Synthesis of Low-Valent Dinuclear Group 14 Compounds with Element–Element Bonds by Transylidation

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1. Experimental Details

1.1 General methods

All experiments and crystallizations were carried out under a dry, oxygen-free argon atmosphere inside the Glovebox or with standard Schlenk techniques. Involved solvents (THF, hexane, toluene, acetonitrile, cyclohexane) were dried using an MBraun SPS-800 or dried in accordance with standard procedures and were stored under molecular sieves prior to use. Glassware was oven-dried at 130 °C prior to use. \(^1\)H, \(^{13}\)C, \(^{31}\)P and \(^{119}\)Sn NMR spectra were recorded on BRUKER Avance-400 spectrometers at 25 °C. All values of the chemical shift are in ppm regarding the \(\delta\)-scale and were referenced to the respective residual solvent signal. All spin-spin coupling constants \((J)\) are printed in Hertz (Hz). To display multiplicities and signal forms correctly the following abbreviations were used: s = singlet, d = doublet, m = multiplet, br = broad signal. Samples for elemental analyses were prepared inside a glovebox and were performed on an Elementar vario MICRO-cube elemental analyzer. Ph\(\text{Y}_2\)Ge, Ph\(\text{Y}_2\)Sn, Cy\(\text{Y}-\text{Li}\) and Cy\(\text{Y}-\text{K}\) were prepared by following literature procedures.\(^{1,2}\) GeCl\(_2\)-dioxane and SnCl\(_2\) (anhydrous) were purchased from Sigma-Aldrich.

1.2 Synthesis of \([2^*][\text{SnCl}_3]\) and Ph\(\text{Y}_2\)GeSnCl\(_2\) (1)

A J.-Young-style NMR tube was filled with SnCl\(_2\) (4 mg, 0.021 mmol) and to this tube a freshly prepared solution of Ph\(\text{Y}_2\)Ge (19.6 mg, 0.021 mmol) in a mixture of solvents C\(_6\)D\(_6\) (0.4 mL) and THF-d\(_8\) (0.1 mL) was added. The reaction mixture was shaken for 10 minutes upon which a colourless precipitate of \([2^*][\text{SnCl}_3]\) formed. The complete consumption of Ph\(\text{Y}_2\)Ge and formation of a mixture of 1 and \([2^*][\text{SnCl}_3]\) were confirmed from the \(^{31}\)P NMR spectrum of the reaction mixture (Figure S1). The reaction mixture was filtered into another J.-Young-style NMR tube and was allowed to stand for 4 hours to let the precipitate \([2^*][\text{SnCl}_3]\) settle down at the bottom of the NMR tube. Subsequently, the solid was separated from the solution and washed with a mixture of C\(_6\)D\(_6\) (0.06 mL) and THF-d\(_8\) (0.06 mL) to remove the impurities [1 and the side product ylide (YH)]. The residue was then dried in vacuo to give \([2^*][\text{SnCl}_3]\) as colorless solid (3 mg, 0.0018 mmol; 26 \% yield). Single crystals of \([2^*][\text{SnCl}_3]\) were grown by slow evaporation technique from its solution in a mixture of C\(_6\)D\(_6\) and THF-d\(_8\) (1:1 ratio).

After \([2^*][\text{SnCl}_3]\) was separated from the reaction mixture, the solution phase of the reaction mixture was filtered into a J.-Young-style NMR tube. The mixture was sonicated for 4 hours in an ultrasound bath thus leading to the conversion of the intermediate SnCl\(_2\) complex (see below) to complex 1 as confirmed by \(^{31}\)P NMR of the solution. The solution was filtered into a glass vial and the solvent was allowed to slowly evaporate thus giving colourless crystals of 1, which were washed with small amounts of benzene to give pure 1 (7 mg, 0.0062 mmol, 89 \%). These crystals were also suitable for single crystal X-ray diffraction analysis.

Yields were calculated according to the following equation:

\[
3 \text{PhYGe} + 3 \text{SnCl}_2 \rightarrow 1 + [2^*][\text{SnCl}_3] + \text{YH} + \text{“SnOCl”}
\]

1 mmol Ph\(\text{Y}\)Ge can only give 0.33 mmol 1 and 0.33 mmol \([2^*][\text{SnCl}_3]\) assuming that both products are formed in a 1:1 ratio as suggested by NMR studies. Thus, 0.33 mmol of 1 corresponds to 100\%.
The same products 1 and [2'][SnCl₃] could be isolated from the reaction of the Ph₂Sn with GeCl₂-dioxane in 1:1 molar ratio. According to ³¹P NMR spectroscopy the same product mixture (i.e. 1:1 ratio of 1 : [2'][SnCl₃] together with ylides) Work-up was performed in the same way as described above.

Characterization of 1:

¹H NMR (400.3 MHz, THF-d₈): δ 2.00 (s, 3H; CH₃), 2.30 (s, 3H; CH₃), 5.94-5.96 (m, 2H, CH₂), 6.06-6.08 (m, 4H, CH₂), 6.47-6.82 (m, 1H, SCHR), 6.96-7.06 (m, 1H, CH₃P), 7.11-7.13 (s, 3H, CH₃), 7.18-7.25 (m, 2H, CH₂), 7.31-7.35 (m, 8H, CH₂), 7.36-7.39 (m, 4H, CH₂), 7.52-7.59 (m, 10H, CH₂).

³¹P NMR (162.05 MHz, THF-d₈): 22.4 (d, 4Jₚp = 3.9 Hz), 27.1 (d, 4Jₚp = 3.9 Hz).

¹¹Sn(¹H) NMR (149.3 MHz, THF-d₈): 63.8.

Anal. Calcd. for C₅₂H₄₄O₄P₄S₂Cl₂Ge₁Sn₁: C, 55.70; H, 3.96. Found: C, 55.35; H, 3.97.

Characterization of [2'][SnCl₃]:

¹H NMR (400.3 MHz, THF-d₈): δ 2.11 (s, 3H; CH₃), 2.18 (s, 6H; CH₃), 6.74-6.76 (m, 4H, CH₂), 6.82-6.84 (m, 4H, CH₂), 6.96-7.06 (m, 10H, CH₂), 7.11-7.13 (s, 3H, CH₃), 7.18-7.25 (m, 2H, CH₂), 7.31-7.35 (m, 8H, CH₂), 7.36-7.39 (m, 4H, CH₂), 7.52-7.59 (m, 10H, CH₂).

¹³C(¹H) NMR (100.6 MHz, THF-d₈): δ 20.3 (CH₃), 20.4 (CH₃), 125.0 (CH₂), 125.1 (CH₂), 126.1 (CH₂), 126.2 (CH₂), 126.8 (d, 1JPC = 102.9 Hz, CPPh₂), 128.3 (d, 1JPC = 73.2 Hz, CPPh₂), 128.4 (d, 3JPC = 12.3 Hz, CPPh₂), 128.7 (d, 3JPC = 12.5 Hz, CPPh₂), 131.3 (d, 4JPC = 2.7 Hz, CPPh₂), 131.8 (d, 4JPC = 2.9 Hz, CPPh₂), 133.4 (d, 2JPC = 10.3 Hz, CPPh₂), 134.2 (d, 2JPC = 10.0 Hz, CPPh₂), 138.8 (C₅C₆), 142.0 (C₅C₆), 146.7 (C₅C₆), 147.3 (C₅C₆). Due to the low
solubility and fluxional behaviour of 1 in solution, it was impossible to detect the quaternary carbon atoms in the $^{13}$C NMR spectrum as well as a signal for the SnCl$_3$ anion in the $^{119}$Sn NMR spectrum.

$^{31}$P($^1$H) NMR (162.05 MHz, THF-d$_6$): 9.9 (br), 13.1 (br).

**Anal. Calcd.** for C$_{78}$H$_{66}$Cl$_9$O$_3$P$_5$S$_3$Ge$_2$Sn$_1$: C, 56.48; H, 4.01. Found: C, 56.86; H, 3.98.

Isolation of intermediate 1-Int

During reaction monitoring we noticed that prior to 1 an intermediate complex 1-Int was formed which upon longer reaction times (or sonication) converted into the final complex 1. This intermediate could be isolated from the reaction mixture. After [2$^+$][SnCl$_3$]$_2$ was separated from the reaction mixture, the solution phase of the reaction mixture was filtered into a glass vial. The solvent was allowed to evaporate, and the obtained residue washed with hexane, thus giving 1-Int as colorless solid (7.6 mg, 0.0068 mmol; 98%). Unfortunately, to obtain single crystal suitable for XRD analysis repeatedly failed. This is probably due to the slow transformation of Int-1 into 1, which complicates crystallization. However, the obtained NMR data as well as elemental analysis suggest that 1-Int is a tautomer, in which the H atom from the C-H activation is located at the other ylide ligand compared to 1. This corroborates with earlier studies by our group on germylene PH$_2$Ge which decomposes via an analogous C-H activation reaction, which according to calculations (as well as the structure of the product) proceeds via addition of the C-H bond across the Ge-C bond to the neighbouring ylide ligand.[2]

Characterization of 1-Int:

$^1$H NMR (400.3 MHz, THF-d$_6$): $\delta$ 2.22 (s, 3H; CH$_3$), 2.30 (s, 3H; CH$_3$), 5.25 (d, $^2$J$_{HH}$ = 10.1 Hz; 1H, SCHP), 6.71-6.73 (d, $^2$J$_{HH}$ = 8.4 Hz, 2H, CH$_{\text{Tol,meta}}$), 6.83-6.85 (d, $^2$J$_{HH}$ = 8.0 Hz, 2H, CH$_{\text{Tol,ortho}}$), 7.00-7.02 (d, $^2$J$_{HH}$ = 8.4 Hz, 2H, CH$_{\text{Tol,cyclo, meta}}$), 7.17-7.20 (m, 4H, CH$_{\text{PPPh,cyclo, ortho, meta, para}}$), 7.28-7.34 (m, 3H, CH$_{\text{PPPh, para}}$), 7.37-7.46 (m, 10H, CH$_{\text{PPPh, ortho}}$), 7.48-7.54 (m, 4H, CH$_{\text{PPPh, meta (two Ph groups)}}$), 7.70-7.72 (d, $^2$J$_{HH}$ = 8.0 Hz, 2H, CH$_{\text{Tol,cyclo, ortho}}$), 7.93-7.98 (m, 6H, CH$_{\text{PPPh, meta}}$), 8.12-8.18 (m, 2H, CH$_{\text{PPPh, meta (two Ph groups)}}$).

$^{13}$C($^1$H) NMR (100.6 MHz, THF-d$_6$): $\delta$ 20.2 (CH$_3$), 20.3 (CH$_3$), 34.3 (br, d, $^1$J$_{PC}$ = 62.0 Hz; PCS), 36.8 (d, $^1$J$_{PC}$ = 98.3 Hz; PHCS), 125.4 (d, $^1$J$_{PC}$ = 137.0 Hz, C$_{\text{PPPh,cyclo,ipso}}$), 127.5 (br, s, CH$_{\text{Tol,ortho}}$), 127.5 (d, $^1$J$_{PC}$ = 61.8 Hz, C$_{\text{PPPh,ipso}}$), 127.6 (d, $^1$J$_{PC}$ = 62.6 Hz, C$_{\text{PPPh,ipso}}$), 127.9 (d, $^1$J$_{PC}$ = 11.9 Hz; CH$_{\text{PPPh,meta}}$), 128.4 (d, $^3$J$_{PC}$ = 12.2 Hz; CH$_{\text{PPPh,meta}}$), 130.1 (d, $^3$J$_{PC}$ = 13.5 Hz; CH$_{\text{PPPh,meta}}$), 131.1 (d, $^4$J$_{PC}$ = 2.3 Hz; CH$_{\text{PPPh,para}}$), 131.4 (d, $^4$J$_{PC}$ = 2.4 Hz; CH$_{\text{PPPh,para}}$), 131.7 (d, $^4$J$_{PC}$ = 2.9 Hz; CH$_{\text{PPPh,para}}$), 133.4 (d, $^2$J$_{PC}$ = 10.4 Hz; CH$_{\text{PPPh,ortho}}$), 133.6 (d, $^2$J$_{PC}$ = 10.9 Hz; CH$_{\text{PPPh,ortho}}$), 134.4 (d, $^2$J$_{PC}$ = 11.2 Hz; CH$_{\text{PPPh,ortho}}$), 134.9 (d, $^3$J$_{PC}$ = 9.9 Hz; CH$_{\text{PPPh,cyclo,GeCCH}}$), 138.1 (CH$_{\text{Tol,meta}}$), 138.5 (CH$_{\text{Tol,para}}$), 138.8 (CH$_{\text{Tol,para}}$), 139.17 (CH$_{\text{Tol,para}}$), 147.2 (br, s, C$_{\text{Tol,ipso}}$), 150.5 (d, $^2$J$_{PC}$ = 17.9 Hz; CH$_{\text{PPPh,cyclo,GeC}}$).

$^{31}$P($^1$H) NMR (162.05 MHz, THF-d$_6$): 18.0, 18.1.

$^{119}$Sn($^1$H) NMR (149.3 MHz, THF-d$_6$): 58.0.

**Anal. Calcd.** for C$_{52}$H$_{44}$O$_4$P$_5$S$_3$Cl$_2$Ge$_1$Sn$_1$: C, 55.70; H, 3.96. Found: C, 55.37; H, 3.94.
1.3 Synthesis of $^{Cy}Y_2$Ge and $^{Cy}Y_2$Sn

Synthesis of $^{Cy}Y_2$Ge

$^{Cy}Y$-$Li$ (197 mg, 0.432 mmol, 2.0 eq.) and GeCl$_2$-dioxane (50 mg, 0.216 mmol, 1.0 eq.) were placed into a Schlenk tube and 20 mL of toluene was added. The reaction mixture was stirred at room temp. for 1h, during which LiCl precipitates out of the solution. The yellow suspension was filtered, and the obtained clear solution was evaporated in vacuo to full dryness (4h, 50 °C, 1 x 10$^{-3}$ mbar). The residue was redissolved in a small amount of ice-cold toluene (5 mL) and filtered again. Removing the solvent in vacuo furnished the title compound as a pale-yellow solid (148 mg, 0.153 mmol, 71 %). X-Ray quality crystals were grown by slow evaporation of a saturated benzene solution.

Characterization of $^{Cy}Y_2$Ge:

$^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) = 1.13 – 1.43 (m, 20H, PCy$_3$-CH$_2$), 1.45 – 1.56 (m, 6H, PCy$_3$-CH$_2$), 1.58 – 1.64 (m, 6H, PCy$_3$-CH$_2$), 1.67 – 1.74 (m, 10H, PCy$_3$-CH$_2$), 1.74 – 1.85 (m, 12H, PCy$_3$-CH$_2$), 1.98 (s, 6H, CH$_3$), 2.20 – 2.34 (m, 6H, PCy$_3$-CH$_2$), 2.49 – 2.62 (m, 6H, PCy$_3$-CH), 6.92 (d, $^3$J$_{HH}$=7.9, 4H, CH$_{Stol,meta}$), 8.36 (d, $^2$J$_{HH}$=7.9, 4H; CH$_{Stol,ortho}$).

$^{13}$C($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) = 21.1 (CH$_3$), 26.7 (PCy$_3$-CH$_2$), 27.0 – 27.8 (m, PCy$_3$-CH$_2$), 28.0 (PCy$_3$-CH$_2$), 28.5 (PCy$_3$-CH$_2$), 34.4 (d, $^1$J$_{PC}$ = 49.8 Hz, PCy$_3$-CH), 47.64 (d, $^3$J$_{PC}$ = 55.6 Hz, PCS), 127.0 (CH$_{Stol,ortho}$), 129.0 (CH$_{Stol,meta}$), 139.2 (CH$_{Stol,para}$), 150.85 (CH$_{Stol,ipso}$).

$^{31}$P($^1$H) NMR (162 MHz, C$_6$D$_6$): $\delta$ (ppm) = 19.7.

Anal. Calcd. for C$_{62}$H$_{90}$O$_4$P$_2$S$_2$Ge$_2$: C, 64.53; H, 8.33; S, 6.62. found: C, 64.57; H, 8.39; S, 6.67

Synthesis of $^{Cy}Y_2$Sn

$^{Cy}Y$-$K$ (257 mg, 0.527 mmol, 2.0 eq.) and finely ground SnCl$_2$ (50 mg, 0.264 mmol, 1.0 eq.) were placed into a Schlenk tube and 20 mL of toluene and a few drops of THF were added. The reaction mixture was stirred at room temp. overnight, during which KCl precipitates out of the solution. The volume of the yellow suspension was reduced to approximately 5 mL, cooled with an ice-bath and filtered, giving a clear slightly yellow solution. Removing the solvent in vacuo furnished the title compound as a pale-yellow solid (201 mg, 0.199 mmol, 75 %). Crystals suitable for XRD analysis were grown by slow evaporation of a saturated benzene solution.

Characterization of $^{Cy}Y_2$Sn:

$^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) = 1.17 – 1.33 (m, 20H, PCy$_3$-CH$_2$), 1.48 – 1.54 (m, 6H, PCy$_3$-CH$_2$), 1.58 – 1.62 (m, 6H, PCy$_3$-CH$_2$), 1.66 – 1.72 (m, 10H, PCy$_3$-CH$_2$), 1.75 – 1.85 (m, 12H, PCy$_3$-CH$_2$), 1.98 (s, 6H, CH$_3$), 2.18 – 2.26 (m, 6H, PCy$_3$-CH$_2$), 2.33 – 2.44 (m, 6H, PCy$_3$-CH), 6.89 (d, $^2$J$_{HH}$=7.9 Hz, 4H; CH$_{Stol,meta}$), 8.24 (d, $^2$J$_{HH}$=7.9 Hz, 4H; CH$_{Stol,ortho}$).
**13C**^1^H NMR (101 MHz, C₆D₆): δ (ppm) = 21.1 (CH₃), 26.7 (PCy₃-CH₂), 27.4 – 27.8 (m, PCy₃-CH₂), 28.0 (PCy₃-CH₂), 28.5 (PCy₃-CH₂), 34.8 (d, J_{PC} = 50.2 Hz, PCy₃-CH₂), 50.4 (d, J_{PC} = 50.5 Hz, PCS), 127.0 (CH₃Stol,ortho), 129.0 (CH₃Stol,meta), 139.2 (CH₃Stol,para), 151.1 (CH₃Stol,pso).

**31P**^1^H NMR (162 MHz, C₆D₆): δ (ppm) = 18.6.

**119Sn**^1^H NMR (149 MHz, C₆D₆): δ (ppm) = −99.4 (t, J_{SnP} = 43.6 Hz).

**Anal. Calcd.** for C₃₂H₈₀O₄P₂S₂Sn₁: C, 61.60; H, 7.95; S, 6.32. found: C, 61.49; H, 8.00; S, 6.23

### 1.4 Synthesis of [CyYSnCl]₂ (3):

A freshly prepared solution of [Cy₂Ge] (51 mg, 0.053 mmol, 1.0 eq. in 0.5 mL C₆D₆) was filtered into a J.-Young-style NMR tube containing finely ground SnCl₂ (10 mg, 0.053 mmol, 1.0 eq.). The tube was placed into an ultra-sound bath and was sonicated for 1h, upon which a white precipitate formed. The reaction mixture was filtered into another NMR tube and the residue was washed with a small amount of C₆D₆ (0.1 mL). The reaction mixture was shaken in THF (0.3 mL), filtered into a glass vial and stored at −30 °C for one week, giving colorless crystals of 3 (15 mg, 0.013 mmol, 47%), suitable for X-ray analyses. The filtrate was identified as 4 (see 1.5 Synthesis of [Cy²(Cl)Ge-Ge(Cl)Cy²] (4):).

**Independent synthesis of 3 starting from the metallated ylide [CyY-K]:**

[CyY-K] (77 mg, 0.16 mmol, 1.0 eq.) and finely ground SnCl₂ (30 mg, 0.16 mmol, 1.0 eq.) were placed into a glass vial and were dissolved in 0.7 mL THF-d₆. The reaction mixture was shaken for 10 min at room temp., filtered into a J.-Young-style NMR tube and analyzed by NMR spectroscopy. The ³¹P{¹H}-NMR spectrum showed the selective formation of 3 and [Cy₂Sn] in a ratio of approximately 1 to 0.5. The addition of another equivalent SnCl₂ yielded full conversion to 3. Upon standing over night, 3 precipitates out of the solution. The solid was filtered off, washed with a small amount of toluene (0.1 mL) and dried in the glovebox atmosphere for 12 h, giving the title compound as a white solid (48 mg, 0.08 mmol, 50%).

Re-dissolving this solid in THF-d₆, gave a mixture of 3 and [Cy₂Sn] in the ³¹P{¹H}-NMR spectrum. When dissolving pure crystals of 3, this product mixture could also be observed, strongly indicating an equilibrium between 3, [Cy₂Sn] and SnCl₂.

NMR data for characterization were collected from a freshly prepared sample of 3 with an excess of SnCl₂ in THF-d₆.

**Characterization of [CyYSnCl]₂ (3):**

**¹H NMR** (400 MHz, THF-d₆): δ (ppm) = 1.09 – 1.32 (m, 10H, PCy₃-CH₂), 1.39 – 1.53 (m, 6H, PCy₃-CH₂), 1.59 – 1.71 (m, 8H, PCy₃-CH₂), 1.73 – 1.81 (m, 6H, PCy₃-CH₂), 2.33 (s, 3H, CH₃), 2.43 – 2.55 (m, 3H, PCy₃-CH), 7.19 (d, J_{HH}= 8.2 Hz, 2H, CH₃Stol,meta), 7.90 (d, J_{HH}= 8.2 Hz, 2H, CH₃Stol,ortho).
Characterization of $^{13}$C\{(H)\} NMR (101 MHz, THF-d$_8$): $\delta$ (ppm) = 21.4 (CH$_3$), 27.1 (d, $^4$J$_{PC} = 1.6$ Hz, PCy$_3$-CH$_2$), 28.1 (d, $^2$J$_{PC} = 12.1$ Hz), 28.6 (d, $^3$J$_{PC} = 3.0$ Hz), 34.6 (d, $^1$J$_{PC} = 49.2$ Hz, PCy$_3$-CH), 127.4 (CH$_{STol,ortho}$), 129.7 (CH$_{STol,meta}$), 140.8 (CH$_{STol,para}$), 149.7 (CH$_{STol,ipso}$). No resonance for the ylidic carbon atom could be detected, probably due broadening and low solubility of the compound.

$^{31}$P\{(H)\} NMR (162 MHz, THF-d$_8$): $\delta$ (ppm) = 24.0 (br).

$^{119}$Sn\{(H)\} NMR (149 MHz, THF-d$_8$): $\delta$ (ppm) = -165.5 (s, br)

Analysis of (see 1.4 independent synthesis of (2)$^{(2)}$ (3)); it was dried in vacuo and subsequently re-dissolved in acetonitrile (0.3 mL). The solution was overlayed with 3 mL of cyclohexane and kept at room temperature for 2 weeks, yielding colourless crystals of 4 (16 mg, 0.014 mmol, 54%), which were suitable for x-ray structure determination.

Independent synthesis of 4 starting from the metallated ylide $^{13}$Y-Li:

![Chemical structure of 4]

$^{1}$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) = 1.09 – 1.30 (m, 16H, PCy$_3$-CH$_2$), 1.44 – 1.84 (m, 44H, PCy$_3$-CH$_2$), 1.95 (s, 3H, CH$_3$), 2.02 (s, 3H, CH$_3$), 2.38 – 2.55 (m, 3H, PCy$_3$-CH), 2.57 – 2.74 (m, 3H, PCy$_3$-CH), 6.86 – 7.13 (m, 4H, CH$_{STol,meta}$), 8.57 (d, $^2$J$_{HH} = 7.9$, 2H, CH$_{STol,ortho}$), 8.64 (d, $^2$J$_{HH} = 7.9$, 2H, CH$_{STol,ortho}$).

$^{13}$C\{(H)\} NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) = 20.9 – 21.4 (m, CH$_3$), 26.1 – 26.4 (m, PCy$_3$-CH$_2$), 27.1 – 27.4 (m, PCy$_3$-CH$_2$), 27.4 – 27.8 (m, PCy$_3$-CH$_2$), 28.0 – 28.2 (m, PCy$_3$-CH$_2$), 33.2 (d, $^1$J$_{PC} = 48.1$ Hz, PCy$_3$-CH), 34.6 (d, $^1$J$_{PC} = 48.3$ Hz, PCy$_3$-CH), 44.0 (d, $^1$J$_{PC} = 49.7$ Hz, PCS), 47.2 (d, $^1$J$_{PC} = 65.8$ Hz, PCS), 129.0 – 129.1 (br, CH$_{STol,ortho}$), 129.1 – 129.2 (br, CH$_{STol,meta}$), 140.7 (CH$_{STol,para}$), 141.1 (CH$_{STol,para}$), 147.1 (CH$_{STol,ipso}$), 147.4 (CH$_{STol,ipso}$).

$^{31}$P\{(H)\} NMR (162 MHz, C$_6$D$_6$): $\delta$ (ppm) = 33.1, 24.1.

Analysis of (C$_{52}$H$_{80}$O$_4$P$_2$S$_2$Ge$_2$Cl$_2$): for C, 56.20; H, 7.26; S, 5.77. found: C, 56.19; H, 7.30; S, 5.67
2. NMR spectra

Figure S1. $^{31}$P($^1$H) NMR spectrum of the reaction mixture of $^{10}$Y$_2$Ge with SnCl$_2$. ([*) signal for YH impurity and (*) signal for unknown impurity].

Figure S2. $^1$H NMR spectrum of 1-Int in THF-$d_8$. 
Figure S3. $^{13}$C{$^1$H} NMR spectrum of 1-Int in THF-$d_8$.

Figure S4. $^{31}$P{$^1$H} NMR spectrum of 1-Int in THF-$d_8$. 
Figure S5. $^{119}$Sn($^1$H) NMR spectrum of 1-Int in THF-d$_8$.

Figure S6. $^1$H NMR spectrum of 1 in THF-d$_8$. 
Figure S7. $^{13}$C($^1$H) NMR spectrum of 1 in THF-d$_8$.

Figure S8. $^{31}$P($^1$H) NMR spectrum of 1 in THF-d$_8$. 
Figure S9. $^{119}\text{Sn}(^{1}H)$ NMR spectrum of 1 in THF-$d_{8}$.

Figure S10. $^{1}H$ NMR spectrum of [2''][SnCl$_{3}$] in THF-$d_{8}$.
**Figure S11.** $^{13}$C($^1$H) NMR spectrum of [2]∗[SnCl$_3$] in THF-$d_8$.

**Figure S12.** $^{31}$P($^1$H) NMR spectrum of [2]∗[SnCl$_3$] in THF-$d_8$. (* signal for YH impurity)
Figure S13. $^1$H NMR spectrum of Cy$_2$Ge in C$_6$D$_6$.

Figure S14. $^{13}$C($^1$H) NMR spectrum of Cy$_2$Ge in C$_6$D$_6$. 
Figure S15. $^{31}P$ (1H) NMR spectrum of $^{\text{Cy}2\text{Ge}}$ in $\text{C}_{6}\text{D}_{6}$.

Figure S16. 1H NMR spectrum of $^{\text{Cy}2\text{Sn}}$ in $\text{C}_{6}\text{D}_{6}$. 
Figure S17. $^{13}$C{\(1\text{H}\)} NMR spectrum of CyY$_2$Sn in C$_6$D$_6$.

Figure S18. $^{31}$P{\(1\text{H}\)} NMR spectrum of CyY$_2$Sn in C$_6$D$_6$. 
Figure S19. $^{119}$Sn($^1$H) NMR spectrum of Cy$_2$Sn in C$_6$D$_6$.

Figure S20. $^1$H NMR spectrum of 3 in THF-$d_8$. Excess SnCl$_2$ present in solution.
Figure S21. $^{13}C(1H)$ NMR spectrum of 3 in THF-$d_8$. Excess SnCl$_2$ present in solution.

The NMR spectra of the dimeric chloro(ylide)stannylene 3 were recorded in the presence of excessive SnCl$_2$ to shift the equilibrium between 3, stannylene CyY$_2$Sn and presumably SnCl$_2$ to the side of 3. This was necessary, since dissolving pure (according to EA), crystalline (XRD) 3 always led to mixtures of 3 and stannylene CyY$_2$Sn. The presence of a mixture of compounds is also confirmed by DFT calculations (see Table S20), which showed that 3 and CyY$_2$Sn→SnCl$_2$ as well as a structure comparable to 4 lie within only 6 kJ/mol of energy.
Figure S22. $^{31}$P($^1$H) NMR spectrum of 3 in THF-$d_8$. Excess SnCl$_2$ present in solution.

Figure S23. $^{119}$Sn($^1$H) NMR spectrum of 3.
Figure S24. $^1$H NMR spectrum of 4 in C$_6$D$_6$.

Figure S25. $^{13}$C($^1$H) NMR spectrum of 4 in C$_6$D$_6$. 

