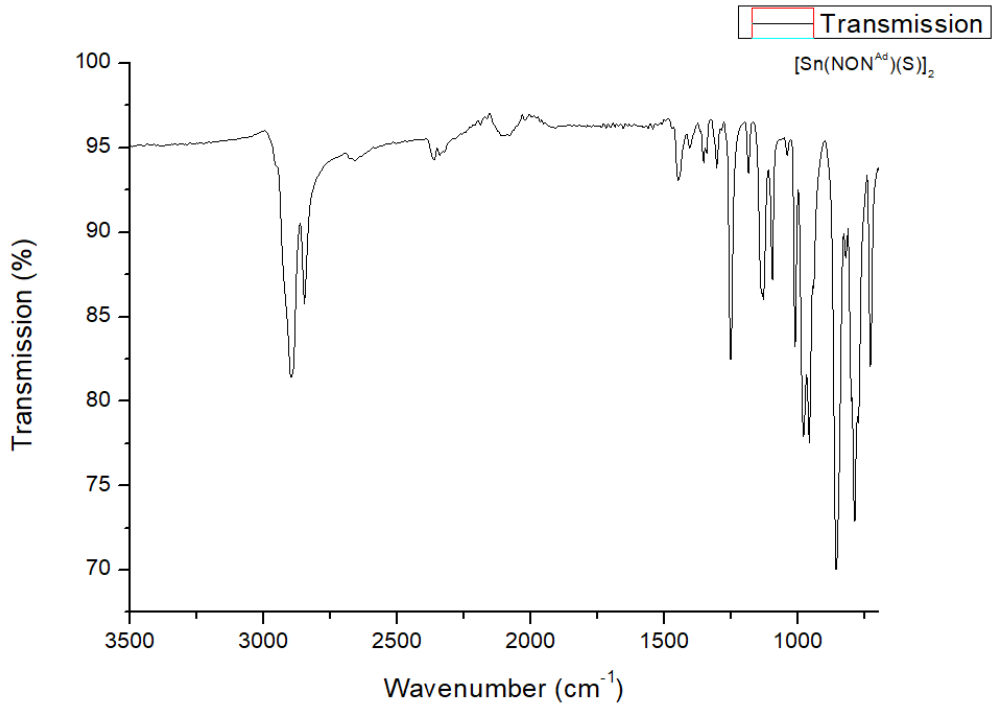
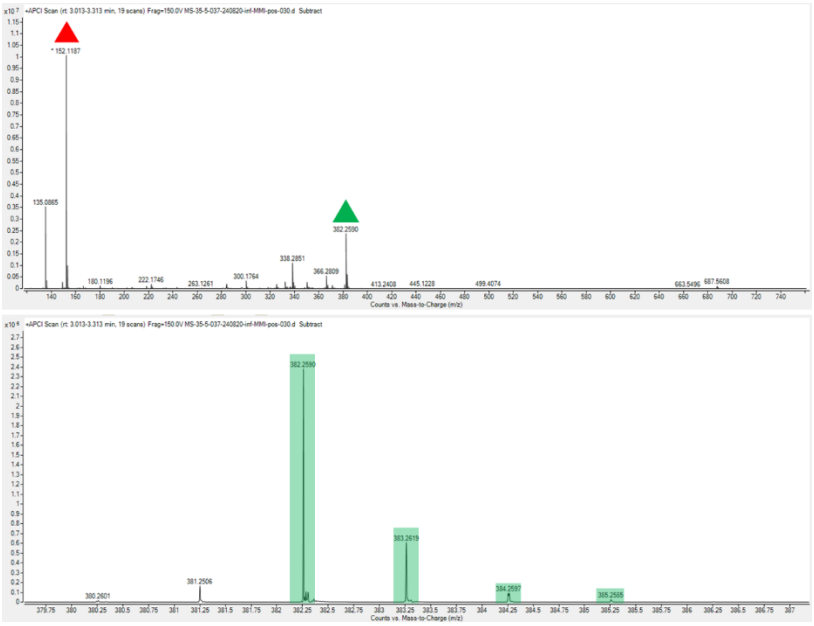
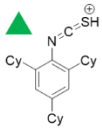


Figure S69: FT-IR spectrum of **7**.



Chemical Formula: $C_{10}H_{18}N^+$
m/z: 152.1434 (100.0%), 153.1468 (10.8%)



Chemical Formula: $C_{25}H_{36}NS^+$
m/z: 382.2563 (100.0%), 383.2597 (27.0%), 384.2521 (4.5%), 384.2631 (3.5%), 385.2555 (1.2%)

Figure S70: HRMS spectrum of an aliquot of the reaction mixture that gave **7**.

2. X-ray Crystallography

General Details

Crystals suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using a Rigaku Xtalab Synergy Dualflex using a graphite monochromator with Cu Kα (1.54180 Å) or Mo Kα (0.71073 Å), or the MX1/MX2 beamlines of the Australian Synchrotron (λ = 0.71090 Å). The software package Blu-Ice[S4] was used for synchrotron data acquisition, while the program XDS[S5] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX-18)[S6] using all unique data. Hydrogen atoms were included in calculated positions (riding model). Crystal data, details of data collections, and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1: Crystallographic Data for Compounds TCHP-MgBr, TCHP-N_3, TCHP-NH-CO-NH-Ad and **1–7**.

Compound	**TCHP-MgBr**	**TCHP-N_3**	**1**	**$[1]_2$**
Empirical formula	$C_{24}H_{35}N_3$	$C_{35.5}H_{55}BrMgO_2$	$C_{24}H_{42}N_2OSi_2Sn$	$C_{48}H_{84}N_4O_2Si_4Sn_2$
Formula weight	365.55	618.01	549.46	1098.93
Temperature	123(2) K	100(2) K	123(2) K	123(2) K
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	*P*2$_1$/*c*	*P*-1	*C*$_2$/*c*	*P*2$_1$/*c*
Unit cell dimensions	a = 14.7377(2) Å α = 90°	a = 11.650(2) Å α = 110.10(3)°	a = 23.4081(3) Å α = 90°	a = 13.88140(10) Å α = 90°
	b = 12.0636(2) Å β = 101.9570(10)°	b = 16.270(3) Å β = 90.20(3)°	b = 9.85020(10) Å β = 117.035(2)°	b = 15.80820(10) Å β = 108.9800(10)°
	c = 12.0363(2) Å γ = 90°	c = 20.410(4) Å γ = 110.90(3)°	c = 24.8391(4) Å γ = 90°	c = 12.12920(10) Å γ = 90°
Volume	2093.50(6) Å^3	3358.7(15) Å^3	5101.44(14) Å^3	2516.92(3) Å^3
Z	4	4	8	2
Density (calculated)	1.160 Mg/m^3	1.222 Mg/m^3	1.431 Mg/m^3	1.450 Mg/m^3
Absorption coefficient	0.516 mm^{-1}	1.271 mm^{-1}	8.997 mm^{-1}	9.118 mm$_{-1}$
F(000)	800	1324	2288	1144
Crystal size	0.530 x 0.430 x 0.250 mm^3	0.150 x 0.130 x 0.080 mm^3	0.400 x 0.300 x 0.300 mm^3	0.230 x 0.100 x 0.080 mm^3
Theta range for data collection	4.780 to 79.941°	1.074 to 26.372°	3.996 to 79.851°	4.378 to 80.466°
Index ranges	-18<=h<=14, -14<=k<=15, -15<=l<=15	-14<=h<=14, -20<=k<=20, -25<=l<=25	-28<=h<=29, -12<=k<=12, -30<=l<=31	-17<=h<=16, -19<=k<=20, -15<=l<=15
Reflections collected	16061	81308	31925	61167
Independent reflections	4482 [R(int) = 0.0294]	13370 [R(int) = 0.0811]	5476 [R(int) = 0.0360]	5471 [R(int) = 0.0611]
Completeness to theta = 67.684°	100.00%	99.50%	100.00%	100.00%
Absorption correction	Gaussian	Semi-empirical from equivalents	Semi-empirical from equivalents	Sphere
Max. and min. transmission	1.000 and 0.238	Value not reported by XDS	1.00000 and 0.50485	0.09790 and 0.01535
Data / restraints / parameters	4482 / 27 / 244	13370 / 2059 / 1180	5476 / 2 / 285	5471 / 0 / 275
Goodness-of-fit on F^2	1.062	1.053	1.044	1.065
Final R indices [I>2sigma(I)]	R_1 = 0.0401, wR_2 = 0.1050	R_1 = 0.0682, wR_2 = 0.1960	R_1 = 0.0254, wR_2 = 0.0675	R1 = 0.0503, wR_2 = 0.1194
R indices (all data)	R_1 = 0.0440, wR_2 = 0.1081	R_1 = 0.1201, wR_2 = 0.2352	R_1 = 0.0258, wR_2 = 0.0679	R1 = 0.0520, wR_2 = 0.1220
Largest diff. peak and hole	0.276 and -0.194 e.Å^{-3}	0.896 and -0.747 e.Å^{-3}	0.760 and -0.765 e.Å^{-3}	2.035 and -0.368 e.Å^{-3}
CCDC Number	2375861	2375864	2375857	2375868

Table S1 (contd.): Crystallographic Data for Compounds TCHP-MgBr, TCHP-N_3, TCHP-NH-CO-NH-Ad and **1–7**.

Compound	**1 + [1]$_2$**	**2**	**3**	**3·THF**
Empirical formula	C_{24} H_{42} N_2 O Si_2 Sn	C_{42} H_{64} N_6 O Si_2 Sn	C_{60} H_{89} N_3 O Si_2 Sn	C_{58} H_{97} N_3 $O_{3.5}$ Si_2 Sn
Formula weight	549.46	843.86	1043.21	1067.25
Temperature	123(2) K	123(2) K	123(2) K	123(2) K
Crystal system	Triclinic	Triclinic	Monoclinic	Orthorhombic
Space group	*P*-1	*P*-1	*P*2$_1$/n	*Pbcn*
Unit cell dimensions	a = 12.0306(2) Å α= 101.088(2)°	a = 10.0691(2) Å α= 100.6960(10)°	a = 12.7009(2) Å α= 90°	a = 25.1156(4) Å α= 90°
	b = 12.4770(2) Å β= 90.514(2)°	b = 12.5740(2) Å β= 91.930(2)°	b = 21.8593(4) Å β= 96.796(2)°	b = 18.2987(2) Å β= 90°
	c = 18.1078(4) Å γ = 107.761(2)°	c = 18.6212(3) Å γ = 93.539(2)°	c = 19.9906(4) Å γ = 90°	c = 24.1950(3) Å γ = 90°
Volume	2533.55(9) Å^3	2309.78(7) Å^3	5511.05(17) Å^3	11119.6(3) Å^3
Z	4	2	4	8
Density (calculated)	1.441 Mg/m^3	1.213 Mg/m^3	1.257 Mg/m^3	1.275 Mg/m^3
Absorption coefficient	9.058 mm^{-1}	5.169 mm^{-1}	0.549 mm^{-1}	4.417 mm^{-1}
F(000)	1144	888	2224	4576
Crystal size	0.314 x 0.124 x 0.081 mm^3	0.400 x 0.300 x 0.300 mm^3	0.400 x 0.300 x 0.300 mm^3	0.190 x 0.170 x 0.120 mm^3
Theta range for data collection	3.868 to 80.021°	3.586 to 80.313°	3.362 to 32.333°	3.503 to 80.617°
Index ranges	-10<=h<=15, -15<=k<=15, -23<=l<=23	-12<=h<=9, -16<=k<=16, -23<=l<=23	-17<=h<=18, -30<=k<=30, -25<=l<=29	-29<=h<=31, -23<=k<=20, -30<=l<=29
Reflections collected	33647	49282	76316	61675
Independent reflections	10624 [R(int) = 0.0370]	9879 [R(int) = 0.0610]	16800 [R(int) = 0.0666]	11906 [R(int) = 0.0684]
Completeness to theta = 67.684°	99.20%	100.00%	99.70%	99.80%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.29927	1.00000 and 0.50616	1.00000 and 0.42137	1.00000 and 0.69084
Data / restraints / parameters	10624 / 0 / 549	9879 / 424 / 570	16800 / 0 / 608	11906 / 273 / 681
Goodness-of-fit on F^2	1.053	1.069	1.035	1.049
Final R indices [I>2sigma(I)]	R_1 = 0.0524, *w*R_2 = 0.1379	R_1 = 0.0362, *w*R_2 = 0.0982	R1 = 0.0393, *w*R_2 = 0.0827	R_1 = 0.0533, *w*R_2 = 0.1398
R indices (all data)	R_1 = 0.0540, *w*R_2 = 0.1389	R_1 = 0.0375, *w*R_2 = 0.1009	R1 = 0.0643, *w*R_2 = 0.0905	R_1 = 0.0667, *w*R_2 = 0.1523
Largest diff. peak and hole	3.476 and -1.398 e.Å^{-3}	1.089 and -1.645 e.Å^{-3}	0.914 and -0.553 e.Å^{-3}	0.977 and -1.927 e.Å^{-3}
CCDC Number	2375866	2375869	2375863	2375858

Table S1 (contd.): Crystallographic Data for Compounds TCHP-MgBr, TCHP-N_3, TCHP-NH-CO-NH-Ad and **1–7**.

Compound	**4**	**5**	**6**	**7**
Empirical formula	C_{48} H_{77} N_3 O Si_2 Sn	C_{49} H_{77} N_3 O_3 Si_2 Sn	C_{66} H_{102} N_4 O_4 Si_4 Sn_2	C_{62} H_{100} N_4 O_2 S_2 Si_4 Sn_2
Formula weight	886.99	931	1365.25	1347.31
Temperature	123(2) K	100(2) K	150(2) K	100(2) K
Crystal system	Triclinic	Orthorhombic	Triclinic	Monoclinic
Space group	*P*-1	*I*222	*P*-1	$P2_1/c$
Unit cell dimensions	a = 11.1935(2) Å α= 76.517(2)°	a = 15.850(3) Å α= 90°	a = 12.0275(3) Å α= 76.540(2)°	a = 15.660(3) Å α= 90°
	b = 12.7879(3) Å β= 79.309(2)°	b = 25.750(5) Å β= 90°	b = 12.2587(2) Å β= 65.263(2)°	b = 17.710(4) Å β= 107.76(3)°
	c = 16.5797(3) Å γ = 82.645(2)°	c = 28.570(6) Å γ = 90°	c = 12.5878(3) Å γ = 87.402(2)°	c = 12.130(2) Å γ = 90°
Volume	2258.83(8) $Å^3$	11660(4) $Å^3$	1636.51(7) $Å^3$	3203.7(12) $Å^3$
Z	2	8	1	2
Density (calculated)	1.304 Mg/m^3	1.061 Mg/m^3	1.385 Mg/m^3	1.397 Mg/m^3
Absorption coefficient	5.288 mm^{-1}	0.514 mm^{-1}	7.149 mm^{-1}	0.964 mm^{-1}
F(000)	944	3952	714	1408
Crystal size	0.180 x 0.070 x 0.020 mm^3	0.080 x 0.050 x 0.020 mm^3	0.310 x 0.130 x 0.100 mm^3	0.100 x 0.080 x 0.040 mm^3
Theta range for data collection	3.568 to 80.621°	1.065 to 26.372°	3.714 to 80.719°	1.365 to 26.371°
Index ranges	-14<=h<=14, -15<=k<=12, -21<=l<=20	-19<=h<=19, -32<=k<=32, -35<=l<=35	-15<=h<=13, -15<=k<=15, -16<=l<=12	-19<=h<=19, -22<=k<=20, -14<=l<=15
Reflections collected	46149	150791	34469	75988
Independent reflections	9606 [R(int) = 0.0653]	11929 [R(int) = 0.1001]	6990 [R(int) = 0.0897]	6512 [R(int) = 0.0419]
Completeness to theta = 67.684°	99.80%	100.00%	99.90%	99.90%
Absorption correction	Gaussian	Semi-empirical from equivalents	Gaussian	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.614	Value not reported by XDS	1.000 and 0.173	Value not reported by XDS
Data / restraints / parameters	9606 / 0 / 503	11929 / 0 / 527	6990 / 0 / 365	6512 / 0 / 348
Goodness-of-fit on F^2	1.04	1.045	1.024	1.1
Final R indices [I>2sigma(I)]	R_1 = 0.0508, wR_2 = 0.1304	R_1 = 0.0787, wR_2 = 0.2127	R_1 = 0.0458, wR_2 = 0.1176	R_1 = 0.0278, wR_2 = 0.0771
R indices (all data)	R_1 = 0.0566, wR_2 = 0.1339	R_1 = 0.0860, wR_2 = 0.2284	R_1 = 0.0470, wR_2 = 0.1192	R_1 = 0.0296, wR_2 = 0.0787
Largest diff. peak and hole	2.159 and -1.465 e.$Å^{-3}$	2.359 and -0.540 e.$Å^{-3}$	2.591 and -1.750 e.$Å^{-3}$	0.980 and -1.131 e.$Å^{-3}$
CCDC Number	2375867	2375860	2375865	2375862

Table S1 (contd.): Crystallographic Data for Compounds TCHP-MgBr, TCHP-N_3, TCHP-NH-CO-NH-Ad and **1–7**.

