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Supporting Information

Isolation of a Diylide-Stabilized Stannylene and Germylene: Enhanced Donor Strength through Coplanar Lone Pair Alignment

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Supporting Information

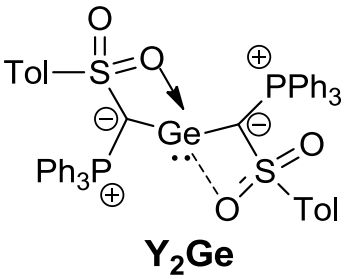
Index

1. Experimental Details

1.1 General methods

All experiments and crystallizations were carried out under a dry, oxygen-free argon atmosphere inside the Glovebox. Involved solvents were dried using an MBraun SPS-800 (THF, toluene, hexane) or dried in accordance with standard procedures. ^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H} and ^{119}Sn NMR spectra were recorded on Avance-400 or Avance-250 spectrometers at 25 °C if not stated otherwise. All values of the chemical shift are in ppm regarding the *δ*-scale. 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. Elemental analyses were performed on an Elementar vario MICRO-cube elemental analyzer. The Sodium Yldiide (**YNa**) was prepared by following the procedure in the literature.[1] $GeCl_2$·dioxane and $SnCl_2$ (anhydrous) were purchased from Sigma-Aldrich.

1.2 Synthesis of Y_2Ge



Y_2Ge

A J-Young NMR tube was filled with **YNa** (39 mg, 0.086 mmol) and $GeCl_2$·dioxane (10 mg, 0.043 mmol) in 2:1 molar ratio. To this mixture, C_6D_6 (0.4 mL) was added and the reaction mixture was shaken for 10 minutes to form a pale-yellow solution. The ^{31}P NMR spectrum of the reaction mixture confirmed the complete consumption of **YNa** and formation of **Y_2Ge** (~95%) (Figure S1). The reaction mixture was filtered into a glass vial to remove the generated NaCl and the clear solution was kept in hexane vapour for two days to yield **Y_2Ge** as pure white solid (25 mg, 63% yield based on Ge). The single crystals were grown from a solution of **Y_2Ge** into a mixture of C_6D_6 and THF (5:1) by vapour diffusion technique with hexane vapour.

^{1}H NMR (400.3 MHz, C_6D_6): *δ* 1.84 (s, 6H; C*H*$_3$), 6.53-6.55 (d, 4H, C*H*$_{STol,meta}$), 6.98-7.07 (m, 18H, C*H*$_{PPh,ortho}$ and C*H*$_{PPh,para}$), 7.70-7.72 (d, 4H; C*H*$_{STol,ortho}$), 7.97-8.02 (m, 12H; C*H*$_{PPh,meta}$). ^{13}C{1H} NMR (100.6 MHz, C_6D_6): *δ* 20.63 (*C*H$_3$), 50.92-51.69 (br, d, $^{1}J_{PC}$ = 77.34 Hz; P*C*S), 126.15 (C*H*$_{STol,ortho}$), 127.56 (C*H*$_{STol,meta}$), 127.99-128.12 (d, $^{3}J_{PC}$ = 12.08 Hz; *C*H$_{PPh,meta}$), 127.80-129.02 (d, $^{1}J_{PC}$ = 122.67 Hz, *C*$_{PPh,ipso}$), 130.99-131.02 (d, $^{4}J_{PC}$ = 2.75 Hz; *C*H$_{PPh,para}$), 134.30-134.41 (d, $^{2}J_{PC}$ = 10.46 Hz; *C*H$_{PPh,ortho}$), 138.25 (*C*$_{STol,para}$), 147.50-147.51 (br, d, $^{3}J_{PC}$ = 1.39 Hz, *C*$_{STol,ipso}$). ^{31}P{^{1}H} NMR (162.05 MHz, C_6D_6): 7.98. Anal. Calcd. for $C_{52}H_{44}GeO_4P_2S_2$: C, 67.04; H, 4.76. Found: C, 66.84; H, 4.70.