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**Table 1**

| Parameter          | Value |
|--------------------|-------|
| 1 Name              | HO_253.21.fld |
| 2 Origin            | Bruker Biospin GmbH |
| 3 Owner             | n/a |
| 4 Site              | n/a |
| 5 Instrument        | spect |
| 6 Author            | n/a |
| 7 Solvent           | CD$_2$D |
| 8 Temperature       | 298.7 |
| 9 Pulse Sequence    | 60G |
| 10 Experiment       | 10 |
| 11 Probe            | 251989B_0002 (PA: T30 45031 88 H 115 D 03 12) |
| 12 Number of Scans  | 16 |
| 13 Receiver Gain    | 9.8 |
| 14 Relaxation Delay | 1.0000 |
| 15 Pulse Width      | 12.0000 |
| 16 Preparation Frequency | 4.0000 |
| 17 Acquisition Time | 4.0000 |
| 18 Acquisition Date | 2020-05-22T16:45:45 |
| 19 Modification Date | 2020-05-22T16:45:56 |
| 20 Class            | n/a |
| 21 Spectrometer Frequency | 800.33 |
| 22 Spectral Width   | 8012.8 |
| 23 Lowest Frequency | 1539.5 |
| 24 Number of Points | 100 |
| 25 Acquired Size    | 32708 |
| 26 Spectral Size    | 80036 |

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**Table 2**

| Parameter          | Value |
|--------------------|-------|
| 1 Name              | HO_253.50.fld |
| 2 Origin            | Bruker Biospin GmbH |
| 3 Owner             | n/a |
| 4 Site              | n/a |
| 5 Instrument        | spect |
| 6 Author            | n/a |
| 7 Solvent           | CD$_2$D |
| 8 Temperature       | 297.2 |
| 9 Pulse Sequence    | 60G |
| 10 Experiment       | 10 |
| 11 Probe            | 251989B_0002 (PA: T30 45031 88 H 115 D 03 12) |
| 12 Number of Scans  | 3100 |
| 13 Receiver Gain    | 120.7 |
| 14 Relaxation Delay | 2.0000 |
| 15 Pulse Width      | 12.0000 |
| 16 Preparation Frequency | 4.3631 |
| 17 Acquisition Time | 4.3631 |
| 18 Acquisition Date | 2020-05-22T16:31:08 |
| 19 Modification Date | 2020-05-22T16:31:08 |
| 20 Class            | n/a |
| 21 Spectrometer Frequency | 100.67 |
| 22 Spectral Width   | 24038.5 |
| 23 Lowest Frequency | 1951.6 |
| 24 Number of Points | 12C |
| 25 Acquired Size    | 32708 |
| 26 Spectral Size    | 80036 |
Figure S26. $^{31}\text{P}^{{1}\text{H}}$ NMR spectrum of 4 in C$_6$D$_6$. 

| Parameter          | Value                                      |
|--------------------|--------------------------------------------|
| Title              | HO_252.20.pdf                              |
| Origin             | Bruker BioSpin GmbH                        |
| Owner              | zneb                              |
| Site               |                                           |
| Instrument         | spect                                   |
| Author             |                                           |
| Solvent            | CD$_2$D$_6$                                |
| Temperature        | 297.2                                     |
| Pulse Sequence     | zg230                                    |
| Experiment         | 10                                        |
| Probe              | Z598398_062002 (PA.TS803050) BB HI P-D-05  |
| Number of Scans    | 138                                       |
| Receiver Gain      | 196.9                                     |
| Relaxation Decay   | 2.0000                                    |
| Pulse Width        | 35.0000                                   |
| Protonation Frequency |                                    |
| Acquisition Time   | 0.5113                                    |
| Acquisition Date   | 2020-05-22T16:47:16                      |
| Modification Date  | 2020-05-22T16:42:35                      |
| Class              |                                           |
| Spectrometer Frequency | 142.66                                |
| Spectral Width     | 541016.6                                  |
| Lowest Frequency   | 22948.5                                   |
| Nucleus            | $^{31}\text{P}$                           |
| Acquired Size      | 32768                                     |
| Spectral Size      | 65536                                     |
3. Crystal Structure Determination

3.1 General information

Data collection of all compounds was conducted with Oxford Synergy. The structures were solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques. The crystals of all compounds were mounted in inert oil (perfluoropolyalkylether). Crystal structure determinations were affected at 100 K. Crystallographic data (including structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1977236 and CCDC-2012933-2012937. Copies of the data can be obtained free of charge on application to Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; [fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk].

3.2 Data collection and refinement details

1: standard refinement

$\text{2SnCl}_3$: The $\text{SnCl}_3$- anions are strongly disordered but could be localized and refined on a 2-fold (ratio 85:15) and a 3-fold (58+32+10) split position. The unit cell contains a total of 6 molecules of benzene, which could not be refined satisfactorily and were masked out with the solvent mask function of Olex2.

$\text{Cy}_2\text{Ge}$: Due to a high residual electron density of 4.9 e/A$^3$ at a distance of 0.93 A$^3$ from the atom Ge1, the germanium layer was split. Starting from this splitted germanium position, the entire molecule was refined at a disordered position. The ratio of the two components after the final refinement is 92:8. The residual electron density was reduced to an acceptable value of 1.8 e/A$^3$. The structure contains 4 strongly disordered molecules of THF, which could not be localized satisfactorily. They were masked out with the solvent mask function of Olex2.

$\text{Cy}_2\text{Sn}$: standard refinement

$\text{(Cy}_2\text{SnCl)}_2$ (3): The structure contained a disordered THF molecule, which was modelled by RIGU instructions. The final occupancies of the two sides were 0.54:0.46.

$\text{Cy}_2\text{Y(Cl)Ge-Ge(Cl)}\text{Cy}_2$ (4): The checkcif report on the initially solved structure gave a B-Alert, obtained from the Hirshfield test for the two Germanium atoms. This was solved by applying EADP instructions on Ge1 and Ge2 as well as on Cl1 and Cl2.
Table S1. Selected bond length and bond angles for $\text{Cy}_2\text{Ge}$, 4 and $2\text{SnCl}_3$.

|                  | $\text{Cy}_2\text{Ge}$ | $\text{Cy}(\text{Cl})_2\text{Ge}(\text{Cl})$ | 4 | $2\text{SnCl}_3$ |
|------------------|-------------------------|---------------------------------|---|------------------|
| P1-C1 [Å]        | 1.709(4)                | 1.743(2)                        | 1.724(5) |                  |
| P2-C27 [Å]       | 1.711(4)                | 1.742(2)                        | 1.740(5) |                  |
| S1-C1 [Å]        | 1.665(4)                | 1.685(2)                        | 1.690(5) |                  |
| S2-C27 [Å]       | 1.657(4)                | 1.660(2)                        | 1.695(5) |                  |
| Ge1-C1 [Å]       | 2.035(3)                | 1.923(2)                        | 1.924(5) |                  |
| Ge1/2-C27 [Å]    | 2.054(3)                | 2.030(2)                        | 1.940(5) |                  |
| Ge2-C53 [Å]      | -                       | -                               | 2.000(6) |                  |
| Ge1-O1 [Å]       | 2.373(3)                | 2.4514(16)                      | -       |                  |
| Ge1-O3 [Å]       | 2.352(3)                | 1.9760(15)                      | -       |                  |
| Ge1-Ge2 [Å]      | -                       | 2.4908(4)                       | 2.4886(8) |                 |
| P1-C1-S1 [°]     | 126.3(2)                | 124.2(1)                        | 116.148(3) |            |
| P2-C27-S2 [°]    | 127.5(2)                | 119.1(1)                        | 115.519(2) |            |
| P3-C53-S3 [°]    | -                       | -                               | 121.992(2) |            |
| C1-Ge1-C27 [°]   | 107.48(14)              | -                               | 118.8(2) |                  |
| C1-Ge1-Ge2 [°]   | -                       | 143.5(1)                        | 130.5(2) |                  |
| C27-Ge2-Ge1 [°]  | -                       | 85.5(1)                         | 104.5(2) |                  |
| Cl1-Ge1-Ge2 [°]  | -                       | 103.8(2)                        | -       |                  |
| Ge1-Ge2-Cl2 [°]  | -                       | 93.2(2)                         | -       |                  |

Table S2. Selected bond lengths and bond angles for $\text{Cy}_2\text{Sn}$ and 3.

|                  | $\text{Cy}_2\text{Sn}$ | $(\text{Cy}\text{SnCl})_2$ (3) |
|------------------|-------------------------|---------------------------------|
| P1-C1 [Å]        | 1.704(3)                | 1.735(5)                        |
| P2-C27 [Å]       | 1.711(3)                | -                               |
| S1-C1 [Å]        | 1.648(3)                | 1.659(5)                        |
| S2-C27 [Å]       | 1.656(3)                | -                               |
| Sn1-C1 [Å]       | 2.240(3)                | 2.191(5)                        |
| Sn1-C27 /Cl1 [Å] | 2.237(3)                | 2.568(12)                       |
| Sn1-Cl1' [Å]     | -                       | 3.0695(11)                      |
| C1-Sn1-C27 [°]   | 103.605(89)             | -                               |
| C1-Sn1-Cl1 [°]   | -                       | 100.9(1)                        |
| P1-C1-S1 [°]     | 126.1(2)                | 123.6(3)                        |
| P2-C27-S2 [°]    | 126.2(1)                | -                               |
Table S3. Data collection and structure refinement details for compounds 1 and [2]SnCl₃.

| Compound | 1 | [2]SnCl₃ |
|----------|---|---------|
| CCDC No. | CCDC 2012934 | CCDC 2012935 |
| Empirical formula | C₆₄H₅₆Cl₂GeO₂P₂S₂Sn | C₇₈H₆₆Cl₃Ge₂O₆P₃S₃Sn₁ |
| Formula weight | 1277.32 | 1658.62 |
| Temperature (K) | 101(2) | 100.00(11) |
| Wavelength | 1.54184 Å | 1.54184 Å |
| Crystal system | Monoclinic | Triclinic |
| Space group | P₂₁/n | P-1 |
| a (Å) | 10.84239(13) | 19.5551(2) |
| b (Å) | 32.4217(4) | 21.5390(2) |
| c (Å) | 16.49907(18) | 23.6054(2) |
| α (°) | 90 | 90.5350(10) |
| β (°) | 96.4751(11) | 113.6730(10) |
| γ (°) | 90 | 107.4850(10) |
| Volume (Å³) | 5762.89(11) | 8588.47(16) |
| Z | 4 | 4 |
| Density (calculated) | 1.472 Mg/m³ | 1.283 Mg/m³ |
| Absorption coefficient | 6.523 mm⁻¹ | 5.548 mm⁻¹ |
| F(000) | 2600.0 | 3360.0 |
| Crystal dimensions (mm³) | 0.53 × 0.136 × 0.015 | 0.325 × 0.039 × 0.033 |
| Theta range (°) | 2.726 to 77.849 | 2.55 to 69 |
| -13 ≤ h ≤ 13, | -23 ≤ h ≤ 23 |
| -40 ≤ k ≤ 40, | -26 ≤ k ≤ 25 |
| -19 ≤ l ≤ 20 | -28 ≤ l ≤ 25 |
| Index ranges | 50007 | 122027 |
| Reflections collected | 12041 reflections | 31844 |
| [R(int) = 0.0584] | [R(int) = 0.0589] |
| Data / restraints / parameters | 12041/0/687 | 31844/247/1751 |
| Goodness-of-fit on F² | 1.083 | 1.045 |
| Final R indices | R₁ = 0.0492, | R₁ = 0.0781, |
| [I>2sigma(I)] | wR₂ = 0.1341 | wR₂ = 0.2279 |
| R indices (all data) | R₁ = 0.0569, | R₁ = 0.0889, |
| | wR₂ = 0.1385 | wR₂ = 0.2404 |
| Largest diff. peak and hole | 2.50 and -2.02 eÅ⁻³ | 2.83 and -2.29 eÅ⁻³ |
**Table S4.** Data collection and structure refinement details for compounds Cy$_2$Ge and Cy$_2$Sn.

| Compound | Cy$_2$Ge | Cy$_2$Sn |
|----------|----------|----------|
| CCDC No. | 1977236  | 2012936  |
| Empirical formula | C$_{52}$ H$_{88}$ O$_4$ P$_2$ S$_2$ Ge | C$_{58}$ H$_{86}$ O$_4$ P$_2$ S$_2$ Sn |
| Formula weight | 967.81 | 1092.01 |
| Temperature (K) | 100.0(2) | 100.01(10) |
| Wavelength | 1.54184 Å | 1.54184 Å |
| Crystal system | Triclinic | Monoclinic |
| Space group | $P\bar{1}$ | $P2_1/n$ |
| a (Å) | 10.3275(3) | 10.94240(10) |
| b (Å) | 12.3453(3) | 26.7086(2) |
| c (Å) | 24.6532(6) | 18.7537(2) |
| α (°) | 89.529(2) | 90 |
| β (°) | 86.210(2) | 95.0080(10) |
| γ (°) | 76.341(2) | 90 |
| Volume (Å$^3$) | 3047.52(14) | 5459.96(9) |
| Z | 2 | 4 |
| Density (calculated) | 1.055 Mg/m$^3$ | 1.328 Mg/m$^3$ |
| Absorption coefficient | 2.089 mm$^{-1}$ | 5.332 mm$^{-1}$ |
| F(000) | 1036.0 | 2312.0 |
| Crystal dimensions (mm$^3$) | 0.185 × 0.031 × 0.019 | 0.128 × 0.111 × 0.048 |
| Theta range (°) | 3.594 to 76.969 | 2.887 to 77.058 |
| Index ranges | -12 ≤ h ≤ 13, -15 ≤ k ≤ 15, -27 ≤ l ≤ 31 | -11 ≤ h ≤ 13, -31 ≤ k ≤ 33, -22 ≤ l ≤ 23 |
| Reflections collected | 42241 | 45191 |
| Independent reflections | 12406 | 11125 |
| [R(int) = 0.0649] | [R(int) = 0.0549] |
| Data / restraints / parameters | 12406/184/733 | 11125/0/606 |
| Goodness-of-fit on F$^2$ | 1.036 | 1.065 |
| Final R indices ($|I|>2\sigma(I)$) | $R_1 = 0.0744$, $wR_2 = 0.2158$ | $R_1 = 0.0416$, $wR_2 = 0.1064$ |
| R indices (all data) | $R_1 = 0.0844$, $wR_2 = 0.2264$ | $R_1 = 0.0464$, $wR_2 = 0.1091$ |
| Largest diff. peak and hole | 1.80 and -0.70 eÅ$^{-3}$ | 0.828 and -1.024 eÅ$^{-3}$ |
Table S5. Data collection and structure refinement details for compounds 3 and 4.

| Compound | 3 | 4 |
|----------|---|---|
| CCDC No. | 2012933 | 2012937 |
| Empirical formula | C$_{30}$H$_{48}$ClO$_3$PSSn | C$_{60}$H$_{95}$Cl$_2$Ge$_2$NO$_4$P$_2$S$_2$ |
| Formula weight | 673.85 | 1236.50 |
| Temperature (K) | 100(2) | 101(2) |
| Wavelength | 1.54184 Å | 1.54184 Å |
| Crystal system | Triclinic | Monoclinic |
| Space group | P-1 | P2$_1$/c |
| a (Å) | 9.0221(3) | 25.4647(2) |
| b (Å) | 11.9787(4) | 15.01930(10) |
| c (Å) | 15.3582(4) | 17.04440(10) |
| α (°) | 67.170(3) | 90 |
| β (°) | 84.700(3) | 107.6870(10) |
| γ (°) | 80.845(3) | 90 |
| Volume (Å$^3$) | 1509.44(9) | 6210.69(8) |
| Z | 2 | 4 |
| Density (calculated) | 1.483 Mg/m$^3$ | 1.322 Mg/m$^3$ |
| Absorption coefficient | 8.921 mm$^{-1}$ | 3.440 mm$^{-1}$ |
| F(000) | 700 | 2616 |
| Crystal dimensions (mm$^3$) | 0.245 × 0.156 × 0.047 | ? |
| Theta range (°) | 3.124 to 67.074 | 3.461 to 77.098 |
| Index ranges | -8 ≤ h ≤ 10 , -14 ≤ k ≤ 14 , -17 ≤ l ≤ 18 | -32 ≤ h ≤ 31 , -16 ≤ k ≤ 18 , -21 ≤ l ≤ 21 |
| Reflections collected | 14458 | 86482 |
| Independent reflections | 5351 | 12974 |
| [R(int) = 0.0495] | [R(int) = 0.0596] |
| Data / restraints / parameters | 5351/70/381 | 12974/0/649 |
| Goodness-of-fit on F$^2$ | 1.037 | 1.033 |
| Final R indices (I>2sigma(I)) | R$_1$ = 0.0691, wR$_2$ = 0.1736 | R$_1$ = 0.0435, wR$_2$ = 0.1143 |
| R indices (all data) | R$_1$ = 0.0724, wR$_2$ = 0.1787 | R$_1$ = 0.0449, wR$_2$ = 0.1154 |
| Largest diff. peak and hole | 2.653 and -0.694 e.Å$^{-3}$ | 1.256 and -1.300 e.Å$^{-3}$ |
3.3 Crystal Structure of 1

Figure S27. ORTEP plot of 1. Ellipsoids drawn at 50% probability level.

Table S6. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for 1. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$ tensor.

| Atom | $x$         | $y$         | $z$         | $U_{eq}$   |
|------|-------------|-------------|-------------|------------|
| Sn1  | 7036.6(2)   | 6776.0(2)   | 3289.3(2)   | 23.92(9)   |
| O1   | 6060(3)     | 7732.7(9)   | 2850.0(17)  | 27.1(6)    |
| S1   | 5171.0(8)   | 7721.8(3)   | 2131.0(5)   | 20.35(17)  |
| P1   | 2860.3(8)   | 7588.8(3)   | 3065.7(5)   | 18.97(18)  |
| Cl1  | 6667.2(10)  | 7121.5(3)   | 4586.9(6)   | 34.0(2)    |
| Ge1  | 4552.4(4)   | 6826.8(2)   | 2737.5(2)   | 17.75(10)  |
| C1   | 3888(3)     | 7418.1(10)  | 2344(2)     | 19.0(7)    |
| C27  | 3774(3)     | 6447.2(11)  | 1928(2)     | 19.4(7)    |
| C2   | 4666(4)     | 8234.0(11)  | 1907(2)     | 23.4(7)    |
| C3   | 3941(4)     | 8309.7(12)  | 1175(2)     | 25.0(7)    |
| O3   | 1652(2)     | 6822.3(8)   | 1729.1(17)  | 24.0(5)    |
| C4   | 3528(4)     | 8708.7(13)  | 999(3)      | 29.0(8)    |
| O4   | 1841(2)     | 6125.5(8)   | 1127.3(16)  | 24.6(5)    |
| Cl2  | 6648.4(9)   | 6067.7(3)   | 3847.2(6)   | 31.3(2)    |
| P2   | 4520.6(8)   | 6158.5(3)   | 1262.5(5)   | 18.68(17)  |
| S2   | 2199.2(8)   | 6412.9(3)   | 1792.3(5)   | 19.38(17)  |
| O2   | 5553(3)     | 7555.5(8)   | 1390.5(17)  | 27.2(6)    |
|   | 4647(4) | 8947.8(13) | 2256(3) | 31.0(9) |
|---|---------|------------|---------|---------|
| C5 | 3862(4) | 9031.2(13) | 1541(3) | 31.2(9) |
| C7 | 5035(4) | 8551.3(12) | 2446(2) | 28.1(8) |
| C21| 3348(4) | 8045.0(12) | 3634(2) | 23.5(7) |
| C8 | 3399(5) | 9464.2(14) | 1362(3) | 40.5(11) |
| C22| 4413(4) | 8021.1(12) | 4188(2) | 25.1(7) |
| C23| 4811(4) | 8366.9(14) | 4644(2) | 31.2(9) |
| C25| 3057(5) | 8750.7(13) | 4013(3) | 34.5(9) |
| C24| 4124(4) | 8730.8(13) | 4552(3) | 32.4(9) |
| C26| 2655(4) | 8407.2(12) | 3546(3) | 27.8(8) |
| C16| 1191(4) | 7831.1(13) | 1751(2) | 29.7(8) |
| C10| 3527(3) | 6825.3(11) | 3652(2) | 20.6(7) |
| C15| 1324(3) | 7672.5(11) | 2536(2) | 21.9(7) |
| C9 | 2843(3) | 7176.9(11) | 3792(2) | 20.1(7) |
| C17| 12(4)  | 7900.0(14) | 1353(3) | 32.2(9) |
| C11| 3519(3) | 6500.6(12) | 4205(2) | 22.0(7) |
| C19| -888(4) | 7650.1(13) | 2518(3) | 29.9(8) |
| C13| 2122(4) | 6873.8(13) | 4978(2) | 24.9(8) |
| C18| -1026(4) | 7812.5(13) | 1738(3) | 31.1(9) |
| C12| 2804(4) | 6518.1(12) | 4845(2) | 25.4(8) |
| C20| 280(4)  | 7579.0(12) | 2917(3) | 27.8(8) |
| C14| 2176(4) | 7210.6(12) | 4469(2) | 24.5(7) |
| C28| 2447(4) | 6189.3(12) | 3059(2) | 24.5(7) |
| C29| 294(4)  | 6387.6(12) | 3700(2) | 26.2(8) |
| C31| 676(4)  | 5803.6(13) | 3962(2) | 32.3(9) |
| C32| 1752(4) | 5614.1(13) | 3573(2) | 28.4(8) |
| C34| 122(5)  | 5595.1(15) | 4656(3) | 39.0(10) |
| C35| 4068(4) | 6269.5(12) | 38(2)   | 25.0(7) |
| C36| 4594(4) | 6044.2(13) | -406(2) | 29.1(8) |
| C37| 4322(4) | 6146.9(14) | -1223(2)| 34.0(9) |
| C38| 3538(5) | 6475.3(15) | -1444(3)| 35.9(10) |
| C46| 7124(4) | 6027.9(12) | 1607(2) | 26.8(8) |
| C39| 3040(4) | 6708.8(14) | -858(2) | 31.3(9) |
| C47| 4373(4) | 5608.6(11) | 1425(2) | 23.0(7) |
| C40| 3321(4) | 6605.1(12) | -38(2)  | 25.0(7) |
| C52| 3718(4) | 5349.3(12) | 859(3)  | 28.3(8) |
| C41| 6148(3) | 6293.7(12) | 1353(2) | 21.9(7) |
| C51| 3509(5) | 4941.1(13) | 1056(3) | 38.1(10) |
| C42| 6401(4) | 6691.9(12) | 1094(2) | 23.3(7) |
| C50| 3949(5) | 4790.7(13) | 1822(3) | 38.3(10) |
| C43| 7621(4) | 6824.3(13) | 1110(2) | 27.4(8) |
| C49| 4621(4) | 5042.6(13) | 2385(3) | 32.3(9) |
| C44| 8588(4) | 6560.9(14) | 1375(2) | 28.2(8) |
| C48| 4832(4) | 5452.2(12) | 2194(2) | 26.7(8) |
| C45| 8346(4) | 6164.9(14) | 1618(3) | 31.3(9) |
| C61| 8214(6) | 4950.3(19) | 2007(4) | 52.7(13) |
| C62| 7961(6) | 4681.4(19) | 1373(4) | 55.8(14) |
The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^* U^{11} + \ldots + 2hk a^* b^* U^{12} ]$

| Atom | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|------|----------|----------|----------|----------|----------|----------|
| Sn1  | 17.96(13)| 30.60(15)| 22.22(14)| 1.46(9)  | -2.03(9) | 0.14(9)  |
| O1   | 19.2(13) | 30.4(14) | 30.0(13) | 1.6(11)  | -4.3(11) | -3.7(11) |
| S1   | 18.2(4)  | 21.2(4)  | 21.3(4)  | 1.3(3)   | 0.3(3)   | -0.7(3)  |
| P1   | 16.7(4)  | 19.8(4)  | 19.7(4)  | 0.0(3)   | -0.7(3)  | 0.4(3)   |
| Cl1  | 37.3(5)  | 40.1(5)  | 22.6(4)  | -3.4(4)  | -5.9(4)  | 5.2(4)   |
| Ge1  | 16.6(2)  | 19.2(2)  | 16.84(19)| 0.37(14)| -0.94(15)| 0.18(14) |
| C1   | 20.1(17) | 15.9(15) | 20.4(16) | 1.0(12)  | -0.1(13)| 2.2(13) |
| C27  | 16.6(16) | 21.5(16) | 19.9(16) | 1.0(13)  | 0.8(12)  | 0.9(13) |
| C2   | 21.9(19) | 24.0(18) | 24.4(18) | 1.1(13)  | 3.0(14)  | -0.7(14)|
| C3   | 26.6(19) | 21.8(17) | 25.9(18) | 0.4(14)  | 0.8(15)  | -2.7(15)|
| O3   | 16.2(13) | 25.0(13) | 30.4(14) | 2.8(10)  | 0.4(10)  | 4.0(10) |
| C4   | 29(2)    | 26.8(19)| 29.9(19)| 5.0(15)  | -0.8(16) | 0.3(16)|
| O4   | 19.6(13) | 29.6(14)| 23.9(12) | -3.4(10) | -0.6(10) | -2.1(10)|
| Cl2  | 30.7(5)  | 31.0(5)  | 30.4(4)  | 3.5(4)   | -4.5(4)  | 0.6(4) |
| P2   | 16.8(4)  | 20.1(4)  | 18.5(4)  | -0.2(3)  | -1.0(3)  | 1.2(3) |
| S2   | 15.9(4)  | 21.1(4)  | 20.7(4)  | 0.1(3)   | -0.1(3)  | -0.3(3)|
| O2   | 30.4(15) | 24.4(13) | 28.0(13) | 0.6(10)  | 8.0(11)  | -0.9(11)|
| C6   | 38(2)    | 25.8(19)| 29.5(19)| -3.0(15)| 6.2(17)  | -6.5(17)|
| C5   | 36(2)    | 24.8(19)| 34(2)    | 5.5(16)  | 11.9(17) | 3.0(16)|
| C7   | 35(2)    | 25.5(19)| 23.9(18)| 0.6(14)  | 2.8(15)  | -1.8(16)|
| C21  | 24.1(18) | 22.8(17)| 23.3(17)| -2.9(14)| 1.7(14)  | -4.3(14)|
| C8   | 53(3)    | 25.2(2)  | 46(3)    | 5.9(18)  | 14(2)    | 7(2) |
| C22  | 22.3(18) | 29.2(19)| 24.1(17)| -4.0(15)| 4.1(14)  | -1.2(15)|
| C23  | 29(2)    | 44(2)    | 20.5(18)| -10.0(16)| 2.3(15)| -11.0(18)|
| C25  | 42(3)    | 23.2(19)| 40(2)    | -4.4(17)| 9.0(19)  | 0.3(17)|
| C24  | 41(2)    | 29(2)    | 28.3(19)| -9.5(16)| 7.9(17)  | -12.6(18)|
| C26  | 27(2)    | 24.7(19)| 32.0(19)| -1.1(15)| 3.7(16)  | -2.6(15)|
| C16  | 26(2)    | 37(2)    | 25.9(19)| 4.6(16)  | 1.5(15)  | 2.1(16)|
| C10  | 16.9(17) | 26.2(18)| 18.0(16)| -1.2(13)| -1.1(13)| -0.4(13)|
| C15  | 19.0(17) | 20.3(16)| 25.1(17)| -1.5(13)| -3.4(14)| 0.5(13)|
| C9   | 20.4(17) | 19.7(16)| 19.1(16)| -1.2(12)| -2.7(13)| -0.1(13)|
| C17  | 27(2)    | 40(2)    | 28.7(19)| 4.6(17)  | -1.8(16)| 8.1(17)|
| C11  | 19.9(17) | 25.7(18)| 19.2(16)| 2.4(13)  | -2.5(13)| -0.5(14)|

Table S7. Anisotropic displacement parameters ($\text{Å}^2 \times 10^{3}$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^* U^{11} + \ldots + 2hk a^* b^* U^{12} ]$. 


| C19 | 17.7(18) | 33(2) | 40(2) | 3.2(17) | 3.9(16) | -0.8(15) |
| C13 | 22.3(19) | 34(2) | 18.3(16) | -3.5(14) | 0.3(14) | -4.3(15) |
| C18 | 21.6(19) | 33(2) | 36(2) | -1.4(17) | -8.9(16) | 2.2(16) |
| C12 | 24.5(19) | 29.8(19) | 20.8(17) | 4.7(14) | 1.8(14) | -3.4(15) |
| C20 | 22.7(19) | 26.8(19) | 34(2) | 6.3(15) | 1.9(15) | 4.0(15) |
| C14 | 23.9(19) | 29.1(19) | 20.1(16) | -3.0(14) | 0.8(14) | 0.3(15) |
| C28 | 14.4(16) | 21.2(17) | 24.0(16) | -1.8(13) | -0.2(13) | -3.3(13) |
| C29 | 22.3(18) | 26.5(18) | 24.2(17) | 0.0(14) | 0.7(14) | -2.6(14) |
| C30 | 16.3(17) | 37(2) | 24.6(17) | -1.0(15) | -0.3(14) | 0.6(15) |
| C31 | 27(2) | 31(2) | 26.2(18) | 0.2(15) | 3.6(15) | -7.9(16) |
| C32 | 38(2) | 23.6(19) | 36(2) | 3.7(16) | 6.9(18) | -4.4(17) |
| C33 | 30(2) | 23.5(18) | 32(2) | -1.0(15) | 5.3(16) | 1.0(16) |
| C34 | 44(3) | 40(2) | 35(2) | 7.1(19) | 14(2) | -2(2) |
| C35 | 21.2(18) | 24.7(17) | 21.0(16) | -0.8(13) | -1.7(13) | -1.5(14) |
| C36 | 32(2) | 31(2) | 23.2(18) | -0.6(15) | 0.0(15) | 4.1(17) |
| C37 | 39(2) | 40(2) | 23.0(19) | -3.4(16) | 4.9(17) | 2.9(19) |
| C38 | 42(3) | 42(2) | 21.6(18) | 2.1(17) | -2.0(17) | -4(2) |
| C46 | 21.7(19) | 27.8(19) | 29.6(19) | -0.1(15) | -2.2(14) | 3.4(15) |
| C39 | 32(2) | 36(2) | 24.5(19) | 8.0(16) | -3.5(16) | 3.6(17) |
| C47 | 19.7(17) | 22.7(17) | 26.3(18) | -0.5(14) | 2.1(14) | 2.1(14) |
| C40 | 22.3(18) | 27.7(19) | 24.5(18) | -0.7(14) | 1.4(14) | 1.1(15) |
| C52 | 29(2) | 24.5(19) | 30.3(19) | -1.4(15) | -3.6(16) | 0.7(15) |
| C41 | 18.2(17) | 27.5(18) | 19.4(16) | -2.6(13) | -1.2(13) | -0.6(14) |
| C51 | 37(2) | 23(2) | 52(3) | -3.4(18) | -5(2) | -5.9(17) |
| C42 | 19.9(18) | 26.7(18) | 23.0(17) | -1.0(14) | 1.3(14) | -0.8(14) |
| C50 | 37(2) | 19.9(19) | 58(3) | 6.2(18) | 5(2) | 4.3(17) |
| C43 | 24(2) | 33(2) | 25.1(18) | 1.1(15) | 3.7(15) | -6.6(16) |
| C49 | 31(2) | 30(2) | 35(2) | 7.3(16) | 1.1(17) | 6.5(17) |
| C44 | 16.3(17) | 41(2) | 27.0(18) | -5.9(16) | 3.3(14) | -0.6(16) |
| C48 | 27(2) | 28.8(19) | 23.9(18) | 1.6(15) | 0.8(15) | -0.1(16) |
| C45 | 20.9(19) | 38(2) | 34(2) | -5.2(17) | -2.0(15) | 5.8(16) |
| C61 | 45(3) | 59(3) | 53(3) | 18(3) | 3(2) | 1(3) |
| C62 | 45(3) | 57(3) | 63(4) | 8(3) | -7(3) | -10(3) |
| C63 | 47(3) | 51(3) | 59(3) | -8(3) | -17(3) | 6(3) |
| C64 | 41(3) | 72(4) | 55(3) | -12(3) | 5(2) | -2(3) |
| C65 | 32(3) | 51(3) | 67(3) | -8(3) | -1(2) | -2(2) |
| C66 | 51(3) | 49(3) | 51(3) | -1(2) | -5(2) | 10(2) |
| C71 | 66(4) | 64(4) | 43(3) | 15(3) | 15(3) | 33(3) |
| C72 | 72(4) | 53(3) | 38(3) | -1(2) | -10(3) | 11(3) |
| C73 | 46(3) | 56(3) | 40(3) | 12(2) | -8(2) | -3(2) |
| C74 | 46(3) | 50(3) | 26(2) | 7.8(18) | 1.9(18) | 9(2) |
| C75 | 46(3) | 42(2) | 32(2) | 12.2(19) | -4.9(19) | 7(2) |
| C76 | 42(3) | 55(3) | 50(3) | 20(2) | 8(2) | 15(2) |
3.4 Crystal Structure of 2'

Figure S28. ORTEP plot of 2'. Ellipsoids drawn at 50% probability level. Only one molecule of the asymmetric unit shown. SnCl$_3$ anion omitted for clarity.