Compound	**TCHP-NH-CO-NH-Ad**	
Empirical formula	C_{35} H_{52} N_2 O	
Formula weight	516.78	
Temperature	123(2) K	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.3416(2) Å	α= 90°
	b = 11.50200(10) Å	β= 95.9520(10)°
	c = 20.3224(2) Å	γ = 90°
Volume	3101.76(6) $Å^3$	
Z	4	
Density (calculated)	1.107 Mg/m^3	
Absorption coefficient	0.494 mm^{-1}	
F(000)	1136	
Crystal size	0.300 x 0.200 x 0.100 mm^3	
Theta range for data collection	3.790 to 80.197°.	
Index ranges	-16<=h<=17, -14<=k<=9, -24<=l<=25	
Reflections collected	33658	
Independent reflections	6652 [R(int) = 0.0534]	
Completeness to theta = 67.684°	100.00%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.72277	
Data / restraints / parameters	6652 / 0 / 351	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R_1 = 0.0619, wR_2 = 0.1750	
R indices (all data)	R_1 = 0.0694, wR_2 = 0.1833	
Largest diff. peak and hole	0.933 and -0.405 $e.Å^{-3}$	
CCDC Number	2375859	

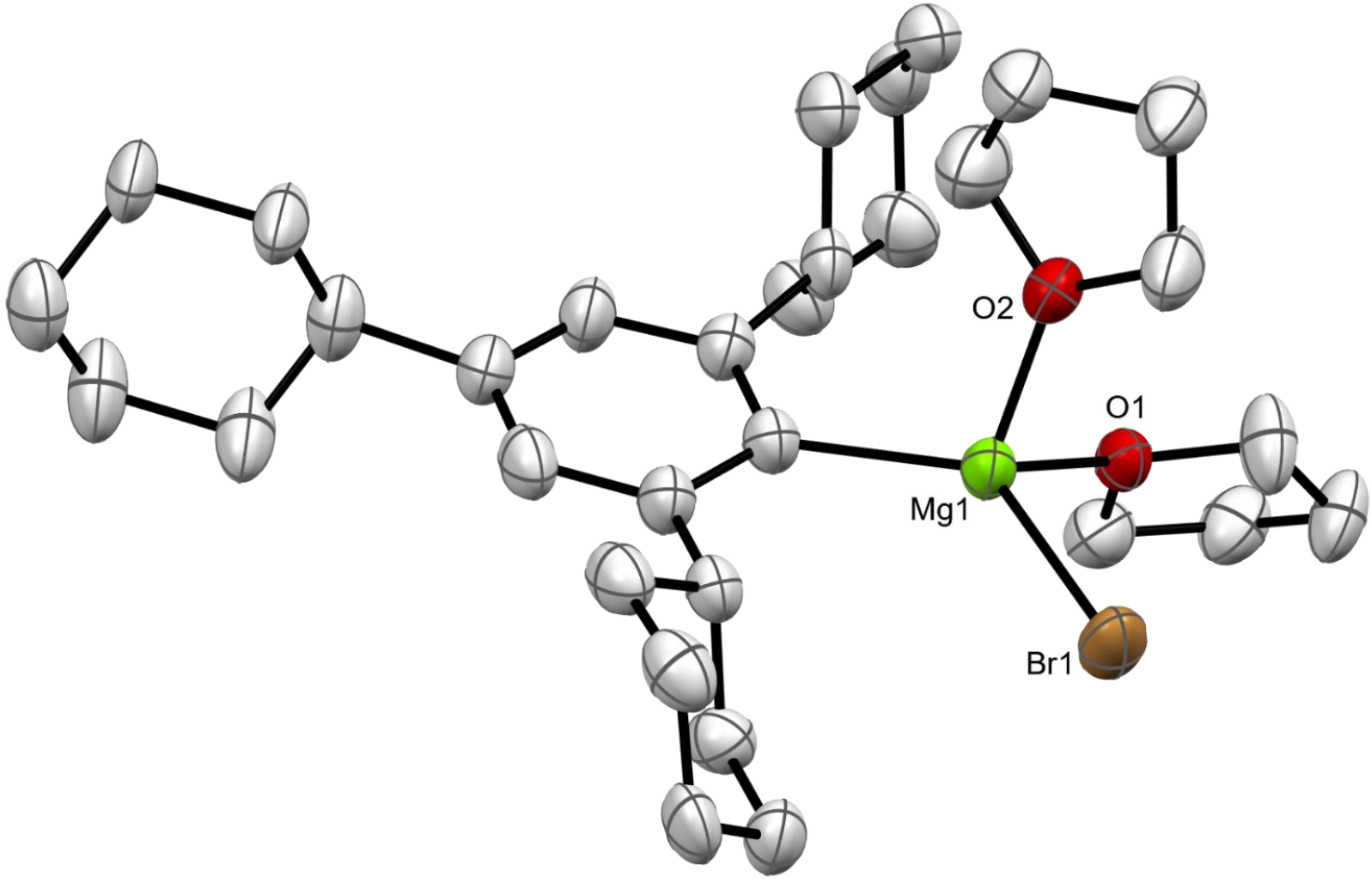


Figure S71: Molecular structure of 2,4,6-tricyclohexylphenyl magnesium bromide (TCHP-MgBr). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted.

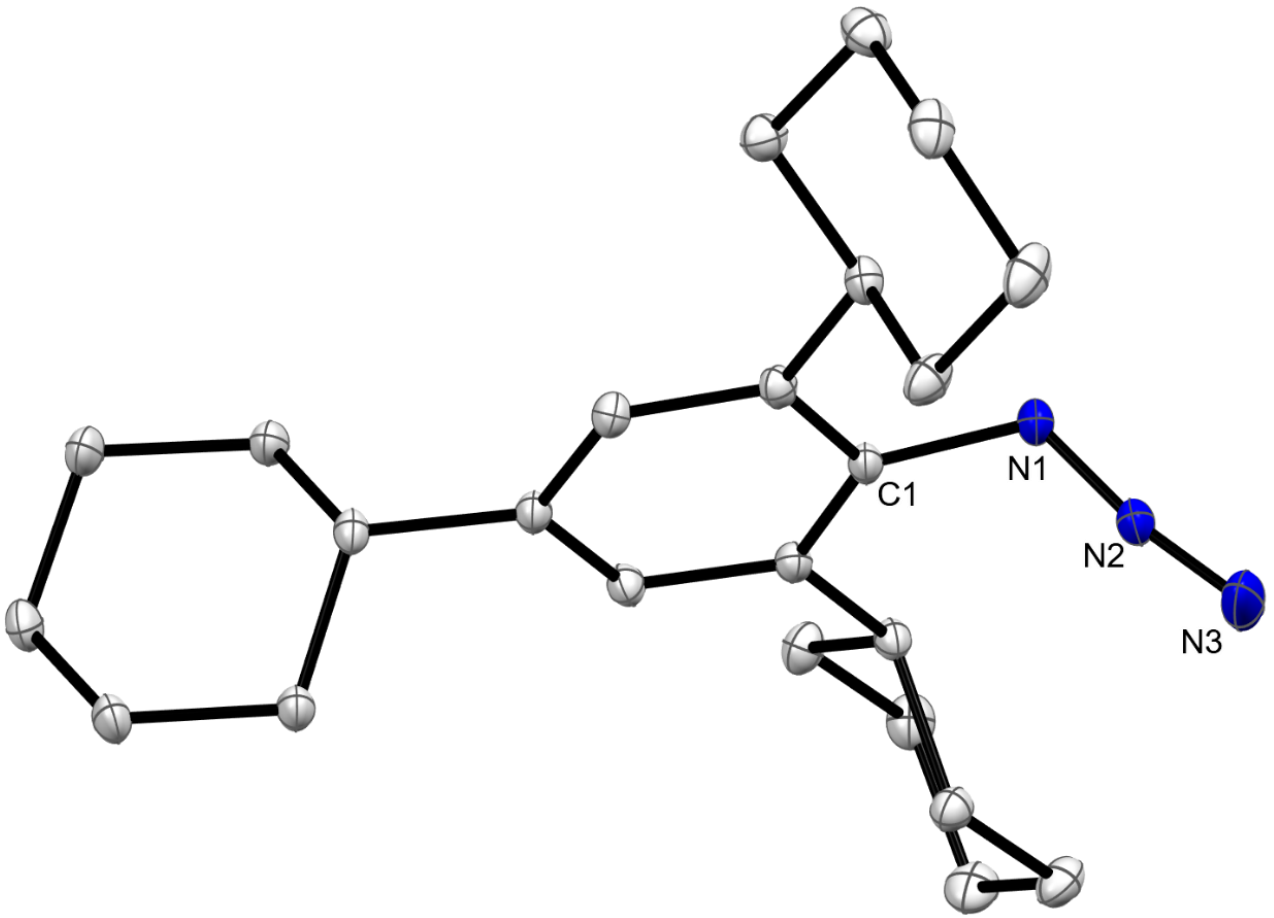


Figure S72: Molecular structure of 2,4,6-tricyclohexylphenyl azide (TCHP-N_3). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted.

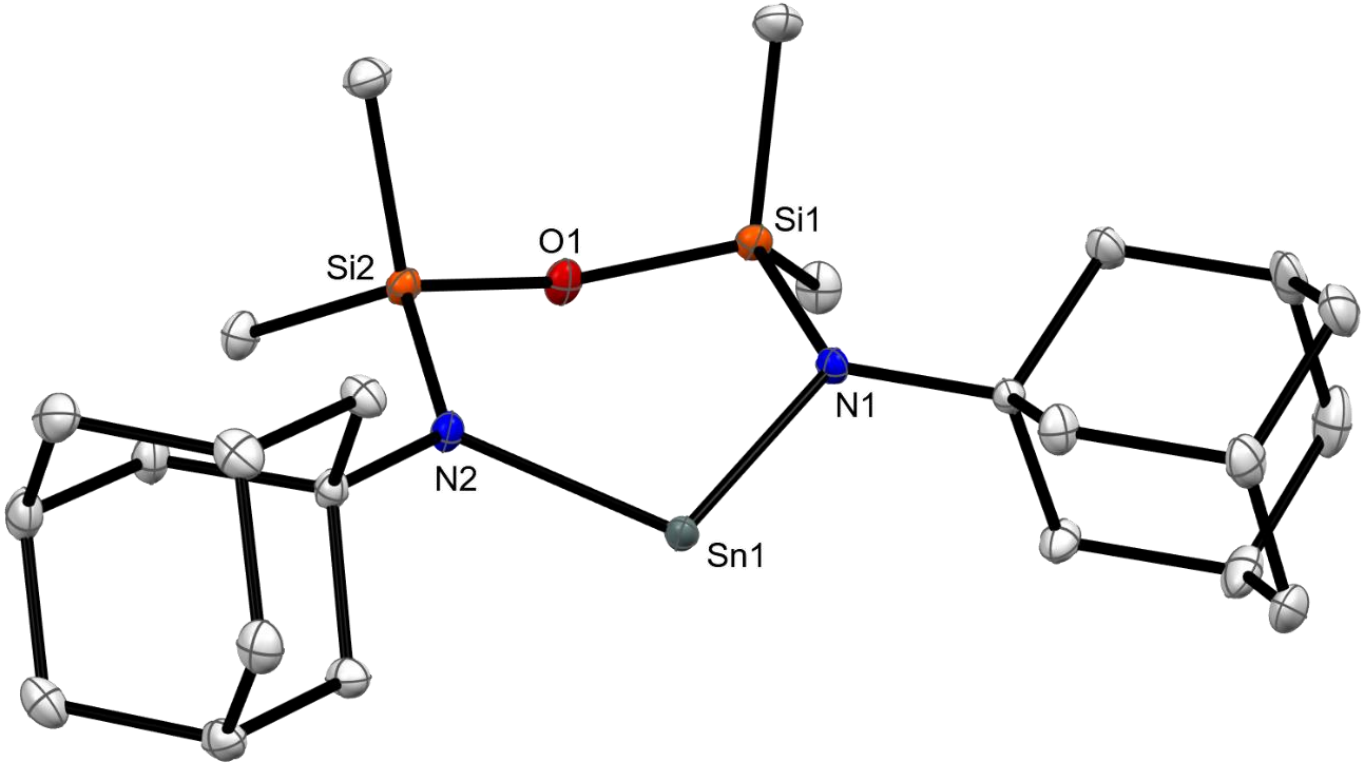


Figure S73: Molecular structure of Sn(NON^{Ad}) (**1**). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted.

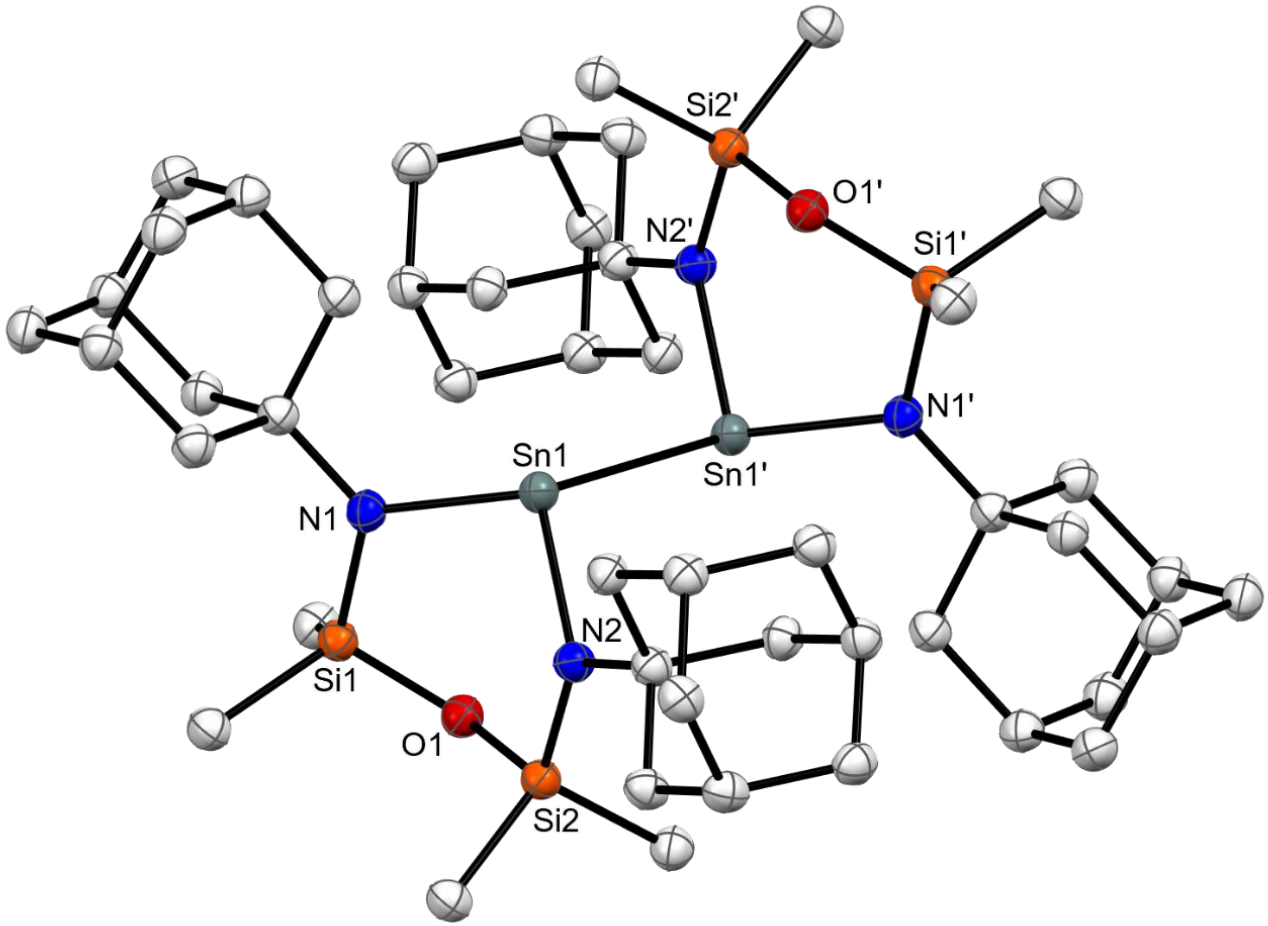


Figure S74: Molecular structure of [Sn(NON^{Ad})]$_2$ ([**1**]$_2$). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted. ‘ = 1-*x*, 1-*y*, -*z*.