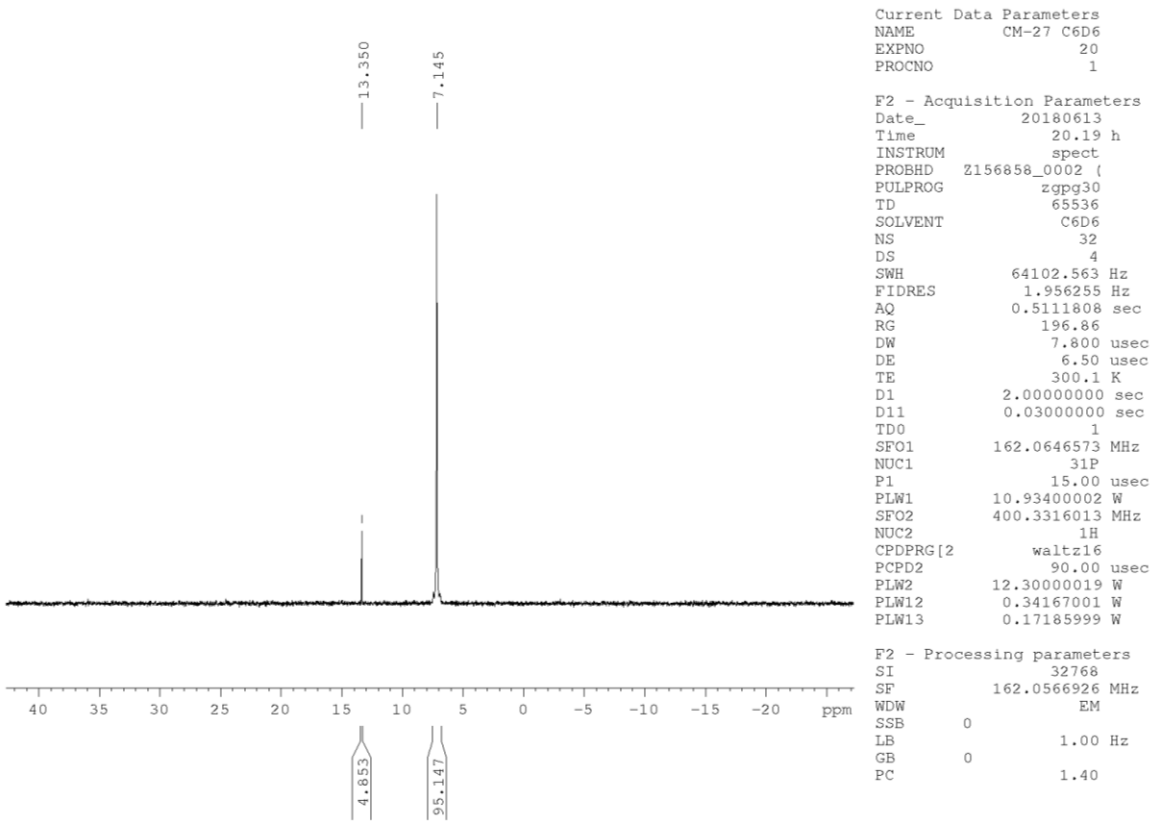


Figure S1. $^{31}P\{^{1}H\}$ spectrum of the reaction mixture of **Y_2Ge**.

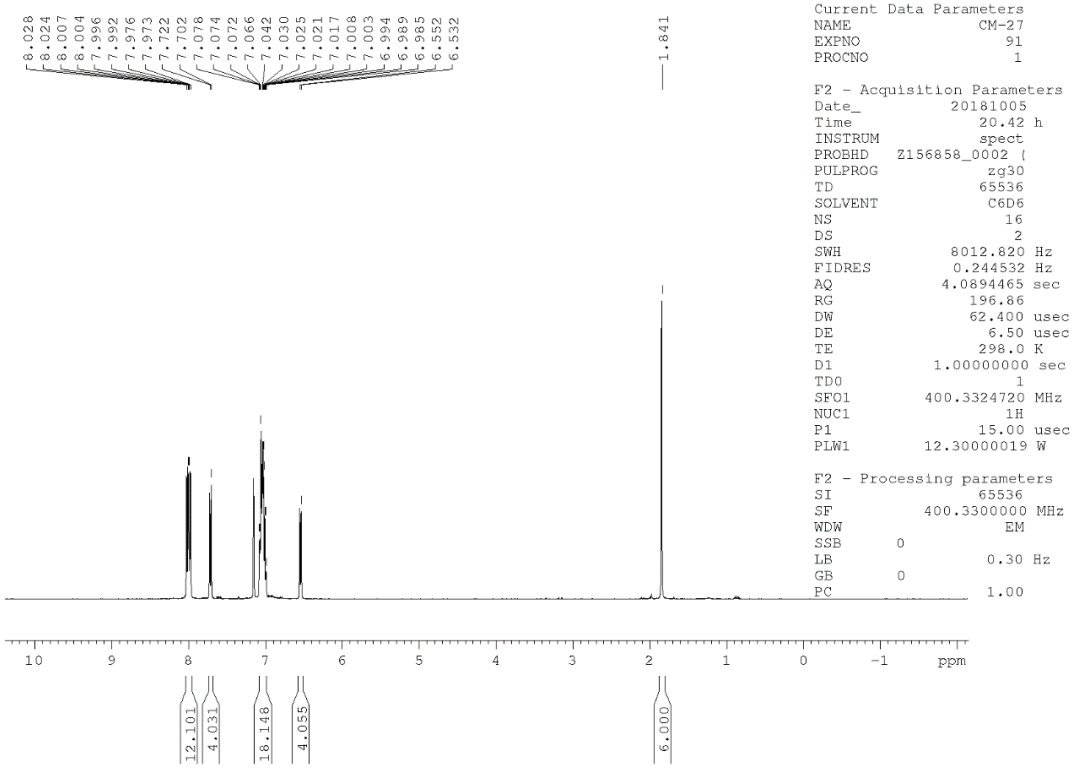


Figure S2. ^{1}H NMR spectrum of **Y_2Ge** in C_6D_6.