Table S8. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2 \times 10^3$) for 2'. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$ tensor.

| Atom  | x     | y     | z     | U(eq) |
|-------|-------|-------|-------|-------|
| Sn1C  | 1877.1(5) | 3422.3(4) | 5227.4(3) | 50.4(2) |
| Cl1C  | 1816.1(18) | 4453.7(13) | 5639.7(13) | 62.4(4) |
| Cl2C  | 1425.7(15) | 2778.2(13) | 5941.9(11) | 62.4(4) |
| Cl3C  | 554.1(14)  | 3135.0(12) | 4342.7(10) | 62.4(4) |
| Sn1D  | 1669(3)   | 3623(3)  | 5120(2)  | 50.4(2) |
| Cl1D  | 308(7)    | 3354(7)  | 4326(5)  | 62.4(4) |
| Cl2D  | 1284(9)   | 2894(7)  | 5817(6)  | 62.4(4) |
| Cl3D  | 1752(11)  | 4597(6)  | 5625(7)  | 62.4(4) |
| Sn2A  | -1489.4(7) | 918.8(6)  | 7977.0(6) | 82.9(3) |
| Cl1A  | -1084(3)  | 2063(2)  | 7808(2)  | 93.4(7) |
| Cl2A  | -613(3)   | 1176(4)  | 9117(2)  | 93.4(7) |
| Cl3A  | -2613(3)  | 1015(4)  | 8179(2)  | 93.4(7) |
| Element | Value | Value | Value | Value |
|---------|-------|-------|-------|-------|
| Sn2B   | -1803.1(12) | 503.7(11) | 8243.6(11) | 82.9(3) |
| Cl1B   | -518(5) | 1232(7) | 9017(4) | 93.4(7) |
| Cl2B   | -1635(4) | 965(4) | 7376(3) | 93.4(7) |
| Cl3B   | -2590(5) | 1105(6) | 8350(4) | 93.4(7) |
| Sn2E   | -1184(4) | 1300(3) | 8423(3) | 82.9(3) |
| Cl1E   | -1262(14) | 535(10) | 7608(10) | 93.4(7) |
| Cl2E   | -970(17) | 2251(9) | 7876(13) | 93.4(7) |
| Cl3E   | -2590(5) | 1105(6) | 8350(4) | 93.4(7) |
| P2     | 4946.3(8) | 7893.4(6) | 1740.1(6) | 32.6(3) |
| O2     | 4771(3) | 7492(2) | 3626.1(19) | 45.1(9) |
| S2     | 5677.9(8) | 9244.9(6) | 8423(3) | 34.1(3) |
| C2     | 6282(4) | 7874(3) | 4281(3) | 44.8(14) |
| Ge2    | 6464.8(4) | 10312.8(3) | 2927.3(3) | 31.58(14) |
| O2'    | 4769(2) | 7402.9(17) | 7128.5(16) | 34.1(8) |
| C2'    | 5805(3) | 7690(3) | 6687(3) | 36.2(11) |
| P2'    | 3535.5(8) | 6671.5(6) | 7558.0(6) | 28.7(3) |
| S2'    | 4052(17) | 5678.7(6) | 8274.6(13) | 31.5(3) |
| Ge2'   | 5334.8(4) | 5192.6(3) | 7940.4(3) | 31.76(14) |
| O4     | 6153(2) | 9907.6(19) | 1999.7(17) | 39.0(8) |
| C3     | 7036(4) | 8055(3) | 4320(3) | 55.0(16) |
| S3     | 7705.3(8) | 9530.8(6) | 3554.3(6) | 35.8(3) |
| P3     | 8340.6(8) | 10938.1(7) | 3620.7(6) | 37.2(3) |
| O3'    | 4166(2) | 6042.4(19) | 8841.2(17) | 38.4(8) |
| C3'    | 5880(4) | 8024(4) | 6213(3) | 57.2(17) |
| P3'    | 7118.0(9) | 5610.8(7) | 8956.0(6) | 36.5(3) |
| S3'    | 6565.9(7) | 6854.6(6) | 8503.4(5) | 30.0(2) |
| C4     | 7635(5) | 8032(3) | 4862(4) | 59.2(18) |
| O4'    | 4629(2) | 5323.3(19) | 8394.7(17) | 36.1(8) |
| C4'    | 6618(5) | 8472(4) | 6311(4) | 65(2) |
| O5'    | 5830(2) | 6801.8(16) | 8051.3(16) | 29.6(7) |
| C5     | 7495(5) | 7808(3) | 5375(3) | 57.4(19) |
| O5    | 6929(2) | 8978.3(18) | 3273.4(18) | 35.5(8) |
| C5'    | 7275(4) | 8579(3) | 6855(4) | 53.5(16) |
| O6'    | 7246(2) | 6997.1(18) | 8386.5(17) | 35.0(8) |
| C6     | 6736(5) | 7596(4) | 5318(3) | 56.0(17) |
| O6    | 8120(2) | 9567(2) | 4221(2) | 46.5(10) |
| C6'    | 7174(5) | 8237(6) | 7313(6) | 112(5) |
| C30    | 4063(4) | 9487(3) | -1(3) | 52.9(16) |
| C29    | 4718(4) | 9367(3) | 432(3) | 45.2(13) |
| C7     | 6112(5) | 7629(3) | 4776(3) | 54.5(16) |
| C7'    | 6439(6) | 7818(6) | 7244(5) | 122(6) |
| C9     | 6018(3) | 9438(3) | 4762(2) | 37.4(11) |
| C9'    | 4178(3) | 5919(2) | 5311(2) | 31.2(10) |
| C8     | 8164(5) | 7783(4) | 5970(3) | 65(2) |
| C8'    | 8068(5) | 9054(4) | 6952(5) | 69(2) |
| C50    | 3216(4) | 7844(3) | 5(3) | 43.7(13) |
| C11    | 7413(4) | 9892(4) | 5420(3) | 55.1(16) |
| C11'   | 2853(4) | 5614(3) | 4499(3) | 51.1(15) |
| C52    | 3625(4) | 7858(3) | 643(3) | 38.5(12) |
|   |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|
| C10 | 6786(4) | 9546(3) | 4848(3) | 42.2(12) |
| C10' | 3378(4) | 5566(3) | 5090(3) | 43.1(13) |
| C12' | 3127(4) | 6016(3) | 4130(3) | 44.2(13) |
| C12 | 7247(5) | 10112(4) | 5883(3) | 63.8(19) |
| C51 | 3557(4) | 7791(3) | -391(3) | 46.2(14) |
| C48 | 4738(4) | 7772(3) | 488(3) | 39.3(12) |
| C14 | 5864(4) | 9667(4) | 5247(3) | 48.2(14) |
| C14' | 4450(4) | 6336(3) | 4936(3) | 46.4(14) |
| C49 | 4325(4) | 7756(3) | -153(3) | 42.2(13) |
| C13 | 6482(5) | 9988(4) | 5808(3) | 66(2) |
| C13' | 3921(4) | 6384(3) | 4350(3) | 50.2(15) |
| C15' | 5812(4) | 6034(3) | 6085(3) | 37.8(12) |
| C15 | 4370(3) | 8622(3) | 4083(2) | 36.9(11) |
| C16' | 5882(5) | 5805(3) | 5558(4) | 53.7(17) |
| C16 | 3615(4) | 8531(4) | 3626(3) | 50.2(15) |
| C40 | 3728(4) | 7828(3) | 2077(3) | 43.8(14) |
| C17 | 3728(4) | 7828(3) | 2077(3) | 43.8(14) |
| C17' | 4323(2) | 7219.2(19) | 5976.5(17) | 38.2(8) |
| C18 | 4865(3) | 6383(2) | 6674(2) | 29.4(10) |
| C19 | 5082(5) | 5835(3) | 5558(4) | 53.7(17) |
| C19' | 7226(5) | 6417(5) | 6657(4) | 71(2) |
| C1 | 5481(3) | 8680(3) | 3510(2) | 33.0(11) |
| Ge1 | 4887.8(3) | 6095.2(3) | 7439.7(2) | 27.46(14) |
| O1 | 5739(2) | 7699.9(18) | 3077.4(17) | 36.4(8) |
| S1 | 5479.1(8) | 7899.6(6) | 3580.0(6) | 34.8(3) |
| P1 | 5236.9(8) | 9107.8(7) | 3979.6(6) | 31.3(3) |
| O1' | 4323(2) | 7219.2(19) | 5976.5(17) | 38.2(8) |
| C1' | 4865(3) | 6383(2) | 6674(2) | 29.4(10) |
| P1' | 4854.2(8) | 5883.1(6) | 6097.6(6) | 29.6(3) |
| S1' | 4863.9(8) | 7172.8(6) | 6593.1(5) | 30.2(2) |
| Ge1 | 5889.7(3) | 9118.9(3) | 2950.0(3) | 28.74(14) |
| O3 | 6064(3) | 9034(2) | 1285.3(19) | 42.6(9) |
| C31' | 1726(4) | 3988(3) | 7645(3) | 43.1(13) |
| C31 | 3518(5) | 9616(3) | 154(3) | 57.3(17) |
| C39' | 2138(4) | 6304(3) | 8511(3) | 42.8(13) |
| C39 | 3098(4) | 7505(4) | 2222(3) | 53.8(16) |
| C33' | 2787(3) | 4850(3) | 8432(3) | 37.7(11) |
| C33 | 4264(4) | 9487(3) | 1217(3) | 44.8(13) |
| C28' | 3126(3) | 5040(3) | 8013(2) | 33.5(11) |
| C28 | 4819(4) | 9372(3) | 1048(3) | 39.7(12) |
| C32' | 2090(4) | 4320(3) | 8235(3) | 42.9(13) |
| C32 | 3617(4) | 9597(3) | 779(3) | 56.0(16) |
| C20 | 6477(4) | 6342(4) | 6623(3) | 49.5(15) |
| C20 | 4459(4) | 8296(3) | 4598(3) | 43.3(13) |
| C36 | 4043(4) | 6827(3) | 2079(3) | 44.3(13) |
| C21 | 5080(3) | 9825(3) | 3632(2) | 35.2(11) |
| C21' | 4574(3) | 5041(2) | 6262(2) | 33.1(10) |
| C22' | 5033(4) | 4647(3) | 6300(3) | 39.7(12) |
| Element | Atomic Number | Atomic Mass | Isotope | Uncertainty |
|---------|---------------|-------------|---------|-------------|
| C22     | 6              | 4536(3)     | 9752(3) | 3004(2)     | 37.0(11)  |
| C46     | 7              | 6396(4)     | 7689(3) | 2237(3)     | 44.2(13)  |
| C44'    | 8              | 4920(4)     | 8714(3) | 8742(3)     | 40.7(12)  |
| C44     | 7              | 6600(5)     | 6997(4) | 1980(3)     | 55.7(17)  |
| C24'    | 6              | 4152(4)     | 3768(3) | 6559(3)     | 46.3(14)  |
| C24     | 7              | 4864(4)     | 10931(3) | 3066(3)     | 43.0(13)  |
| C46     | 7              | 5397(4)     | 11015(3) | 3684(3)     | 44.0(13)  |
| C44'    | 8              | 5309(4)     | 6795(3) | 1491(3)     | 41.7(13)  |
| C44     | 7              | 5503(5)     | 6697(4) | 3966(3)     | 39.1(12)  |
| C24'    | 6              | 4152(4)     | 3768(3) | 6559(3)     | 46.3(14)  |
| C24     | 7              | 4864(4)     | 10931(3) | 3066(3)     | 43.0(13)  |
| C46     | 7              | 5397(4)     | 11015(3) | 3684(3)     | 44.0(13)  |
| C44'    | 8              | 5309(4)     | 6795(3) | 1491(3)     | 41.7(13)  |
| C44     | 7              | 5503(5)     | 6697(4) | 3966(3)     | 39.1(12)  |

... (remaining elements)
| Atom     | U_{11}  | U_{22}  | U_{33}  | U_{23}  | U_{12}  |
|----------|---------|---------|---------|---------|---------|
| C38'     | 1423(4) | 5898(3) | 8066(3) | 46.7(14)|         |
| C38      | 2949(4) | 6852(4) | 2297(3) | 58.7(18)|         |
| C37'     | 1335(4) | 5700(3) | 7474(3) | 48.5(14)|         |
| C37      | 3416(5) | 6510(3) | 2229(3) | 55.0(17)|         |
| C65      | 10150(4)| 10594(4)| 3396(5)| 70(2)   |         |
| C63      | 10397(4)| 10535(4)| 4456(4)| 70(2)   |         |
| C25'     | 3692(4) | 4160(3) | 6519(3) | 44.0(13)|         |
| C26'     | 3897(3) | 4791(3) | 6375(3) | 36.2(11)|         |
| C72      | 8558(4) | 12159(3)| 3194(4)| 48.7(15)|         |
| C72'     | 7040(4) | 4400(3) | 9414(3) | 47.0(14)|         |
| C48'     | 2726(4) | 6171(3) | 6296(3) | 40.4(12)|         |
| C75      | 7990(5) | 11449(4)| 5120(3)| 56.7(16)|         |
| C75'     | 8437(8) | 6810(5) | 10632(4)| 100(4) |         |
| C45'     | 4128(4) | 8555(3) | 8376(3) | 39.0(12)|         |
| C62      | 9736(4) | 10698(3)| 4372(3) | 53.4(16)|         |
| C40'     | 2782(3) | 6534(3) | 8356(3) | 35.4(11)|         |
| C78      | 9156(4) | 11876(3)| 4700(4) | 56.9(16)|         |
| C78'     | 8549(4) | 6664(4) | 9520(3) | 53.8(16)|         |
| C42'     | 4881(3) | 7651(3) | 8399(2) | 33.4(11)|         |
| C43'     | 5306(4) | 8260(3) | 8761(3) | 42.1(12)|         |
| C43      | 5813(4) | 6438(3) | 1566(3) | 49.5(15)|         |
| C77      | 9238(5) | 12173(4)| 5264(4) | 67(2)   |         |
| C77'     | 9106(5) | 7139(5) | 9991(5) | 79(3)   |         |
| C76      | 8667(5) | 11961(4)| 5470(3) | 61.9(18)|         |
| C76'     | 9049(6) | 7224(5) | 10552(4)| 89(3)  |         |
| C74      | 7897(4) | 11144(3)| 4565(3) | 48.2(14)|         |
| C74'     | 7846(5) | 6309(4) | 10159(3)| 65(2)  |         |
| C46'     | 3694(3) | 7932(3) | 8019(2) | 33.9(11)|         |
| C45      | 6893(4) | 7325(4) | 2313(3) | 53.2(15)|         |
| C59      | 8080(5) | 9295(4) | 2601(4) | 64(2)  |         |
| C59'     | 7331(5) | 7679(4) | 9497(3) | 58.7(17)|         |
| C64      | 10595(5)| 10482(5)| 3972(5) | 78(3)  |         |
| C73'     | 7905(4) | 6227(3) | 9600(3) | 49.5(15)|         |
| C73      | 8470(4) | 11352(3)| 4345(3) | 44.1(13)|         |
| C70'     | 6272(5) | 3982(3) | 9999(3) | 56.3(18)|         |
| C70      | 8283(4) | 12282(4)| 2118(4) | 60.1(19)|         |
| C50'     | 2231(5) | 6787(4) | 5484(3) | 57.9(18)|         |
| C69      | 7933(4) | 11611(4)| 1950(4) | 55.9(17)|         |
| C51'     | 2597(5) | 7357(4) | 5912(3) | 53.7(17)|         |
| C53'     | 6347(3) | 5879(3) | 8517(2) | 31.4(10)|         |
| C53      | 7537(3) | 10218(3)| 3315(3) | 36.0(11)|         |
| C54'     | 6708(4) | 7106(3) | 9215(2) | 39.6(12)|         |
| C54      | 8240(4) | 9262(3) | 3206(4) | 52.3(17)|         |
| C57      | 6874(6) | 7741(6) | 10307(4)| 92(3)  |         |
| C57      | 9087(8) | 8789(5) | 2703(9) | 119(5) |         |

**Table S9.** Anisotropic displacement parameters (Å²×10³) for 2+. The anisotropic displacement factor exponent takes the form: \(-2p^2 [ h^2 a^*2 U^{11} + ... + 2 h k a^* b^* U^{12} ]\)
| Atom  | U11   | U22   | U33   | U23   | U13   | U12   |
|-------|-------|-------|-------|-------|-------|-------|
| Sn1C  | 48.3(4)| 58.8(4)| 43.1(3)| 2.2(3)| 23.1(3)| 11.3(3)|
| Cl1C  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Cl2C  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Cl3C  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Sn1D  | 48.3(4)| 58.8(4)| 43.1(3)| 2.2(3)| 23.1(3)| 11.3(3)|
| Cl1D  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Cl2D  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Cl3D  | 58.7(8)| 68.9(9)| 49.9(6)| 10.7(6)| 20.3(5)| 11.7(6)|
| Sn2A  | 70.7(6)| 78.6(6)| 93.9(7)| -18.9(5)| 32.6(5)| 21.7(5)|
| Cl1A  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl2A  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl3A  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Sn2B  | 70.7(6)| 78.6(6)| 93.9(7)| -18.9(5)| 32.6(5)| 21.7(5)|
| Cl1B  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl2B  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl3B  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Sn2E  | 70.7(6)| 78.6(6)| 93.9(7)| -18.9(5)| 32.6(5)| 21.7(5)|
| Cl1E  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl2E  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| Cl3E  | 64.9(10)| 109.4(15)| 85.4(16)| 10.0(13)| 21.5(10)| 15.5(10)|
| P2    | 43.9(7)| 30.5(6)| 29.5(6)| 7.1(5)| 20.1(6)| 14.0(5)|
| O2    | 63.3(3)| 38.2(2)| 45.2(2)| 11.8(17)| 36.2(1)| 12.1(19)|
| S2    | 44.6(7)| 33.7(6)| 32.7(6)| 10.4(5)| 23.4(6)| 14.8(5)|
| C2    | 62.4(2)| 35.3(6)| 36.3(6)| 14(2)| 19(3)| 17(3)|
| Ge2   | 33.0(3)| 31.3(3)| 35.6(3)| 7.9(2)| 17.7(2)| 13.1(2)|
| O2'   | 48.2(2)| 33.9(18)| 30.0(17)| 8.8(14)| 22.2(16)| 18.5(16)|
| C2'   | 44.3(2)| 30.2(2)| 44(3)| 13(2)| 25(3)| 18(2)|
| P2'   | 32.3(6)| 33.8(6)| 26.2(6)| 7.4(5)| 15.0(5)| 15.7(5)|
| S2'   | 36.4(6)| 37.6(6)| 28.6(6)| 12.2(5)| 19.1(5)| 15.8(5)|
| Ge2'  | 38.9(3)| 33.1(3)| 31.4(3)| 9.9(2)| 18.9(3)| 17.3(2)|
| O4    | 49.2(2)| 38.2(3)| 35.5(19)| 10.7(15)| 24.3(18)| 14.3(17)|
| C3    | 57.4(4)| 44(3)| 56(4)| 28(3)| 20(3)| 10(3)|
| S3    | 34.1(6)| 34.9(6)| 47.5(7)| 15.6(5)| 21.6(6)| 17.5(5)|
| P3    | 30.2(7)| 35.1(7)| 48.1(8)| 16.1(6)| 17.0(6)| 12.6(5)|
| O3'   | 47.2(2)| 44(2)| 30.5(18)| 9.5(15)| 22.3(17)| 15.5(17)|
| C3'   | 55.4(4)| 74.5(4)| 44(3)| 19(3)| 30(3)| 9(3)|
| P3'   | 40.2(7)| 40.3(7)| 34.7(7)| 14.7(5)| 16.7(6)| 19.6(6)|
| S3'   | 36.5(6)| 33.2(6)| 27.9(5)| 9.0(4)| 18.1(5)| 15.5(5)|
| C4    | 54.4(2)| 43(3)| 70(4)| 22(3)| 18(3)| 12(3)|
| O4'   | 41.2(2)| 46(2)| 38.5(19)| 18.8(16)| 26.3(17)| 24.2(17)|
| C4'   | 59.4(4)| 86(5)| 59(4)| 23(4)| 42(4)| 12(4)|
| O5    | 35.2(18)| 28.5(16)| 31.8(17)| 6.9(13)| 17.3(15)| 15.3(14)|
| C5    | 87.5(5)| 30(3)| 42(3)| 6(2)| 14(3)| 21(3)|
| O5'   | 40.2(2)| 32.9(18)| 45(2)| 14.0(15)| 24.7(17)| 17.1(16)|
| C5'   | 56.4(2)| 43(3)| 84(5)| 23(3)| 43(4)| 27(3)|
| O6    | 35.5(19)| 38.7(19)| 38.3(19)| 11.5(15)| 20.9(16)| 15.2(15)|
| O6'   | 76.5(5)| 54(4)| 40(3)| 18(3)| 25(3)| 25(3)|
| O6    | 40.2(2)| 41(2)| 61(3)| 22.4(19)| 21(2)| 16.7(17)|
|    |    |    |    |    |    |
|----|----|----|----|----|----|
| C6' | 44(4) | 107(8) | 117(8) | 78(7) | -7(5) |-13(5) |
| C30 | 61(4) | 45(3) | 34(3) | 11(2) | 9(3) | 7(3) |
| C29 | 56(4) | 40(3) | 38(3) | 10(2) | 23(3) | 9(3) |
| C7  | 80(5) | 51(4) | 44(3) | 21(3) | 31(3) | 30(3) |
| C7' | 67(6) | 118(8) | 99(7) | 90(7) | -11(5) | -19(5) |
| C9  | 36(3) | 50(3) | 26(2) | 6(2) | 10(2) | 18(2) |
| C9' | 43(3) | 27(2) | 28(2) | 4.5(18) | 18(2) | 14(2) |
| C8  | 79(5) | 49(4) | 53(4) | 2(3) | 10(4) | 27(4) |
| C8' | 57(4) | 59(4) | 100(6) | 20(4) | 45(4) | 16(3) |
| C50 | 43(3) | 39(3) | 39(3) | 5(2) | 9(3) | 11(2) |
| C11 | 38(3) | 60(4) | 52(4) | 16(3) | 4(3) | 16(3) |
| C11' | 47(4) | 55(4) | 52(4) | 16(3) | 22(3) | 17(3) |
| C52 | 44(3) | 35(3) | 38(3) | 3(2) | 17(2) | 15(2) |
| C10 | 42(3) | 46(3) | 41(3) | 15(2) | 17(3) | 20(3) |
| C10' | 48(3) | 46(3) | 48(3) | 18(3) | 28(3) | 22(3) |
| C12' | 51(3) | 48(3) | 35(3) | 5(2) | 18(3) | 19(3) |
| C12 | 62(5) | 74(5) | 34(3) | 8(3) | 1(3) | 20(4) |
| C51 | 65(4) | 38(3) | 34(3) | 7(2) | 17(3) | 20(3) |
| C48 | 52(3) | 39(3) | 35(3) | 9(2) | 23(3) | 21(2) |
| C14 | 52(4) | 67(4) | 32(3) | 6(3) | 18(3) | 29(3) |
| C14' | 48(3) | 49(3) | 33(3) | 6(2) | 19(3) | 0(3) |
| C49 | 66(4) | 34(3) | 33(3) | 4(2) | 24(3) | 20(3) |
| C13 | 79(5) | 84(5) | 31(3) | 0(3) | 20(3) | 29(4) |
| C13' | 64(4) | 50(3) | 34(3) | 9(3) | 25(3) | 11(3) |
| C15 | 46(3) | 35(3) | 48(3) | 13(2) | 32(3) | 17(2) |
| C15 | 42(3) | 47(3) | 34(3) | 11(2) | 24(2) | 20(2) |
| C16' | 65(4) | 42(3) | 70(4) | -1(3) | 49(4) | 11(3) |
| C16 | 44(3) | 72(4) | 41(3) | 24(3) | 22(3) | 22(3) |
| C40 | 46(3) | 47(3) | 37(3) | 3(2) | 19(3) | 11(3) |
| C17' | 78(5) | 47(4) | 97(6) | 4(4) | 68(5) | 13(3) |
| C17 | 37(3) | 81(5) | 46(3) | 12(3) | 16(3) | 13(3) |
| C18 | 51(4) | 74(4) | 52(4) | 20(3) | 35(3) | 20(3) |
| C18' | 66(5) | 80(5) | 107(7) | 47(5) | 65(5) | 45(4) |
| C19 | 51(4) | 64(4) | 49(3) | 25(3) | 36(3) | 26(3) |
| C19' | 45(4) | 118(7) | 63(4) | 45(5) | 27(4) | 35(4) |
| C1  | 46(3) | 34(3) | 30(2) | 12(2) | 24(2) | 18(2) |
| Ge1' | 34.2(3) | 29.5(3) | 26.9(3) | 8.2(2) | 18.1(2) | 14.5(2) |
| O1  | 52(2) | 32.4(18) | 36.0(19) | 11.0(15) | 25.6(17) | 18.4(16) |
| S1  | 46.8(7) | 31.8(6) | 33.6(6) | 10.8(5) | 23.8(6) | 13.9(5) |
| P1  | 34.1(6) | 40.1(7) | 26.6(6) | 8.9(5) | 16.8(5) | 16.0(5) |
| O1' | 51(2) | 44(2) | 31.4(18) | 15.9(15) | 21.4(17) | 26.2(18) |
| C1' | 36(3) | 34(2) | 24(2) | 8.5(18) | 17(2) | 14(2) |
| P1' | 37.4(7) | 28.6(6) | 29.7(6) | 5.9(5) | 20.4(5) | 11.9(5) |
| S1' | 41.3(7) | 31.0(6) | 29.1(6) | 10.7(4) | 20.7(5) | 18.5(5) |
| Ge1 | 34.5(3) | 29.9(3) | 28.9(3) | 7.6(2) | 18.2(2) | 13.5(2) |
| O3  | 53(2) | 49(2) | 42(2) | 12.5(17) | 32.9(19) | 19.6(19) |
| C31' | 39(3) | 49(3) | 48(3) | 16(3) | 23(3) | 17(3) |
| C31 | 57(4) | 49(4) | 51(4) | 12(3) | 8(3) | 16(3) |
| C39' | 51(3) | 43(3) | 50(3) | 10(2) | 32(3) | 20(3) |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| C39 | 45 | 64(4) | 56(4) | 1(3) | 27(3) | 15(3) |
| C33' | 41(3) | 45(3) | 36(3) | 15(2) | 22(2) | 18(2) |
| C33 | 55(4) | 41(3) | 42(3) | 9(2) | 23(3) | 18(3) |
| C28' | 37(3) | 34(3) | 39(3) | 11(2) | 22(2) | 15(2) |
| C28 | 51(3) | 28(3) | 38(3) | 12(2) | 19(3) | 10(2) |
| C32' | 46(3) | 46(3) | 52(3) | 18(3) | 35(3) | 17(3) |
| C32 | 49(4) | 51(4) | 64(4) | 4(3) | 14(3) | 24(3) |
| C20' | 45(3) | 74(4) | 44(3) | 27(3) | 26(3) | 28(3) |
| C20 | 41(3) | 60(4) | 41(3) | 18(3) | 24(3) | 23(3) |
| C36 | 57(4) | 39(3) | 39(3) | 5(2) | 25(3) | 12(3) |
| C21 | 40(3) | 43(3) | 33(3) | 8(2) | 23(2) | 17(2) |
| C21' | 42(3) | 31(2) | 28(2) | 3.5(19) | 18(2) | 11(2) |
| C22' | 50(3) | 35(3) | 44(3) | 6(2) | 29(3) | 16(2) |
| C22 | 38(3) | 44(3) | 33(3) | 7(2) | 17(2) | 16(2) |
| C46 | 54(4) | 49(3) | 46(3) | 9(3) | 32(3) | 24(3) |
| C44' | 48(3) | 34(3) | 43(3) | 4(2) | 21(3) | 14(2) |
| C44 | 68(5) | 61(4) | 60(4) | 12(3) | 33(4) | 43(4) |
| C24' | 66(4) | 28(3) | 48(3) | 5(2) | 28(3) | 14(3) |
| C24 | 56(4) | 42(3) | 48(3) | 13(2) | 31(3) | 27(3) |
| C25 | 59(4) | 39(3) | 47(3) | 4(2) | 31(3) | 22(3) |
| C42 | 58(4) | 34(3) | 42(3) | 6(2) | 28(3) | 18(3) |
| C26 | 45(3) | 49(3) | 35(3) | 6(2) | 24(2) | 21(3) |
| C27' | 36(3) | 36(3) | 33(2) | 15(2) | 21(2) | 18(2) |
| C27 | 43(3) | 32(2) | 31(2) | 10(2) | 23(2) | 15(2) |
| C55 | 66(5) | 58(4) | 149(9) | 48(5) | 69(6) | 38(4) |
| C55' | 51(3) | 61(4) | 35(3) | 10(3) | 22(3) | 32(3) |
| C29' | 46(3) | 46(3) | 37(3) | 12(2) | 25(3) | 15(3) |
| C68 | 46(3) | 52(3) | 59(4) | 27(3) | 32(3) | 28(3) |
| C68' | 62(4) | 47(3) | 33(3) | 13(2) | 22(3) | 20(3) |
| C52' | 48(3) | 54(3) | 38(3) | 16(2) | 23(3) | 31(3) |
| C47' | 34(3) | 52(3) | 27(2) | 9(2) | 14(2) | 24(2) |
| C47 | 57(3) | 28(2) | 33(3) | 7(2) | 27(3) | 10(2) |
| C41' | 40(3) | 30(2) | 31(2) | 9.6(19) | 21(2) | 17(2) |
| C41 | 44(3) | 38(3) | 42(3) | 12(2) | 26(3) | 19(2) |
| C56 | 89(7) | 73(6) | 225(15) | 58(7) | 115(9) | 52(5) |
| C56' | 59(4) | 110(6) | 39(3) | 3(4) | 23(3) | 46(4) |
| C30' | 42(3) | 49(3) | 42(3) | 6(2) | 18(3) | 14(3) |
| C23' | 67(4) | 34(3) | 51(3) | 10(2) | 33(3) | 24(3) |
| C23 | 48(3) | 50(3) | 36(3) | 15(2) | 20(3) | 27(3) |
| C58 | 93(7) | 87(7) | 141(10) | -31(6) | 91(8) | -6(6) |
| C58' | 63(5) | 94(6) | 72(5) | -40(5) | 18(4) | 12(5) |
| C34' | 47(4) | 64(4) | 69(5) | 8(3) | 31(4) | 2(3) |
| C34 | 95(7) | 98(7) | 71(6) | 17(5) | 2(5) | 50(6) |
| C69' | 69(4) | 43(3) | 35(3) | 8(2) | 24(3) | 11(3) |
| C67' | 55(4) | 35(3) | 33(3) | 9(2) | 14(3) | 15(3) |
| C67 | 31(3) | 43(3) | 59(4) | 23(3) | 22(3) | 19(2) |
| C66' | 56(4) | 72(5) | 86(5) | 22(4) | 31(4) | 40(4) |
| C65' | 89(7) | 93(6) | 128(9) | 47(6) | 69(7) | 65(6) |
| C64' | 99(7) | 79(6) | 120(8) | 25(5) | 82(7) | 48(5) |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C63' | 71(5) | 67(4) | 72(5) | 19(4) | 48(4) | 32(4) |
| C62' | 57(4) | 43(3) | 54(4) | 14(3) | 36(3) | 20(3) |
| C61' | 46(3) | 49(3) | 60(4) | 21(3) | 28(3) | 30(3) |
| C61 | 26(3) | 42(3) | 62(4) | 21(3) | 17(3) | 11(2) |
| C71 | 53(4) | 55(4) | 102(6) | 43(4) | 45(4) | 30(3) |
| C71' | 99(6) | 40(3) | 32(3) | 11(2) | 18(3) | 30(4) |
| C60' | 79(7) | 220(16) | 90(8) | -81(10) | 31(6) | 17(8) |
| C60 | 185(16) | 111(10) | 320(30) | 23(13) | 205(19) | 54(11) |
| C35' | 31(3) | 35(3) | 38(3) | 9(2) | 19(2) | 17(2) |
| C35 | 49(3) | 38(3) | 60(4) | 5(2) | 18(2) | 19(2) |
| C36' | 38(3) | 47(3) | 36(3) | 6(2) | 18(2) | 19(2) |
| C36 | 70(4) | 38(3) | 56(4) | 9(3) | 19(3) | 9(3) |
| C37 | 45(4) | 81(5) | 111(7) | 45(5) | 50(4) | 34(4) |
| C37' | 42(4) | 69(5) | 87(6) | 46(4) | 15(4) | 20(3) |
| C25' | 52(3) | 33(3) | 50(3) | 10(2) | 29(3) | 9(2) |
| C26' | 43(3) | 32(3) | 39(3) | 8(2) | 23(2) | 12(2) |
| C72 | 37(3) | 40(3) | 75(4) | 20(3) | 26(3) | 17(2) |
| C72' | 65(4) | 47(3) | 35(3) | 12(2) | 16(3) | 33(3) |
| C72 | 42(3) | 55(3) | 32(3) | 7(2) | 18(2) | 24(3) |
| C75 | 67(4) | 52(4) | 51(4) | 15(3) | 27(3) | 19(3) |
| C75' | 147(10) | 64(5) | 35(4) | 9(3) | 8(5) | 6(6) |
| C75 | 52(3) | 34(3) | 42(3) | 10(2) | 24(3) | 24(2) |
| C40' | 41(3) | 55(4) | 65(4) | 31(3) | 20(3) | 20(3) |
| C78 | 37(3) | 39(3) | 35(3) | 9(2) | 19(2) | 13(2) |
| C78 | 44(4) | 49(4) | 67(4) | 6(3) | 18(3) | 9(3) |
| C78' | 41(3) | 61(4) | 54(4) | 17(3) | 13(3) | 20(3) |
| C42' | 36(3) | 42(3) | 29(2) | 5(2) | 15(2) | 20(2) |
| C43' | 38(3) | 49(3) | 37(3) | 3(2) | 14(2) | 16(2) |
| C43 | 67(4) | 36(3) | 56(4) | 8(3) | 34(3) | 20(3) |
| C77 | 55(4) | 56(4) | 67(5) | -5(3) | 9(4) | 10(3) |
| C77' | 50(4) | 72(5) | 87(6) | 28(5) | 11(4) | 7(4) |
| C76 | 74(5) | 57(4) | 47(4) | 6(3) | 18(4) | 22(4) |
| C76' | 92(7) | 71(5) | 53(5) | 16(4) | 3(4) | -3(5) |
| C74 | 53(4) | 45(3) | 51(3) | 21(3) | 24(3) | 20(3) |
| C74' | 81(5) | 54(4) | 36(3) | 12(3) | 14(3) | 3(4) |
| C46' | 34(3) | 42(3) | 34(3) | 13(2) | 16(2) | 21(2) |
| C45 | 50(4) | 57(4) | 64(4) | 10(3) | 28(3) | 28(3) |
| C59 | 62(4) | 61(4) | 81(5) | -4(4) | 52(4) | 5(3) |
| C59' | 60(4) | 56(4) | 54(4) | -10(3) | 24(3) | 13(3) |
| C64 | 40(4) | 90(6) | 121(7) | 57(6) | 40(5) | 38(4) |
| C73' | 46(3) | 46(3) | 44(3) | 17(3) | 7(3) | 16(3) |
| C73 | 38(3) | 40(3) | 46(3) | 13(2) | 13(3) | 10(2) |
| C70' | 93(5) | 41(3) | 36(3) | 14(2) | 31(3) | 18(3) |
| C70 | 52(4) | 70(5) | 84(5) | 50(4) | 43(4) | 35(4) |
|   | C50' | C69 | C51' | C53' | C53 | C54' | C54 | C57' | C57 |
|---|------|-----|------|------|-----|------|-----|------|-----|
|   | 63(4)| 49(4)| 71(4)| 38(3)| 36(3)| 43(3)| 43(3)| 80(6)| 113(9) |
|   | 97(6)| 76(5)| 80(5)| 34(3)| 35(3)| 49(3)| 39(3)| 138(9)| 67(6) |
|   | 30(3)| 62(4)| 37(3)| 31(2)| 41(3)| 29(3)| 95(5)| 60(5)| 238(17) |
|   | 22(3)| 37(4)| 24(3)| 12(2)| 15(2)| 2(2)| 17(3)| -32(5)| 20(8) |
|   | 17(3)| 31(3)| 29(3)| 18(2)| 19(2)| 16(2)| 47(4)| 19(5)| 139(12) |
|   | 53(4)| 36(3)| 54(4)| 19(2)| 19(2)| 16(2)| 17(3)| 54(6)| 23(6) |
3.5 Crystal Structure of $^{65}$Y$_2$Ge