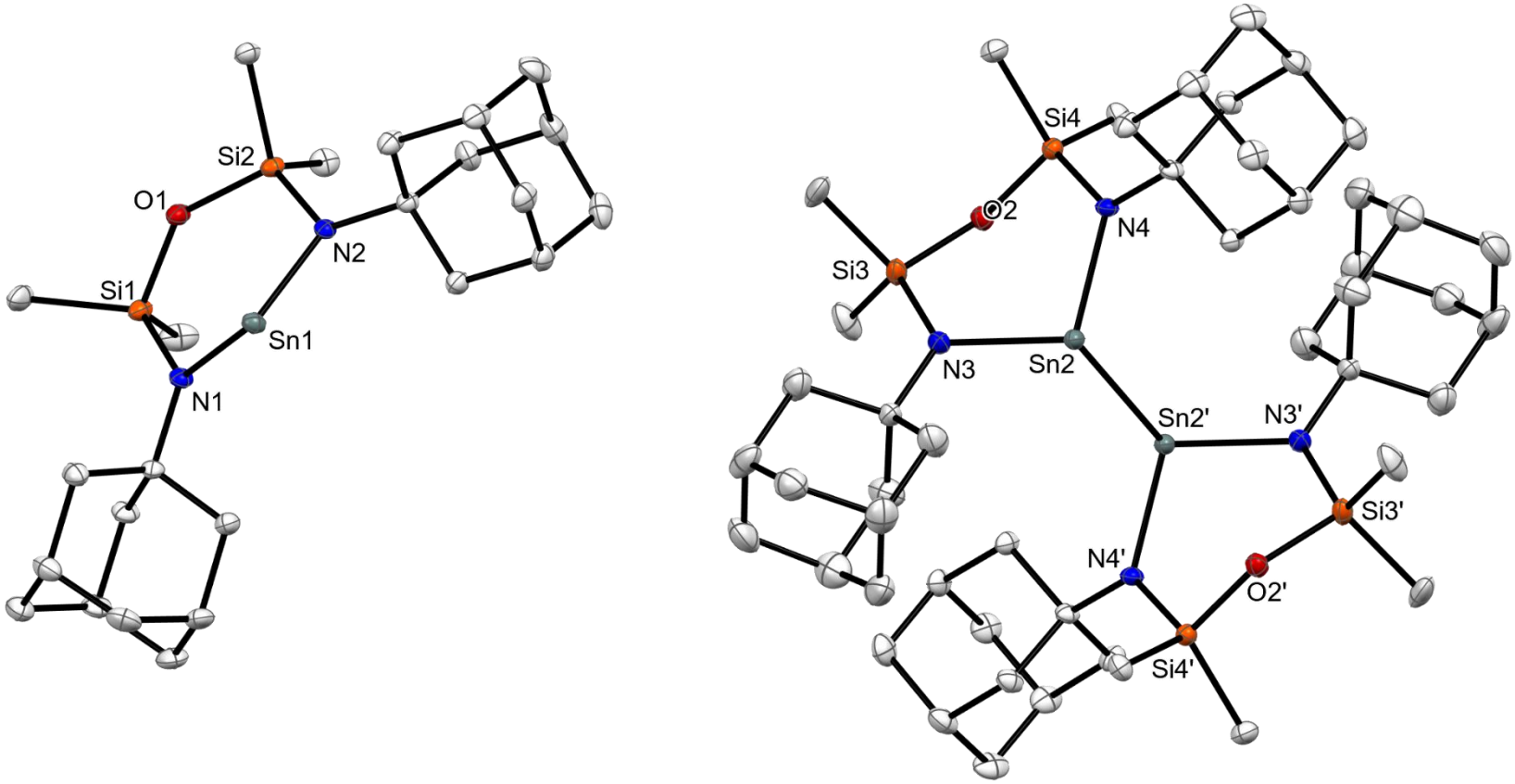


Figure S75: Molecular structure of co-crystallised Sn(NON^{Ad}) + [Sn(NON^{Ad})]$_2$ (**1** + [**1**]$_2$). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted. ‘ = 2-*x*, 1-*y*, 1-*z*.

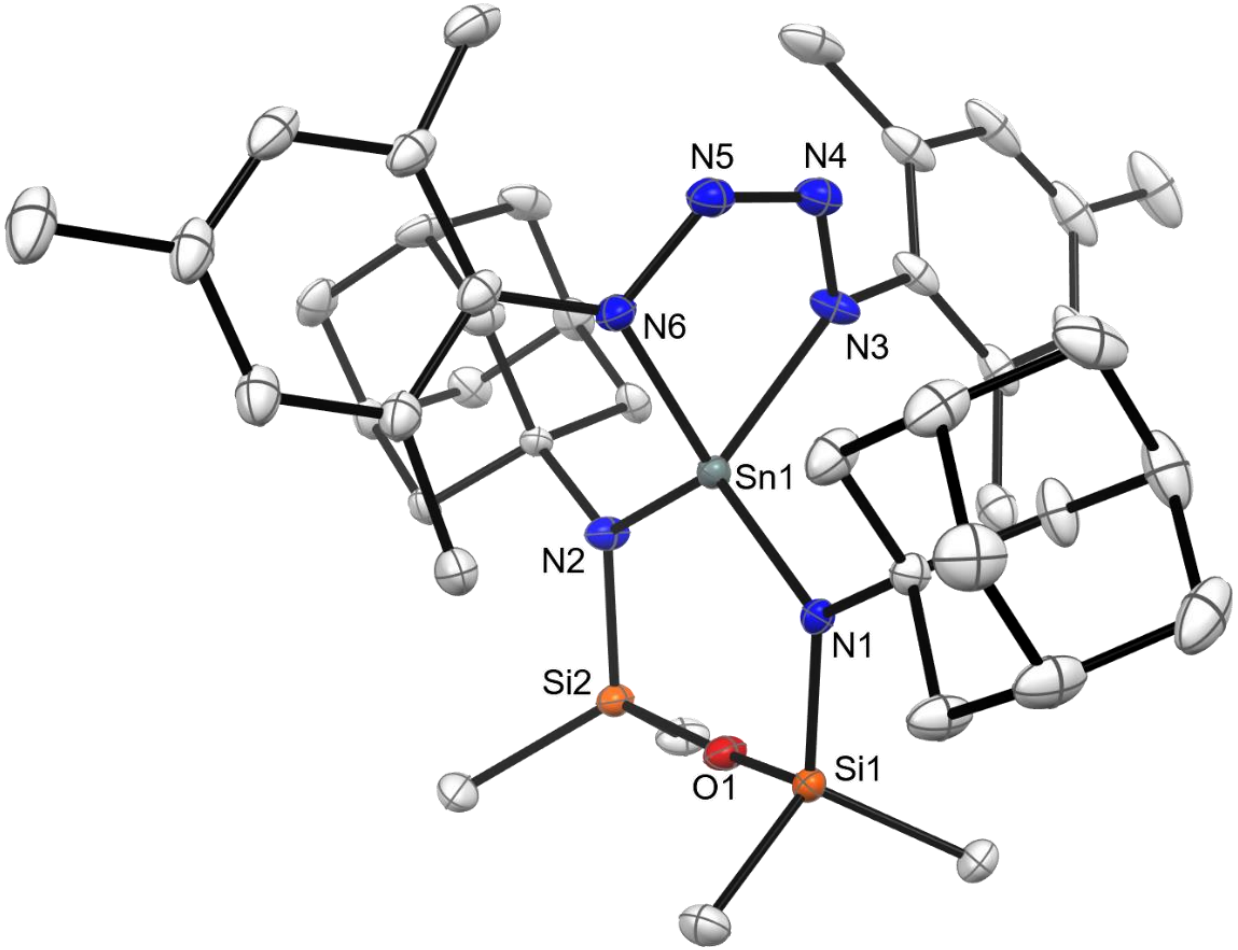


Figure S76: Molecular structure of Sn(NON^{Ad})(Mes_2N_4) (**2**). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted.

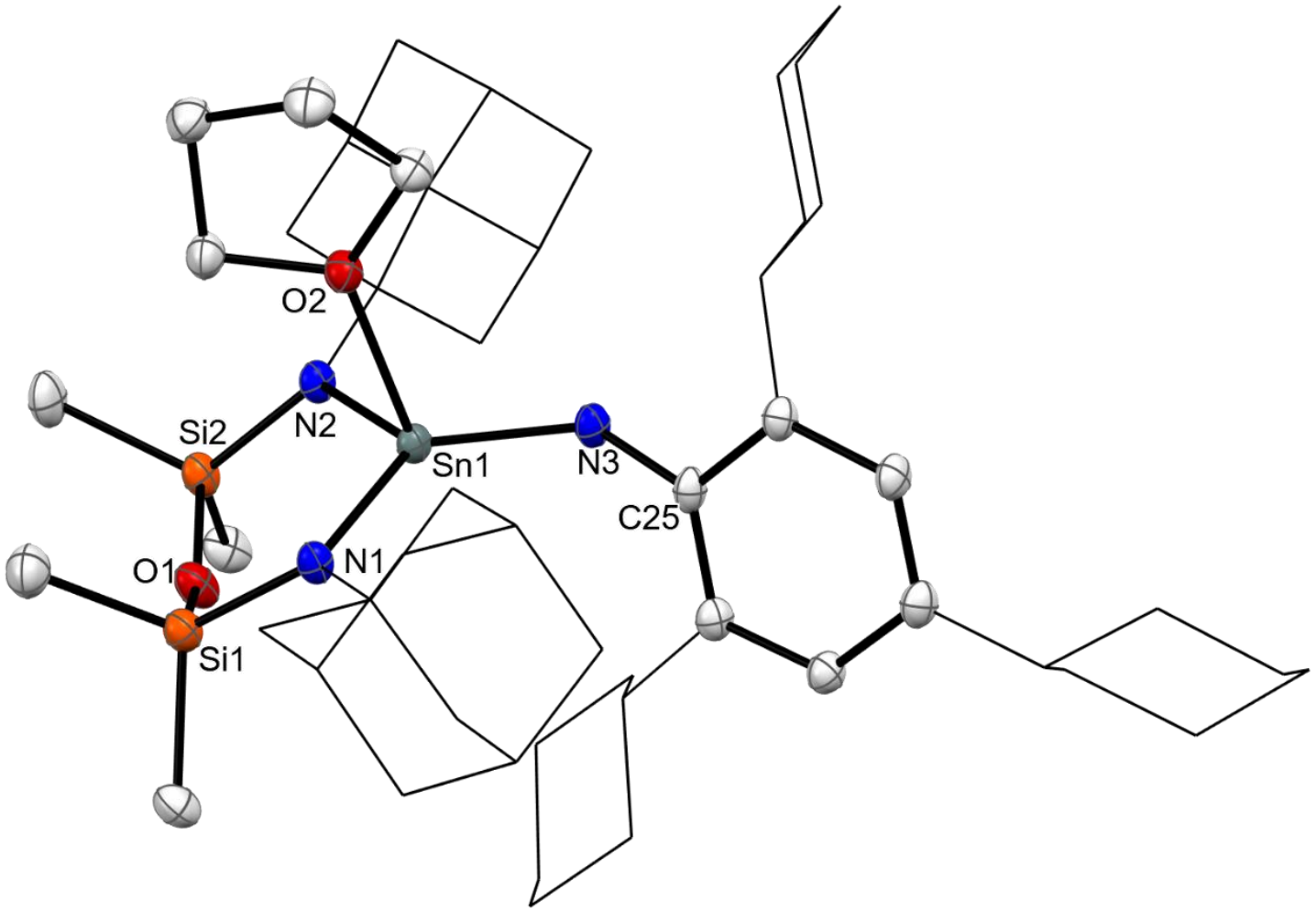


Figure S77: Molecular structure of (NON^{Ad})(THF)Sn=N(TCHP) (**3**·THF). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted; cyclohexyl and adamantyl groups shown in wireframe for clarity.

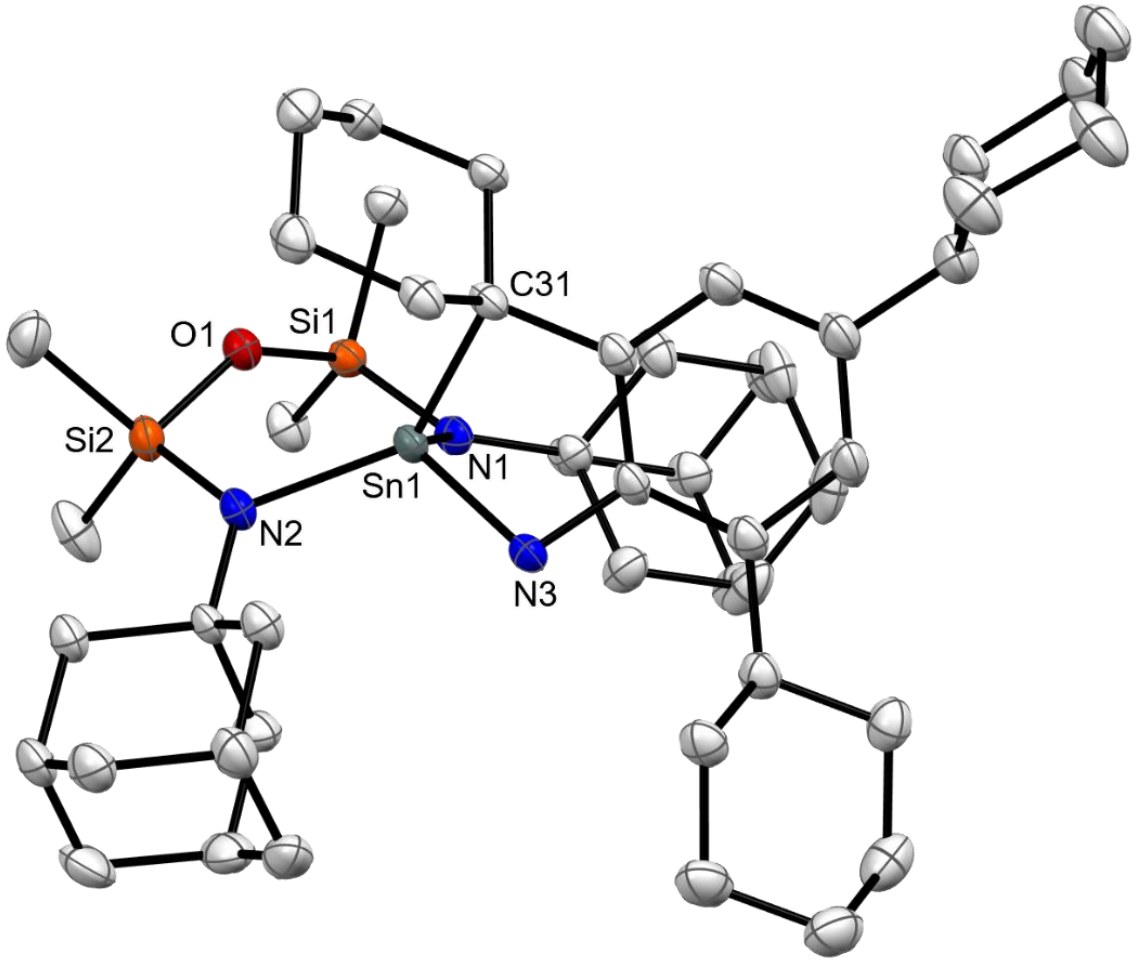


Figure S78: Molecular structure of Sn(NON^{Ad})(NTCHP*) (**4**). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted.