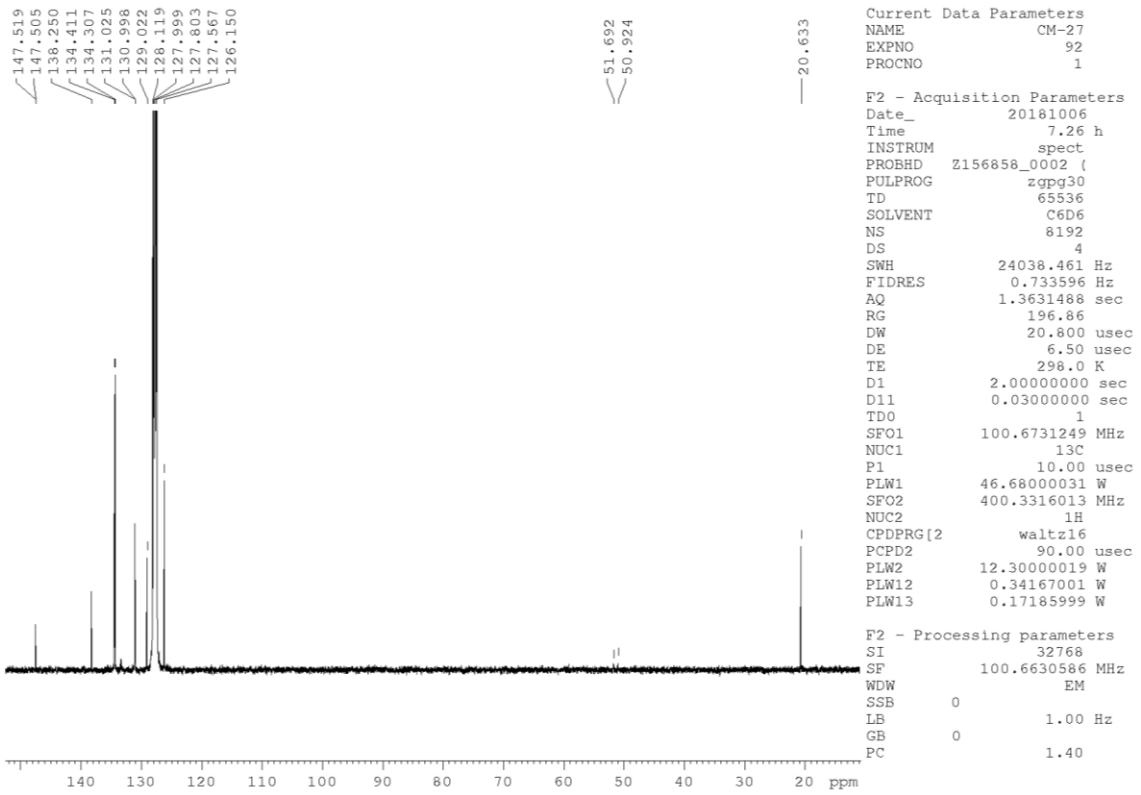


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **Y_2Ge** in C_6D_6.

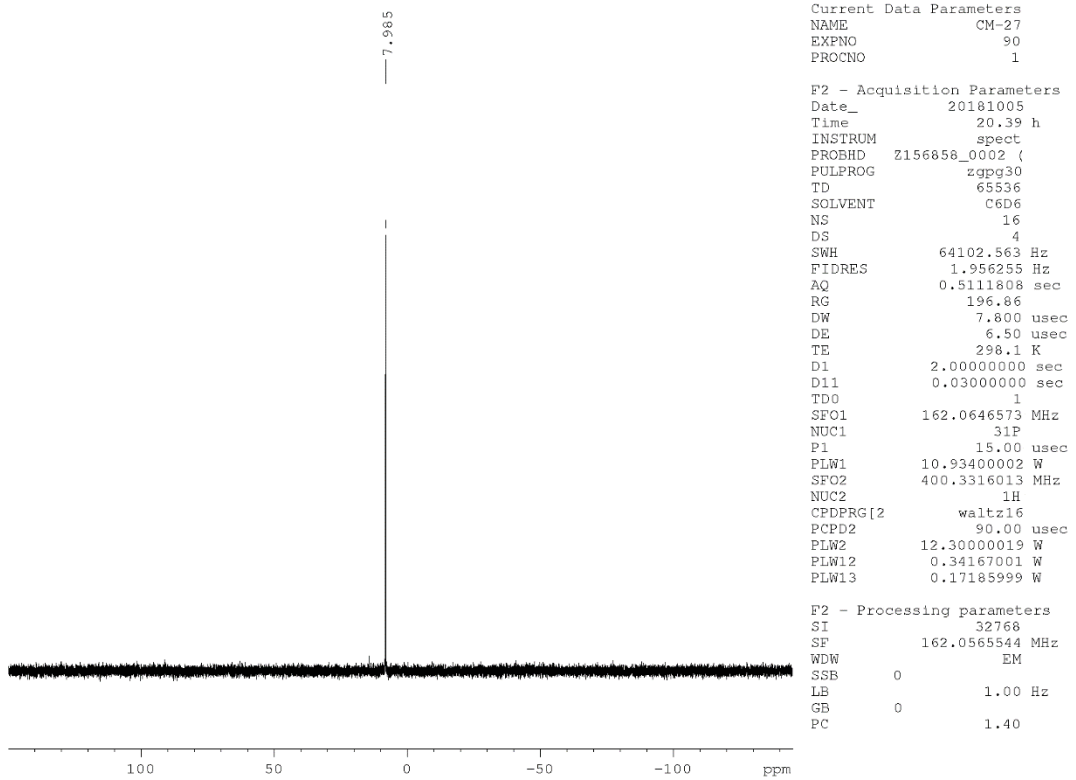
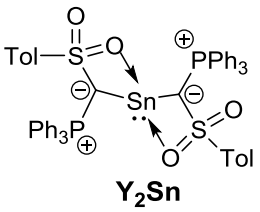


Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum of **Y_2Ge** in C_6D_6.