Figure S29. ORTEP plot of $^{65}$Y$_2$Ge. Ellipsoids drawn at 50% probability level.

Table S10. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2\times 10^3$) for $^{65}$Y$_2$Ge. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$ tensor.

| Atom | x    | y    | z    | U(eq)   |
|------|------|------|------|---------|
| Ge(1)| 7916.4(5) | 3810.9(4) | 2871.5(2) | 31.43(17) |
| S(1) | 6484.5(13) | 4696.7(13) | 3839.2(4) | 28.6(3)  |
| P(2) | 6341.5(12) | 5763.9(10) | 1974.5(4) | 25.5(2)  |
| S(2) | 7179.1(10) | 3257.3(9)  | 1856.6(4) | 29.7(2)  |
| P(1) | 5789.8(15) | 2509.2(15) | 3632.0(7) | 30.9(3)  |
| O(1) | 5197(3)    | 5216(3)   | 4103.4(14)| 37.4(6)  |
| O(4) | 6111(3)    | 3084(3)   | 1541.7(11)| 37.4(6)  |
| O(2) | 7134(3)    | 5377(2)   | 3457.5(11)| 37.0(6)  |
| O(3) | 7672(3)    | 2405(2)   | 2275.6(12)| 38.3(6)  |
| C(3) | 7125(4)    | 4633(4)   | 4913.1(15)| 30.0(9)  |
| C(35) | 5490(4) | 5737(3)   | 1342.5(14)| 29.4(7)  |
| C(2) | 7589(4)    | 4409(3)   | 4379.5(14)| 28.4(7)  |
| C(27) | 6884(3) | 4437(3)   | 2209.6(13)| 25.4(7)  |
| C(41) | 7692(4)    | 6483(3)   | 1808.4(16)| 30.0(8)  |
| C(9)  | 5389(5)    | 2443(4)   | 4370.9(16)| 37.5(9)  |
| C(42) | 8545(4)    | 6475(4)   | 2297.9(16)| 31.9(9)  |
| C(47) | 5255(4)    | 6646(3)   | 2500.6(15)| 30.6(8)  |
| C(5)  | 9325(5)    | 3801(5)   | 5215.7(16)| 34.5(8)  |
| C(40) | 4162(4)    | 5394(4)   | 1435.7(15)| 32.5(8)  |
| Atom  | X     | Y     | Z     | u     | v     | w     |
|-------|-------|-------|-------|-------|-------|-------|
| C(4)  | 7991(5) | 4325(5) | 5325.8(14) | 33.3(8) |
| C(6)  | 9774(4) | 3594(5) | 4670.5(16) | 36.4(9) |
| C(1)  | 6558(4) | 3562(3) | 3467.2(14) | 27.6(7) |
| C(15) | 4184(4) | 2663(3) | 3316.0(16) | 34.1(8) |
| C(52) | 4194(4) | 6115(4) | 2766.9(15) | 32.2(11) |
| C(14) | 6628(6) | 2006(9) | 4698.8(18) | 40.8(10) |
| C(51) | 6628(6) | 2006(9) | 4698.8(18) | 40.8(10) |
| C(21) | 6854(5) | 1194(4) | 3355(2)   | 39.7(9) |
| C(36) | 5287(4) | 6783(3) | 988.2(17) | 35.4(9) |
| C(7)  | 8919(4) | 3882(4) | 4255.3(15) | 34.6(8) |
| C(46) | 10514(4) | 6598(4) | 1660.8(19) | 41.8(11) |
| C(28) | 8573(4) | 3097(4) | 1361.9(16) | 34.4(8) |
| C(32) | 9678(4) | 6573(4) | 1178.0(19) | 39.1(11) |
| C(26) | 8309(5) | 1024(5) | 3467(3)   | 44.5(14) |
| C(43) | 9654(5) | 7081(5) | 2160.3(18) | 40.3(11) |
| C(39) | 3675(4) | 5132(4) | 891.2(17)  | 40.5(10) |
| C(31) | 10749(4) | 3005(4) | 616.0(16)  | 40.6(10) |
| C(33) | 9863(4) | 2949(5) | 1542.8(16) | 36.0(9) |
| C(8)  | 10244(5) | 3452(5) | 5663.5(18) | 44.5(11) |
| C(22) | 6322(8)  | 162(4)  | 3506(3)   | 47.4(11) |
| C(37) | 4794(4) | 6543(4) | 441.0(16) | 41.3(10) |
| C(49) | 3875(9) | 8546(5) | 2792(3)   | 46.1(14) |
| C(10) | 4298(5) | 1822(4) | 4546(2)   | 45.6(13) |
| C(38) | 3508(5) | 6104(4) | 513.4(18) | 43.6(11) |
| C(24) | 8629(9) | -1031(5) | 3334(4)   | 59.1(16) |
| C(13) | 6249(9) | 2185(8) | 5306.9(19) | 52.4(13) |
| C(25) | 9152(7) | -4(6)   | 3168(4)   | 52.3(16) |
| C(20) | 4369(4) | 2713(4) | 2697.5(17) | 40.4(10) |
| C(12) | 5141(9) | 1596(4) | 5483.9(19) | 61.4(15) |
| C(23) | 7189(10) | -882(4) | 3224(2)   | 58.3(13) |
| C(34) | 11193(5) | 3003(6) | 215(2)    | 57.4(14) |
| C(19) | 3031(5) | 2890(5) | 2435(2)   | 50.8(12) |
| C(18) | 2020(5) | 3928(5) | 2662(2)   | 48.0(12) |
| C(17) | 1831(5) | 3870(5) | 3272(2)   | 45.9(11) |
| C(11) | 3934(7) | 1968(5) | 5156(2)   | 57.6(16) |
| Ge(1A) | 7279(7) | 3748(4) | 2726(2)   | 31.43(17) |
| O(2A) | 6900(30) | 5292(16) | 3329(7)   | 37.0(6) |
| O(3A) | 7160(30) | 2354(12) | 2163(6)   | 38.3(6) |
| C(27A) | 6280(20) | 4430(11) | 2074(5)   | 25.4(7) |
| C(1A) | 6100(20) | 3565(18) | 3389(5)   | 27.6(7) |
| S(1A) | 6320(20) | 4650(16) | 3754(6)   | 28.6(3) |
| S(2A) | 6873(15) | 3232(11) | 1737(4)   | 29.7(2) |
|        |        |        |        |        |
|--------|--------|--------|--------|--------|
| P(2A)  | 6132(18)| 5796(11)| 1876(6)| 25.5(2) |
| P(1A)  | 5570(20)| 2449(18)| 3658(8)| 30.9(3) |
| O(1A)  | 5090(30)| 5260(30)| 4055(13)| 37.4(6) |
| C(2A)  | 7490(30)| 4310(30)| 4249(9)| 28.4(7) |
| C(7A)  | 8840(30)| 3890(50)| 4102(12)| 34.6(8) |
| O(4A)  | 5970(30)| 3030(20)| 1333(10)| 37.4(6) |
| C(28A) | 8430(20)| 3110(40)| 1357(9)| 34.4(8) |
| C(15A) | 3940(30)| 2430(30)| 3363(12)| 34.1(8) |
| C(21A) | 6710(40)| 1160(20)| 3410(20)| 39.7(9) |
| C(3A)  | 7160(40)| 4730(60)| 4779(11)| 30.0(9) |
| C(6A)  | 9740(30)| 3650(70)| 4504(14)| 36.4(9) |
| C(29A) | 8570(30)| 3050(60)| 801(9)| 39.3(10) |
| C(33A) | 9600(30)| 3080(60)| 1629(12)| 36.0(9) |
| C(40A) | 4100(40)| 5470(40)| 1258(14)| 32.5(8) |
| C(36A) | 5060(50)| 7090(30)| 957(15)| 35.4(9) |
| C(42A) | 8360(40)| 6260(60)| 2330(13)| 31.9(9) |
| C(46A) | 8650(40)| 5710(50)| 1347(18)| 34.9(11) |
| C(52A) | 3980(50)| 6170(40)| 2660(20)| 32.2(11) |
| C(48A) | 4560(90)| 7900(20)| 2260(30)| 39.6(12) |
| C(37A) | 4600(50)| 6980(40)| 383(12)| 41.3(10) |
| C(14A) | 6470(50)| 2010(100)| 4715(14)| 40.8(10) |
| C(10A) | 4050(60)| 2020(70)| 4617(16)| 45.6(13) |
| C(16A) | 2980(40)| 3590(50)| 3490(20)| 37.9(10) |
| C(20A) | 4240(30)| 2320(40)| 2735(12)| 40.4(10) |
| C(26A) | 8140(40)| 1010(50)| 3540(50)| 44.5(14) |
| C(22A) | 6200(70)| 100(20)| 3530(30)| 47.4(11) |
| C(13A) | 6170(80)| 2260(90)| 5322(13)| 52.4(13) |
| C(4A)  | 8010(40)| 4340(70)| 5184(11)| 33.3(8) |
| C(5A)  | 9340(40)| 3780(70)| 5055(13)| 34.5(8) |
| C(30A) | 9740(30)| 2950(60)| 511(11)| 44.7(12) |
| C(32A) | 10790(30)| 3010(50)| 1333(14)| 36.8(9) |
| C(39A) | 3610(40)| 5390(40)| 698(15)| 40.5(10) |
| C(43A) | 9490(50)| 6870(60)| 2240(20)| 40.3(11) |
| C(45A) | 9770(40)| 6330(60)| 1253(18)| 39.1(11) |
| C(51A) | 3190(60)| 6870(50)| 3140(20)| 38.1(12) |
| C(49A) | 3770(110)| 8590(30)| 2740(40)| 46.1(14) |
| C(38A) | 3340(40)| 6480(40)| 416(16)| 43.6(11) |
| C(11A) | 3780(80)| 2190(70)| 5225(18)| 57.6(16) |
| C(17A) | 1690(40)| 3730(60)| 3200(20)| 45.9(11) |
| C(19A) | 2920(40)| 2440(40)| 2460(16)| 50.8(12) |
| C(25A) | 9040(60)| 1070| 3240(60)| 52.3(16) |
| C(23A) | 7120(90)| -910(30)| 3243.81| 58.3(13) |
| C(12A) | 5010(100)| 1761.2| 5535(12)| 61.4(15) |
| C(8A)  | 10300(50)| 3470(80)| 5488(18)| 44.5(11) |
| C(31A) | 10920(30)| 2900(50)| 777(15)| 40.6(10) |
The anisotropic displacement parameters (Å$^2\times10^3$) for $\text{O}_2\text{Y}_2\text{Ge}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 h^2 a^2 U_{11} + \ldots + 2 h k a^* b^* U_{12}^2$

| Atom     | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|----------|----------|----------|----------|----------|----------|----------|
| Ge(1)    | 36.5(3)  | 35.8(2)  | 20.4(2)  | 1.32(16) | 3.58(19) | -6.93(19) |
| S(1)     | 30.3(6)  | 31.9(4)  | 23.1(5)  | 0.2(4)   | 3.7(4)   | -7.8(4)   |
| P(2)     | 22.7(6)  | 32.2(4)  | 20.1(6)  | 1.0(4)   | 2.3(3)   | -4.2(4)   |
| S(2)     | 28.8(6)  | 35.5(4)  | 23.7(5)  | -1.7(4)  | 2.5(3)   | -6.0(4)   |
| P(1)     | 31.8(8)  | 31.0(5)  | 28.3(4)  | -0.6(3)  | 11.9(4)  | -8.0(4)   |
| O(1)     | 32.7(14) | 42.1(14) | 31.9(13) | -4.6(11) | 4.8(11)  | 0.5(11)   |
| O(4)     | 36.7(15) | 48.5(16) | 28.1(14) | -12.2(12)| 2.7(13)  | -13.2(12) |
| O(2)     | 45.6(17) | 41.3(14) | 28.6(13) | 5.1(11)  | -4.9(12) | -19.0(12) |
| O(3)     | 40.2(16) | 38.8(14) | 33.4(14) | -0.7(11) | 7.1(12)  | -7.0(12)  |
| C(3)     | 30.6(17) | 31.2(19) | 26.8(18) | -1.4(18) | 6.4(16)  | -6.6(14)  |
| C(35)    | 28.1(17) | 36(2)    | 20.4(16) | 2.2(13)  | 2.9(13)  | -2.2(15)  |
| C(2)     | 31.9(17) | 31.6(17) | 22.9(17) | -0.6(14) | 1.7(14)  | -11.1(14) |
| C(27)    | 22.4(16) | 31.8(16) | 20.1(14) | 1.0(12)  | 0.4(12)  | -3.4(13)  |
| C(41)    | 28.9(16) | 29(2)    | 30.2(16) | 0.4(14)  | 7.1(13)  | -5.7(14)  |
| C(9)     | 44.2(2)  | 32.5(18) | 33.5(17) | -0.2(14)| 17.8(15)| -10.0(17) |
| C(42)    | 25.5(19) | 40(3)    | 32.0(17) | 0.6(15)  | 2.4(14)  | -12.1(14) |
| C(47)    | 26.7(18) | 37.1(18) | 25.7(17) | -0.2(13)| 5.2(14)  | -4.8(14)  |
| C(5)     | 38.2(19) | 34.7(18) | 31(2)    | -1(2)    | -0.3(18)| -11.3(15) |
| C(40)    | 29.0(17) | 45(2)    | 21.6(19) | -2.0(17)| 1.6(15)  | -5.9(15)  |
| C(4)     | 42(2)    | 35.5(18) | 22.7(18) | -3(2)    | 6.1(17)| -11.4(15) |
| C(6)     | 30.6(18) | 44(2)    | 32(2)    | -1(2)   | 5.5(17)  | -4.3(15)  |
| C(1)     | 23.1(17) | 31.3(16) | 27.2(16) | 0.7(13)  | 5.3(13)  | -5.9(14)  |
| C(15)    | 31.2(19) | 38(2)    | 35.7(18) | -5.3(15)| 10.9(15) | -16.6(15) |
| C(52)    | 30(2)    | 38.5(19) | 26(2)    | -1.7(16)| 3.6(16)  | -4.8(16)  |
| C(14)    | 62(3)    | 32.9(18) | 28.4(17) | -0.3(14)| 13.3(17) | -17(2)     |
| C(51)    | 32(2)    | 46(2)    | 30(2)    | 0.3(18)  | 8.1(18)  | 0.7(18)   |
| C(21)    | 46(2)    | 37.7(19) | 30.9(19) | 0.8(14)  | 11.8(16) | -4.9(16)  |
| C(36)    | 34(2)    | 38(2)    | 30.0(17) | 4.7(16) | 0.1(15)  | -1.7(18)  |
| C(7)     | 32.5(18) | 44(2)    | 25.8(19) | -5(2)    | 8.3(15)  | -8.9(15)  |
| C(46)    | 33.4(18) | 39(3)    | 29.1(17) | 0.6(17)  | 6.7(14)  | -5.6(17)  |
| C(28)    | 32.9(18) | 37.1(18) | 28.5(16) | -2.5(13)| 4.7(14)  | -0.5(15)  |
| C(32)    | 30.0(18) | 52(2)    | 26(2)    | -6.3(19)| 1.9(15)  | -5.8(17)  |
| C(45)    | 31.9(19) | 47(3)    | 35(2)    | 6.3(18)  | 9.7(15)  | -6.5(18)  |
| C(48)    | 39(2)    | 35.8(19) | 39(3)    | -1.0(15)| 9(2)     | -2.8(16)  |
| C(50)    | 36(2)    | 45(2)    | 35(3)    | -2.6(19)| 3(2)     | 6.9(17)   |
|  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| C(30) | 38(2) | 70(3) | 22.3(17) | -0.5(18) | 1.0(16) | -6(2) |
| C(29) | 32(2) | 52(3) | 32.5(18) | -4.8(16) | 1.8(14) | -8.0(19) |
| C(16) | 34(2) | 40(2) | 38(2) | -2.3(16) | 8.6(16) | -10.2(17) |
| C(44) | 29.2(18) | 52(3) | 44(3) | 4.3(19) | 8.1(17) | -11.7(18) |
| C(26) | 49(3) | 31.9(19) | 46(4) | -0.8(18) | 12(2) | -2.0(18) |
| C(43) | 33(2) | 53(3) | 39(2) | -1.5(19) | 3.5(17) | -19.0(18) |
| C(39) | 35(2) | 59(3) | 27(2) | -4.4(18) | -1.4(17) | -8.8(19) |
| C(31) | 39(2) | 57(3) | 24.5(19) | -0.8(19) | 5.7(16) | -10.2(19) |
| C(33) | 35(2) | 46(2) | 23.6(17) | -3.7(16) | 6.9(14) | -5(2) |
| C(8) | 49(2) | 46(2) | 38(2) | 0(3) | -9(2) | -10.4(19) |
| C(22) | 62(3) | 34(2) | 45(2) | -6.4(17) | 10(2) | -11.9(19) |
| C(37) | 39(2) | 53(3) | 26.6(17) | 8.7(18) | 0.4(15) | 0(2) |
| C(49) | 46(3) | 42(2) | 45(3) | -9.4(18) | 8(2) | -2.1(18) |
| C(10) | 52(3) | 39(3) | 44(2) | 4.1(18) | 19.5(19) | -13(2) |
| C(38) | 40(2) | 61(3) | 26.6(19) | 0.8(19) | -8.4(16) | -3(2) |
| C(24) | 85(4) | 39(2) | 42(3) | -8.2(18) | -2(3) | 8(2) |
| C(13) | 88(4) | 40(3) | 29.9(18) | -1.1(16) | 17(2) | -23(2) |
| C(25) | 52(3) | 50(2) | 42(4) | -1(2) | 8(2) | 10(2) |
| C(20) | 34(2) | 48(3) | 39(2) | -6.8(18) | 8.1(16) | -13.2(18) |
| C(12) | 109(5) | 46(2) | 34(2) | -3.2(18) | 28(3) | -36(3) |
| C(23) | 79(4) | 38(2) | 53(2) | -10.7(19) | 7(2) | -7(2) |
| C(34) | 40(2) | 105(4) | 29(2) | -6(2) | 7.8(18) | -23(3) |
| C(19) | 42(2) | 65(3) | 49(2) | -12(2) | 0.5(19) | -21(2) |
| C(18) | 36(2) | 61(3) | 51(3) | -5(2) | -3.0(18) | -18(2) |
| C(17) | 35(2) | 51(3) | 54(3) | -5(2) | 5.4(18) | -15.6(19) |
| C(11) | 79(4) | 42(3) | 50(3) | -2(2) | 37(3) | -21(3) |
| Ge(1A) | 36.5(3) | 35.8(2) | 20.4(2) | 1.32(16) | 3.58(19) | -6.93(19) |
| O(2A) | 45.6(17) | 41.3(14) | 28.6(13) | 5.1(11) | -4.9(12) | -19.0(12) |
| O(3A) | 40.2(16) | 38.8(14) | 33.4(14) | -0.7(11) | 7.1(12) | -7.0(12) |
| C(27A) | 22.4(16) | 31.8(16) | 20.1(14) | 1.0(12) | 0.4(12) | -3.4(13) |
| C(1A) | 23.1(17) | 31.3(16) | 27.2(16) | 0.7(13) | 5.3(13) | -5.9(14) |
| S(1A) | 30.3(6) | 31.9(4) | 23.1(5) | 0.2(4) | 3.7(4) | -7.8(4) |
| S(2A) | 28.8(6) | 35.5(4) | 23.7(5) | -1.7(4) | 2.5(3) | -6.0(4) |
| P(2A) | 22.7(6) | 32.2(4) | 20.1(6) | 1.0(4) | 2.3(3) | -4.2(4) |
| P(1A) | 31.8(8) | 31.0(5) | 28.3(4) | -0.6(3) | 11.9(4) | -8.0(4) |
| O(1A) | 32.7(14) | 42.1(14) | 31.9(13) | -4.6(11) | 4.8(11) | 0.5(11) |
| C(2A) | 31.9(17) | 31.6(17) | 22.9(17) | -0.6(14) | 1.7(14) | -11.1(14) |
| C(7A) | 32.5(18) | 44(2) | 25.8(19) | -5(2) | 8.3(15) | -8.9(15) |
| O(4A) | 36.7(15) | 48.5(16) | 28.1(14) | -12.2(12) | 2.7(13) | -13.2(12) |
| C(28A) | 32.9(18) | 37.1(18) | 28.5(16) | -2.5(13) | 4.7(14) | -0.5(15) |
| C(35A) | 28.1(17) | 36(2) | 20.4(16) | 2.2(13) | 2.9(13) | -2.2(15) |
| C(41A) | 28.9(16) | 29(2) | 30.2(16) | 0.4(14) | 7.1(13) | -5.7(14) |
| C(47A) | 26.7(18) | 37.1(18) | 25.7(17) | -0.2(13) | 5.2(14) | -4.8(14) |
| C(9A) | 44(2) | 32.5(18) | 33.5(17) | -0.2(14) | 17.8(15) | -10.0(17) |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| C(15A) | 31.2(19) | 38(2) | 35.7(18) | -5.3(15) | 10.9(15) | -16.6(15) |
| C(21A) | 46(2) | 37.7(19) | 30.9(19) | 0.8(14) | 11.8(16) | -4.9(16) |
| C(3A) | 30.6(17) | 31.2(19) | 26.8(18) | -1.4(18) | 6.4(16) | -6.6(14) |
| C(6A) | 30.6(18) | 44(2) | 32(2) | -1(2) | 5.5(17) | -4.3(15) |
| C(29A) | 32(2) | 52(3) | 32.5(18) | -4.8(16) | 1.8(14) | -8.0(19) |
| C(33A) | 35(2) | 46(2) | 23.6(17) | -3.7(16) | 6.9(14) | -5(2) |
| C(40A) | 29.0(17) | 45(2) | 21.6(19) | -2.0(17) | 1.6(15) | -5.9(15) |
| C(36A) | 34(2) | 38(2) | 30.0(17) | 4.7(16) | 0.1(15) | -1.7(18) |
| C(42A) | 25.5(19) | 40(3) | 32.0(17) | 0.6(15) | 2.4(14) | -12.1(14) |
| C(46A) | 33.4(18) | 39(3) | 29.1(17) | 0.6(17) | 6.7(14) | -5.6(17) |
| C(52A) | 30(2) | 38.5(19) | 26(2) | -1.7(16) | 3.6(16) | -4.8(16) |
| C(48A) | 39(2) | 35.8(19) | 39(3) | -1.0(15) | 9(2) | -2.8(16) |
| C(37A) | 39(2) | 53(3) | 26.6(17) | 8.7(18) | 0.4(15) | 0(2) |
| C(14A) | 62(3) | 32.9(18) | 28.4(17) | -0.3(14) | 13.3(17) | -17(2) |
| C(10A) | 52(3) | 39(3) | 44(2) | 4.1(18) | 19.5(19) | -13(2) |
| C(16A) | 34(2) | 40(2) | 38(2) | -2.3(16) | 8.6(16) | -10.2(17) |
| C(20A) | 34(2) | 48(3) | 39(2) | -6.8(18) | 8.1(16) | -13.2(18) |
| C(26A) | 49(3) | 31.9(19) | 46(4) | -0.8(18) | 12(2) | -2.0(18) |
| C(22A) | 62(3) | 34(2) | 45(2) | -6.4(17) | 10(2) | -11.9(19) |
| C(13A) | 88(4) | 40(3) | 29.9(18) | -1.1(16) | 17(2) | -23(2) |
| C(4A) | 42(2) | 35.5(18) | 22.7(18) | -3(2) | 6.1(17) | -11.4(15) |
| C(5A) | 38.2(19) | 34.7(18) | 31(2) | -1(2) | -0.3(18) | -11.3(15) |
| C(30A) | 38(2) | 70(3) | 22.3(17) | -0.5(18) | 1.0(16) | -6(2) |
| C(32A) | 30.0(18) | 52(2) | 26(2) | -6.3(19) | 1.9(15) | -5.8(17) |
| C(39A) | 35(2) | 59(3) | 27(2) | -4.4(18) | -1.4(17) | -8.8(19) |
| C(43A) | 33(2) | 53(3) | 39(2) | -1.5(19) | 3.5(17) | -19.0(18) |
| C(45A) | 31.9(19) | 47(3) | 35(2) | 6.3(18) | 9.7(15) | -6.5(18) |
| C(51A) | 32(2) | 46(2) | 30(2) | 0.3(18) | 8.1(18) | 0.7(18) |
| C(49A) | 46(3) | 42(2) | 45(3) | -9.4(18) | 8(2) | -2.1(18) |
| C(38A) | 40(2) | 61(3) | 26.6(19) | 0.8(19) | -8.4(16) | -3(2) |
| C(11A) | 79(4) | 42(3) | 50(3) | -2(2) | 37(3) | -21(3) |
| C(17A) | 35(2) | 51(3) | 54(3) | -5(2) | 5.4(18) | -15.6(19) |
| C(19A) | 42(2) | 65(3) | 49(2) | -12(2) | 0.5(19) | -21(2) |
| C(25A) | 52(3) | 50(2) | 42(4) | -1(2) | 8(2) | 10(2) |
| C(23A) | 79(4) | 38(2) | 53(2) | -10.7(19) | 7(2) | -7(2) |
| C(12A) | 109(5) | 46(2) | 34(2) | -3.2(18) | 28(3) | -36(3) |
| C(8A) | 49(2) | 46(2) | 38(2) | 0(3) | -9(2) | -10.4(19) |
| C(31A) | 39(2) | 57(3) | 24.5(19) | -0.8(19) | 5.7(16) | -10.2(19) |
| C(44A) | 29.2(18) | 52(3) | 44(3) | 4.3(19) | 8.1(17) | -11.7(18) |
| C(50A) | 36(2) | 45(2) | 35(3) | -2.6(19) | 3(2) | 6.9(17) |
| C(18A) | 36(2) | 61(3) | 51(3) | -5(2) | -3.0(18) | -18(2) |
| C(24A) | 85(4) | 39(2) | 42(3) | -8.2(18) | -2(3) | 8(2) |
| C(34A) | 40(2) | 105(4) | 29(2) | -6(2) | 7.8(18) | -23(3) |
3.6 Crystal Structure of \( ^{\text{Cy}}Y_2\text{Sn} \)