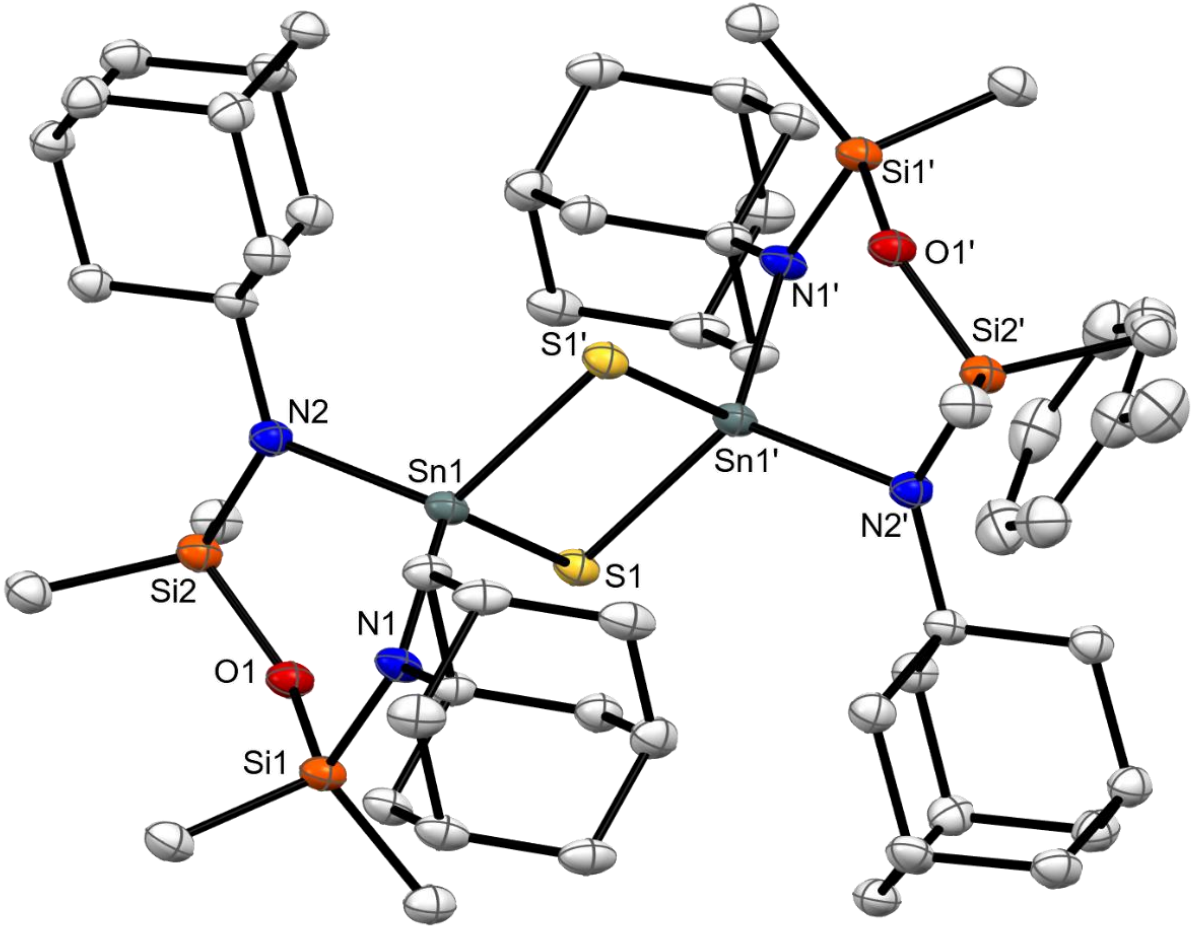


Figure S79: Molecular structure of [Sn(NON^{Ad})(μ-S)]$_2$ (**7**). Thermal ellipsoids shown at 20% probability; hydrogen atoms omitted. ‘ = -*x* 1-*y* 1-*z*.

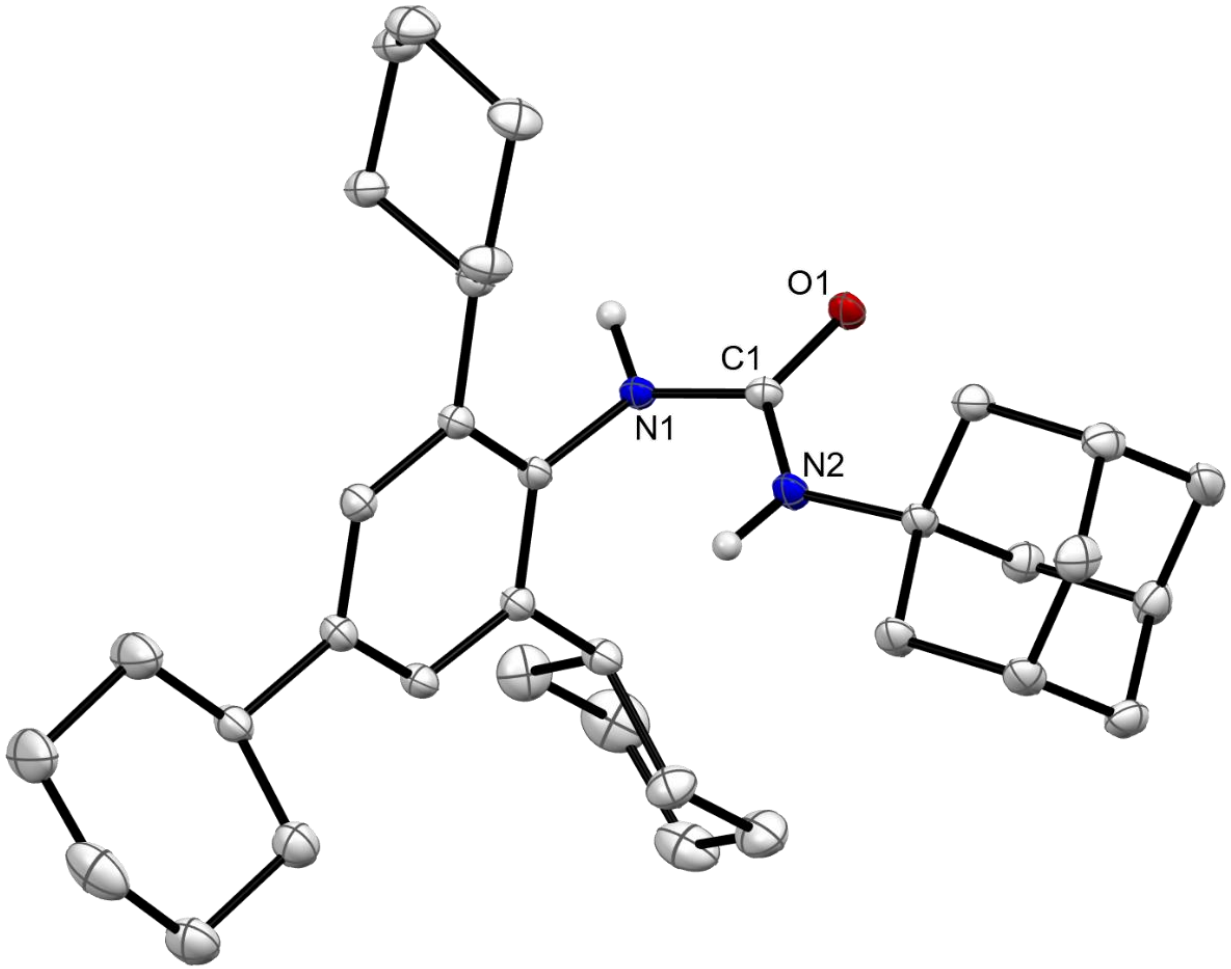


Figure S80: Molecular structure of 1-(1-adamantyl)-3-(2,4,6-tricyclohexylphenyl)urea (TCHP-NH-CO-NH-Ad). Thermal ellipsoids shown at 20% probability; hydrogen atoms except H1 and H2 omitted.

3. Computational

3.1 General Details

DFT calculations were run using Gaussian 09 (Revision D.01)[S7] using the M06-2X functional and an ultrafine integration grid (keyword int=ultrafine).[S8] Geometry optimisation and frequency calculations were carried out using BS1, with and without dispersion corrections (keyword: empiricaldisperion = gd3). Single point frequency calculations were then carried out at BS2 to obtain the final free energies.[S9] The M06-2X functional and BS2 were tested against the solid-state date (**Table S2**) and have recently been used by Fischer, Aldridge and co-workers in a related stannaimine project.[S10]

BS1 was built as follows. Sn centres were described with Stuttgart SDDAll RECPs and associated basis sets, while 6-31g**was used for all other atoms (C, H, N, O, Si, S).[S11]–[S13]

BS2 was built as follows. Sn centres were described with Stuttgart SDDAll RECPs and associated basis sets, while def2-SVP was used for all other atoms (C, H, N, O, Si, S).[S14]

Geometry optimisations were performed without symmetry constraints (keyword = nosymm). Frequency analyses for all stationary points were performed to confirm their nature of the structures as minima (no imaginary frequency). Single point solvent corrections (benzene, epsilon = 2.2706) were applied using the polarised continuum model (PCM) to free energies.[S15] Gaussview 5.0.9 was used to visualise the various properties of compounds.[S16]

Natural Bond Orbital (NBO) analysis was carried out in NBO 6.0.[S17],[S18] A full NBO analysis for select stationary points was carried out and the relevant NPA charges and Wiberg Bond Indices recorded (**Figure S85**). ETS-NOCV calculations were performed using DFT as implemented in ORCA 4.2.1.[S19],[S20] The optimised geometry of stannaimine complex **3** from the Gaussian 09 calculation detailed above was used as the input geometry. Single point calculations were performed using the M06-2X functional on the relevant fragments (**Figure S87**). The def2-tzvpp basis set was used for all atoms.[S14] Graphical surface representations were plotted using Avogadro 1.2.0 (**Figure S88**).

3.2 Computed Structures

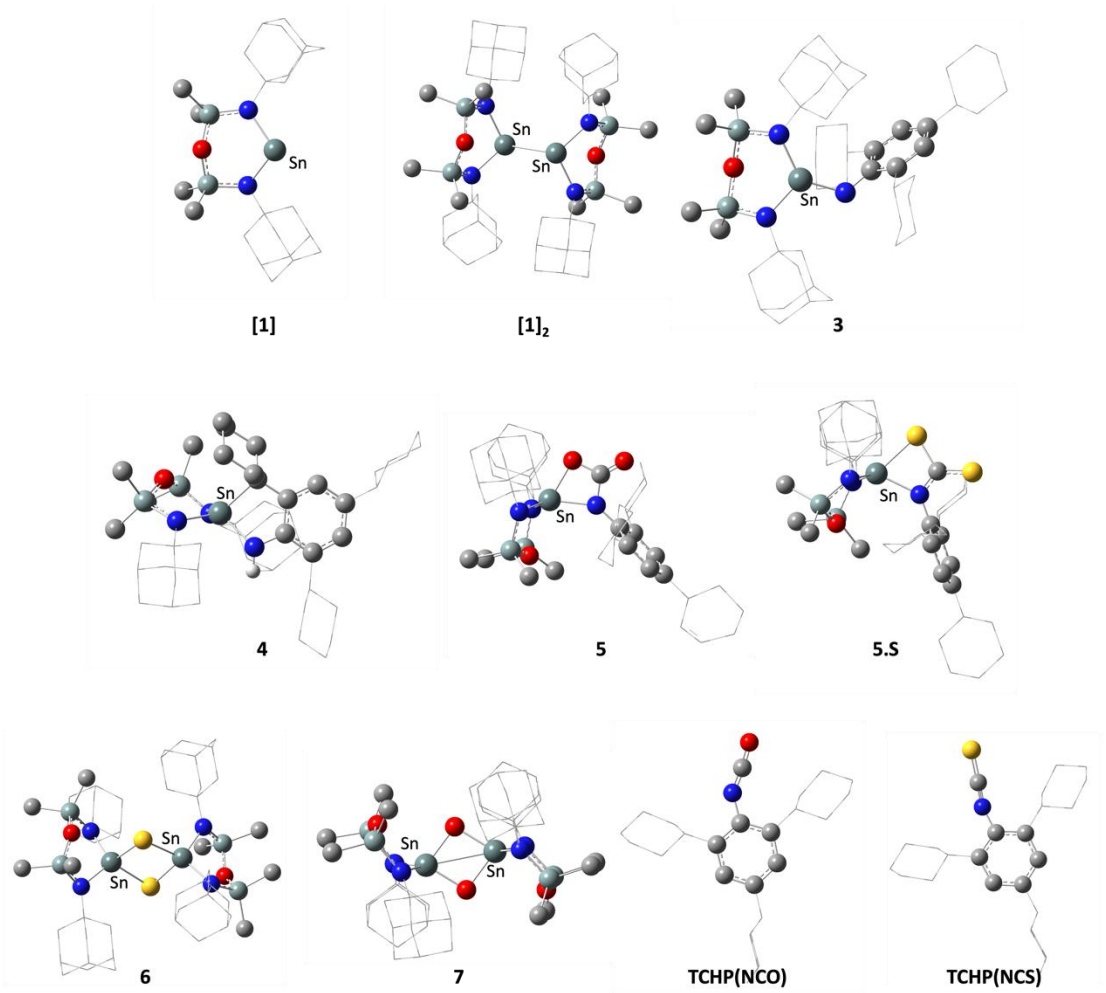


Figure S81: Structures of all stationary point minima as calculated by DFT (grey = carbon, white = hydrogen, red = oxygen, blue = nitrogen, yellow = sulphur, teal = silicon or tin, labelled). Most hydrogen atoms omitted and adamantly/cyclohexyl units shown in wireframe for clarity.

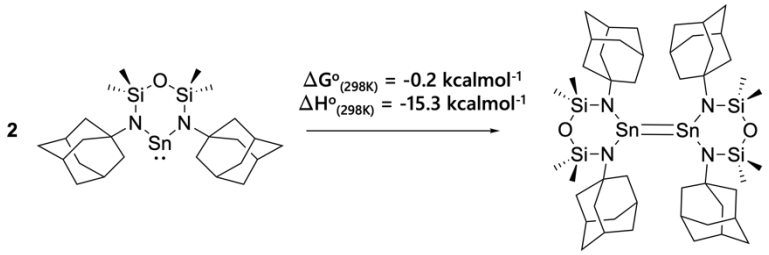


Figure S82: Equilibria for monomer-dimer relationship of **1**/[**1**]$_2$ (M06-2X).