1.3 Synthesis of Y_2Sn



Y_2Sn

A J-Young NMR tube was filled with **YNa** (47 mg, 0.104 mmol) and $SnCl_2$ (10 mg, 0.052 mmol) in 2:1 molar ratio. To this mixture, C_6D_6 (or Toluene-d_8) and THF-d_8 were added in 4:1 (v/v, total 0.5 mL) and the reaction mixture was shaken for 10 minutes to form a pale-yellow solution. The ^{31}P NMR spectrum of the reaction mixture confirmed the complete consumption of **YNa** and the formation of **Y_2Sn** (~98%) (Figure S5). The reaction mixture was filtered into a glass vial to remove the formed NaCl. The vial with the obtained clear solution was kept in a vial filled with hexane for 24 hours to yield **Y_2Sn** as pure colorless solid (35 mg, 68% yield based on Sn). The single crystals of **Y_2Sn** were grown by a similar technique like in case of **Y_2Ge**.

^1H NMR (250.13 MHz, C_6D_6): δ 1.96 (s, 6H; C*H*$_3$), 6.63-6.66 (d, 4H, C*H*$_{STol,meta}$), 7.09-7.23 (m, 18H, C*H*$_{PPh,ortho}$ and C*H*$_{PPh,para}$), 7.80-7.83 (d, 4H; C*H*$_{STol,ortho}$), 8.07-8.17 (m, 12H; C*H*$_{PPh,meta}$). $^{13}C\{^1H\}$ NMR (100.6 MHz, THF-d_8): δ 20.14 (*C*H$_3$), 52.78-53.42 (br, d, $^1J_{PC}$ = 64.29 Hz; P*C*S), 125.75 (C*H*$_{STol,ortho}$), 127.56 (C*H*$_{STol,meta}$), 127.89-128.02 (d, $^3J_{PC}$ = 12.01 Hz; *C*H$_{PPh,meta}$), 128.57-129.48 (d, $^1J_{PC}$ = 90.77 Hz, *C*$_{PPh,ipso}$), 130.82-130.85 (d, $^4J_{PC}$ = 2.71 Hz; *C*H$_{PPh,para}$), 133.88-133.98 (d, $^2J_{PC}$ = 10.28 Hz; *C*H$_{PPh,ortho}$), 138.09 (*C*$_{STol,para}$), 147.73-147.75 (br, d, $^3J_{PC}$ = 1.82 Hz, *C*$_{STol,ipso}$). $^{31}P\{^1H\}$ NMR (101.25 MHz, C_6D_6): 6.88 (s + $d_{satellite}$, $^2J_{SnP}$ = 51.10 Hz). ^{119}Sn NMR (149.3 MHz, THF-d_8): -122.23. Anal. Calcd. for $C_{52}H_{44}O_4P_2S_2Sn$: C, 63.88; H, 4.54. Found: C, 63.38; H, 4.33.