Figure S30. ORTEP plot of \( ^{\text{Cy}}Y_2\text{Sn} \) containing one benzene molecule. Ellipsoids drawn at 50% probability level.

Table S12. Atomic Coordinates (\( \times 10^4 \)) and Equivalent Isotropic Displacement Parameters (\( \text{Å}^2 \times 10^3 \)) for \( ^{\text{Cy}}Y_2\text{Sn} \). \( U_{\text{eq}} \) is defined as 1/3 of the trace of the orthogonalised \( U_{ij} \) tensor.

| Atom | \( x \)   | \( y \)   | \( z \)   | \( U_{\text{eq}} \) |
|------|-----------|-----------|-----------|-----------------|
| Sn(1) | 2834(1)   | 6615(1)   | 7989(1)   | 28(1)           |
| O(1)  | 4885(2)   | 6241(1)   | 8072(1)   | 32(1)           |
| S(1)  | 5234(1)   | 6474(1)   | 7396(1)   | 27(1)           |
| P(1)  | 3658(1)   | 6950(1)   | 6202(1)   | 25(1)           |
| C(1)  | 3937(2)   | 6723(1)   | 7050(1)   | 27(1)           |
| C(13) | 6066(3)   | 7495(1)   | 4755(2)   | 39(1)           |
| C(12) | 6586(3)   | 7955(1)   | 5150(2)   | 37(1)           |
| C(11) | 6696(3)   | 7872(1)   | 5961(2)   | 35(1)           |
| C(10) | 5466(3)   | 7715(1)   | 6221(2)   | 30(1)           |
| C(9)  | 5005(3)   | 7232(1)   | 5835(2)   | 30(1)           |
| C(8)  | 8764(3)   | 8168(1)   | 8242(2)   | 41(1)           |
| C(7)  | 7437(3)   | 6972(1)   | 7408(2)   | 31(1)           |
| C(6)  | 8231(3)   | 7365(1)   | 7600(2)   | 33(1)           |
| C(5)  | 7926(3)   | 7733(1)   | 8077(2)   | 33(1)           |
| C(3)  | 6005(3)   | 7301(1)   | 8197(2)   | 32(1)           |
|   |   |   |   |   |
|---|---|---|---|---|
| O(3) | 800(2) | 6624(1) | 7294(1) | 33(1) |
| C(46) | 902(3) | 4688(1) | 7012(2) | 39(1) |
| C(19) | 1500(3) | 5822(1) | 5189(2) | 42(1) |
| C(30) | -2405(3) | 5744(1) | 8466(2) | 32(1) |
| C(48) | 4102(3) | 4548(1) | 8021(2) | 30(1) |
| C(25) | 1352(3) | 8045(1) | 6930(2) | 31(1) |
| C(47) | -1564(3) | 5742(1) | 7957(2) | 31(1) |
| P(2) | 2241(1) | 5281(1) | 8064(1) | 24(1) |
| O(2) | 5899(2) | 6156(1) | 6936(1) | 34(1) |
| S(2) | 565(1) | 6080(1) | 7414(1) | 27(1) |
| C(2) | 6316(2) | 6947(1) | 7699(2) | 28(1) |
| C(49) | 5397(3) | 4433(1) | 7823(2) | 33(1) |
| C(26) | 2582(3) | 7809(1) | 6790(2) | 32(1) |
| C(45) | -309(4) | 4419(2) | 6810(2) | 54(1) |
| C(20) | 1959(3) | 7321(1) | 5024(2) | 35(1) |
| C(41) | 585(3) | 4838(1) | 7805(2) | 30(1) |
| C(18) | 2490(3) | 5439(1) | 5059(2) | 41(1) |
| C(4) | 6805(3) | 7689(1) | 8382(2) | 34(1) |
| O(4) | -7(2) | 5811(1) | 6802(1) | 35(1) |
| C(50) | 5512(3) | 4489(1) | 7026(2) | 33(1) |
| C(27) | 1911(2) | 5876(1) | 7771(1) | 25(1) |
| C(40) | 1312(3) | 5445(1) | 9373(2) | 32(1) |
| C(35) | 2459(2) | 5249(1) | 9050(1) | 27(1) |
| C(39) | 1448(3) | 5412(1) | 10184(2) | 38(1) |
| C(34) | -3228(3) | 6059(1) | 9594(2) | 40(1) |
| C(38) | 2578(3) | 5696(1) | 10493(2) | 39(1) |
| C(33) | -447(3) | 6400(1) | 8626(2) | 32(1) |
| C(37) | 3730(3) | 5512(1) | 10178(2) | 35(1) |
| C(32) | -1301(3) | 6386(1) | 9126(2) | 33(1) |
| C(15) | 3112(3) | 6476(1) | 5532(1) | 28(1) |
| C(42) | 903(3) | 4367(1) | 8272(2) | 37(1) |
| C(23) | 522(3) | 7827(1) | 5667(2) | 40(1) |
| C(36) | 3597(3) | 5538(1) | 9359(1) | 30(1) |
| C(31) | -2295(3) | 6056(1) | 9055(2) | 32(1) |
| C(51) | 5115(3) | 5010(1) | 6773(2) | 35(1) |
| C(28) | -569(2) | 6078(1) | 8042(2) | 29(1) |
| C(44) | -462(4) | 3963(2) | 7280(2) | 58(1) |
| C(21) | 2361(3) | 7379(1) | 6251(1) | 28(1) |
| C(17) | 3660(3) | 5694(1) | 4868(2) | 39(1) |
| C(16) | 4117(3) | 6087(1) | 5421(2) | 34(1) |
| C(43) | -317(3) | 4103(1) | 8070(2) | 46(1) |
| C(22) | 1750(3) | 7583(1) | 5541(2) | 33(1) |
| C(53) | -1366(4) | 6476(2) | 5288(3) | 70(1) |
| C(54) | -2304(4) | 6134(2) | 5205(3) | 67(1) |
| C(55) | -2913(4) | 6060(2) | 4544(2) | 59(1) |
Table S 13. Anisotropic displacement parameters (Å$^2 \times 10^3$) for $\text{O}_2\text{Y}_2\text{Sn}$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^2U_{11} + ... + 2hk a^* b^* U_{12}]$

| Atom  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|-------|----------|----------|----------|----------|----------|----------|
| Sn(1) | 33(1)    | 22(1)    | 28(1)    | 0(1)     | 6(1)     | -2(1)    |
| O(1)  | 34(1)    | 27(1)    | 34(1)    | 6(1)     | 3(1)     | -5(1)    |
| S(1)  | 29(1)    | 22(1)    | 30(1)    | 1(1)     | 3(1)     | -1(1)    |
| P(1)  | 31(1)    | 20(1)    | 26(1)    | 1(1)     | 6(1)     | 1(1)     |
| C(1)  | 29(1)    | 26(1)    | 26(1)    | 3(1)     | 8(1)     | -3(1)    |
| C(13) | 48(2)    | 33(2)    | 38(2)    | 7(1)     | 15(1)    | 3(1)     |
| C(12) | 34(2)    | 35(2)    | 44(2)    | 10(1)    | 12(1)    | -1(1)    |
| C(11) | 33(2)    | 32(2)    | 41(2)    | 8(1)     | 5(1)     | -1(1)    |
| C(10) | 33(1)    | 26(1)    | 33(1)    | 4(1)     | 6(1)     | 0(1)     |
| C(9)  | 33(1)    | 24(1)    | 33(1)    | 3(1)     | 9(1)     | 2(1)     |
| C(8)  | 45(2)    | 34(2)    | 44(2)    | -1(1)    | 2(1)     | -8(1)    |
| C(7)  | 32(1)    | 25(1)    | 37(2)    | 0(1)     | 4(1)     | 1(1)     |
| C(6)  | 29(1)    | 31(2)    | 40(2)    | 3(1)     | 4(1)     | -1(1)    |
| C(5)  | 37(2)    | 26(1)    | 33(1)    | 3(1)     | -2(1)    | -2(1)    |
| C(3)  | 32(1)    | 30(1)    | 34(1)    | 0(1)     | 6(1)     | -1(1)    |
| O(3)  | 37(1)    | 27(1)    | 34(1)    | 7(1)     | 8(1)     | 4(1)     |
| C(46) | 45(2)    | 38(2)    | 32(2)    | -10(1)   | 4(1)     | -8(1)    |
| C(19) | 49(2)    | 35(2)    | 39(2)    | -7(1)    | -4(1)    | -4(1)    |
| C(30) | 27(1)    | 29(1)    | 41(2)    | -1(1)    | 2(1)     | -3(1)    |
| C(48) | 37(2)    | 23(1)    | 30(1)    | 1(1)     | 4(1)     | 1(1)     |
| C(25) | 47(2)    | 25(1)    | 44(2)    | -5(1)    | 17(1)    | 0(1)     |
| C(47) | 30(1)    | 22(1)    | 27(1)    | 0(1)     | 6(1)     | 0(1)     |
| C(24) | 42(2)    | 35(2)    | 52(2)    | 0(1)     | 16(1)    | 11(1)    |
| C(14) | 47(2)    | 27(1)    | 31(1)    | 2(1)     | 11(1)    | -1(1)    |
| C(52) | 41(2)    | 29(1)    | 26(1)    | 2(1)     | 7(1)     | 8(1)     |
| C(29) | 30(1)    | 30(1)    | 33(1)    | -1(1)    | 1(1)     | 1(1)     |
| P(2)  | 29(1)    | 21(1)    | 24(1)    | 0(1)     | 4(1)     | -1(1)    |
| O(2)  | 34(1)    | 27(1)    | 40(1)    | -4(1)    | 6(1)     | 2(1)     |
| S(2)  | 29(1)    | 26(1)    | 28(1)    | 2(1)     | 4(1)     | 1(1)     |
| C(2)  | 31(1)    | 22(1)    | 32(1)    | 3(1)     | 0(1)     | 0(1)     |
| C(49) | 36(2)    | 25(1)    | 35(2)    | -1(1)    | 3(1)     | 6(1)     |
| C(26) | 41(2)    | 23(1)    | 35(1)    | -2(1)    | 8(1)     | 1(1)     |
| C(45) | 54(2)    | 62(2)    | 46(2)    | -24(2)   | 0(2)     | -15(2)   |
| C(20) | 39(2)    | 30(1)    | 30(1)    | -4(1)    | 4(1)     | -2(1)    |
| C(41) | 31(1)    | 27(1)    | 31(1)    | -2(1)    | 4(1)     | -2(1)    |
| C(18) | 65(2)    | 26(2)    | 31(2)    | -7(1)    | -2(1)    | -2(1)    |
| C(4)  | 42(2)    | 30(2)    | 30(1)    | -1(1)    | 2(1)     | 0(1)     |
| O(4)  | 33(1)    | 42(1)    | 31(1)    | 1(1)     | 2(1)     | 0(1)     |
| C(50) | 37(2)    | 27(1)    | 36(2)    | -1(1)    | 8(1)     | 4(1)     |
| C    |      |      |      |      |      |      |
|------|------|------|------|------|------|------|
| (27) | 26   | 20   | 30   | -1   | 7    | -3   |
| (40) | 32   | 36   | 29   | 2    | 6    | 1    |
| (35) | 31   | 26   | 25   | 0    | 5    | 0    |
| (39) | 36   | 50   | 28   | 3    | 8    | 5    |
| (34) | 39   | 40   | 42   | 3    | 11   | -6   |
| (38) | 41   | 50   | 27   | -5   | 5    | 7    |
| (33) | 30   | 29   | 37   | -1   | 6    | 0    |
| (37) | 38   | 38   | 28   | -2   | 1    | 0    |
| (32) | 32   | 32   | 34   | -5   | 5    | -2   |
| (15) | 40   | 24   | 21   | 0    | 5    | 1    |
| (42) | 41   | 25   | 45   | 1    | 10   | -5   |
| (23) | 37   | 39   | 45   | 0    | 4    | 10   |
| (36) | 33   | 33   | 24   | -1   | 2    | 0    |
| (31) | 31   | 28   | 38   | 2    | 7    | -1   |
| (51) | 45   | 25   | 36   | -1   | 15   | 4    |
| (28) | 28   | 32   | 31   | 2    | 1    | 4    |
| (44) | 52   | 47   | 75   | -26  | 13   | -23  |
| (21) | 32   | 21   | 31   | 1    | 7    | 0    |
| (17) | 60   | 28   | 31   | -2   | 10   | 5    |
| (16) | 44   | 24   | 34   | -2   | 11   | 2    |
| (43) | 48   | 31   | 62   | -3   | 15   | -11  |
| (22) | 37   | 30   | 32   | 2    | 4    | 5    |
| (53) | 48   | 97   | 63   | 5    | -6   | 18   |
| (54) | 65   | 61   | 75   | 16   | 15   | 20   |
| (55) | 60   | 47   | 73   | -11  | 14   | 0    |
| (56) | 56   | 56   | 53   | -22  | 8    | 2    |
| (57) | 57   | 53   | 57   | -10  | 18   | 5    |
| (58) | 39   | 76   | 71   | -20  | 4    | -4   |
3.7 Crystal Structure of (\(\text{CyYSnCl})_2\) (3)

Figure S31. ORTEP plot of 3 containing one THF molecule (disordered). Ellipsoids drawn at 50% probability level.

Table S14. Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

| Atom  | x     | y     | z     | U(eq) |
|-------|-------|-------|-------|-------|
| Sn(1) | 5562(1)| 8057(1)| 768(1)| 52(1) |
| P(1)  | 2455(1)| 7821(1)| 2484(1)| 43(1) |
| O(1)  | 6999(4)| 6879(3)| 2139(3)| 59(1) |
| Cl(1) | 6712(1)| 9977(1)| 560(1)| 58(1) |
| S(1)  | 5696(1)| 6813(1)| 2826(1)| 48(1) |
| C(1)  | 4336(5)| 7721(4)| 2126(3)| 48(1) |
| C(2)  | 6199(5)| 7445(4)| 3624(4)| 47(1) |
| O(2)  | 5405(4)| 5584(3)| 3436(3)| 54(1) |
| C(3)  | 6220(6)| 6748(5)| 4584(4)| 54(1) |
| C(4)  | 6486(6)| 7274(5)| 5211(4)| 54(1) |
| C(5)  | 6759(6)| 8479(5)| 4886(4)| 55(1) |
| C(6)  | 6751(6)| 9156(5)| 3914(4)| 54(1) |
| C(7)  | 6475(5)| 8653(5)| 3275(4)| 49(1) |
| C(8)  | 6992(7)| 9054(6)| 5562(5)| 66(1) |
| C(9)  | 2174(5)| 7255(4)| 3781(3)| 45(1) |
| C(10) | 2534(5)| 8147(4)| 4216(3)| 46(1) |
| C(11) | 2495(6)| 7544(5)| 5294(3)| 51(1) |
| C(12) | 970(6)| 7138(5)| 5669(4)| 56(1) |
| C(13) | 591(5)| 6267(4)| 5240(3)| 50(1) |
| C(14) | 621(5)| 6836(4)| 4167(3)| 47(1) |
| C(15) | 1586(5)| 9415(4)| 1917(3)| 44(1)|
Table S15. Anisotropic displacement parameters (Å$^2\times10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2p^2 [ h^2 a^2 U_{11} + ... + 2 h k a^* b^* U_{12}^* ]$

| Atom   | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|--------|----------|----------|----------|----------|----------|----------|
| Sn(1)  | 53(1)    | 56(1)    | 50(1)    | -25(1)   | 10(1)    | -12(1)   |
| P(1)   | 44(1)    | 42(1)    | 43(1)    | -17(1)   | 5(1)     | -8(1)    |
| O(1)   | 50(2)    | 65(2)    | 64(2)    | -31(2)   | 10(2)    | -6(2)    |
| Cl(1)  | 59(1)    | 62(1)    | 55(1)    | -22(1)   | 5(1)     | -21(1)   |
| S(1)   | 45(1)    | 48(1)    | 52(1)    | -22(1)   | 4(1)     | -5(1)    |
| C(1)   | 50(2)    | 48(2)    | 46(2)    | -19(2)   | 2(2)     | -6(2)    |
| C(2)   | 42(2)    | 52(2)    | 50(2)    | -24(2)   | 2(2)     | -3(2)    |
| C(3)   | 58(2)    | 48(2)    | 56(2)    | -20(2)   | -1(2)    | -7(1)    |
| C(4)   | 52(2)    | 50(2)    | 60(3)    | -21(2)   | -4(2)    | -1(2)    |
| C(5)   | 46(2)    | 52(2)    | 53(2)    | -23(2)   | 3(2)     | -6(2)    |
| C(6)   | 42(2)    | 56(2)    | 53(2)    | -22(2)   | 8(2)     | 3(2)     |
| C(7)   | 53(3)    | 54(2)    | 52(3)    | -22(2)   | -8(2)    | 3(2)     |
| C(8)   | 69(3)    | 68(3)    | 69(3)    | -38(3)   | -9(3)    | 4(2)     |
| C(9)   | 46(2)    | 43(2)    | 45(2)    | -17(2)   | 4(2)     | -8(2)    |
| C(10)  | 47(2)    | 43(2)    | 47(2)    | -16(2)   | 3(2)     | -8(2)    |
| C(11)  | 53(2)    | 56(2)    | 46(2)    | -21(2)   | 4(2)     | -12(2)   |
| C(12)  | 55(2)    | 61(3)    | 45(2)    | -20(2)   | 7(2)     | -14(2)   |
| C(13)  | 53(2)    | 61(3)    | 45(2)    | -12(2)   | 7(2)     | -11(2)   |
| C(14)  | 46(2)    | 45(2)    | 49(2)    | -19(2)   | 5(2)     | -9(2)    |
| C(15)  | 49(2)    | 39(2)    | 43(2)    | -14(2)   | 2(2)     | -9(2)    |
| C(16)  | 47(2)    | 46(2)    | 51(2)    | -19(2)   | 1(2)     | -9(2)    |
3.8 Crystal Structure of CyY(Cl)Ge-Ge(Cl)Cy (4)

Figure S 32. ORTEP plot of 4 containing non-coordinating solvent molecules (acetonitrile and cyclohexane). Ellipsoids drawn at 50% probability level.
Table S 16. Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 4. Ueq is defined as 1/3 of of the trace of the orthogonalised Uij tensor.

| Atom | x    | y    | z    | U(eq) |
|------|------|------|------|-------|
| Ge(1)| 3181(1) | 4050(1) | 6613(1) | 15(1) |
| C(1) | 3648(1) | 3232(2) | 6267(1) | 15(1) |
| Cl(1)| 3694(1) | 5138(1) | 7372(1) | 24(1) |
| S(1) | 3882(1) | 2571(1) | 7099(1) | 16(1) |
| P(1) | 3715(1) | 2994(1) | 5301(1) | 13(1) |
| O(1) | 3602(1) | 2937(1) | 6321(2) | 50(1) |
| N(1) | 2454(1) | -505(2) | 6321(2) | 50(1) |
| Ge(2)| 2280(1) | 4187(1) | 6895(1) | 15(1) |
| P(2) | 1762(1) | 6118(1) | 6387(1) | 13(1) |
| O(2) | 3823(1) | 1622(1) | 6944(1) | 23(1) |
| S(2) | 2494(1) | 5446(1) | 5464(1) | 13(1) |
| Cl(2)| 1869(1) | 3054(1) | 5959(1) | 24(1) |
| C(2) | 4604(1) | 2741(2) | 7583(1) | 20(1) |
| C(3) | 4815(1) | 3598(2) | 7707(2) | 23(1) |
| O(3) | 5374(1) | 3725(2) | 8082(2) | 27(1) |
| C(4) | 6334(1) | 3156(3) | 8783(2) | 41(1) |
| O(4) | 4314(1) | 2264(2) | 5421(1) | 16(1) |
| C(5) | 4797(2) | 2997(2) | 8346(2) | 29(1) |
| C(6) | 5510(1) | 2149(2) | 8213(2) | 30(1) |
| C(7) | 4951(1) | 2009(2) | 7835(2) | 25(1) |
| C(8) | 5342(1) | 2063(2) | 5952(2) | 21(1) |
| C(9) | 5329(1) | 1491(2) | 5204(2) | 23(1) |
| C(10)| 4769(1) | 1047(2) | 4850(2) | 20(1) |
| C(11)| 4298(1) | 1722(2) | 4643(1) | 19(1) |
| C(12)| 3751(1) | 4037(1) | 4767(1) | 14(1) |
| C(13)| 4151(1) | 4736(2) | 5281(1) | 18(1) |
| C(14)| 4376(1) | 3156(3) | 8783(2) | 41(1) |
| C(15)| 4874(1) | 2747(2) | 5736(2) | 18(1) |
| C(16)| 5342(1) | 2063(2) | 5952(2) | 21(1) |
| C(17)| 5329(1) | 1491(2) | 5204(2) | 23(1) |
| C(18)| 4769(1) | 1047(2) | 4850(2) | 20(1) |
| C(19)| 4298(1) | 1722(2) | 4643(1) | 19(1) |
| C(20)| 3751(1) | 4037(1) | 4767(1) | 14(1) |
| C(21)| 4151(1) | 4736(2) | 5281(1) | 18(1) |
| C(22)| 4376(1) | 3156(3) | 8783(2) | 41(1) |
| C(23)| 4874(1) | 2747(2) | 5736(2) | 18(1) |
| C(24)| 5342(1) | 2063(2) | 5952(2) | 21(1) |
| C(25)| 5329(1) | 1491(2) | 5204(2) | 23(1) |
Table S17. Anisotropic displacement parameters (Å²×10³) for 4. The anisotropic displacement factor exponent takes the form: 

\[-2p²[h²a²U₁₁ + ... + 2hk a²b² U₁₂]\]

| Atom | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   |
|------|-------|-------|-------|-------|-------|-------|
| Ge(1) | 18(1) | 15(1) | 14(1) | 1(1)  | 8(1)  | 2(1)  |
| C(1)  | 18(1) | 14(1) | 14(1) | 1(1)  | 7(1)  | 4(1)  |
| Cl(1) | 27(1) | 18(1) | 24(1) | -4(1) | 5(1)  | 1(1)  |
| S(1)  | 20(1) | 16(1) | 14(1) | 3(1)  | 7(1)  | 3(1)  |
| P(1)  | 16(1) | 12(1) | 13(1) | 0(1)  | 6(1)  | 1(1)  |
| O(1)  | 22(1) | 24(1) | 15(1) | 2(1)  | 10(1) | 4(1)  |
| N(1)  | 54(2) | 44(2) | 53(2) | -7(1) | 18(2) | -8(1) |
| Ge(2) | 18(1) | 15(1) | 14(1) | 1(1)  | 8(1)  | 2(1)  |
| P(2)  | 14(1) | 14(1) | 12(1) | -1(1) | 5(1)  | 1(1)  |
| O(2)  | 32(1) | 15(1) | 22(1) | 4(1)  | 11(1) | 3(1)  |
| S(2)  | 16(1) | 13(1) | 13(1) | 1(1)  | 7(1)  | 1(1)  |
| Cl(2) | 27(1) | 18(1) | 24(1) | -4(1) | 5(1)  | 1(1)  |
| C(2)  | 20(1) | 26(1) | 14(1) | 3(1)  | 6(1)  | 6(1)  |
| C(3)  | 22(1) | 27(1) | 19(1) | 2(1)  | 7(1)  | 4(1)  |
| O(3)  | 18(1) | 18(1) | 14(1) | 2(1)  | 7(1)  | 5(1)  |
| C(4) | 22(1) | 38(2) | 21(1) | -2(1) | 8(1) | 2(1) |
|------|-------|-------|-------|-------|------|------|
| O(4) | 22(1) | 14(1) | 20(1) | 0(1)  | 10(1)| -2(1)|
| C(5) | 21(1) | 51(2) | 16(1) | 2(1)  | 8(1) | 9(1) |
| C(6) | 29(1) | 44(2) | 19(1) | 7(1)  | 10(1)| 20(1)|
| C(7) | 30(1) | 28(1) | 18(1) | 6(1)  | 11(1)| 11(1)|
| C(8) | 21(1) | 72(2) | 27(1) | -1(1) | 5(1) | 9(1) |
| C(9) | 19(1) | 12(1) | 17(1) | 0(1)  | 7(1) | 3(1) |
| C(10)| 18(1) | 16(1) | 21(1) | -2(1) | 9(1) | 1(1) |
| C(11)| 19(1) | 20(1) | 25(1) | -1(1) | 8(1) | 3(1) |
| C(12)| 23(1) | 21(1) | 29(1) | -1(1) | 14(1)| 6(1) |
| C(13)| 27(1) | 16(1) | 22(1) | -2(1) | 11(1)| 6(1) |
| C(14)| 24(1) | 16(1) | 17(1) | -2(1) | 7(1) | 4(1) |
| C(15)| 17(1) | 12(1) | 13(1) | 1(1)  | 6(1) | 1(1) |
| C(16)| 21(1) | 15(1) | 17(1) | -2(1) | 5(1) | -2(1)|
| C(18)| 25(1) | 15(1) | 22(1) | 4(1)  | 9(1) | -1(1)|
| C(17)| 26(1) | 13(1) | 22(1) | -2(1) | 7(1) | -1(1)|
| C(19)| 26(1) | 17(1) | 15(1) | 3(1)  | 8(1) | 1(1) |
| C(20)| 23(1) | 14(1) | 15(1) | 1(1)  | 9(1) | 1(1) |
| C(21)| 20(1) | 15(1) | 15(1) | -3(1) | 7(1) | -1(1)|
| C(22)| 17(1) | 20(1) | 24(1) | -6(1) | 5(1) | 0(1) |
| C(23)| 20(1) | 25(1) | 30(1) | -9(1) | 2(1) | 2(1) |
| C(24)| 24(1) | 28(1) | 36(2) | -10(1)| 9(1) | -8(1)|
| C(25)| 30(1) | 20(1) | 24(1) | -4(1) | 7(1) | -7(1)|
| C(26)| 28(1) | 19(1) | 20(1) | -1(1) | 7(1) | -6(1)|
| C(53)| 53(2) | 61(3) | 57(2) | -2(2) | 0(2) | 3(2) |
| C(52)| 29(1) | 18(1) | 16(1) | 0(1)  | 6(1) | 6(1) |
| C(51)| 40(2) | 20(1) | 23(1) | 4(1)  | 9(1) | 8(1) |
| C(50)| 42(2) | 29(1) | 20(1) | 7(1)  | 6(1) | 13(1)|
| C(49)| 34(1) | 32(1) | 14(1) | 1(1)  | 4(1) | 9(1) |
| C(48)| 21(1) | 22(1) | 16(1) | -1(1) | 3(1) | 4(1) |
| C(47)| 18(1) | 17(1) | 14(1) | 1(1)  | 5(1) | 4(1) |
| C(46)| 19(1) | 24(1) | 21(1) | -6(1) | 9(1) | -3(1)|
| C(45)| 22(1) | 31(1) | 27(1) | -8(1) | 10(1)| -10(1)|
| C(44)| 19(1) | 41(2) | 32(1) | -10(1)| 12(1)| -9(1)|
| C(43)| 21(1) | 36(1) | 28(1) | -10(1)| 15(1)| -5(1)|
| C(42)| 19(1) | 26(1) | 23(1) | -6(1) | 10(1)| 0(1) |
| C(41)| 15(1) | 21(1) | 16(1) | -4(1) | 6(1) | -2(1)|
| C(40)| 16(1) | 18(1) | 15(1) | -2(1) | 6(1) | -2(1)|
| C(39)| 21(1) | 22(1) | 21(1) | -4(1) | 7(1) | -5(1)|
| C(38)| 21(1) | 28(1) | 19(1) | -4(1) | 1(1) | -5(1)|
| C(37)| 27(1) | 22(1) | 13(1) | 0(1)  | 3(1) | -4(1)|
| C(36)| 22(1) | 18(1) | 16(1) | 1(1)  | 5(1) | -2(1)|
| C(35)| 14(1) | 15(1) | 13(1) | -2(1) | 4(1) | 0(1) |
| C(34)| 42(2) | 58(2) | 19(1) | 1(1)  | 1(1) | -5(2)|
| C(33)| 21(1) | 19(1) | 17(1) | 1(1)  | 9(1) | 2(1) |
| C(32)| 20(1) | 24(1) | 22(1) | -4(1) | 6(1) | 0(1) |
| C(31)| 27(1) | 32(1) | 17(1) | -1(1) | 4(1) | 5(1) |
| C(30)| 35(1) | 31(1) | 16(1) | 6(1)  | 9(1) | 1(1) |
| C(29)| 26(1) | 21(1) | 18(1) | 2(1)  | 9(1) | 0(1)|
|     | C(28) | C(27) | C(54) | C(55) | C(56) | C(57) | C(58) | C(59) | C(60) |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 20  | 17    | 44    | 52    | 52    | 73    | 51    | 50    | 33    | 30    |
| 15  | 14    | 51    | 50    | 50    | 51    | 42    | 49    | 28    | 38    |
| 15  | 14    | 70    | 116   | 61    | 61    | 61    | 41    | 41    | 35    |
| 0   | 2     | -16   | 34    | 34    | -3    | -3    | 4    | 10    | 8     |
| 7   | 8     | -1    | 47    | 47    | 24    | 24    | 12    | 6     | 8     |
| 4   | 2     | 5     | 15    | 15    | 0     | 0     | 7     | -1    | -5    |
4. Computational studies