Table S2. Comparison of DFT calculated structures to solid-state data (Å); DFT(disp) includes dispersion corrections in the geometry optimisation calculation.

		Sn=N	Sn–Sn	Sn–N	N–Si
1	XRD	-	-	2.093, 2.092	1.724, 1.725
	DFT	-	-	2.118, 2.129	1.737, 1.739
	DFT(disp)	-	-	2.117, 2.129	1.738, 1.737
[1]$_2$	XRD	-	3.145	2.091, 2.095	1.720, 1.725
	DFT	-	3.202	2.114, 2.114	1.735, 1.736
	DFT(disp)	-	3.190	2.113, 2.113	1.736, 1.736
3	XRD	1.934	-	2.046, 2.027	1.733, 1.731
	DFT	1.917	-	2.044, 2.030	1.749, 1.747
	DFT(disp)	1.917	-	2.044, 2.030	1.749, 1.747
4	XRD	2.062	-	2.090, 2.053	1.714, 1.718
	DFT	2.077	-	2.093, 2.062	1.741, 1.741
	DFT(disp)	2.078	-	2.092, 2.060	1.741, 1.740
5	XRD	2.087	-	2.014, 2.036	1.740, 1.732
	DFT	2.067	-	2.026, 2.026	1.744, 1.740
	DFT(disp)	2.065	-	2.026, 2.026	1.744, 1.740

3.3 Molecular Orbitals

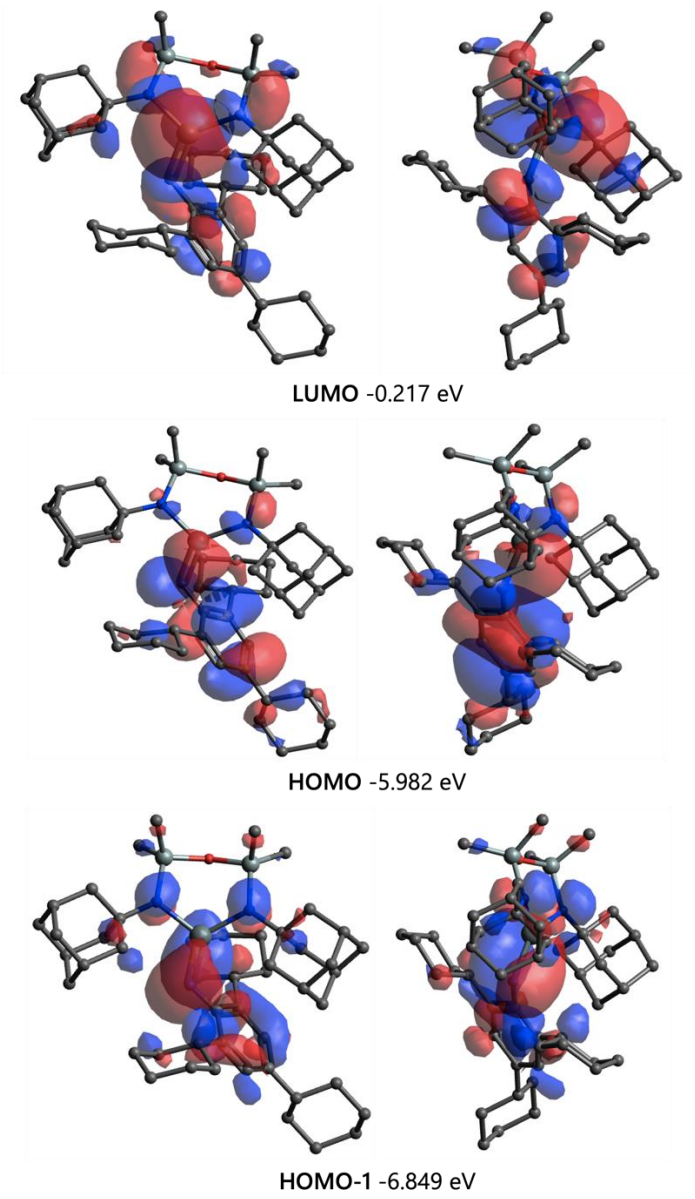


Figure S83: Selected molecular orbitals of the optimised structure of stannaimine complex **3**. HOMO-LUMO gap = 5.77 eV.

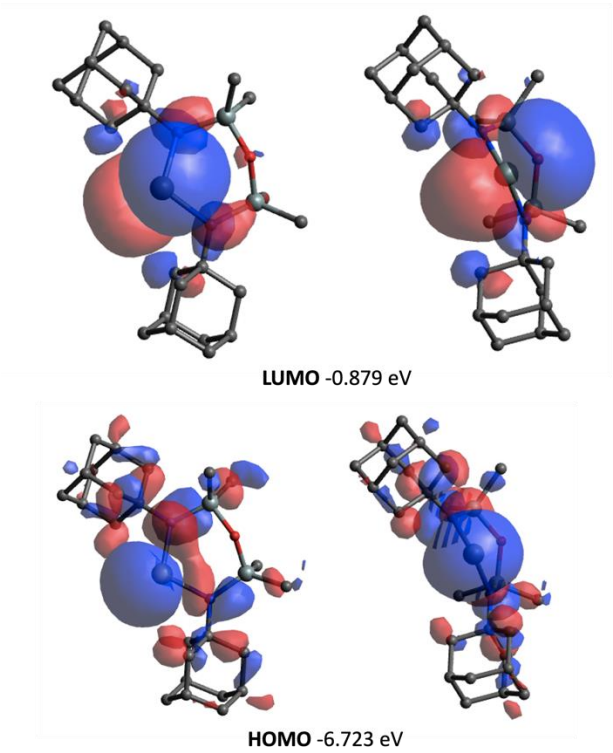


Figure S84: Selected molecular orbitals of the optimised structure of stannylene monomer complex **1**. HOMO-LUMO gap = 5.84 eV.

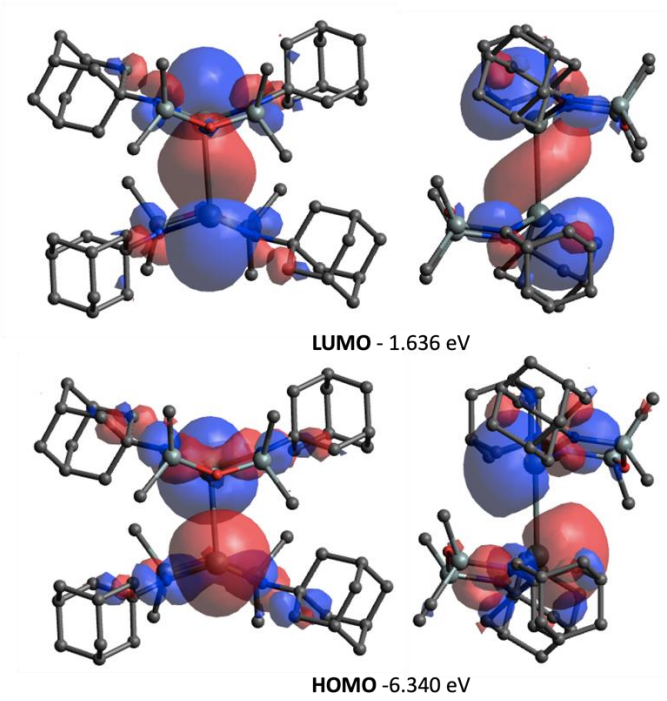


Figure S85: Selected molecular orbitals of the optimised structure of stannylene dimer complex **[1]**$_2$. HOMO-LUMO gap = 4.70 eV.

3.4 Natural Bond Orbital (NBO) Analysis

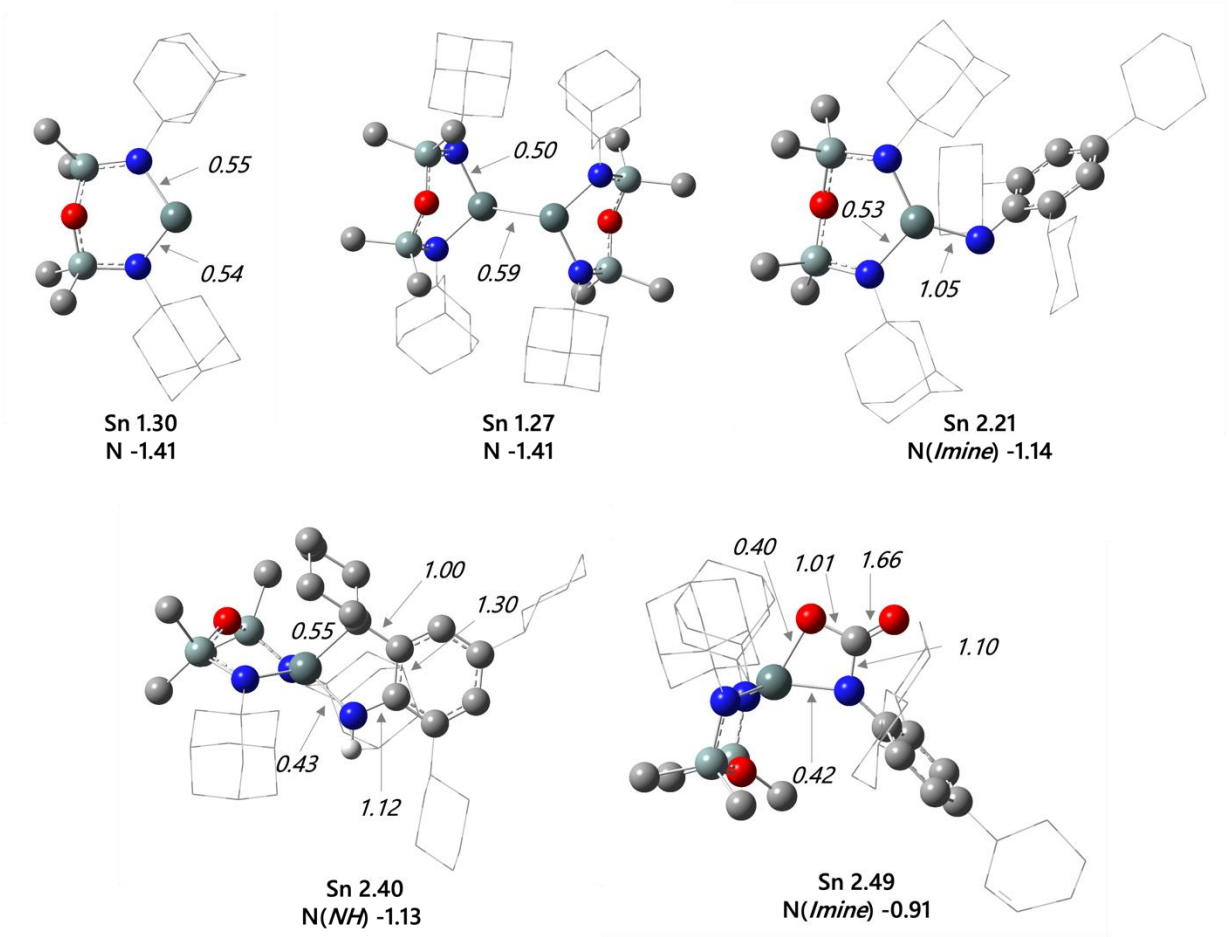


Figure S86: Select DFT optimised structures with NBO analysis annotated; Select Natural Population Analysis (NPA) Charges shown in bold, and Wiberg Bond Indices (WBI) annotated in italics.

3.5 DFT Calculated Thermodynamics

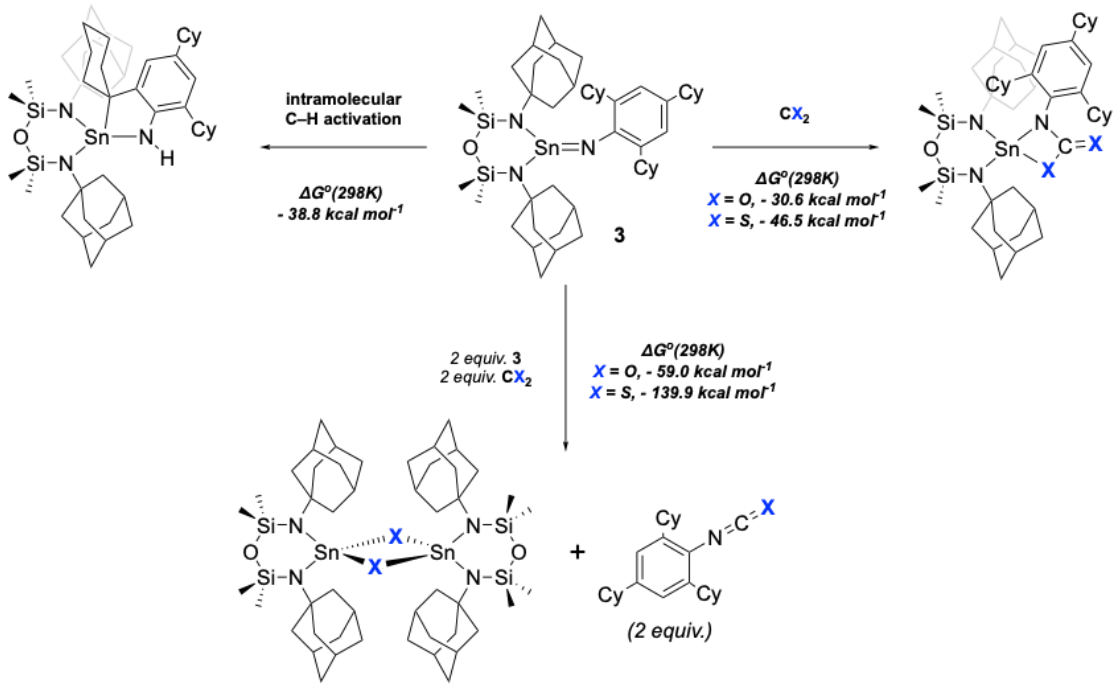


Figure S87: DFT calculated thermodynamics (298.15 K and 1 atm) for intramolecular C–H activation and [2+2] cycloaddition reactions with CO_2 and CS_2 of stannaimine **3** (Gibbs Free Energy, M06-2X).

3.6 Extended Transition State- Natural Orbital Chemical Valence (ETS-NOCV) Calculations

Stannaimine complex **3** was fragmented at the Sn=N bond and submitted for ETS-NOCV calculations as described above. The total orbital interaction energy (ΔE_{ORB}) was calculated as -243.7 kcal mol^{-1}.

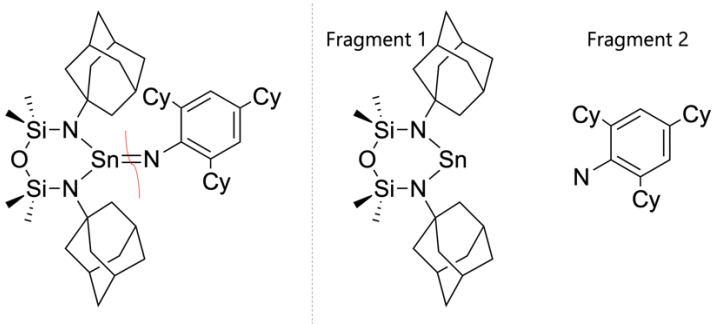


Figure S88: Fragments of stannaimine complex **3** used for ETS-NOCV calculations.