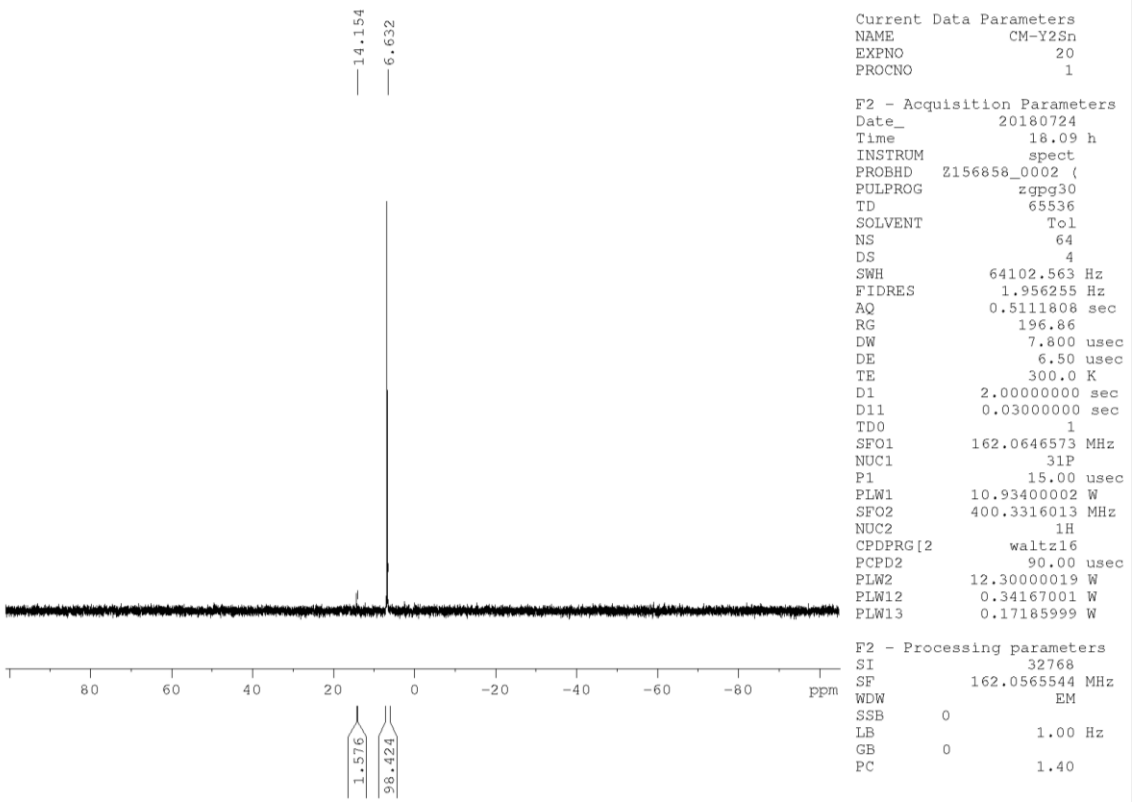


Figure S5. $^{31}P\{^1H\}$ spectra of the reaction mixture of **Y_2Sn**.

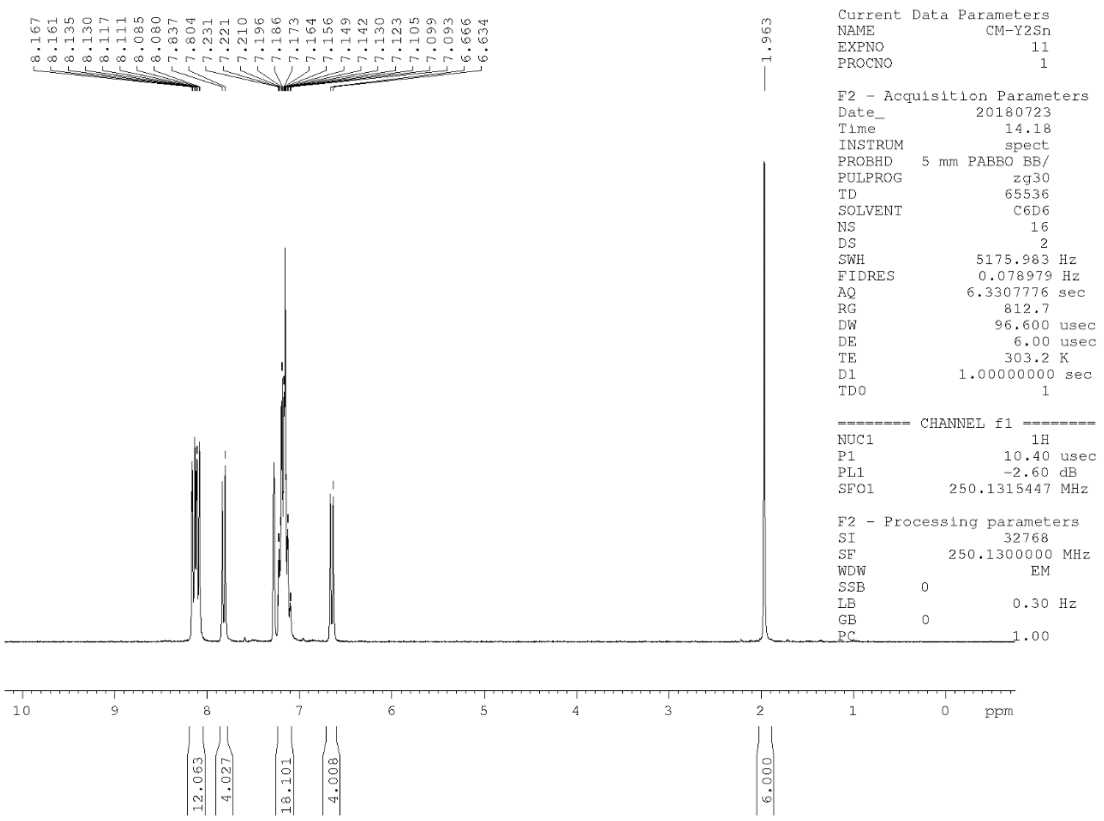


Figure S6. ^{1}H spectrum of **Y_2Sn** in C_6D_6.