4.1 General

All computational studies were carried out without symmetry restrictions. If it was not possible to obtain starting coordinates from crystal structures GaussView 6.0\textsuperscript{4} were used. Calculations were performed with the Gaussian16 Revision C.01\textsuperscript{5} program packages using Density-Functional Theory (DFT).\textsuperscript{6,7} Energy optimizations were carried out with the PW6B95D3 functional\textsuperscript{8} and def2svp basis set\textsuperscript{9} as well as the MWB46 ECP\textsuperscript{10} as implemented in Gaussian for Sn together with GRIMMES D3 dispersion correction with Becke-Johnson damping.\textsuperscript{11–13} To determine the nature of the structure harmonic vibrational frequency analyses were performed on the same level of theory.\textsuperscript{14} No imaginary frequencies were observed for the ground states; for transition states, one imaginary frequency corresponding to the translational motion was observed. Single point energies were calculated on PW6B95D3\textsuperscript{8}/def2tzvp\textsuperscript{9} level of theory as with the MWB46 ECP\textsuperscript{10} as implemented in Gaussian for Sn. Additionally, single point energies were calculated on the same level of theory with the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM)\textsuperscript{15} as implemented in Gaussian16 with the parameters for benzene.

NBO Analysis was performed with NBO Version 7.\textsuperscript{16} Chemcraft 3D\textsuperscript{17} and Gimp\textsuperscript{18} were used for graphical representation.

4.2 Molecular Orbitals and Results of the NBO-Analysis

Table S18. Results of the NBO-Analysis.

|       | Ph₂Ge=GePh₂ | Ph₃Ge–GePh₃ | A  | 1        | [2]\textsuperscript{*} | 4\textsuperscript{Ge} |
|-------|-------------|-------------|----|----------|------------------------|----------------------|
| WBI   |             |             |    |          |                        |                      |
| Ge₁–Ge₂/Sn₁ | 1.5281 | 0.8627 | 1.6676 | 0.6452 | 0.8607 | 0.8290 |
| Ge₁–C\textsuperscript{Ge₁} | 0.7721/0.8070 | 0.7762/0.7762/0.7763 | – | 0.5121/0.7631/0.7089 | 0.7645/0.7885 | 0.7068\textsuperscript{(5)} |
| Ge₂–C\textsuperscript{Ge₂} | 0.8100/0.7813 | 0.7761/0.7763/0.7763 | – | – | – | 0.7048 | 0.6305\textsuperscript{(3)} |
| Ge–O | – | – | – | 0.0112/0.0160/0.0086 | 0.3542/0.2859 | 0.1954/0.3121 |
| Natural Charge | Ge₁ | 0.78173 | 1.24444 | 0.26266 | 0.92517 | 1.32014 | 1.25887\textsuperscript{(5)} |
| Ge₂/Sn | 0.84758 | 1.24454 | -0.14200 | 0.87908 | 0.65312 | 0.50782\textsuperscript{(2)} |
| C\textsuperscript{Ge₁} | -0.45955/-0.45885 | -0.46437/-0.46475/-0.46472 | – | -1.23357/-1.44737/-0.40469 | -1.46075/-1.48094 | -1.49519 |
| C\textsuperscript{Ge₂} | -0.47039/-0.47018 | -0.46481/-0.46447/-0.46470 | – | – | -1.46819 | -1.46766 |
| O    | – | – | – | -0.92789/-0.95030/-0.99573 | -0.98459/-0.98950 | -0.94562/-1.01424 |
**Figure S33.** Comparison of the HOMO-LUMO levels of different ylide-substituted germynes and stannynes and their singlet-triplet gaps in kJ/mol.

### 4.3 Energies and Coordinates of the Optimized Structures of the Ge-Compounds

**Figure S34.** Investigated isomers of 3 and 4.
Table S19. Energies of the optimized Structures of the Ge-Compounds. Relative energies (ΔG) are given relative to the first structure given in each category. The energy of those structures are set to zero.

| Structure | E(SCF) | Corr(H) | Corr(G) | E(PCM) | ΔG(PCM) [hartree] | ΔG(PCM) [kJ/mol] |
|-----------|--------|---------|---------|--------|------------------|------------------|
| (Ph₂Ge)₂ | -5084.18770936 | 0.392157 | 0.307273 | - | - | - |
| (Ph₃Ge)₂ | -5548.34833675 | 0.587108 | 0.479221 | - | - | - |
| A       | -6453.72159711 | 1.216888 | 1.054843 | - | - | - |
| 1       | -6795.91590497 | 0.895647 | 0.732740 | - | - | - |
| [2]⁺     | -9845.74258788 | 1.332986 | 1.123628 | - | - | - |
| 3⁴Ge    | -8892.24737179 | 1.323003 | 1.144771 | -8892.25706278 | 0 | 0 |
| 4⁴Ge    | -8892.27755833 | 1.323466 | 1.148761 | -8892.28720095 | -0.026 | -68.652 |
| 4-Iso¹⁴Ge | -8892.23902140 | 1.324133 | 1.145467 | -8892.24958397 | 0.008 | 21.463 |
| 4-Iso²⁴Ge | -8892.25124484 | 1.323057 | 1.147097 | -8892.26267838 | -0.003 | -8.637 |
| 4-Iso³⁴Ge | -8892.27475103 | 1.323532 | 1.149772 | -8892.28338626 | -0.021 | -55.982 |
| 4-Iso⁴⁴Ge | -8892.23700441 | 1.322967 | 1.149584 | -8892.24574550 | 0.016 | 42.350 |
| Cy₂Y²Ge (S = 0) | -5892.98407039 | 1.313253 | 1.151770 | - | 0 | 0 |
| Cy₂Y²Ge (S = 1) | -5892.92161406 | 1.313788 | 1.151351 | - | 0.062 | 162.259 |
| Ph₂Y²Ge (S = 0) | -5871.21690208 | 0.885744 | 0.731721 | - | 0.068 | 179.191 |
| Ph₂Y²Ge (S = 1) | -5871.14951494 | 0.886187 | 0.732584 | - | 0.068 | 179.191 |

Structure of Ph₂Ge=GePh₂
E = -5084.18770936
Ge -1.045619 -0.162993 0.600251
Ge 1.001678 0.182284 -0.431078
C -2.379036 1.216259 0.173842
C -2.698867 2.196432 1.119481
C -3.010610 1.264461 -1.075301
C -3.622818 3.196021 0.828808
H -2.218336 2.183512 2.097928
C -3.931780 2.264151 -1.368716
H -2.776610 0.514745 -1.830371
C -4.239610 3.231589 -0.416762
H -3.860757 3.949464 1.577817
H -4.409176 2.290529 -2.346877
H -4.960076 4.014328 -0.647262
C 1.838232 1.923876 -0.175337
C 3.206172 2.108644 -0.411227
C 1.060337 3.042687 0.153791
C 3.782956 3.370351 -0.303251
H 3.831084 1.259066 -0.684564
C 1.636992 4.300610 0.266519
H -0.009358 2.929963 0.326627
C 3.001127 4.467617 0.039785
H 4.848443 3.495647 -0.488662
H 1.018818 5.156682 0.531324
Figure S35. Calculated Structure of Ph₂Ge=GePh₂.

Structure of Ph₂Ge=GePh₃
E = -5548.34833675
Ge -0.016496 -0.004372 -1.213789
Ge 0.018520 0.003773 1.213843
C -1.835324 -0.078156 1.810583
C -2.733129 0.910078 1.386030
C -2.325818 -1.153847 2.555212
C -4.085183 0.823534 1.699728
H -2.376268 1.753829 0.794631
C -3.679347 -1.242775 2.867366
H -1.654536 -1.934574 2.893506
C -4.561004 -0.256374 2.438370
H -4.770026 1.599032 1.360805
H -4.046925 -2.087436 3.447812
H -5.620145 -0.328119 2.679682
C 1.030281 -1.562553 1.783943
C 2.217452 -1.447898 2.511575
C 0.619546 -2.834965 1.365279
Figure S36. Calculated Structure of Ph₃Ge–GePh₃.

Structure of A
E = -6453.72159711
Ge 0.521738 0.000122 0.000007
B -0.171512 1.903007 -0.121027
B -0.170788 1.903074 0.120494
Ge 2.835980 0.000851 0.001293
N 0.795031 -2.967177 -0.023497
C 0.180952 -4.175775 0.279423
C 2.192717 -2.879316 -0.236631
N -1.380928 -2.583047 0.507332
C -1.110479 3.945240 0.598307
C -2.657186 -2.076493 0.868654
N 0.794069 2.967352 0.022689
C 0.179525 4.175812 -0.279894
C 2.191707 2.880042 0.236264
N -1.381988 2.582650 -0.507393
C -1.111916 3.944915 -0.598474
C -2.658072 2.075644 -0.868733
H 0.714190 -5.117632 0.228234
H -1.875608 -4.654017 0.888480
C 2.693172 -2.782434 -1.555156
C 3.062069 -2.941209 0.874819
C 4.074166 -2.828206 -1.738815
C 1.739247 -2.685005 -2.725683
C 4.938676 -2.959887 -0.658411
H 4.481450 -2.761797 -2.744399
C 4.438733 -3.001503 0.631989
H 6.012833 -3.004473 -0.826615
H 5.124141 -3.071561 1.473848
C 2.533659 -2.993394 2.294027
C 2.302740 -1.885523 -3.890310
C 1.284604 -4.074098 -3.172870
H 0.857519 -2.144696 -2.360501
H 2.634649 -0.894935 -3.559328
H 1.532445 -1.747015 -4.658411
H 3.148424 -2.391334 -4.373678
Figure S37. Calculated structure of A. H-Atoms are omitted for clarity.
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Sn      | -6.795    | 0.9159    | 0.0497    |
| Cl      | -0.900    | 0.6912    | -0.403    |
| Ge      | 0.344     | -0.3117   | -0.7259   |
| O       | 2.701     | 1.2110    | -3.2145   |
| C       | -1.490    | -0.3662   | 0.2701    |
| C       | 1.849     | 2.9011    | 0.0067    |
| C       | 3.663     | 2.2481    | 0.3927    |
| P       | -2.421    | 1.1637    | 0.1866    |
| C       | -1.370    | 2.3269    | -0.6986   |
| C       | -3.978    | 1.0614    | -0.7194   |
| C       | -2.826    | 1.7007    | 1.8622    |
| C       | 1.630     | -0.1015   | 0.6968    |
| C       | -0.092    | 1.8724    | -0.9959   |
| P       | 2.959     | -1.1819   | 0.8178    |
| S       | 1.450     | 0.9539    | 2.0248    |
| C       | 0.751     | 2.7449    | 1.6930    |
| O       | 0.053     | 0.9461    | 2.4932    |
| C       | -1.831    | 3.5958    | -1.0447   |
| O       | 2.524     | 0.6418    | 2.9971    |
| C       | 2.930     | 2.2831    | 2.6681    |
| C       | 2.890     | -2.3843   | -0.5381   |
| C       | 4.567     | -0.3491   | 0.8037    |
| C       | 1.741     | 2.6378    | 1.5044    |
| C       | -0.971    | 4.4459    | 1.7181    |
| C       | 0.319     | 4.0172    | 2.0336    |
| C       | -3.922    | 0.9055    | -2.1091   |
| C       | -5.206    | 1.1420    | -0.0590   |
| C       | -5.108    | 0.8027    | -2.8245   |
| C       | -6.334    | 0.8719    | -2.1686   |
| C       | -6.384    | 1.0501    | -0.7893   |
| C       | -3.184    | 0.7434    | 2.8126    |
| C       | -3.538    | 1.1400    | 4.0948    |
| C       | -2.830    | 3.0538    | 2.1997    |
| C       | -3.534    | 2.4890    | 4.4339    |
| C       | -3.181    | 3.4435    | 3.4867    |
| C       | -3.617    | 2.7825    | 1.6792    |
| C       | -4.868    | 2.0643    | -0.2679   |
| C       | -4.805    | -0.3097   | 2.3220    |
| C       | -6.040    | 2.8966    | 1.6892    |
| C       | -7.315    | -3.250    | 2.3929    |
| C       | -6.049    | 2.3888    | 0.3900    |
| C       | 1.850     | -2.2699    | 3.1475    |
| C       | 3.954     | -3.2183    | 2.4320    |
| C       | 1.802     | -3.1865    | 4.1917    |
| C       | 2.827     | -4.1103    | 4.3622    |
| C       | 3.905     | -4.1262    | 3.4817    |
| C       | 1.790     | -3.2481    | -0.5151   |
| C       | 3.867     | -2.5324    | -1.5209   |
| C       | 1.658     | -4.2362    | 1.4805    |
| C       | 2.635     | -4.3825    | -2.4616   |
| C       | 3.734     | -3.5328    | 2.4793    |
| C       | 5.339     | -0.2325    | 1.9601    |
| C       | 4.942     | 0.3292    | -0.3616    |
| C       | 6.502     | 0.5288    | 1.9386    |
| C       | 6.894     | 1.1749    | 0.7709    |
| C       | 6.113     | 1.0767    | -0.3772   |
Figure S38. Calculated structure of 1. H-Atoms are omitted for clarity.

**Structure of [2]**

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 2.133766 | -1.111100 | -0.416770 |
| S    | 1.961377  | -0.731511  | 1.211811  |
| Ge   | 0.808222  | -0.794499  | -1.879885 |
| P    | 3.695356  | -1.700885  | -0.873057 |
| O    | 0.571430  | -0.090055  | 1.373886  |
| C    | 1.808862  | -2.187285  | 2.214406  |
| S    | -1.835158 | -2.356150  | -0.570888 |
| Ge   | -0.571381 | 0.353901   | -0.179473 |
| P    | -3.466525 | -0.630832  | 1.098157  |
| O    | 3.032156  | 0.077866   | 1.809945  |
| C    | 2.475905  | -2.250204  | 3.428693  |
| H    | 3.116824  | -1.427043  | 3.733802  |
| S    | -1.346171 | 2.706132   | 1.614087  |
Figure S39. Calculated structure of [2]+. H-Atoms are omitted for clarity.
Figure S40. HOMO of [2]+. H-Atoms are omitted for clarity.

Structure of 3Ge
E = -8892.24737179
O -2.520049 -1.204751 -2.783517
Cl -0.069919 -1.640720 -0.776514
S -3.708240 -0.895268 -1.887462
C -2.986240 0.179395 -0.827966
C -4.130165 -2.433151 -1.083859
O -4.941208 -0.484803 -2.576995
P -3.891894 1.270355 0.150865
C -5.347793 -3.030385 -1.375112
C -3.263403 -2.987003 -0.145353
C -5.609803 0.643801 0.401407
C -3.040029 1.568259 1.742217
C -4.061109 2.912011 -0.668311
C -5.710045 -4.192850 -0.701793
C -3.640591 -4.145329 0.514023
C -5.673827 -0.512949 1.403018
C -6.662025 1.703135 0.742238
C -2.485270 0.301931 2.393264
C -3.836654 2.417804 2.731727
C -4.738778 2.729071 -2.028050
C -2.711173 3.611566 -0.830853
C -4.869664 -4.765064 0.252842
C -7.060071 -1.141814 1.400347
C -8.051579 1.073315 0.764448
C -1.626993 0.681403 3.593346
C -2.973653 2.771511 3.937624
C -4.888258 4.054271 -2.760777
C -2.857274 4.929450 -1.581975
C -5.258904 -6.015788 0.981378
C -8.128728 -0.107606 1.721639
C -2.407160 1.521015 4.595601
C -3.541138 4.741026 -2.927946
|   | X      | Y      | Z      |
|---|--------|--------|--------|
| H | -1.869062 | 5.389118 | -1.709708 |
| H | -3.448814 | 5.627710 | -0.969669 |
| H | -5.204216 | -5.875810 | 2.068160 |
| H | -4.581989 | -6.843071 | 0.731010 |
| H | -6.277471 | -6.327807 | 0.729357 |
| H | -7.985293 | 0.252145 | 2.752348 |
| H | -9.127938 | -0.560385 | 1.687232 |
| H | -1.767109 | 1.795589 | 5.443531 |
| H | -3.235482 | 0.924166 | 5.009262 |
| H | -2.901173 | 4.121393 | -3.574004 |
| H | 5.882451 | 2.212495 | 2.606368 |
| H | 2.409548 | 2.586446 | 0.123766 |
| H | 5.796712 | -0.326328 | 0.778538 |
| H | 2.269233 | -1.964754 | -1.726897 |
| H | 4.666816 | -3.515984 | -0.240944 |
| H | 6.757897 | 4.375062 | 1.711403 |
| H | 3.274495 | 4.733340 | -0.770687 |
| H | 5.015866 | 1.373688 | -0.897769 |
| H | 5.639188 | 0.359240 | -2.194326 |
| H | 6.549220 | -2.001663 | -1.665526 |
| H | 6.617837 | -2.540700 | 0.009431 |
| H | 1.969006 | 0.437141 | -1.683680 |
| H | 3.455774 | 0.691781 | -2.596745 |
| H | 4.942911 | -1.472935 | -3.124801 |
| H | 4.386898 | -3.036895 | -2.529613 |
| H | 3.886438 | -2.315637 | 2.462537 |
| H | 5.521035 | -2.467717 | 1.881033 |
| H | 2.219883 | -3.705440 | 2.462537 |
| H | 1.895441 | -3.039482 | 0.954897 |
| H | 7.301774 | 1.559091 | 0.069333 |
| H | 7.270446 | 2.127449 | -1.598726 |
| H | 8.265536 | -0.816103 | 0.567734 |
| H | 8.844952 | -1.799929 | -0.773296 |
| H | 1.511124 | 0.706285 | -4.130688 |
| H | 1.007193 | -0.871180 | -3.537248 |
| H | 2.437472 | -2.949472 | -4.053388 |
| H | 3.935239 | -2.764743 | -4.965056 |
| H | 4.983358 | -3.01062 | 3.460545 |
| H | 5.319316 | -4.959240 | 1.861401 |
| H | 1.673929 | -5.494972 | 0.974380 |
| H | 3.311571 | -5.684307 | 0.355723 |
| H | 5.651104 | 5.967930 | -1.244294 |
| H | 4.934834 | 6.830358 | 0.117232 |
| H | 6.597678 | 6.228518 | 0.233547 |
| H | 8.177343 | -0.044163 | -2.390537 |
| H | 9.250990 | 0.639337 | -1.173638 |
| H | 2.202633 | -1.113427 | -5.701039 |
| H | 3.616221 | -0.301736 | -5.032684 |
| H | 3.297311 | -6.042303 | 2.807986 |
| H | 2.547174 | -4.466660 | 3.054750 |
| Ge | -1.214155 | 0.253522 | -1.794980 |
| Ge | 1.043617 | -0.331796 | 1.509628 |
Figure S41. Calculated Structure of 3\textsuperscript{Ge}. H-Atoms are omitted for clarity.

Structure of 4\textsuperscript{Ge}
E = -8892.27755833
Ge 1.424570 -1.188913 -1.882166
Cl 0.887098 0.819050 -2.967611
Ge -0.665246 -1.032402 -0.544628
P 3.899451 -1.043859 0.164383
C 4.773273 -1.278303 -1.434592
C 3.834327 -2.703068 0.959111
C 4.846305 0.038735 1.313870
O 1.837250 0.214322 2.348540
S 1.545830 0.501685 0.932775
O 0.041471 0.454439 0.615265
C 1.859983 2.252540 0.765487
S -3.205517 -1.389487 -1.610775
O -3.934376 -0.791422 -2.735945
O -2.065942 -2.320472 -1.905626
C -2.449527 -0.319245 -0.538906
C -4.418461 -2.390910 -0.763673
Cl -0.532435 -2.594134 1.083120
P -3.114940 1.192721 -0.029346
C -2.465174 1.629942 1.623910
C -2.706247 2.613468 -1.123777
C -4.955999 1.043198 -0.052952
C 2.273982 5.001523 0.558412
C 2.477073 6.480720 0.429765
C 4.709631 -0.084044 -2.389863
C 6.203404 -1.797413 -1.298568
C 5.244158 -0.495973 -3.755761
C 6.662377 -1.042118 -3.658083
C 6.749872 -2.193846 -2.665864
C 5.324369 1.328840 0.646446
C 5.997760 -0.615034 2.080939
C 5.822001 2.307965 1.699427
C 6.948885 1.691086 2.516752
C 6.532033 0.359564 3.127315
C 3.098431 -2.622277 2.298380
C 3.165849 -3.747334 0.064602
C 3.123000 -5.107572 0.751424
C 2.423630 -5.030521 2.100239
C 3.070553 -3.978630 2.988972
Figure S42. Calculated Structure of $^{4}\text{Ge}$. H-Atoms are omitted for clarity.

Figure S43. HOMO-3 of $^{4}\text{Ge}$. H-Atoms are omitted for clarity.

Figure S44. HOMO of $^{4}\text{Ge}$. H-Atoms are omitted for clarity.
Figure S45. LUMO of 4\textsuperscript{Ge}. H-Atoms are omitted for clarity.

Figure S46. LUMO+4 of 4\textsuperscript{Ge}. H-Atoms are omitted for clarity.

Structure of 4-Iso1\textsuperscript{Ge}

\begin{verbatim}
E = -8892.23902140
O  -1.864137 1.103499 2.775056
Cl  0.890903 2.673749 0.747677
S  -3.088132 1.040179 1.949488
C  -2.774357 -0.200290 0.801424
Cl  2.616917 1.112117
O  -4.379438 0.903608 2.642886
P  -4.075746 -0.88461 -0.139510
C  -4.065207 3.518688 1.632427
C  -2.386743 2.914295 0.026294
C  -5.367798 0.394322 -0.443313
C  -3.436527 -1.570108 -1.715802
C  -4.935183 -2.286060 0.701128
C  -4.114322 4.833098 1.049521
C  -2.449805 4.173719 -0.548425
C  -4.961881 1.343253 -1.571872
C  -6.794838 -0.108312 -0.672330
C  -2.423643 -0.695431 -2.454528
C  -4.511465 -2.106922 -2.661337
C  -5.437144 -1.865073 2.082088
C  -4.084522 -3.550095 0.810121
C  -3.311407 5.154823 -0.046233
C  -5.896926 2.541499 -1.619343
C  -7.750309 1.080145 -0.751367
C  -1.759693 -1.515504 -3.551790
\end{verbatim}
|    |    |    |    |
|----|----|----|----|
| H  | -8.771138 | 0.721999 | -0.937100 |
| H  | -1.020424 | -0.901650 | -4.079091 |
| H  | -1.187533 | -2.325853 | -3.078886 |
| H  | -3.374835 | -3.794713 | -3.348209 |
| H  | -4.613779 | -3.264245 | -4.483781 |
| H  | -6.556896 | -2.660835 | 3.740174 |
| H  | -7.129568 | -3.197979 | 2.163390 |
| H  | -4.221075 | -5.597118 | 1.574623 |
| H  | -5.709429 | -4.961354 | 0.849066 |
| H  | -3.554830 | 6.452243 | -1.749479 |
| H  | -2.401728 | 7.038248 | -0.549676 |
| H  | -4.140220 | 7.137940 | -0.221544 |
| H  | -7.435909 | 1.626007 | -2.808575 |
| H  | -8.018740 | 2.949198 | -1.804336 |
| H  | -2.309276 | -2.694547 | -5.284691 |
| H  | -3.289919 | -1.252624 | -5.044259 |
| H  | -5.966162 | -5.065951 | 3.308813 |
| H  | -4.532426 | -4.064184 | 3.524339 |
| H  | 4.095314 | -3.330436 | -2.639239 |
| H  | 1.859726 | -2.099075 | 0.800624 |
| H  | 5.268958 | -0.942286 | -0.912838 |
| H  | 3.161745 | 2.351354 | 1.530146 |
| H  | 5.733898 | 2.521995 | -0.495750 |
| H  | 4.419154 | -5.584557 | -1.620118 |
| H  | 2.170212 | -4.332001 | 1.815527 |
| H  | 4.312802 | -1.736037 | 1.288159 |
| H  | 5.585511 | -0.852247 | 2.124493 |
| H  | 7.127064 | 0.718841 | 0.859022 |
| H  | 7.011228 | 0.825849 | -0.906143 |
| H  | 2.103130 | 0.209891 | 2.107707 |
| H  | 3.576867 | -0.309638 | 2.929095 |
| H  | 5.727025 | 1.203344 | 2.717388 |
| H  | 5.625759 | 2.699707 | 1.789401 |
| H  | 3.942435 | 1.626988 | -2.802313 |
| H  | 5.534965 | 1.002653 | -2.499002 |
| H  | 3.768147 | 3.861801 | 0.229642 |
| H  | 2.864969 | 3.315130 | -1.169977 |
| H  | 6.022312 | -3.092232 | 0.099239 |
| H  | 6.192523 | -3.245637 | 1.844642 |
| H  | 7.694643 | -1.498648 | -1.177660 |
| H  | 8.901396 | -0.622124 | -0.241780 |
| H  | 1.991140 | 0.683490 | 4.548866 |
| H  | 1.899369 | 2.151886 | 3.586685 |
| H  | 4.059289 | 3.665118 | 3.421367 |
| H  | 5.525776 | 3.135853 | 4.243019 |
| H  | 5.612242 | 2.748144 | -4.257090 |
| H  | 6.529754 | 3.273449 | -2.848238 |
| H  | 3.806040 | 5.572180 | -1.552330 |
| H  | 5.430464 | 4.988638 | -1.205565 |
| H  | 3.899811 | -6.388101 | 1.810987 |
| H  | 2.545787 | -7.002495 | 0.861612 |
| H  | 4.189934 | -7.091463 | 0.207725 |
| H  | 8.028759 | -1.588473 | 1.860300 |
| H  | 8.422992 | -2.881369 | 0.732189 |
| H  | 3.466592 | 2.472466 | 5.503661 |
| H  | 4.399092 | 1.067610 | 4.998267 |
| H  | 5.101859 | 5.134585 | -3.655494 |
| H  | 3.672783 | 4.109246 | -3.547732 |
| Ge | -0.927336 | -0.701662 | 1.085484 |
| Ge | 0.793529 | 0.779938 | -0.538806 |
Figure S47. Calculated Structure of 4-Iso\textsuperscript{1}Ge. H-Atoms are omitted for clarity.