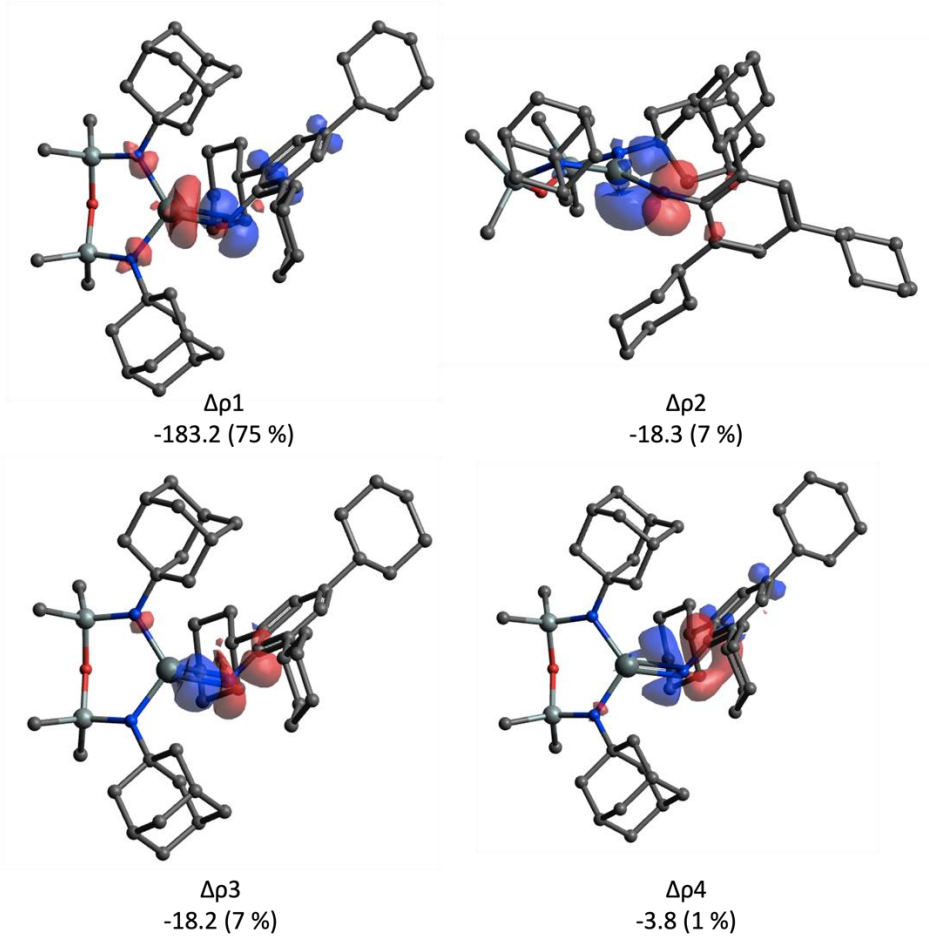


Figure S89: Plots all energies in kcal mol^{-1} with the percentage contribution to the overall orbital interaction energy (ΔE_{ORB} = -243.7 kcal mol^{-1}) shown in brackets. Charge flow is from red to blue (isovalue = 0.01)

3.7 Cartesian Coordinates

1-dimer.log

SCF (M06-2X) = -3411.35344291

E(SCF)+ZPE(0 K)= -3410.085398

H(298 K)= -3410.027845

G(298 K)= -3410.173291

Lowest Frequency = -164.0660 cm^{-1}

Sn	6.934149	8.181986	1.576564
Si	9.181429	5.880193	2.175967
Si	6.192778	5.170017	2.632549
O	7.680073	5.228062	1.894274
N	8.878209	7.589199	2.159697
N	5.682506	6.829298	2.612779
C	9.894752	8.606320	2.470156
C	4.312671	7.267368	2.923857
C	3.661054	6.343209	3.975615
H	4.282247	6.342926	4.880481
H	3.633286	5.313538	3.595293
C	3.419651	7.267583	1.665591
H	3.876371	7.917852	0.902909
H	3.403738	6.251038	1.249921
C	4.306908	8.696617	3.511868
H	4.948093	8.711601	4.403219
H	4.739069	9.397125	2.782268
C	2.881918	9.162180	3.848595
H	2.922641	10.178499	4.256805
C	11.299102	8.155745	2.010776
H	11.561087	7.212236	2.508611
H	11.274100	7.961778	0.931529
C	9.953522	8.879527	3.989191

H	8.958973	9.208030	4.321849
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C	2.262532	8.212384	4.882400
H	1.246885	8.541908	5.134276
H	2.850356	8.226945	5.808548
C	6.397553	4.430136	4.347715
H	7.080139	3.574933	4.306198
H	5.446709	4.079973	4.759632
H	6.813829	5.164672	5.043381
C	12.367003	9.207644	2.340777
H	13.345244	8.841583	2.007094
C	2.030342	9.152679	2.569764
H	2.449356	9.847809	1.832303
H	1.012185	9.492536	2.796929
C	12.392963	9.447162	3.857694
H	13.162421	10.187880	4.108438
H	12.653638	8.516900	4.378397
C	1.379667	6.774084	3.024015
H	0.349987	7.074950	3.253550
H	1.338583	5.756262	2.614314
C	2.228994	6.791402	4.304510
H	1.798592	6.102902	5.040841
C	1.991676	7.731015	1.989894
H	1.386121	7.721002	1.073778
C	9.857022	5.217289	3.799635
H	9.248540	5.556743	4.643057
H	10.889028	5.533005	3.983244
H	9.842808	4.122326	3.790593
C	10.206229	5.242607	0.738966
H	10.203000	4.147822	0.742094
H	11.244332	5.584219	0.741782
H	9.737110	5.569463	-0.196558

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H	5.266098	4.337823	0.508712
H	4.117858	3.971050	1.810062
H	5.583831	2.998852	1.617217
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H	11.030194	10.112648	5.404839
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H	9.509594	9.771955	0.688915
H	8.613776	10.328093	2.108162
C	10.652130	11.007356	2.080430
H	10.392613	11.934862	1.556279
C	12.027634	10.514280	1.612733
H	12.790887	11.274507	1.820374
H	12.018893	10.346970	0.526911
C	10.680279	11.253881	3.596491
H	11.428392	12.018709	3.839374
H	9.706660	11.632399	3.932175
Sn	6.947252	7.626215	-1.576576
Si	4.699961	9.927997	-2.175986
Si	7.688611	10.638191	-2.632552
O	6.201312	10.580136	-1.894287
N	5.003189	8.218992	-2.159704
N	8.198889	8.978911	-2.612788
C	3.986649	7.201864	-2.470156
C	9.568728	8.540849	-2.923862
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H	10.248109	10.494685	-3.595281
C	10.461742	8.540629	-1.665591
H	10.005021	7.890353	-0.902915
H	10.477649	9.557171	-1.249915
C	9.574498	7.111603	-3.511882

H	8.933318	7.096624	-4.403236
H	9.142337	6.411089	-2.782289
C	10.999492	6.646048	-3.848606
H	10.958775	5.629731	-4.256823
C	2.582296	7.652440	-2.010786
H	2.320310	8.595943	-2.508633
H	2.607293	7.846419	-0.931542
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H	4.922437	6.600135	-4.321837
H	3.708091	7.867164	-4.513143
C	11.618879	7.595853	-4.882402
H	12.634529	7.266335	-5.134274
H	11.031060	7.581296	-5.808552
C	7.483846	11.378083	-4.347713
H	6.801252	12.233280	-4.306195
H	8.434690	11.728257	-4.759620
H	7.067582	10.643550	-5.043389
C	1.514400	6.600534	-2.340779
H	0.536156	6.966597	-2.007104
C	11.851062	6.655544	-2.569771
H	11.432047	5.960407	-1.832316
H	12.869222	6.315693	-2.796933
C	1.488446	6.360998	-3.857693
H	0.718992	5.620274	-4.108431
H	1.227771	7.291252	-4.378409
C	12.501730	9.034145	-3.024003
H	13.531413	8.733284	-3.253535
H	12.542809	10.051964	-2.614295
C	11.652409	9.016832	-4.304502
H	12.082813	9.705338	-5.040826
C	11.889720	8.077204	-1.989890
H	12.495271	8.087213	-1.073772

C	4.024377	10.590887	-3.799663
H	4.632870	10.251431	-4.643078
H	2.992375	10.275162	-3.983280
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H	9.763521	11.837162	-1.810044
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C	2.866797	5.866478	-4.322178
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H	4.371805	6.036252	-0.688899
H	5.267629	5.480099	-2.108136
C	3.229277	4.800831	-2.080403
H	3.488795	3.873331	-1.556239
C	1.853769	5.293908	-1.612718
H	1.090520	4.533677	-1.820353
H	1.862505	5.461232	-0.526898
C	3.201135	4.554287	-3.596461
H	2.453025	3.789454	-3.839338
H	4.174757	4.175767	-3.932136

1.log

SCF (M06-2X) = -1705.66513850

E(SCF)+ZPE(0 K)= -1705.031382

H(298 K)= -1705.003575

G(298 K)= -1705.086061

Lowest Frequency = -168.0352 cm^{-1}

Si	10.123145	5.274257	12.338220
Si	8.492886	3.975373	14.575407
O	9.849421	4.543682	13.806626
N	10.058389	3.948213	11.217417
N	7.853017	2.821685	13.442086
C	10.409279	4.025863	9.787642
C	6.716324	1.935824	13.762156
C	9.113686	3.222493	16.180024
H	9.838236	2.430301	15.968142
H	8.316002	2.794854	16.795011
H	9.620068	3.988607	16.775980
C	8.774188	6.547491	12.022115
H	7.803556	6.049804	11.925446
H	8.953050	7.102749	11.095466
H	8.706314	7.273739	12.838545
C	11.262152	2.814549	9.344777
H	12.173304	2.789608	9.955917
H	10.718616	1.880790	9.536832
C	5.749098	2.605403	14.763004
H	6.282582	2.833822	15.695004
H	5.402649	3.556852	14.340352
C	11.776058	6.136736	12.542695
H	11.774783	6.634893	13.517441
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H	7.863586	0.095748	13.674519
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H	10.537393	2.942720	5.957451

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H	4.158133	0.495259	11.871762
C	11.604195	2.888464	7.848148
H	12.198331	2.009860	7.571660
C	11.229763	5.293105	9.466239
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C	5.896094	1.619904	12.489913
H	5.561597	2.567158	12.047511
H	6.537164	1.120616	11.749883
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C	10.270346	5.414972	7.148902
H	9.675335	6.296982	7.417169
H	10.504793	5.492076	6.080009
C	9.130899	4.061731	8.917980
H	8.520102	4.919701	9.228719
H	8.538947	3.155679	9.119322
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H	6.677071	5.207318	15.787518
H	6.801761	5.765247	14.112797
C	5.993618	-0.318013	14.696645
H	6.361056	-1.256404	15.127807
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H	3.902698	2.207825	15.806812
C	5.217955	-0.612634	13.403572
H	5.868783	-1.126331	12.684800
H	4.374657	-1.281624	13.615384
C	12.405399	4.165635	7.564779
H	13.346434	4.152510	8.128365

H	12.662734	4.221863	6.499716
C	5.065745	0.383399	15.698969
H	4.219833	-0.268660	15.949734
H	5.607267	0.588470	16.631179
C	11.567083	5.385092	7.970127
H	12.138650	6.302957	7.790566
C	3.773174	1.397536	13.802949
H	2.911930	0.755336	14.025426
H	3.384345	2.329247	13.373845
Sn	9.097247	2.167047	11.843197

3.log

SCF (M06-2X) = -2694.88265967

E(SCF)+ZPE(0 K)= -2693.698919

H(298 K)= -2693.649034

G(298 K)= -2693.778210

Lowest Frequency = -177.8429 cm^{-1}

Sn	4.923360	9.462930	3.828141
Si	4.644781	11.533062	6.203248
Si	2.070167	10.541184	4.701171
O	3.258113	10.674010	5.863058
N	6.116613	8.041218	3.347284
N	5.706683	10.978867	4.928223
N	2.957876	9.809027	3.386221
C	5.725937	6.899621	2.655025
C	7.166509	11.202659	4.874848
C	4.976421	5.853625	3.270521
C	7.514328	12.546307	5.545426
H	7.185804	12.536063	6.593543
H	6.972722	13.352699	5.033999

C	2.356227	9.148856	2.212380
C	1.992103	7.683361	2.517580
H	1.304987	7.652854	3.373719
H	2.904055	7.144684	2.803101
C	4.492910	6.025541	4.694187
H	4.059875	7.040144	4.777371
C	6.150776	6.726451	1.308895
C	3.332796	9.163866	1.019212
H	4.243711	8.603860	1.278073
H	3.615711	10.203669	0.803784
C	5.848524	5.541809	0.637195
H	6.176466	5.412154	-0.391035
C	7.650950	11.270842	3.412192
H	7.440318	10.310865	2.916378
H	7.092220	12.059799	2.890751
C	7.935166	10.072496	5.588301
H	7.594806	10.015160	6.631084
H	7.690141	9.118469	5.101265
C	6.945926	7.831856	0.648799
H	6.487946	8.786715	0.955086
C	1.403367	12.242803	4.294018
H	1.137831	12.779059	5.210705
H	0.508356	12.184752	3.668066
H	2.150167	12.833446	3.755539
C	9.163720	11.534856	3.348440
H	9.479217	11.577629	2.300188
C	1.362970	7.007052	1.291280
H	1.121461	5.966244	1.538207
C	1.079692	9.897493	1.779976
H	0.353792	9.901777	2.604646
H	1.334882	10.941851	1.557634
C	5.117579	4.515279	1.231268

C	5.648946	5.966829	5.707572
H	6.057268	4.946807	5.702356
H	6.445898	6.641372	5.383477
C	4.772473	3.256390	0.466805
H	5.230853	3.336443	-0.530654
C	0.441012	9.222152	0.554905
H	-0.468720	9.769207	0.281974
C	4.689532	4.698235	2.547918
H	4.111106	3.909892	3.022470
C	9.899782	10.391573	4.062717
H	10.983715	10.552468	4.008017
H	9.681856	9.439613	3.562400
C	8.393230	7.867459	1.171401
H	8.369473	7.909929	2.265102
H	8.890265	6.929784	0.885112
C	9.028730	12.803786	5.499936
H	9.242490	13.756570	5.997771
C	4.998696	0.732605	0.331152
H	5.485853	0.787805	-0.652087
H	5.399206	-0.154962	0.832207
C	1.433474	9.249676	-0.615560
H	0.982782	8.782612	-1.499768
H	1.674012	10.286944	-0.880604
C	0.740451	9.462132	5.451837
H	1.168028	8.503386	5.759803
H	-0.092120	9.260437	4.772204
H	0.335313	9.951503	6.343295
C	3.372885	5.073533	5.124408
H	3.750435	4.041745	5.131943
H	2.548621	5.107352	4.400840
C	6.945252	7.795383	-0.882746
H	5.915001	7.759691	-1.258641

H	7.442312	6.879530	-1.230988
C	2.708165	8.495818	-0.214668
H	3.431706	8.522192	-1.037490
C	5.151402	11.009368	7.926150
H	4.357927	11.267151	8.634868
H	6.074751	11.483641	8.269895
H	5.294324	9.925329	7.962267
C	9.485847	12.867342	4.037268
H	10.563951	13.063706	3.989006
H	8.979947	13.692254	3.520133
C	9.157730	9.058571	0.590977
H	8.683210	9.985539	0.943874
H	10.189702	9.071437	0.961040
C	0.087601	7.765591	0.895681
H	-0.384985	7.286138	0.029659
H	-0.637807	7.738686	1.719159
C	2.367009	7.037963	0.129570
H	3.279621	6.496476	0.410398
H	1.940036	6.537732	-0.749390
C	9.133477	9.047805	-0.938930
H	9.675056	8.163040	-1.300572
H	9.654747	9.924357	-1.338424
C	9.449132	10.329051	5.530553
H	9.973862	9.514953	6.042855
C	2.872403	5.426434	6.527364
H	2.426643	6.431047	6.505650
H	2.078415	4.736183	6.831026
C	5.340701	1.991552	1.130829
H	4.921345	1.901515	2.142544
H	6.424478	2.096040	1.248718
C	7.694973	8.998122	-1.460166
H	7.686975	8.960448	-2.554710