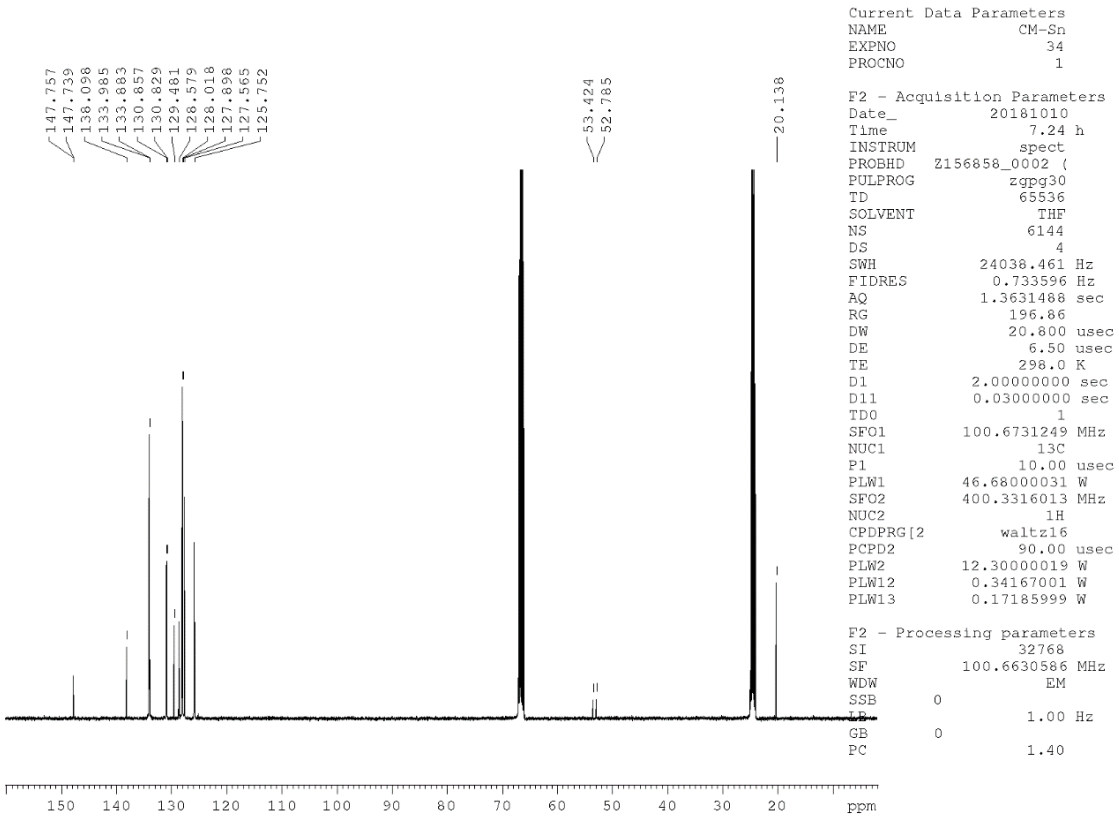


Figure S7. $^{13}C\{^{1}H\}$ spectrum of **Y_2Sn** in THF-d_8

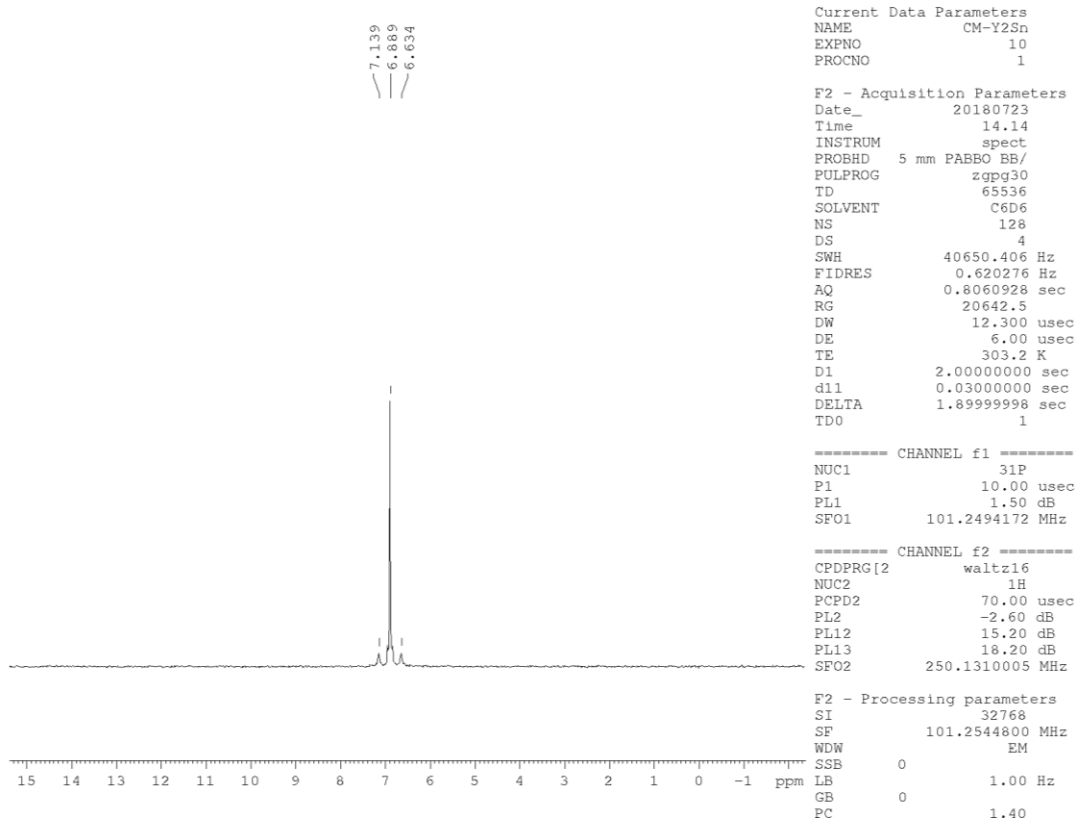


Figure S8. $^{31}P\{^{1}H\}$ spectrum of **Y_2Sn** in C_6D_6.