Structure of 4-Iso\textsuperscript{2}Ge

E = -8892.25124484
O -1.025235 0.825184 2.076610
Cl 0.084704 1.047458 -2.701297
S -2.489546 0.944170 1.617143
C -2.541089 -0.361124 0.591356
C -2.591651 2.490492 0.736376
O -3.476976 1.060900 2.698195
P -3.962254 -1.171361 0.075046
C -3.118933 3.609801 1.367736
C -2.183152 2.541617 -0.590361
C -5.405004 -0.033557 0.184423
C -3.652090 -1.841909 -1.598917
C -4.358926 -2.612426 1.152699
C -3.231484 4.794821 0.647768
C -2.307549 3.727199 -1.295754
C -5.432391 1.000304 -0.942941
C -6.777424 -0.692278 0.332710
C -3.056049 -0.825945 -2.571629
C -4.849992 -2.579489 -2.205499
C -4.430530 -2.142337 2.607323
C -3.348110 -3.749213 0.994175
C -2.830199 4.874543 -0.688493
C -6.468849 2.074042 -0.646855
C -7.838111 0.372470 0.598351
C -2.660452 -1.511329 -3.871535
C -4.443891 -3.246174 -3.517546
C -4.729359 -3.295436 3.554718
C -3.639498 -4.890093 1.959034
C -2.932302 6.157205 -1.455541
C -7.849153 1.457564 -0.469519
C -3.840542 -2.244252 -4.493644
C -3.703183 -4.407883 3.400435
O 2.607066 -0.846683 -3.221048
Cl 0.193771 -2.299727 -1.674857
S 3.524541 -0.357048 -2.193763
C 2.603169 -0.002940 -0.790010
C 4.558594 -1.744379 -1.733256
O 4.468589 0.723483 -2.540038
P 3.217251 0.999567 0.482402
| H   | -3.534413 | -2.754393 | -5.415708 |
|-----|-----------|-----------|-----------|
| H   | -4.614041 | -1.515498 | -4.783698 |
| H   | -3.934902 | -5.243518 | 4.073032  |
| H   | -2.714253 | -4.028641 | 3.698965  |
| H   | 6.343907  | -0.812592 | -2.444771 |
| H   | 2.896203  | -2.883913 | -0.982735 |
| H   | 5.322240  | 0.943760  | -0.536102 |
| H   | 1.408606  | 0.663035  | 1.912780  |
| H   | 3.278654  | 3.344424  | 1.020394  |
| H   | 7.794346  | -2.730327 | -1.748497 |
| H   | 4.328477  | -4.788725 | -0.276924 |
| H   | 5.216589  | -1.152867 | 0.832213  |
| H   | 5.405045  | -0.190152 | 2.301199  |
| H   | 5.388207  | 2.424356  | 2.138886  |
| H   | 5.316743  | 3.157640  | 0.536493  |
| H   | 2.247517  | -1.620164 | 1.531633  |
| H   | 3.655532  | -1.306003 | 2.533252  |
| H   | 3.987941  | 1.150949  | 3.463292  |
| H   | 2.805365  | 2.380074  | 3.038142  |
| H   | 2.531107  | 2.561333  | -1.839256 |
| H   | 4.111676  | 3.093227  | -1.333811 |
| H   | 0.966335  | 2.695147  | 1.624328  |
| H   | 0.606939  | 2.327784  | -0.056523 |
| H   | 7.430440  | -0.346538 | 0.029449  |
| H   | 7.570807  | -1.145575 | 1.590119  |
| H   | 7.481187  | 2.236756  | -0.080339 |
| H   | 7.625716  | 3.161063  | 1.411788  |
| H   | 1.942644  | -2.445280 | 3.876302  |
| H   | 0.752883  | -1.215663 | 3.466241  |
| H   | 1.057432  | 1.192430  | 4.329433  |
| H   | 2.442328  | 1.573991  | 5.351780  |
| H   | 2.839093  | 4.940586  | -2.406994 |
| H   | 3.191691  | 5.341483  | -0.727064 |
| H   | -0.259821 | 4.541642  | 0.565426  |
| H   | 1.347923  | 5.075103  | 1.048178  |
| H   | 6.686066  | -5.275912 | 0.538552  |
| H   | 6.780295  | -5.945678 | -1.090970 |
| H   | 8.086950  | -4.826149 | -0.669425 |
| H   | 7.597187  | 1.062643  | 2.741368  |
| H   | 8.881827  | 0.996331  | 1.538049  |
| H   | 1.662259  | -0.776005 | 5.721927  |
| H   | 3.304666  | -0.743007 | 5.085730  |
| H   | 0.816261  | 5.878636  | -1.259828 |
| H   | 0.553663  | 4.205241  | -1.773115 |
| Ge  | -0.680222 | -1.016249 | 1.012927  |
| Ge  | 0.709020  | -0.204919 | -0.946502 |
Figure S48. Calculated Structure of 4-Iso2Ge. H-Atoms are omitted for clarity.

Structure of 4-Iso3Ge

| Element | X    | Y    | Z    |
|---------|------|------|------|
|          | 0.645431 | -0.301974 | -2.005708 |
|          | -0.556956 | -0.212121 | 2.175070 |
| C        | -1.612884 | 0.254399  | 0.032746 |
| C        | 1.689081  | 0.397669  | 0.059346 |
| S        | 1.950386  | 0.393364  | -1.586947 |
| O        | 2.277572  | 1.658668  | -2.260410 |
| C        | 3.231403  | -0.731291 | -2.091803 |
| P        | -2.722956 | 0.650619  | -1.220355 |
| C        | -4.097677 | 1.616438  | -0.473899 |
| C        | -3.464222 | -0.852082 | -1.987379 |
| C        | -1.878228 | 1.533297  | -2.581853 |
| S        | -1.868228 | 0.375954  | 1.684283 |
|          | -2.274683 | 1.688348  | 2.208073 |
| P        | -3.125605 | -0.727540 | 2.315540 |
| C        | 2.568823  | 1.307637  | 1.224720 |
| C        | 4.325671  | 1.402559  | 0.701073 |
| C        | 1.950670  | 3.031545  | 1.392026 |
| C        | 2.347450  | 0.530388  | 2.866378 |
| C        | 4.135640  | -0.356050 | -3.075815 |
| C        | 5.126598  | -1.256687 | -3.452816 |
| C        | -3.711017 | 3.067356  | -0.180423 |
| C        | -5.459077 | 1.540238  | -1.164129 |
| C        | 3.293851  | -1.984575 | -1.498995 |
| C        | -2.452195 | 1.575945  | -2.874972 |
| C        | -3.974041 | 1.775964  | -0.882672 |
| C        | 5.033697  | 0.053310  | 0.838022 |
| C        | 5.178295  | 2.503427  | 1.333352 |
| C        | -2.993099 | -2.899275 | -3.401025 |
| C        | -0.971617 | 2.669379  | -2.118994 |
| C        | -2.839430 | 1.977220  | -3.684265 |
| C        | 5.217344  | -2.520866 | -2.866824 |
| C        | 4.283791  | -2.869484 | -1.883292 |
| C        | 6.280331  | -3.492715 | -3.280427 |
| C        | -4.755628 | 3.707695  | 0.720056 |
| C        | 2.154381  | 3.833511  | 0.105621 |
| C        | 0.466746  | 3.007696  | 1.751822 |
| C        | -0.216053 | 3.254897  | -3.303059 |
| C        | 6.378525  | 0.092826  | 0.128071 |
| C        | -1.168539 | 3.716197  | -4.396988 |
| C        | 2.421003  | -0.992389 | 2.847839 |
| Component | X         | Y         | Z         |
|-----------|-----------|-----------|-----------|
| C         | 3.219676  | 1.108365  | 3.979955  |
| C         | -6.512017 | 2.205057  | -0.279283 |
| C         | -4.552388 | -3.067066 | -1.440921 |
| C         | -4.371251 | -0.217422 | 2.661069  |
| C         | -2.879546 | -2.094033 | 2.389066  |
| C         | -3.903985 | -2.953793 | 2.750052  |
| C         | -5.183446 | -2.471368 | 3.056363  |
| C         | -3.516393 | -3.791361 | -2.286242 |
| C         | -2.067709 | 2.575855  | -4.854123 |
| C         | -5.392656 | -1.091853 | 3.015909  |
| C         | 1.590261  | 5.243113  | 0.238216  |
| C         | 1.949940  | -1.542543 | 4.184514  |
| C         | -6.139737 | 3.634743  | 0.090174  |
| C         | -6.287042 | -3.417913 | 3.413408  |
| C         | 2.765462  | 0.549245  | 5.325738  |
| C         | 6.538542  | 2.554692  | 0.643482  |
| C         | 2.770824  | -0.974745 | 5.334344  |
| C         | 7.252051  | 1.208951  | 0.685737  |
| C         | 1.174900  | 5.222493  | 0.621831  |
| H         | -4.215210 | 1.111612  | 0.494783  |
| H         | -4.307569 | -0.510710 | -2.606937 |
| H         | -1.208596 | 0.758065  | -2.982037 |
| H         | 4.227245  | 1.631613  | -0.375005 |
| H         | 2.527531  | 3.492459  | 2.210633  |
| H         | 1.300004  | 0.773577  | 3.089785  |
| H         | 4.057115  | 0.629885  | -3.526635 |
| H         | 5.844799  | -0.971161 | -4.220254 |
| H         | -2.722092 | 3.109133  | 0.287557  |
| H         | -3.660056 | 3.622734  | -1.128224 |
| H         | -5.417428 | 2.048028  | -2.139747 |
| H         | -5.748679 | 0.503469  | -1.354991 |
| H         | 2.796877  | -2.265761 | -0.708790 |
| H         | -2.159352 | -0.943809 | -3.721653 |
| H         | -1.530602 | -1.768342 | -2.306405 |
| H         | -3.118146 | -2.028205 | -0.243006 |
| H         | -4.700689 | -1.264460 | -0.233702 |
| H         | 5.196033  | -0.150253 | 1.906526  |
| H         | 4.407851  | -0.757508 | 0.453584  |
| H         | 4.689688  | 3.481618  | 1.266253  |
| H         | 5.316957  | 2.292307  | 2.402509  |
| H         | -3.802870 | -2.699727 | -4.120621 |
| H         | -2.192557 | -3.411096 | -3.948587 |
| H         | -0.279359 | 2.289114  | -1.358469 |
| H         | -1.565686 | 3.459803  | -1.64920  |
| H         | -3.458258 | 1.136890  | -4.027536 |
| H         | -3.528314 | 2.736331  | -3.284846 |
| H         | 4.320565  | -3.848841 | -1.408790 |
| H         | 6.977829  | -3.047492 | -3.997214 |
| H         | 6.856115  | -3.842207 | -2.414503 |
| H         | 5.836178  | -4.381076 | -3.747858 |
| H         | -4.746292 | 3.184067  | 1.688059  |
| H         | -4.481658 | 4.749433  | 0.929680  |
| H         | 1.651828  | 3.307154  | -0.715265 |
| H         | 3.212923  | 3.875684  | -0.178659 |
| H         | 0.271633  | 2.441972  | 2.667979  |
| H         | -0.064948 | 2.473603  | 0.950895  |
| H         | 0.418289  | 4.083158  | -2.959575 |
| H         | 0.469439  | 2.494336  | -3.696575 |
| H         | 6.207352  | 0.248287  | -0.947215 |
H 6.881307 -0.877886 0.224341
H -1.795390 4.539148 -4.018313
H -0.606986 4.120608 -5.248808
H 3.447175 -1.328921 2.651275
H 1.809886 -1.401706 2.045425
H 4.268892 0.826013 3.808948
H 3.183262 2.059782 3.994018
H -6.616017 1.608692 0.640526
H -7.489022 2.177886 -0.778575
H -4.883665 -3.701539 -0.610094
H -5.443706 -2.845305 -2.048676
H -4.525750 0.858808 2.663762
H -1.892190 -2.481483 2.152283
H -3.706142 -4.023829 2.795986
H -2.670102 -4.088081 -1.648650
H -3.932867 -4.717009 -2.702823
H -1.450104 1.789221 -5.312307
H -2.768110 2.916766 -5.627547
H -6.370917 -0.692375 3.280052
H 2.158218 5.794035 1.004260
H 1.735189 5.784924 -0.705737
H 2.002487 -2.637853 4.162225
H 0.889779 -1.277665 4.311078
H -6.151926 4.255153 -0.819260
H -6.894685 4.059982 0.763895
H -6.010455 -4.036234 4.276485
H -7.210338 -2.884252 3.660189
H -6.504117 -4.104134 2.584701
H 3.404229 0.942773 6.127236
H 1.746461 0.910204 5.530543
H 6.388939 2.854322 -0.404816
H 7.160984 3.333008 1.103804
H 2.398847 -1.346612 6.297860
H 3.809477 -1.329543 5.245118
H 7.509497 0.973317 1.729933
H 8.201721 1.266770 0.138577
H -1.175869 4.330346 2.122268
H 0.367564 4.919229 2.739427
H -0.457641 4.768884 -0.197956
H -0.262589 6.245190 0.743822
Ge -0.241531 -3.348172 0.125406
Ge 0.085647 -0.745282 0.021247
Cl 0.390922 -3.670277 -2.037951
Cl 1.768705 -3.893961 1.090280
Figure S49. Calculated structure of 4-Iso$^3$Ge. H-Atoms are omitted for clarity.

Structure of 4-Iso$^4$Ge
E = -8892.23700441
O 1.080834 -2.054890 1.293130
C -1.469384 -0.493561 0.375672
C 1.757192 -0.134864 -0.056407
S 2.255452 -1.652925 0.394948
O 2.649027 -2.636763 -0.624468
C 3.630431 -1.665119 1.550455
P -2.237482 -2.013702 0.181373
C -3.876227 -1.815329 -0.645297
C -2.631803 -2.686831 1.850441
C -1.213391 -3.281140 -0.664893
S -1.655063 0.875897 -0.500507
O -1.192387 0.940436 -1.898266
C -3.310548 1.543691 -0.545748
P 2.591333 0.793414 -1.251519
C 4.403946 0.712780 -0.889220
C 2.498226 0.261985 -3.017795
C 1.908154 2.492502 -1.255008
C 4.687318 -2.540890 1.346405
C 5.732750 -2.571465 2.264695
C -3.790554 -1.465266 -2.133178
C -4.937276 -2.892741 -0.403457
C 3.602599 -0.831419 2.664830
C -1.395181 -3.016809 2.684505
C -3.533109 -1.718488 2.619790
C 4.764119 1.475649 0.384696
C 5.397286 1.058899 -1.998348
C -1.792978 -3.601123 4.033605
C -0.511287 -2.730866 -1.908136
C -1.985761 -4.566084 -0.961392
C 5.733980 -1.741580 3.385755
C 4.649908 -0.873790 3.570733
C 6.870370 -1.755328 4.362607
C -5.142781 -0.960544 -2.621406
C 2.995323 -1.160455 -3.259403
C 1.138020 0.458557 -3.679274
C 0.348443 -3.809677 -2.558223
C 6.158975 1.093160 0.853425
Figure S50. Calculated structure of 4-Iso4Ge. H-Atoms are omitted for clarity.

Structure of CyY2Ge (S = 0)
E = -5892.98407039
Ge -0.065984 -0.842581 1.073563
O -0.683347 1.277189 1.951242
O 0.474179 -2.098312 -0.825761
C 1.563353 -0.098325 0.071336
C -1.696070 -0.036155 0.136546
S -1.972701 1.240736 1.155528
O -2.457867 2.505534 0.571072
C -3.205022 0.841082 2.394976
P 2.684080 1.148818 0.414656
C 3.946649 1.213035 -0.921498
C 3.605681 0.887721 1.993323
C 1.820236 2.746178 0.645814
S 1.786927 -1.359574 -0.991512
O 2.227054 -1.052734 -2.363137
C 2.994109 -2.549142 -0.411623
P -2.622644 -0.387225 -1.258612
C -4.386591 0.098518 -1.029991
C -2.039587 0.496193 -2.766981
C -2.442517 -2.170513 -1.646950
C -4.264651 1.702637 2.629023
C -5.235947 1.348524 3.563005
C 3.375961 1.796302 -2.215798
C 5.301575 1.841880 -0.600678
C -3.094304 -0.357822 3.095513
C 2.674664 0.969665 3.204975
C 4.316264 -0.463102 1.954121
C -5.111043 -0.808765 -0.032851
C -5.217815 0.240879 -2.307537
C 3.414326 0.649639 4.498814
C 0.770892 3.037789 -0.420444
C 2.763944 3.930703 0.849511
C -5.158009 0.148643 4.267301
C -4.066062 -0.695741 4.021311
C -6.207325 -0.238456 5.265611
C 4.323532 1.515801 -3.370346
C -2.216912 2.008632 -2.626099
C -0.569110 0.175796 -3.024942
C -0.009507 4.290159 -0.049720
C -6.485147 -0.245327 0.302355
C 0.916020 5.482865 0.138251
C -2.498602 -3.095663 -0.431478
C -3.337105 -2.689593 -2.771127
C 6.262109 1.589001 -1.760391
C 5.065876 -0.755661 3.244988
C 4.253116 -2.600799 -0.992552
C 2.689724 -3.343133 0.691621
C 3.671226 -4.155482 1.235400
C 4.964717 -4.191128 0.697851
C 4.122613 -0.695632 4.436943
C 1.974418 5.188987 1.192318
C 5.232248 -3.413739 -0.428977
C -1.696578 2.741970 -3.856480
C -2.050152 -4.493227 -0.838516
C 5.706568 2.087591 -3.088835
C 6.026443 -5.041967 1.327100
C -2.895747 -4.092055 -3.176095
C -6.600130 0.795834 -1.979211
C -2.892307 -5.039653 -1.983867
C -7.325450 -0.64298 -0.953576
C -0.042564 2.894159 3.281655
C -1.254390 2.573670 1.572355
C -4.288834 1.098957 -0.574310
C -2.651781 0.130344 -3.607499
C -1.402106 -2.208048 -1.995235
C -4.318260 2.635334 2.072478
C -6.074368 2.020082 3.744533
C 2.384919 1.375019 -2.414512
C 3.263469 2.883936 -2.095608
C 5.187794 2.923101 -0.440934
C 5.724552 1.428373 0.322282
C -2.256683 -1.026775 2.894159
C 2.221721 1.964574 3.281655
C 1.841482 0.262737 3.066588
C 3.551821 -1.234960 1.808996
C 4.990472 -0.532898 1.090147
C -5.235836 -1.803478 -0.485314
C -4.512461 -0.946043 0.873956
C -4.722698 0.892039 -3.035257
C -5.327427 -0.740672 -2.78926
C 4.158380 1.438459 4.690724
C 2.709704 0.677078 5.339631
C 0.110166 2.168719 -0.516139
C 1.252176 3.187530 -1.394020
C 3.502028 3.721303 1.635594
C 3.329735 4.107078 -0.077352
C -3.983537 -1.636059 4.565391
C -6.994815 0.518964 5.334190
C -6.678478 -1.92501 4.996337
C -5.774306 -0.366702 6.266024
C 4.379578 0.426567 -3.514111
C 3.916864 1.932671 -4.300819
C -1.674044 2.337146 -1.731667
C -3.264354 2.276689 -2.441614
C -0.391890 -0.899014 -3.127789
C 0.003249 0.490575 -2.139588
C -0.768381 4.494424 -0.815985
Figure S51. Calculated structure of Cy$_2$Ge (S = 0). H-Atoms are omitted for clarity.

Figure S52. HOMO of Cy$_2$Ge (S = 0). H-Atoms are omitted for clarity.
Figure S53. LUMO of Cy₂Ge (S = 0). H-Atoms are omitted for clarity.

Figure S54. LUMO+4 of Cy₂Ge (S = 0). H-Atoms are omitted for clarity.

Structure of Cy₂Ge (S = 1)
E = -5892.92161406
Ge 0.055331 0.687166 0.575754
O 1.141808 -1.737981 2.212335
O -0.991616 1.919952 -2.036870
C -1.613266 0.165333 -0.240295
C 1.702896 -0.240785 0.159005
Figure S55. Calculated structure of $^\text{Cy}Y_2\text{Ge}$ ($S = 1$). H-Atoms are omitted for clarity.

Structure of $^\text{Ph}Y_2\text{Ge}$ ($S = 0$)

E = -3796.60415202
Sn -0.052882 -0.019635 -1.748421
O -1.084867 -2.157203 -0.831607
C -1.728924 0.160684 -0.273968
C 1.725322 -0.244079 -0.353312
O 0.901374 2.051574 -0.795756
S -2.163284 -1.431650 -0.066590
C -3.680449 -1.747378 -0.963375
O -2.435555 -1.883888 1.309064
P -2.471894 1.416004 0.576551
C -4.247410 1.107735 0.822567
C -2.257085 2.927323 -0.401691
C -1.799590 1.751340 2.222986
C 4.003726 1.143970 -2.007469
H 3.437605 0.282635 -2.357230
C 3.537752 1.865744 -0.915893
Figure S56. Calculated Structure of $^\text{Ph}Y_2\text{Ge}$ ($S = 0$). H-Atoms are omitted for clarity.
Figure S57. HOMO of $^{\text{Ph}}\text{Y}_2\text{Ge} \ (S = 0)$. H-Atoms are omitted for clarity.

Figure S58. LUMO of $^{\text{Ph}}\text{Y}_2\text{Ge} \ (S = 0)$. H-Atoms are omitted for clarity.
Figure S59. LUMO+16 of $\text{PhY}_2\text{Ge}$ ($S = 0$). H-Atoms are omitted for clarity.

Structure of $\text{PhY}_2\text{Ge}$ ($S = 1$)

\[
\begin{align*}
E &= -376.52238437 \\
\text{Sn} &= -0.042900 \quad -0.200585 \quad -1.510317 \\
O &= -1.447040 \quad -2.515438 \quad 0.293138 \\
C &= -1.799740 \quad -0.016442 \quad -0.294597 \\
C &= 1.801247 \quad -0.124285 \quad -0.405107 \\
O &= 1.250978 \quad 2.404098 \quad -0.226209 \\
S &= -2.343885 \quad -1.386096 \quad 0.569780 \\
C &= -3.939377 \quad -1.834436 \quad -0.100718 \\
O &= -2.595984 \quad -1.011718 \quad 1.979342 \\
P &= -2.471036 \quad 1.511554 \quad 0.116857 \\
C &= -4.265862 \quad 1.442220 \quad 0.443760 \\
C &= -2.174455 \quad 2.616272 \quad -1.289349 \\
C &= -1.791094 \quad 2.315734 \quad 1.588491 \\
C &= 4.328958 \quad 1.320412 \quad -1.590581 \\
H &= 3.717102 \quad 0.618906 \quad -2.154759 \\
C &= 3.827129 \quad 1.866015 \quad -0.417725 \\
C &= 5.619259 \quad 1.635352 \quad -1.992979 \\
S &= 2.222631 \quad 1.401884 \quad 0.230681 \\
P &= 4.592978 \quad 2.750912 \quad 0.334537 \\
C &= -6.261533 \quad -2.330890 \quad 0.209812 \\
H &= -7.115059 \quad -2.460451 \quad 0.874407 \\
C &= -5.020358 \quad -2.011152 \quad 0.748619 \\
C &= -6.437778 \quad -2.472180 \quad -1.166696 \\
H &= -4.877053 \quad -1.877741 \quad 1.818037 \\
C &= -4.079171 \quad -1.995660 \quad -1.475382 \\
O &= 2.462542 \quad 1.294182 \quad 1.689994 \\
C &= -5.324071 \quad -2.308117 \quad -1.998854 \\
C &= -7.791645 \quad -2.755757 \quad -1.745040 \\
H &= 6.021408 \quad 1.185830 \quad -2.900193 \\
C &= 6.418132 \quad 2.503365 \quad -1.244126 \\
C &= 7.833780 \quad 2.779188 \quad -1.651919 \\
C &= 5.877186 \quad 3.067773 \quad -0.086376 \\
P &= 2.539645 \quad -1.525675 \quad 0.272180 \\
C &= 2.045603 \quad -2.927015 \quad -0.759344 \\
C &= 2.052669 \quad -1.916592 \quad 1.971056
\end{align*}
\]
C 0.306622 -1.881828 3.634207
H -0.709483 -1.606491 3.907628
H 0.787063 -2.820736 5.510741
H 4.352408 -0.064064 1.954122
C 6.335487 -0.364438 1.169000
H 6.794353 0.321664 1.877897
C 7.113397 -1.003215 0.208768
H 8.186356 -0.823033 0.167794
C 6.519100 -1.878014 -0.693768
H 7.124957 -2.393971 -1.436117
H 4.694955 -2.790776 -1.359088

Figure S60. Calculated structure of Ph₂Ge (S = 1). H-Atoms are omitted for clarity.

4.5 Optimized Structures of the Sn-Compounds

Table S20. Energies of the optimized Structures of the Sn-Compounds. Relative energies (ΔG) are given relative to the first structure given in each category. The energy of those structures are set to zero.

|                  | E(SCF)  | Corr(H) | Corr(G) | E(PCM)  | ΔG [hartree] | ΔG [kJ/mol] |
|------------------|---------|---------|---------|---------|-------------|-------------|
| 3 Sn             | -4743.03508401 | 1.322371 | 1.143393 | -4743.04607679 | 0           | 0           |
| 4 Sn             | -4743.04000668 | 1.323067 | 1.146404 | -4743.04994506 | -0.000857   | -2.250762   |
| 4-iso1 Sn        | -4743.01448532 | 1.322765 | 1.140225 | -4743.02514692 | 0.017762    | 46.633790   |
| 4-iso2 Sn        | -4743.00987714 | 1.322558 | 1.142533 | -4743.02203394 | 0.023183    | 60.866573   |
| 4-iso3 Sn        | -4743.04261415 | 1.323040 | 1.146776 | -4743.05199407 | -0.002534   | -6.653752   |
| 4-iso4 Sn        | -4743.02037103 | 1.322336 | 1.143960 | -4743.03040689 | 0.016237    | 42.629981   |
| Cy₂SnCl (S = 0)  | -2371.49531249 | 0.660056 | 0.558560 | –        | 0.0081602   | 214.246799  |
| Cy₂SnCl (S = 1)  | -2371.41054621 | 0.659467 | 0.555708 | –        | 0.000816    | 214.246799  |
| Cy₂Sn (S = 0)    | -3818.37212370 | 1.313265 | 1.152236 | –        | 0           | 0           |
| Cy₂Sn (S = 1)    | -3818.29445342 | 1.313075 | 1.149112 | –        | 0.074262    | 194.975795  |
| Ph₂Sn (S = 0)    | -3796.60415202 | 0.885692 | 0.731914 | –        | 0           | 0           |
| Ph₂Sn (S = 1)    | -3796.52238437 | 0.885401 | 0.730000 | –        | 0.079854    | 209.655758  |
**Structure of 3^n**

| Atom | COORDS | E   |
|------|--------|-----|
| O    | 2.511100 0.903519 -2.936627 | -4743.03508401 |
| Cl   | -0.066273 1.578660 -0.755737 | 0.903519 |
| S    | 3.723342 0.698742 -2.058609 | -0.837408 |
| C    | 3.105025 -0.269160 -0.837408 | -0.837408 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
| P    | 4.111948 -1.135306 0.248923 | -1.135306 |
| C    | 5.358768 2.882396 -1.732650 | 2.882396 |
| C    | 3.236120 2.962338 -0.573814 | 2.962338 |
| S    | 3.723342 0.698742 -2.058609 | -0.573814 |
| C    | 3.105025 -0.269160 -0.837408 | -0.573814 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
| P    | 4.111948 -1.135306 0.248923 | -1.135306 |
| C    | 5.358768 2.882396 -1.732650 | 2.882396 |
| C    | 3.236120 2.962338 -0.573814 | 2.962338 |
| S    | 3.723342 0.698742 -2.058609 | -0.573814 |
| C    | 3.105025 -0.269160 -0.837408 | -0.269160 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
| P    | 4.111948 -1.135306 0.248923 | -1.135306 |
| C    | 5.358768 2.882396 -1.732650 | 2.882396 |
| C    | 3.236120 2.962338 -0.573814 | 2.962338 |
| S    | 3.723342 0.698742 -2.058609 | -0.573814 |
| C    | 3.105025 -0.269160 -0.837408 | -0.269160 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
| P    | 4.111948 -1.135306 0.248923 | -1.135306 |
| C    | 5.358768 2.882396 -1.732650 | 2.882396 |
| C    | 3.236120 2.962338 -0.573814 | 2.962338 |
| S    | 3.723342 0.698742 -2.058609 | -0.573814 |
| C    | 3.105025 -0.269160 -0.837408 | -0.269160 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
| P    | 4.111948 -1.135306 0.248923 | -1.135306 |
| C    | 5.358768 2.882396 -1.732650 | 2.882396 |
| C    | 3.236120 2.962338 -0.573814 | 2.962338 |
| S    | 3.723342 0.698742 -2.058609 | -0.573814 |
| C    | 3.105025 -0.269160 -0.837408 | -0.269160 |
| C    | 4.132134 2.316371 -1.421528 | -0.269160 |
| O    | 4.947019 0.239878 -2.738810 | 0.239878 |
|    |        |        |        |        |        |        |        |        |        |
|----|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|    | C      | -3.129018 | 5.078337 | 0.737078 |
|    | C      | -5.214486 | -6.073979 | -0.334392 |
|    | C      | -8.376958 | -0.505022 | -1.458752 |
|    | C      | -2.849348 | 0.701256 | 4.746264 |
|    | C      | -3.676560 | 5.090452 | 2.156105 |
|    | H      | 6.031643 | 2.352063 | -0.722228 |
|    | H      | 2.272472 | 2.506338 | -0.353598 |
|    | H      | 6.005472 | -0.155829 | 0.722228 |
|    | H      | 2.458718 | 1.720827 | 1.70827 |
|    | H      | 5.030579 | -3.360061 | 0.395988 |
|    | H      | 6.673703 | 4.546832 | -1.389821 |
|    | H      | 2.902456 | 4.681477 | 0.655575 |
|    | H      | 5.124548 | 1.552467 | 0.887497 |
|    | H      | 5.728878 | 0.585147 | 2.229408 |
|    | H      | 6.743635 | -1.767842 | 1.769916 |
|    | H      | 6.894357 | -2.315906 | 0.103200 |
|    | H      | 2.102478 | 0.536491 | 1.579218 |
|    | H      | 3.549793 | 0.873553 | 2.523673 |
|    | H      | 5.080387 | -1.248945 | 3.176135 |
|    | H      | 4.564632 | -2.842695 | 2.627884 |
|    | H      | 4.167446 | -2.359559 | -2.361551 |
|    | H      | 5.808106 | -2.379830 | -1.783195 |
|    | H      | 2.619639 | -3.694266 | 0.834931 |
|    | H      | 2.218726 | -3.127608 | -0.775708 |
|    | H      | 7.438384 | 1.789524 | 0.008252 |
|    | H      | 7.322276 | 2.391408 | 1.657346 |
|    | H      | 8.497718 | -0.546070 | -0.413351 |
|    | H      | 9.059438 | -1.492177 | 0.961690 |
|    | H      | 1.574213 | 0.894387 | 4.011905 |
|    | H      | 1.124725 | -0.721281 | 3.471657 |
|    | H      | 2.579907 | -2.735533 | 4.102094 |
|    | H      | 4.050928 | -2.484020 | 5.040795 |
|    | H      | 5.374147 | -4.325534 | -3.264222 |
|    | H      | 5.755428 | -4.880606 | -1.636471 |
|    | H      | 2.156403 | -5.585535 | -0.690541 |
|    | H      | 3.807590 | -5.645218 | -0.082170 |
|    | H      | 5.125854 | 6.034513 | 1.427304 |
|    | H      | 4.551753 | 6.877806 | -0.011455 |
|    | H      | 6.242810 | 6.357823 | 0.087199 |
|    | H      | 8.268667 | 0.262377 | 2.527510 |
|    | H      | 9.366463 | 0.950567 | 1.343230 |
|    | H      | 2.270249 | -0.838932 | 5.668308 |
|    | H      | 3.682006 | -0.025623 | 4.997617 |
|    | H      | 3.790691 | -6.121803 | -2.513878 |
|    | H      | 2.951843 | -4.604417 | -2.827351 |
|    | H      | -6.031524 | -2.351939 | 2.402366 |
|    | H      | -2.272099 | 2.506399 | 0.353966 |
|    | H      | -6.005417 | 0.155270 | 0.722333 |
|    | H      | -2.458831 | 1.845046 | -1.720557 |
|    | H      | -5.031278 | 3.359781 | -0.395767 |
|    | H      | -6.673541 | 4.546999 | 1.389665 |
|    | H      | -2.902040 | -4.81527 | -0.655253 |
|    | H      | -5.124372 | 1.552605 | -0.887790 |
|    | H      | -5.728938 | -0.585105 | -2.229470 |
|    | H      | -6.743959 | 1.767662 | -1.769462 |
|    | H      | -6.894722 | 2.315324 | -0.102613 |
|    | H      | -2.102485 | -0.536440 | -1.579106 |
|    | H      | -3.549791 | -0.873645 | -2.523536 |
|    | H      | -5.080508 | 1.248933 | -3.175991 |
|    | H      | -4.564709 | 2.842678 | -2.627763 |
Figure S61. Calculated structure of 3\textsuperscript{Sn}. H-Atoms are omitted for clarity.