H	7.174401	9.921403	-1.170109
C	4.271996	13.366783	6.145830
H	4.110686	13.704050	5.118210
H	5.085729	13.959987	6.571834
H	3.365596	13.579669	6.721794
C	3.254877	3.109041	0.261624
H	2.767773	3.061692	1.246050
H	2.865741	4.003665	-0.238101
C	4.013066	5.408870	7.548199
H	4.393668	4.382439	7.639616
H	3.642858	5.699074	8.537123
C	9.764929	11.664469	6.220950
H	10.845639	11.852003	6.205427
H	9.456382	11.624906	7.273563
C	5.159400	6.323964	7.111473
H	5.984350	6.274512	7.829992
H	4.804423	7.366669	7.108302
C	3.487406	0.598447	0.132867
H	3.256605	-0.292719	-0.460227
H	3.008154	0.461881	1.112056
C	2.910862	1.848673	-0.535008
H	1.825515	1.756177	-0.648651
H	3.328500	1.938953	-1.547202

4.log

SCF (M06-2X) = -2694.94794248

E(SCF)+ZPE(0 K)= -2693.762543

H(298 K)= -2693.711684

G(298 K)= -2693.843578

Lowest Frequency = -170.6268 cm^{-1}

Sn	5.160233	9.006947	3.584742
Si	3.075442	9.197780	1.228254
Si	4.411874	11.783428	2.300874
O	4.194631	10.438661	1.331128
N	3.350658	8.380306	2.740699
N	5.164426	11.065614	3.696521
N	5.546358	8.196625	5.458512
H	4.910935	8.260946	6.243188
C	6.936070	7.833978	3.056781
C	3.536778	8.229453	-0.310488
H	3.506143	8.888100	-1.184631
H	2.855139	7.393781	-0.497319
H	4.550330	7.825135	-0.229696
C	2.730311	7.082817	3.081573
C	6.793473	6.688605	4.052806
C	5.481739	11.771917	4.950810
C	1.332628	6.967124	2.435871
H	0.710856	7.806785	2.771996
H	1.420414	7.035825	1.342634
C	6.099222	6.924393	5.270751
C	0.665601	5.627579	2.789948
H	-0.318708	5.584098	2.309398
C	6.479417	4.627504	5.905307
H	6.349379	3.812207	6.612212
C	6.010980	7.022035	8.452596
H	6.898529	6.447954	8.751713
H	6.377646	7.913326	7.930998
C	5.646102	13.284892	4.694901
H	4.729237	13.694765	4.251527
H	6.461073	13.433905	3.975095
C	7.160931	8.590789	0.642182
H	7.202310	8.237656	-0.394269

H	6.288996	9.257819	0.709079
C	3.581637	5.895013	2.587745
H	3.713170	5.981701	1.500129
H	4.578564	5.945156	3.045262
C	5.937414	5.879205	6.203447
C	5.184336	6.145707	7.491132
H	4.269169	6.710258	7.235411
C	6.809319	11.277646	5.562822
H	7.612319	11.440364	4.831175
H	6.744186	10.201942	5.759944
C	7.299888	5.416953	3.802985
H	7.808349	5.228976	2.861203
C	6.987380	7.399083	1.589350
H	7.849747	6.731575	1.440260
H	6.093640	6.816995	1.330432
C	5.496706	12.947130	1.317379
H	6.491014	12.510685	1.179715
H	5.613748	13.923713	1.793608
H	5.057039	13.102413	0.327209
C	1.361059	9.923841	0.983766
H	0.935763	10.306486	1.914670
H	0.668384	9.183112	0.574884
H	1.419689	10.752257	0.269691
C	8.201609	8.654277	3.390808
H	8.174859	8.986312	4.434963
H	9.060395	7.969430	3.307606
C	8.411780	9.838385	2.443705
H	9.346971	10.352036	2.692938
H	7.602374	10.568427	2.588261
C	7.154231	4.367779	4.714996
C	4.352345	11.577302	5.983042
H	4.227867	10.501657	6.174022

H	3.411458	11.938270	5.547084
C	8.426253	9.381680	0.983348
H	8.527515	10.243302	0.314904
H	9.303975	8.742798	0.815156
C	7.258688	13.516574	6.602187
H	7.485120	14.053596	7.531774
H	8.089224	13.697815	5.908855
C	4.698280	4.893748	8.228534
H	4.115736	4.259799	7.549147
H	5.564278	4.303299	8.557315
C	5.947176	14.038586	6.000925
H	6.039937	15.108139	5.779947
C	0.503530	5.517589	4.312339
H	0.019476	4.567256	4.569497
H	-0.142329	6.324327	4.681129
C	7.120752	12.013554	6.875396
H	8.057837	11.624471	7.289476
C	1.541256	4.472160	2.283155
H	1.642209	4.528225	1.191561
H	1.065010	3.511988	2.517421
C	2.539709	6.946209	4.604449
H	1.935152	7.791620	4.959841
H	3.515461	7.002543	5.092331
C	2.924469	4.553225	2.944101
H	3.558731	3.735245	2.583268
C	4.802928	13.815093	7.000768
H	3.862598	14.205778	6.591401
H	5.006879	14.362897	7.929001
C	7.645083	2.973506	4.392061
H	7.545123	2.366409	5.304718
C	6.770525	2.316409	3.309590
H	6.822241	2.929864	2.398437

H	5.723978	2.326965	3.635904
C	2.774756	4.456510	4.469870
H	3.764919	4.512447	4.941816
H	2.329005	3.491820	4.744483
C	5.200902	7.408941	9.691142
H	5.810940	8.012938	10.371017
H	4.353922	8.038984	9.383199
C	3.868564	5.275586	9.457114
H	2.967048	5.811842	9.129562
H	3.527644	4.374099	9.976558
C	5.978715	11.775961	7.875750
H	5.883360	10.702197	8.085492
H	6.201381	12.276056	8.826514
C	1.886035	5.606225	4.971037
H	1.785028	5.544031	6.062208
C	4.662807	12.313697	7.293216
H	3.847096	12.151181	8.007180
C	2.736846	12.563515	2.642043
H	2.210341	12.769449	1.704389
H	2.815803	13.506953	3.189860
H	2.118110	11.883637	3.236165
C	9.578634	1.500302	3.674621
H	9.512120	0.899646	4.592152
H	10.630222	1.494603	3.369306
C	8.704757	0.860489	2.593589
H	8.832688	1.415908	1.654302
H	9.027109	-0.167975	2.400135
C	9.123421	2.929939	3.976708
H	9.739584	3.377591	4.763707
H	9.264636	3.544835	3.077354
C	4.667993	6.167708	10.410479
H	5.517037	5.594244	10.806556

H	4.052597	6.456429	11.268846
C	7.228515	0.890867	2.995174
H	7.087082	0.264298	3.886506
H	6.607113	0.458601	2.203789

5.log

SCF (M06-2X) = -2882.10313299

E(SCF)+ZPE(0 K)= -2880.926677

H(298 K)= -2880.873854

G(298 K)= -2881.011467

Lowest Frequency = -166.1643 cm^{-1}

Sn	12.849436	11.905155	16.569296
Si	12.055770	14.461588	15.126236
Si	14.062229	14.493505	17.566623
O	12.508506	9.893395	16.640607
O	13.951552	8.445570	15.635238
N	13.443647	12.982104	18.179730
N	14.292188	10.763140	15.630032
O	13.508319	14.353050	15.979889
C	16.792117	11.245832	12.929685
H	16.834421	11.387970	11.853670
C	12.515624	14.627477	13.326724
H	13.200559	13.817085	13.058074
H	13.020276	15.578689	13.132390
H	11.644235	14.564458	12.667547
N	11.404702	12.908165	15.564117
C	10.181273	12.240628	15.107553
C	17.987718	11.255229	13.642365
C	13.236796	10.519861	21.101690
H	13.187469	9.425662	21.113528

C	13.290296	11.002103	19.645874
H	14.158435	10.571144	19.128230
H	12.392278	10.650866	19.115546
C	16.718603	9.058945	17.427708
H	15.874097	8.608949	16.900125
H	17.630128	8.641349	16.975540
C	13.959009	9.530178	12.395579
H	14.789319	9.137559	11.790659
H	13.921832	8.928964	13.308811
C	17.942724	11.065296	15.019635
H	18.879568	11.066046	15.568408
C	16.745491	10.584641	17.194332
H	15.827907	11.014914	17.625741
C	15.561740	11.065411	13.560999
C	16.739781	10.874429	15.702279
C	13.367212	12.535694	19.573931
C	15.921271	14.549578	17.433520
H	16.260227	13.693275	16.838400
H	16.407410	14.498054	18.412112
H	16.255080	15.462361	16.931073
C	15.538478	10.880945	14.959598
C	14.617322	12.999328	20.342039
H	14.674421	14.097829	20.317725
H	15.505194	12.615146	19.826560
C	13.631857	9.572464	15.930772
C	10.493282	11.236831	13.985064
H	11.213769	10.495085	14.361036
H	10.979100	11.776277	13.160458
C	17.893368	10.849374	19.442835
H	18.755393	11.293009	19.952479
H	16.998241	11.295102	19.894857
C	12.650725	9.410872	11.610523

H	12.475427	8.365309	11.336348
H	11.817630	9.707209	12.260108
C	14.568731	12.525805	21.801775
H	15.470687	12.867389	22.322259
C	14.497340	10.992060	21.840038
H	15.391007	10.558349	21.372740
H	14.474184	10.645126	22.880250
C	7.246680	11.833451	15.265554
H	6.322024	11.346512	14.932541
H	6.975991	12.538179	16.061775
C	19.774984	10.045066	12.361956
H	18.944986	9.607749	11.791786
H	19.988691	9.360510	13.189050
C	14.287931	10.997442	12.741077
H	13.462621	11.383745	13.359188
C	17.856810	9.336970	19.668035
H	17.794757	9.112756	20.738884
H	18.796204	8.897739	19.305396
C	17.937951	11.189374	17.950988
H	17.976694	12.274849	17.800279
H	18.873020	10.778663	17.549448
C	11.056570	15.927359	15.718834
H	10.625194	15.737395	16.705520
H	10.235940	16.144127	15.028552
H	11.684677	16.821737	15.780718
C	11.990842	11.107901	21.781304
H	11.934122	10.764241	22.821325
H	11.084941	10.756752	21.272092
C	8.234990	11.593240	12.972063
H	7.319320	11.109745	12.610497
H	8.681151	12.123991	12.121253
C	19.315122	11.400931	12.925124

H	20.055721	11.730370	13.669834
C	9.513623	11.484370	16.273567
H	9.296614	12.200417	17.077568
H	10.210417	10.729028	16.664886
C	12.648790	10.294885	10.361397
H	13.397211	9.916340	9.651721
H	11.678162	10.240867	9.856342
C	12.991691	11.746335	10.706726
H	13.028747	12.356148	9.797654
H	12.198773	12.170966	11.338640
C	12.121027	13.111213	20.274940
H	11.226664	12.789284	19.723638
H	12.155189	14.207182	20.225975
C	16.685775	8.704321	18.915363
H	15.741545	9.059471	19.352922
H	16.693083	7.616501	19.038669
C	8.579170	9.786787	14.684340
H	7.672327	9.266166	14.353019
H	9.275275	9.028834	15.062762
C	13.369882	16.023402	18.389876
H	13.649845	16.916168	17.821418
H	13.764588	16.142403	19.403892
H	12.279608	15.984744	18.455162
C	19.260582	12.437671	11.826024
H	18.713887	13.351875	12.049882
C	13.320945	13.115451	22.478237
H	13.279408	12.799682	23.527739
H	13.372499	14.211732	22.470013
C	8.230453	10.783579	15.801171
H	7.779626	10.249594	16.644925
C	7.891340	12.586785	14.092556
H	7.197562	13.346252	13.714534

C	14.328066	11.822926	11.447238
H	14.605809	12.862155	11.659280
H	15.102920	11.422874	10.780598
C	9.175418	13.278728	14.578216
H	8.943618	13.994629	15.377596
H	9.627078	13.838858	13.746254
C	12.059447	12.642120	21.738146
H	11.170132	13.065722	22.218432
C	20.620621	11.066411	10.231217
H	20.040212	10.467684	9.515341
H	21.524299	11.379510	9.695921
C	19.822189	12.281287	10.626860
H	19.716089	13.070082	9.884965
C	9.215133	10.537407	13.503874
H	9.465341	9.828536	12.705885
C	20.987363	10.215529	11.448558
H	21.790905	10.711769	12.007155
H	21.371591	9.241669	11.130126

6.log

SCF (M06-2X) = -3561.68188406

E(SCF)+ZPE(0 K)= -3560.405706

H(298 K)= -3560.345784

G(298 K)= -3560.497760

Lowest Frequency = -176.8582 cm^{-1}

Sn	5.783124	6.821843	1.258884
Si	5.220793	9.772819	1.843521
Si	3.017876	7.553466	2.353507
O	7.077002	5.374480	0.835297
O	3.922073	8.744215	1.598309

N	4.210696	6.288156	2.437689
N	6.521147	8.613882	1.888947
C	4.027561	4.901422	2.877718
C	3.720037	3.968108	1.688638
H	2.836914	4.347583	1.154842
H	4.572725	4.004013	0.992365
C	7.904902	8.871904	2.311416
C	2.867380	4.817639	3.887424
H	1.940644	5.178651	3.417819
H	3.088313	5.477133	4.736504
C	2.421002	8.186010	4.011961
H	3.247307	8.238110	4.726662
H	1.644269	7.545163	4.438580
H	2.001840	9.191006	3.898012
C	3.505206	2.523432	2.163779
H	3.273703	1.882544	1.303257
C	5.260404	10.889390	0.347121
H	6.102674	11.586642	0.362248
H	4.335468	11.467565	0.261766
H	5.351703	10.260904	-0.544482
C	5.109722	2.932596	4.049566
H	6.030160	2.586871	4.533224
C	5.301900	4.381389	3.572981
H	6.143847	4.429573	2.867759
H	5.530024	5.041073	4.420644
C	10.300519	8.046041	2.262385
H	10.947888	7.238774	1.901744
C	2.662452	3.373263	4.367727
H	1.830519	3.346981	5.080892
C	2.339142	2.479356	3.161609
H	2.169229	1.448052	3.494539
H	1.416182	2.821650	2.675834

C	4.789899	2.030925	2.846068
H	5.621489	2.047938	2.130392
H	4.664849	0.993156	3.179693
C	3.945426	2.875537	5.049188
H	3.804209	1.847709	5.405950
H	4.169875	3.497304	5.924770
C	8.854005	7.756865	1.835784
H	8.788580	7.659681	0.743568
H	8.533934	6.792523	2.252449
C	4.969819	10.761864	3.414785
H	4.923081	10.111935	4.292918
H	4.029542	11.319384	3.350316
H	5.773697	11.487924	3.573176
C	10.372260	8.120793	3.794501
H	11.403764	8.315207	4.113973
H	10.070503	7.160441	4.230123
C	1.590415	7.182436	1.204974
H	0.939633	8.054902	1.092857
H	0.977273	6.345822	1.553896
H	1.990767	6.926026	0.218718
C	8.397576	10.209785	1.723655
H	7.742385	11.023305	2.068694
H	8.317429	10.165259	0.629170
C	9.839994	10.505374	2.159226
H	10.158222	11.462607	1.730319
C	9.446624	9.239389	4.293262
H	9.486805	9.293688	5.387356
C	8.004379	8.947189	3.849680
H	7.652022	7.994710	4.268089
H	7.332098	9.730947	4.218654
C	10.758628	9.381416	1.660524
H	11.796941	9.588062	1.948487