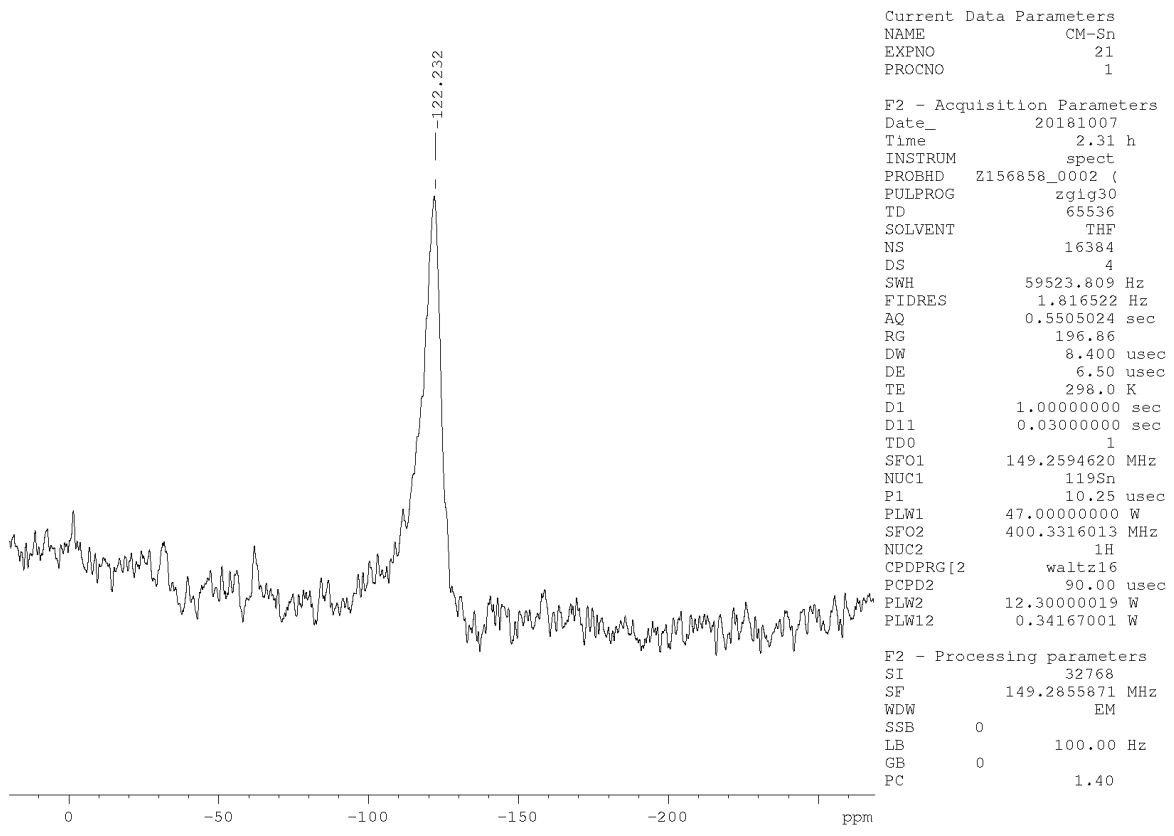
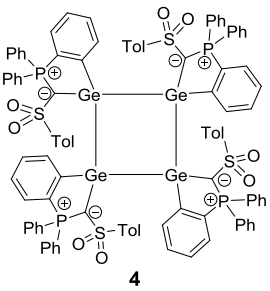


Figure S9. ^{119}Sn spectrum of **Y_2Sn** in THF-d_8.

1.4 Synthesis of Y_4G_4 (4)



4

In a J-Young NMR tube **Y_2Ge** (25mg, 0.027 mmol) was dissolved in toluene-d_8 (0.4 mL). The solution was heated to 90 ˚C for 1 hour. During heating, the colour of the solution changed from a pale-yellow to intense yellow and yellow solid precipitated from the solution. The complete consumption of **Y_2Ge** and liberation of the ylide (**Y**) was confirmed by ^{31}P NMR spectroscopy of the reaction mixture. The yellow solid was separated by decanting/removing of the supernatant yellow solution (containing **Y** and other side products along with some amount of **4**). The solid was again dissolved in toluene (0.4 mL) by heating at 90 ˚C and the solution was cooled to room temperature and allowed to stand overnight to get single crystals of **4** (9 mg, 33% yield base on **Y**). The single crystals were suitable for X-Ray structure determination and other characterizations.