Structure of 4\textsuperscript{Sn}

\[ E = -4743.0400668 \]

\begin{align}
\text{C} & : 2.439702 -0.335417 -0.143913 \\
\text{Cl} & : 1.306450 1.097698 -3.236980 \\
\text{P} & : 3.395379 -0.877901 0.390616 \\
\text{O} & : 5.060661 -0.978328 -1.109647 \\
\text{S} & : 3.948193 -2.584616 1.085159 \\
\text{O} & : 4.772121 0.185506 1.680675 \\
\text{O} & : 1.694023 0.109441 2.373340 \\
\text{S} & : 1.499041 0.485862 0.960505 \\
\text{O} & : 0.050489 0.439720 0.503042 \\
\text{C} & : 1.803101 2.248703 0.931621 \\
\text{S} & : -3.653883 -1.428622 -1.502159 \\
\text{O} & : -4.513020 -0.881687 -2.561346 \\
\text{O} & : -2.582895 -2.410682 -1.911611
\end{align}
Figure S62. Calculated structure of $4^{\text{Sn}}$. H-Atoms are omitted for clarity.

Structure of $4$-Iso$1^{\text{Sn}}$

$E = -4743.01448532$

$O -2.656956 1.407322 2.939542$

$Cl 1.537975 3.143683 0.764776$

$S -3.664304 1.411437 1.827757$

$C -3.190669 0.059525 0.914873$

$C -3.324028 2.925836 0.943152$

$O -5.091976 1.486604 2.164331$

$P -4.244401 -0.719828 -0.210970$

$C -4.369367 3.758788 0.575985$

$C -2.006748 3.272535 0.663576$

$C -5.174530 0.556016 -1.164990$

$C -3.262926 -1.827301 -1.303778$

$C -5.518737 -1.832710 0.529462$

$C -4.088244 4.931903 -0.119750$

$C -1.740509 4.440908 -0.028912$

$C -4.247086 1.301720 -2.128678$

$C -6.445913 0.081393 -1.872798$

$C -1.921101 -1.294002 -1.799259$

$C -4.073522 -2.416884 -2.460770$

$C -6.451204 -1.086551 1.482685$

$C -4.914559 -3.047027 1.234473$

$C -2.778874 5.285932 -0.442700$
Figure S63. Calculated structure of 4-Iso$^{1}$Sn. H-Atoms are omitted for clarity.

**Structure of 4-Iso$^{2}$Sn**

E = -4743.00987714

O -1.414014 0.667113 2.453522
Cl 0.195483 1.218206 -2.739365
S -2.782631 0.892712 1.813835
C -2.840639 -0.369826 0.726277
C -2.630751 2.461627 0.980888
O -3.903382 1.063792 2.750608
P -4.264268 -0.934479 -0.042527
C -3.236519 3.590309 1.512827
C -1.909480 2.528913 -0.205617
C -5.571037 0.365242 -0.057409
C -3.797391 -1.550353 -1.703505
C -4.991951 -2.366364 0.863174
C -3.115293 4.800278 0.835085
C -1.796498 3.737845 -0.869241
C -5.317157 1.464345 -1.091544
C -7.014086 -0.132843 -0.163713
C -2.995896 -0.543231 -2.528215
C -4.955134 -2.142648 -2.504424
C -5.267980 -1.958355 2.311938
C -4.086837 -3.596961 0.808488
C -2.398528 4.895591 -0.359385
C -6.266827 2.631591 -0.863651
C -7.983008 1.029968 0.031091
C -2.491208 -1.187247 -3.811508
C -4.441920 -2.770852 -3.795936
C -5.844796 -3.112981 3.118570
C -4.657962 -4.745181 1.631319
C -2.272997 6.197012 -1.091657
C -7.715768 2.172225 -0.938905
C -3.638428 -1.774223 -4.621088
C -4.929794 -4.327492 3.068729
O 2.576645 -1.121607 -2.930701
Cl -0.026005 -2.533168 -1.452555
S 3.666957 -0.683628 -2.045220
C 2.892928 -0.069237 -0.658906
C 4.512254 -2.173297 -1.530379
O 4.728764 0.193103 -2.573367
| x     | y     | z     |
|-------|-------|-------|
| 3.596628 | 1.073409 | 0.413218 |
| 5.889524  | -2.265052  | -1.646012  |
| 3.764951  | -3.229697  | -1.014830  |
| 6.534546  | -3.16718  | -1.201273  |
| 4.420946  | -4.367845  | -0.577197  |
| 5.786716  | -0.373837  | 1.397670  |
| 6.224392  | 2.066535  | 0.930244  |
| 2.620865  | -0.484415  | 2.608239  |
| 3.230912  | 1.915260  | 3.083175  |
| 3.756280  | 2.988792  | -1.557974  |
| 1.882186  | 3.293772  | 0.093907  |
| 5.816370  | -4.478979  | -0.655159  |
| 7.280172  | -0.658762  | 1.318203  |
| 7.719586  | 1.768512  | 0.883592  |
| 1.703442  | -0.409292  | 3.825864  |
| 2.315723  | 1.906118  | 4.301702  |
| 3.554904  | 4.413276  | -2.052514  |
| 1.695542  | 4.720335  | -0.409292  |
| 6.506630  | -5.721037  | -0.176838  |
| 8.090605  | 5.505573  | 4.883040  |
| 2.110786  | 4.854523  | -1.866235  |
| -3.804534  | 3.506052  | 2.436201  |
| -1.464468  | 1.632077  | -0.625603  |
| -5.444892  | 0.808206  | 0.943833  |
| -3.091683  | -2.360514  | -1.451743  |
| -9.415142  | -2.611237  | 0.363193  |
| -3.592791  | 5.690578  | 1.242213  |
| -1.232218  | 3.768102  | -1.800946  |
| -4.275277  | 1.798149  | -1.061889  |
| -5.492899  | 1.054974  | -2.096855  |
| -7.178652  | -0.591894  | -1.149328  |
| -7.224745  | -0.903673  | 0.585260  |
| -2.159692  | -0.162854  | -1.933534  |
| -3.618025  | 0.322874  | -2.783521  |
| -5.667655  | -1.341240  | -2.752708  |
| -5.508252  | -2.885443  | -1.913060  |
| -4.324609  | 1.622099  | 2.763680  |
| -5.930939  | -1.084781  | 2.355147  |
| -3.932526  | -3.924277  | -0.226814  |
| -3.095700  | -3.327337  | 1.206972  |
| -6.064081  | 0.369993  | 0.124763  |
| -6.070463  | 3.420405  | -1.60808  |
| -7.880387  | 1.399825  | 1.062308  |
| -9.015502  | 0.671708  | -0.669998  |
| -1.933825  | -0.443222  | -4.392262  |
| -1.771069  | 1.976014  | -3.555188  |
| -3.802202  | -3.629342  | -3.542170  |
| -5.285208  | -3.168349  | -4.375587  |
| -6.006377  | -2.792912  | 4.155481  |
| -6.833545  | -3.384642  | 2.717459  |
| -3.969970  | -5.599329  | 1.598283  |
| -5.597311  | -5.083653  | 1.167695  |
| -2.714506  | 6.129388  | -2.094000  |
| -1.218863  | 6.471524  | -1.227734  |
| -2.770070  | 7.011919  | -0.555936  |
| -7.932079  | 1.834149  | -1.964049  |
**Figure S64.** Calculated structure of 4-Iso2^Sn. H-Atoms are omitted for clarity.

**Structure of 4-Iso3^Sn**

\[
\begin{align*}
E &= -4743.04261415 \\
O &= 0.728651 -0.018356 -2.120828 \\
O &= -0.709008 -0.022512 2.261505 \\
C &= -1.755476 0.445822 0.083495 \\
C &= 1.789752 0.611742 0.004700 \\
S &= 2.006970 0.669727 -1.647617 \\
O &= 2.336517 1.968734 -2.254720 \\
C &= 3.310557 -0.425656 -2.167858 \\
P &= -2.835828 0.853231 -1.181325 \\
C &= -4.275173 1.757094 -0.475324 \\
C &= -3.499708 -0.658126 -2.005889 \\
C &= -1.960002 1.779021 -2.493862 \\
S &= -2.002879 0.572224 1.728597 \\
O &= -2.411780 1.881310 2.257069 \\
C &= -3.261810 -0.552537 2.320009 \\
P &= 2.667518 1.467498 1.198481 \\
C &= 4.428260 1.655003 0.710869 \\
C &= 2.007359 3.161663 1.483258 \\
P &= 2.415331 0.554800 2.764203 \\
C &= 4.338992 0.043966 -2.970658 \\
C &= 5.369967 -0.824970 -3.318057 \\
C &= -3.949788 3.216675 -0.150375 \\
C &= -5.600776 1.641839 -1.226922 \\
C &= 3.3287785 -1.744517 -1.727002 \\
P &= -2.457575 -1.350451 -2.884780 \\
C &= -4.011360 1.619388 -0.934871 \\
C &= 5.180182 0.323400 0.755037 \\
C &= 5.216441 2.730313 1.460977 \\
P &= -2.992300 -2.650647 -3.472061 \\
C &= -1.071840 2.905896 -1.972719 \\
P &= -2.889074 2.238310 -3.617323 \\
C &= 5.381061 -2.148647 -2.876825 \\
C &= 4.320178 -2.594629 -2.077479 \\
C &= 6.491829 -3.082616 -3.250644 \\
C &= -5.063913 3.825962 0.687001 \\
C &= 2.176349 4.020479 0.228870 \\
C &= 0.531121 3.091461 1.873111 \\
C &= -0.298944 3.542173 -3.119238 \\
C &= 6.558771 0.472567 0.128005 \\
P &= -1.227764 4.022214 -4.224799 \\
C &= 2.671273 -0.949421 2.686097 \\
C &= 3.095904 1.148036 3.995321 \\
\end{align*}
\]
Figure S65. Calculated structure of 4-Iso3Sn. H-Atoms are omitted for clarity.
Structure of 4-Iso4^Sn
E = -4743.02037103
O 1.845390 -2.157509 1.590039
C -1.381497 -0.732288 0.370241
C 2.170390 -0.304905 -0.025047
S 2.863641 -1.696901 0.565310
O 3.341150 -2.706702 -0.397353
C 4.318917 -1.335396 1.553815
P -2.292341 -2.162492 0.542877
C -3.459035 -2.347300 -0.865383
C -3.343016 -2.259009 2.060261
C -1.064580 -3.518272 0.700015
S -1.899651 0.799425 0.167060
O -0.668763 1.610391 -0.075398
C -3.046650 1.139065 -1.158085
P 2.719865 0.495222 -1.433730
C 4.554871 0.386858 1.581853
C 2.053551 -0.208414 -3.008702
C 2.088832 2.214126 -1.389239
C 5.479439 -2.068686 1.357149
C 6.610225 -1.771697 2.113621
C -2.806041 -2.226692 -2.240440
C -4.433420 -3.522636 -0.841016
C 4.273089 -0.327188 3.512270
C -2.480019 -1.941936 3.284685
C -4.546137 -1.314712 1.987726
C 5.245229 1.331365 -0.597310
C 5.147643 0.549364 -2.981507
C -3.294825 -1.951741 4.570881
C -0.161517 -3.635679 -0.529826
C -1.667978 -4.864207 1.104138
C 6.596591 -0.753082 3.065165
C 5.405522 -0.039743 3.255451
C 7.819827 -0.415242 3.862858
C -3.873864 -1.982240 -3.294939
C 2.351103 -1.702369 -3.106032
C 0.556223 0.059660 -3.122344
C 0.899086 -4.708707 -0.325149
C 6.741895 1.063712 -0.551801
C 0.270356 -6.049386 0.017434
C 2.288801 2.988943 -0.085566
C 2.492894 3.054011 -2.600248
C -5.511292 -3.303441 -1.899290
C -5.349958 -1.335687 3.282357
C -2.542664 1.471252 -2.408351
C -4.415274 1.149672 -0.920623
C -5.282621 1.462308 -1.960322
C -4.803501 1.782962 -3.231631
C -4.476763 -0.998207 4.480943
C -0.587558 -5.926694 1.267331
C -3.419531 1.783658 -3.435034
C 1.760696 -2.312580 -4.368682
C 1.478847 4.278657 -0.132814
C -4.911247 -3.098677 -3.285522
C -5.737658 2.129530 -4.350210
C 1.683593 4.346124 -2.633330
C 6.654460 0.310262 -2.946639
C 1.842460 5.130482 -1.339004
C 7.357690 1.206504 -1.936539
C -0.053088 -0.591655 -4.357120
Figure S66. Calculated structure of 4-IsoSn. H-Atoms are omitted for clarity.

Structure of CyYSnCl (S = 0)
E = -2371.49531249
Sn -0.941752 -2.860154 -0.201223
O 0.702018 -2.478388 -1.788157
Cl 0.599129 -3.446442 1.686378
S 0.793845 -0.960150 -1.634724
C -0.297122 -0.715609 -0.401769
C 2.471080 -0.656987 -1.106608
O 0.640808 -0.171936 -2.866190
P -0.901199 0.803157 0.078289
C 3.270686 0.195256 -0.281854
C 2.936825 -1.242610 0.067799
C 0.282807 2.170904 1.554466
Figure S67. Calculated Structure of \( \text{CyYSnCl (S = 0)} \). H-Atoms are omitted for clarity.

Figure S68. HOMO-1 of \( \text{CyYSnCl (S = 0)} \). H-Atoms are omitted for clarity.
Figure S69. HOMO of $^6\text{CyYSnCl}$ ($S = 0$). H-Atoms are omitted for clarity.

Figure S70. LUMO of $^6\text{CyYSnCl}$ ($S = 0$). H-Atoms are omitted for clarity.

Structure of $^6\text{CySnCl}$ ($S = 1$)

\begin{verbatim}
E = -2371.41054621
Sn -1.811460 -2.516443 -0.438237
O 0.306514 -1.818519 -2.965991
Cl -0.051142 -3.710116 0.946643
S 0.613212 -0.616184 -2.205669
C 0.392834 -0.627385 -0.755215
C 2.241707 -0.752563 -1.515805
O 0.541892 0.692955 -2.883042
P -0.569825 0.867717 0.179959
C 3.215710 0.162591 -1.894312
\end{verbatim}
Figure S71. Calculated structure of $^{29}$Y$_2$SnCl ($S = 1$). H-Atoms are omitted for clarity.

**Structure of $^{29}$Y$_2$Sn ($S = 0$)**

E = -3818.37212370
Sn 0.074030 0.711870 1.416159
O 0.960641 -1.578327 1.864308
C 1.842314 0.028909 0.194377
O -0.576970 2.184960 -0.484527
C -1.708782 0.075543 0.148982
S 2.185269 -1.382863 0.991458
P 2.674452 0.560330 -1.199660
S -1.865560 1.446354 -0.779211
P -2.804604 -1.231378 0.217705
O 2.635920 -2.539801 0.193503
C 3.510710 -1.157538 2.182179
C 4.463051 0.118679 -1.130415
O 2.037627 -0.150195 -2.775859
C 2.401721 2.367220 -1.355823
O -2.235672 1.290135 -2.197903
C -3.123016 2.541782 -0.123903
C -1.850624 -2.779679 0.458214
C -3.880996 -1.257639 -1.273418
C -3.960989 -1.159012 1.660072
C 4.566269 -2.055531 2.214364
C 3.477261 -0.074248 3.056432
C 5.211833 0.945759 -0.084036
H 4.422202 -0.925927 -0.776193
C 5.224913 0.135016 -2.457017
C 0.559105 0.183148 -2.951791
H 2.619640 0.315808 -3.587477
C 2.228222 -1.666582 -2.823979
C 2.555266 3.168831 -0.063377
H 1.327052 2.392310 -1.582662
C 3.151817 3.041936 -2.502334
C -4.346390 2.654961 -0.767697
C -2.911918 3.156228 1.107900
C -2.728648 -4.026694 0.556712
| Atom  | X      | Y      | Z      |
|-------|--------|--------|--------|
| C     | -1.362861 | -2.605370 | 1.430912 |
| C     | -0.709772  | -2.975209  | -0.538591 |
| C     | -3.098355  | -1.652846  | -2.523828 |
| H     | -4.124963  | -0.187844  | -1.374846 |
| C     | -5.202774  | -2.020471  | -1.211416 |
| C     | -4.796425  | 0.117465   | 1.589895  |
| H     | -4.624738  | -2.034039  | 1.581371  |
| C     | -3.198229  | -1.229621  | 2.983294  |
| H     | 4.559827   | -2.898407  | 1.527633  |
| C     | 5.607775   | -1.853334  | 3.116939  |
| H     | 2.645693   | 0.629574   | 3.030896  |
| C     | 4.519133   | 0.115408   | 3.948235  |
| C     | 6.617222   | 0.400178   | -0.224843 |
| H     | 5.272687   | 0.117465   | -0.441894 |
| H     | 4.655201   | 0.970274   | 0.859370  |
| H     | 1.697216   | -2.106602  | -1.971256 |
| C     | 2.003757   | 4.573635   | -0.272048 |
| H     | 2.026228   | 2.671360   | 0.756570  |
| H     | 3.611553   | 3.224985   | 0.232993  |
| C     | 2.619862   | 4.455904   | -2.710340 |
| H     | 4.224555   | 3.090852   | -2.261318 |
| H     | 3.061413   | 2.465777   | -3.432107 |
| C     | -5.384896  | 3.340419   | -0.143627 |
| H     | -4.472032  | 2.202638   | -1.749159 |
| H     | -1.940267  | 3.071987   | 1.593334  |
| C     | -3.951414  | 3.842396   | 1.714058  |
| H     | -3.220826  | -4.194470  | -0.413443 |
| H     | -3.527187  | -3.891961  | 1.298127  |
| C     | -1.895297  | -5.253926  | 0.907260  |
| C     | -0.089122  | -2.071473  | -0.561481 |
| C     | -1.110160  | -3.120500  | -1.548675 |
| C     | 0.112101   | -4.197683  | -0.153634 |
| C     | -2.128957  | -1.146701  | -2.527406 |
| C     | -2.916126  | -2.737546  | -2.499423 |
| C     | -3.898335  | -1.309111  | -3.768128 |
| C     | -5.010657  | -3.101147  | -1.157903 |
| C     | -5.779987  | -1.757342  | -0.317450 |
| C     | -6.021010  | -1.704513  | -2.461616 |
| H     | -4.106446  | 0.967855   | 1.578203  |
| C     | -5.364106  | 0.168209   | 0.652343  |
| C     | -5.727189  | 0.268174   | 2.783608  |
| C     | -4.124572  | -1.054021  | 4.180822  |
| H     | -2.661309  | -2.181960  | 3.070613  |
| H     | -2.434687  | -0.435420  | 2.989669  |
| H     | 6.440829   | -2.555072  | 3.138926  |
| C     | 5.606641   | -0.767903  | 3.990728  |
| H     | 4.494692   | 0.967555   | 4.626675  |
| C     | 7.393566   | 0.378444   | -1.184297 |
| H     | 6.545829   | -0.618936  | 0.530504  |
| H     | 7.144022   | 0.998597   | 0.879557  |
| H     | 6.580988   | -1.455549  | -1.964475 |
| H     | 7.187783   | -0.366855  | -3.208905 |
Figure S72. Calculated Structure of $\text{CyY}_2\text{Sn} (S = 0)$. H-Atoms are omitted for clarity.

Figure S73. HOMO of $\text{CyY}_2\text{Sn} (S = 0)$. H-Atoms are omitted for clarity.
Figure S74. LUMO of Cy₂Sn (S = 0). H-Atoms are omitted for clarity.

Figure S75. LUMO+4 of Cy₂Sn (S = 0). H-Atoms are omitted for clarity.

Structure of Cy₂Sn (S = 1)
E = -3818.2945342
Sn 0.109228 0.351898 1.204868
O 1.428127 -2.514606 1.275044
C 1.917178 -0.227744 0.165292
O -1.021230 2.623620 -0.641506
C -1.703713 0.232660 0.046604
S 2.492808 -1.774537 0.574965
Figure S76. Calculated structure of $^8$Y$_2$Sn (S = 1). H-Atoms are omitted for clarity.

Structure of $^{76}$Y$_2$Sn (S = 0)
E = -3796.60415202
Sn -0.052882 -0.019635 -1.748421
O -1.084867 -2.157203 -0.831607
C -1.728924 0.160684 -0.273968
C 1.725332 -0.244079 -0.353312
O 0.901374 2.051574 -0.795756
S -2.163284 -1.431650 -0.66590
C -3.680449 -1.747378 -0.963375
O -2.435555 -1.888388 1.309064
P -2.471894 1.416004 0.576551
C -4.247410 1.107735 0.822567
C -2.257085 2.927323 -0.401691
C -1.799590 1.751340 2.222986
C 4.003726 1.143970 -2.007469
H 3.437605 0.282635 -2.357230
C 3.537752 1.865744 -0.915893
C 5.202265 1.505171 -2.604942
S 2.035116 1.367320 -0.071217
C 4.253220 2.952339 -0.429303
C -5.948274 -2.516377 -1.018214
H -6.797914 -2.975985 -0.514502
C -4.754103 -2.343788 -0.323748
C -6.082058 -2.099860 -2.341103

H 1.359633 6.192010 0.144166
H 3.039468 5.672259 0.044530
C -6.803263 4.038459 2.304247
H -1.365994 -5.157619 -2.334775
H -0.102715 -6.064941 -1.506293
H -6.789635 -1.410779 -3.871066
H -5.869028 -2.811312 -3.332887
H -3.232135 -0.047068 4.823273
H -4.558536 -0.950243 5.550426
H 6.646550 -1.364086 5.652954
H 7.135603 0.096388 4.792762
H 7.855749 -1.464810 4.360766
H -6.947717 3.461281 3.227076
H -7.737840 4.000246 1.735522
H -6.629557 5.080107 2.601889

Figure S76. Calculated structure of $^8$Y$_2$Sn (S = 1). H-Atoms are omitted for clarity.
Figure S77. Calculated structure of Ph$_2$Y$_2$Sn ($S = 0$). H-Atoms are omitted for clarity.
Figure S78. HOMO of $\text{Ph}_2\text{Y}_2\text{Sn}$ ($S = 0$). H-Atoms are omitted for clarity.

Figure S79. LUMO of $\text{Ph}_2\text{Y}_2\text{Sn}$ ($S = 0$). H-Atoms are omitted for clarity.
Figure S80. LUMO+16 of $^{\text{Pb}Y_2\text{Sn}}$ (S = 0). H-Atoms are omitted for clarity.

**Structure of $^{\text{Pb}Y_2\text{Sn}}$ (S = 1)**

$E = -3796.52238437$

$\text{Sn} = -0.042900 -0.200585 -1.510317$

$\text{O} = -1.447040 -2.515438 0.293138$

$\text{C} = -1.799740 -0.016442 -0.294597$

$\text{C} = 1.801247 -0.124285 -0.405107$

$\text{O} = 1.250978 2.404098 -0.226209$

$\text{S} = -2.343885 -1.386096 0.569780$

$\text{C} = -3.939377 -1.834436 -0.010718$

$\text{O} = -2.595984 -1.011718 1.979342$

$\text{P} = -2.471036 1.511554 0.116857$

$\text{C} = -4.265862 1.442220 0.443760$

$\text{C} = -2.174455 2.616272 -1.289349$

$\text{C} = -1.791094 2.315734 1.588491$

$\text{C} = 4.328958 1.320412 -1.500581$

$\text{H} = 3.717102 0.818906 -2.154759$

$\text{C} = 3.827129 1.868015 -0.417725$

$\text{C} = 5.619259 1.635352 -1.992979$

$\text{S} = 2.222631 1.401864 0.230681$

$\text{C} = 4.592978 2.750912 0.334537$

$\text{C} = -6.261533 -2.330890 0.209812$

$\text{H} = -7.115059 -2.460451 0.874407$

$\text{C} = -5.020358 -2.011152 -0.748619$

$\text{C} = -6.437778 -2.472180 -1.166696$

$\text{H} = -4.877053 -1.877741 1.818037$

$\text{C} = -4.079171 -1.995660 -1.475382$

$\text{O} = 2.462542 1.294182 1.689994$

$\text{C} = -5.324071 -2.308117 -1.998854$

$\text{C} = -7.791645 -2.755757 -1.745040$

$\text{H} = 6.021408 1.185830 -2.900193$

$\text{C} = 6.418132 2.503365 -1.244126$

$\text{C} = 7.833780 2.779188 -1.651919$

$\text{C} = 5.877186 3.067773 -0.086376$

$\text{P} = 2.539645 -1.525675 0.272180$
C 2.045603 -2.927015 -0.759344
C 2.052669 -1.916592 1.971056
C 4.359682 -1.445108 0.296889
H -3.213438 -1.861393 -2.122309
H -5.439055 -2.429089 -3.075564
H -8.309148 -1.820644 -2.002753
H -8.428102 -3.293852 -1.034153
H -7.722219 -3.350923 -2.662450
C -4.709975 1.252093 1.755467
C -5.194233 1.459907 -0.599860
H -3.987723 1.193283 -2.565403
C -6.067778 1.112162 2.016861
C -6.988551 1.142415 -0.333493
H -6.404752 0.969337 3.041716
H -7.263773 1.327051 -1.153800
H -4.866144 1.601770 -1.625634
C -1.532771 3.842487 -1.127912
C -2.541424 2.187070 -2.571387
H -1.182888 4.150321 -0.146435
C -1.286676 4.644736 -2.237710
H -0.767501 5.591938 -2.105845
C -1.681357 4.231991 -3.503479
C -1.485105 4.863509 -4.367972
C -2.308934 2.999400 -3.670840
H -2.598776 2.662393 -4.664068
H -1.819518 4.051638 3.258158
C -2.285190 4.932180 3.696811
C -0.649366 3.529617 3.809497
C -2.392381 3.449681 2.466008
H -0.202318 4.009233 4.678657
C -0.050714 2.408096 3.251049
H 0.878366 2.004570 3.644751
C -0.627622 1.799427 2.143014
H -0.159945 0.932223 1.691850
H -2.982330 1.199677 -2.702363
H -3.308310 3.853900 1.716801
H 8.485601 1.938577 -1.374057
H 8.227200 3.676962 -1.163628
H 7.923096 2.910735 -2.736503
H 6.482109 3.753167 0.506392
H 4.187214 3.152649 1.260234
C 1.390395 -0.426550 -0.210651
C 2.273048 -2.866786 -2.140740
H 1.169600 -4.056343 0.853019
C 0.970599 -5.063147 -1.038475
H 0.437032 -5.908065 -0.609053
C 1.214269 -5.011416 -2.404163
C 1.870407 -3.912892 -2.956668
H 2.051450 -3.864779 -4.028519
H 0.882800 -5.824844 -3.046890
H 2.754376 -1.989002 -2.570059
C 2.886654 -2.612287 2.848887
C 0.768405 -1.552767 2.367655
H 3.890341 -2.901304 2.542873
C 2.427421 -2.928675 4.122013
H 3.076980 -3.463640 4.812275
C 1.140702 -2.565096 4.513331
C 4.965706 -0.585797 1.221636
Figure S81. Calculated structure of Ph$_2$Sn (S = 1). H-Atoms are omitted for clarity.
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