H	10.727933	9.329821	0.563988
C	9.900854	10.579131	3.693001
H	10.923807	10.807743	4.016803
H	9.255962	11.390641	4.054225
Sn	6.785202	5.449495	-1.159451
Si	7.804163	2.631924	-1.641679
Si	9.677631	5.162072	-2.117836
O	5.395016	6.801809	-0.724222
O	8.929931	3.846619	-1.398337
N	8.316728	6.231918	-2.252643
N	6.366887	3.591990	-1.882341
C	8.200520	7.552691	-2.876672
C	8.178344	8.677489	-1.822111
H	9.111189	8.626293	-1.242711
H	7.345221	8.503530	-1.125001
C	5.046580	3.131756	-2.323724
C	9.386935	7.804419	-3.825578
H	10.328541	7.742811	-3.259462
H	9.406342	7.019147	-4.591657
C	10.451040	4.609349	-3.731456
H	9.681111	4.407472	-4.482172
H	11.138842	5.354800	-4.139743
H	11.016327	3.686386	-3.565241
C	8.038746	10.053833	-2.489045
H	8.011510	10.832901	-1.716433
C	7.809575	1.664921	-0.043468
H	7.038628	0.890355	-0.006955
H	8.781722	1.192746	0.127765
H	7.628583	2.375212	0.770883
C	6.772992	9.006621	-4.388344
H	5.845105	9.036061	-4.970669
C	6.902173	7.636493	-3.706502

H	6.041100	7.482494	-3.039167
H	6.911497	6.826983	-4.448787
C	2.602479	3.761516	-2.566476
H	1.880363	4.568229	-2.397575
C	9.270672	9.183875	-4.492899
H	10.133051	9.336351	-5.152123
C	9.240531	10.281381	-3.418239
H	9.170405	11.267080	-3.894715
H	10.171802	10.264936	-2.837484
C	6.741165	10.100074	-3.310546
H	5.874894	9.946299	-2.656774
H	6.629454	11.086579	-3.777681
C	7.974940	9.235379	-5.315661
H	7.886104	10.209153	-5.813117
H	7.997991	8.468605	-6.100117
C	3.992092	4.233621	-2.119447
H	3.961990	4.533582	-1.065004
H	4.284435	5.126263	-2.693481
C	8.299406	1.563988	-3.097125
H	8.286598	2.132441	-4.031137
H	9.313356	1.182281	-2.939219
H	7.636047	0.700942	-3.213363
C	2.642239	3.399764	-4.057988
H	1.651515	3.066248	-4.391049
H	2.905764	4.284284	-4.650835
C	10.957914	5.759622	-0.894715
H	11.813465	5.082190	-0.819815
H	11.330636	6.758633	-1.144607
H	10.474078	5.813579	0.086575
C	4.613967	1.883446	-1.530726
H	5.347307	1.080251	-1.696186
H	4.631142	2.122513	-0.459093

C	3.224656	1.404445	-1.974883
H	2.940786	0.520542	-1.391330
C	3.675981	2.287059	-4.283309
H	3.716529	2.030167	-5.348134
C	5.061017	2.772550	-3.824187
H	5.374241	3.658493	-4.391838
H	5.808785	1.991103	-4.003792
C	2.201481	2.526484	-1.746093
H	1.200588	2.187955	-2.041228
H	2.158924	2.783647	-0.679279
C	3.271681	1.047681	-3.469102
H	2.290180	0.686220	-3.800098
H	3.991097	0.236115	-3.637265

7.log

SCF (M06-2X) = -4207.58242154

E(SCF)+ZPE(0 K)= -4206.308722

H(298 K)= -4206.248625

G(298 K)= -4206.399595

Lowest Frequency = -185.9090 cm^{-1}

Sn	5.767025	7.059689	1.386744
Si	4.659540	9.716259	2.514808
Si	2.794000	7.250921	2.162625
O	3.581200	8.675012	1.762459
N	4.184355	6.226812	2.407975
N	6.162134	8.888502	2.205253
C	4.227512	4.863381	2.956503
C	4.345445	3.792290	1.850911
H	3.468881	3.883021	1.193172
H	5.236219	3.977583	1.236258

C	7.539557	9.346540	2.425777
C	2.936847	4.566142	3.747227
H	2.068076	4.657634	3.078278
H	2.823658	5.309320	4.545483
C	1.684685	7.562204	3.641166
H	2.248713	7.672115	4.570580
H	0.948278	6.765969	3.777622
H	1.138156	8.495247	3.464964
C	4.413319	2.382872	2.458954
H	4.527474	1.644034	1.655920
C	4.449806	11.375794	1.680542
H	4.912099	12.193768	2.238851
H	3.380312	11.589595	1.589260
H	4.875993	11.354077	0.673442
C	5.460740	3.315018	4.544149
H	6.316935	3.245014	5.224425
C	5.409487	4.724415	3.937592
H	6.351787	4.923505	3.411458
H	5.296843	5.487224	4.719375
C	9.796990	9.750238	1.340904
H	10.347660	9.683474	0.394054
C	2.969814	3.153348	4.352875
H	2.035732	2.980473	4.899768
C	3.117419	2.111117	3.234936
H	3.135877	1.102305	3.665617
H	2.256754	2.160550	2.555163
C	5.615464	2.289326	3.411320
H	6.545726	2.483112	2.863817
H	5.683533	1.276120	3.826761
C	4.161620	3.042015	5.314139
H	4.189832	2.039906	5.759672
H	4.051736	3.761777	6.134864

C	8.351886	9.284595	1.117243
H	7.846592	9.900034	0.359241
H	8.366413	8.252341	0.747565
C	4.242826	9.823583	4.340186
H	4.382227	8.844166	4.809486
H	3.205952	10.138372	4.496196
H	4.889324	10.537029	4.860086
C	10.459479	8.842580	2.389233
H	11.502062	9.146992	2.544475
H	10.468023	7.805398	2.030474
C	1.773317	6.756098	0.675626
H	0.925952	7.429867	0.517393
H	1.382846	5.737827	0.786904
H	2.406488	6.780760	-0.218252
C	7.561614	10.806818	2.916651
H	6.981442	10.892307	3.846285
H	7.088626	11.446725	2.162323
C	9.005044	11.280498	3.157896
H	8.983488	12.317063	3.513434
C	9.684348	8.932427	3.713719
H	10.158237	8.287966	4.462693
C	8.237206	8.472217	3.487161
H	8.231345	7.424667	3.154020
H	7.656144	8.524319	4.417553
C	9.792693	11.200982	1.841463
H	10.820411	11.550656	1.999809
H	9.336217	11.856613	1.089060
C	9.676749	10.385796	4.209435
H	10.702960	10.729132	4.389747
H	9.137464	10.454566	5.162581
Sn	6.853749	5.498799	-1.410222
Si	7.361897	2.480366	-1.683863

Si	9.617273	4.577505	-2.401378
O	8.685980	3.488522	-1.538904
N	8.443589	5.844358	-2.658535
N	6.083056	3.657342	-1.881787
C	8.711474	7.173067	-3.226234
C	8.972465	8.213350	-2.119748
H	9.815690	7.871889	-1.501562
H	8.090058	8.266383	-1.471207
C	4.709522	3.324590	-2.299323
C	9.945747	7.124735	-4.149581
H	10.824515	6.791389	-3.580013
H	9.767994	6.393268	-4.948354
C	10.239270	3.762328	-3.968643
H	9.434929	3.668059	-4.703785
H	11.054438	4.328178	-4.428069
H	10.614580	2.759630	-3.739293
C	9.249152	9.598847	-2.718228
H	9.423872	10.317148	-1.906920
C	7.283142	1.544976	-0.068679
H	6.462020	0.824150	-0.028796
H	8.220925	1.011143	0.112959
H	7.146260	2.270714	0.740297
C	7.785083	9.032231	-4.679832
H	6.914920	9.345367	-5.267650
C	7.518140	7.642633	-4.082094
H	6.613269	7.685894	-3.462523
H	7.345611	6.901315	-4.872970
C	2.286559	4.076525	-2.370340
H	1.618050	4.902448	-2.101150
C	10.232669	8.510544	-4.751535
H	11.118752	8.442682	-5.393171
C	10.487272	9.521167	-3.622976

H	10.707762	10.507546	-4.049543
H	11.362654	9.216621	-3.035009
C	8.029134	10.037996	-3.543415
H	7.144138	10.093213	-2.896906
H	8.197375	11.038809	-3.960442
C	9.024812	8.965899	-5.582452
H	9.224355	9.950354	-6.023650
H	8.851658	8.266054	-6.409446
C	3.718516	4.448456	-1.961388
H	3.766173	4.674040	-0.887619
H	4.009997	5.363513	-2.491581
C	7.618661	1.319034	-3.132126
H	7.705919	1.871087	-4.072144
H	8.547094	0.758610	-2.978831
H	6.807477	0.592214	-3.238282
C	2.242477	3.841807	-3.887231
H	1.223352	3.581581	-4.199281
H	2.521504	4.761326	-4.416182
C	11.023446	5.036829	-1.257493
H	11.631338	4.155792	-1.029104
H	11.683149	5.804168	-1.672609
H	10.606937	5.413688	-0.317314
C	4.239064	2.041499	-1.582931
H	4.918421	1.212509	-1.827720
H	4.296476	2.204666	-0.498917
C	2.814072	1.658668	-2.006335
H	2.517834	0.741427	-1.484288
C	3.211054	2.707957	-4.253032
H	3.192219	2.540002	-5.336067
C	4.638004	3.088003	-3.823060
H	4.968793	4.002385	-4.333690
H	5.337257	2.291393	-4.101644

C	1.854958	2.798705	-1.638956
H	0.827479	2.533023	-1.916929
H	1.867735	2.963234	-0.552923
C	2.784165	1.424130	-3.524410
H	1.774729	1.131944	-3.839187
H	3.459029	0.599645	-3.788555
S	5.320178	7.346655	-1.031228
S	7.595024	5.509160	0.970677

co2.log

SCF (M06-2X) = -188.371533571

E(SCF)+ZPE(0 K)= -188.359587

H(298 K)= -188.356045

G(298 K)= -188.380274

Lowest Frequency = 694.7538 cm^{-1}

C	0.234483	1.165517	0.000000
O	1.397336	1.165517	0.000000
O	-0.928370	1.165517	0.000000

cs2.log

SCF (M06-2X) = -834.162742185

E(SCF)+ZPE(0 K)= -834.155647

H(298 K)= -834.151640

G(298 K)= -834.178545

Lowest Frequency = 416.9051 cm^{-1}

C	0.234483	1.165517	0.000000
S	1.788861	1.165517	0.000000
S	-1.319895	1.165517	0.000000

TCHP_CO2.log

SCF (M06-2X) = -1102.46745722

E(SCF)+ZPE(0 K)= -1101.907684

H(298 K)= -1101.884005

G(298 K)= -1101.959142

Lowest Frequency = -53.5775 cm^{-1}

N	5.925868	8.064660	3.379827
C	5.663631	6.899849	2.645009
C	4.917841	5.893869	3.282744
C	4.470474	6.089979	4.716230
H	4.184470	7.145613	4.825712
C	6.119596	6.764458	1.322082
C	5.816859	5.577826	0.653929
H	6.151601	5.446892	-0.370794
C	6.934102	7.865085	0.677153
H	6.493440	8.828911	0.975654
C	5.087976	4.552926	1.253439
C	5.634119	5.834311	5.693194
H	5.939212	4.782690	5.598369
H	6.496860	6.445612	5.409999
C	4.773112	3.281763	0.495600
H	5.224634	3.369759	-0.503818
C	4.647182	4.731342	2.566572
H	4.069440	3.943555	3.040538
C	8.393019	7.846426	1.177195
H	8.429548	7.824938	2.271857
H	8.854417	6.910197	0.834103
C	5.080041	0.768341	0.372976
H	5.565161	0.834111	-0.610465

H	5.508917	-0.102945	0.878585
C	3.260747	5.241106	5.122407
H	3.524181	4.175751	5.071010
H	2.433834	5.401324	4.421499
C	6.926927	7.854874	-0.855973
H	5.896787	7.838403	-1.228474
H	7.416774	6.941557	-1.219593
C	9.173761	9.046450	0.638611
H	8.734068	9.965390	1.048844
H	10.210456	9.008514	0.988050
C	9.127845	9.092227	-0.890418
H	9.664154	8.220970	-1.290584
H	9.647551	9.981552	-1.261012
C	2.831159	5.560283	6.556298
H	2.515986	6.610753	6.613935
H	1.963006	4.953351	6.832986
C	5.384151	2.040607	1.166895
H	4.969316	1.942881	2.179708
H	6.464510	2.179173	1.281462
C	7.686101	9.066160	-1.404117
H	7.672292	9.053577	-2.498696
H	7.172555	9.984912	-1.090780
C	3.260095	3.087749	0.299880
H	2.779279	3.023334	1.285867
H	2.838736	3.967241	-0.198557
C	3.981938	5.323276	7.537003
H	4.234060	4.254008	7.539216
H	3.673911	5.578238	8.556232
C	5.220206	6.128084	7.136705
H	6.050816	5.915402	7.817649
H	4.999350	7.199865	7.231191
C	3.573512	0.585991	0.176980

H	3.371316	-0.313288	-0.413809
H	3.099822	0.435956	1.156787
C	2.956310	1.815108	-0.493404
H	1.874342	1.688790	-0.603446
H	3.367910	1.916557	-1.506861
C	6.504469	9.116055	3.361007
O	7.033468	10.161554	3.453002

TCHP_CS2.log

SCF (M06-2X) = -1425.37352488

E(SCF)+ZPE(0 K)= -1424.816405

H(298 K)= -1424.792130

G(298 K)= -1424.870113

Lowest Frequency = -53.7001 cm^{-1}

N	5.940858	8.047301	3.307555
C	5.658282	6.880653	2.614911
C	4.914290	5.879876	3.264522
C	4.477536	6.087461	4.698965
H	4.179089	7.141301	4.799814
C	6.115060	6.748993	1.290944
C	5.809540	5.561797	0.627740
H	6.140591	5.427023	-0.397556
C	6.927913	7.857626	0.658251
H	6.484910	8.814554	0.972598
C	5.080545	4.539531	1.234876
C	5.652796	5.855333	5.668919
H	5.966919	4.805706	5.583522
H	6.509343	6.470285	5.373857
C	4.762795	3.267117	0.480812
H	5.210781	3.353094	-0.520161

C	4.642296	4.717474	2.550072
H	4.065880	3.929781	3.025501
C	8.382414	7.839533	1.170692
H	8.402724	7.838005	2.265655
H	8.848083	6.899681	0.842950
C	5.069931	0.754347	0.361379
H	5.552451	0.818916	-0.623353
H	5.500459	-0.115945	0.867134
C	3.280500	5.230178	5.123868
H	3.556493	4.167657	5.080293
H	2.446205	5.374552	4.428369
C	6.925512	7.849435	-0.874409
H	5.896603	7.838093	-1.250894
H	7.412547	6.934104	-1.237449
C	9.169670	9.033312	0.627243
H	8.730880	9.956334	1.029386
H	10.203914	8.993988	0.983629
C	9.132268	9.073165	-0.901929
H	9.663501	8.196419	-1.297054
H	9.660192	9.957293	-1.273347
C	2.859639	5.560373	6.557858
H	2.531632	6.607292	6.606009
H	2.001471	4.945838	6.848164
C	5.376332	2.027470	1.153029
H	4.964214	1.930910	2.167030
H	6.456998	2.166223	1.264148
C	7.692305	9.056644	-1.420325
H	7.680915	9.044281	-2.514942
H	7.183371	9.977997	-1.107407
C	3.248806	3.073404	0.291072
H	2.771341	3.009709	1.278697
H	2.825532	3.952062	-0.207152

C	4.021255	5.348867	7.531607
H	4.285707	4.282695	7.545445
H	3.718352	5.613349	8.549803
C	5.246870	6.162920	7.111730
H	6.085706	5.967573	7.787447
H	5.016054	7.233456	7.194684
C	3.562870	0.571547	0.170074
H	3.359313	-0.328229	-0.419348
H	3.092056	0.422100	1.151336
C	2.943209	1.799691	-0.499793
H	1.860949	1.673243	-0.605979
H	3.351317	1.900334	-1.514676
C	6.389108	9.103420	3.595769
S	6.978132	10.516761	4.031604

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