^1H NMR (400.3 MHz, THF-d_8): δ 1.79 (s, 12H; CH_3), 5.63-5.65 (d, 8H, C$H_{STol,meta}$), 6.11-6.13 (d, 8H; C$H_{STol,ortho}$), 6.84-6.87 (m, 16H, C$H_{PPh,ortho}$), 7.08-7.18 (m, 16H; C$H_{PPh,meta}$), 7.26-7.44 (m, 20H, C$H_{PPh,para}$ and C$H_{PPhcyclo,ortho,meta\ and\ para}$), 9.65-9.68 (d, 4H, C$H_{PPhcyclo,\ GeCCH}$). $^{13}C\{^1H\}$ NMR (100.6 MHz, THF-d_8): δ 20.03 (CH_3), 37.07-37.88 (br, d, $^1J_{PC}$ = 81.27 Hz; P*C*S), 124.52 (C$H_{STol,ortho}$), 126.66-127.65 (d, $^1J_{PC}$ = 100.7 Hz, $C_{PPh,ipso}$), 127.42-128.31 (d, $^1J_{PC}$ = 89.7 Hz, $C_{PPhcyclo,ipso}$), 127.90-128.01 (d, $^2J_{PC}$ = 11.19 Hz; $CH_{PPh,ortho}$), 128.57-128.70 (d, $^3J_{PC}$ = 12.93 Hz; $CH_{PPh,meta}$), 130.78-130.81 (d, $^4J_{PC}$ = 3.11 Hz; $CH_{PPh,para}$), 130.87.-130.90 (d, $^4J_{PC}$ = 2.70 Hz; $CH_{PPhcyclo,para}$), 133.80-133.91 (d, $^2J_{PC}$ = 10.82 Hz; $CH_{PPhcyclo,ortho}$), 135.43 (C$H_{STol,meta}$), 136.17 ($C_{STol,para}$), 141.24-141.36 (br, d, $^3J_{PC}$ = 12.10 Hz; $CH_{PPhcyclo,meta\ and\ GeCCH}$), 147.28 ($C_{STol,ipso}$), 151.78-151.98 (d, $^2J_{PC}$ = 20.73 Hz; $CH_{PPhcyclo,GeC}$). $^{31}P\{^1H\}$ NMR (162.05 MHz, THF-d_8): 15.73. Anal. Calcd. for $C_{104}H_{84}Ge_4O_8P_4S_4$: C, 62.32; H, 4.22. Found: C, 61.44; H, 3.88.

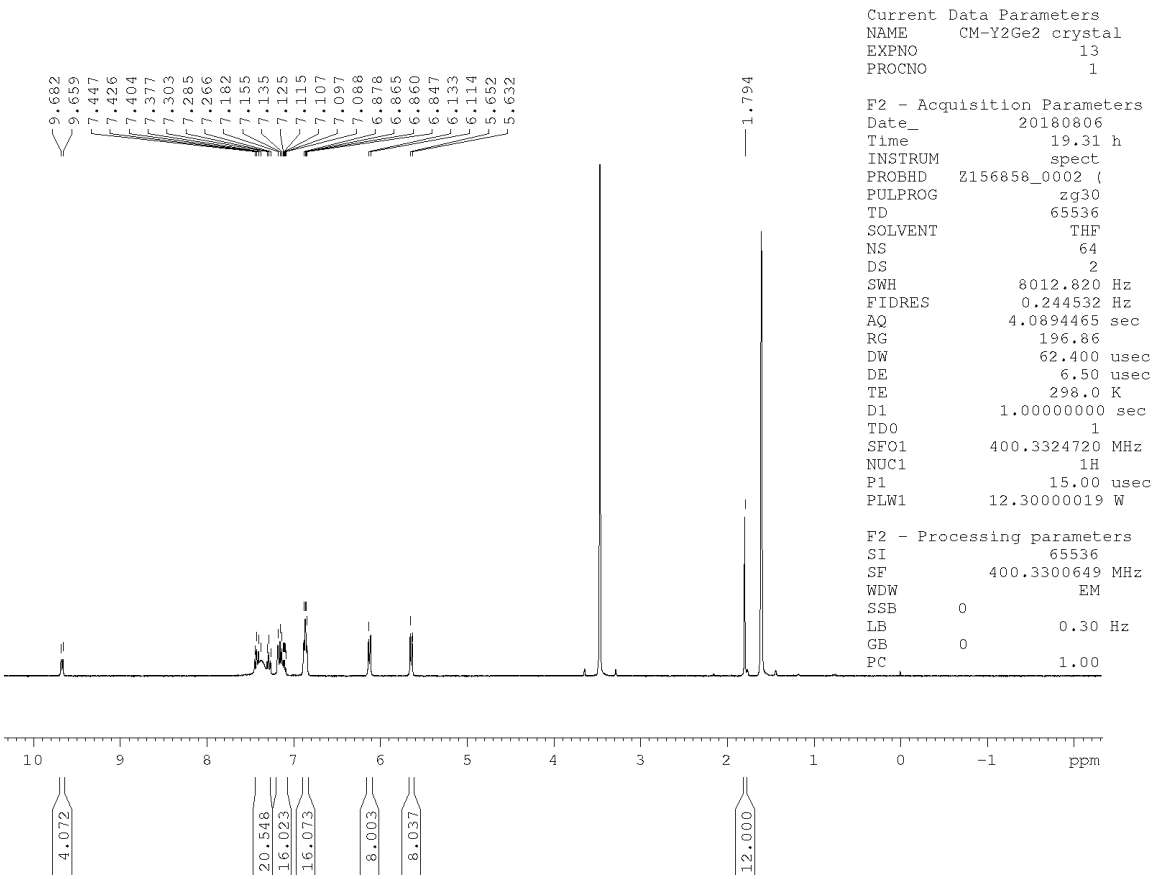


Figure S10. ^{1}H spectrum of **4** in THF-d_8.

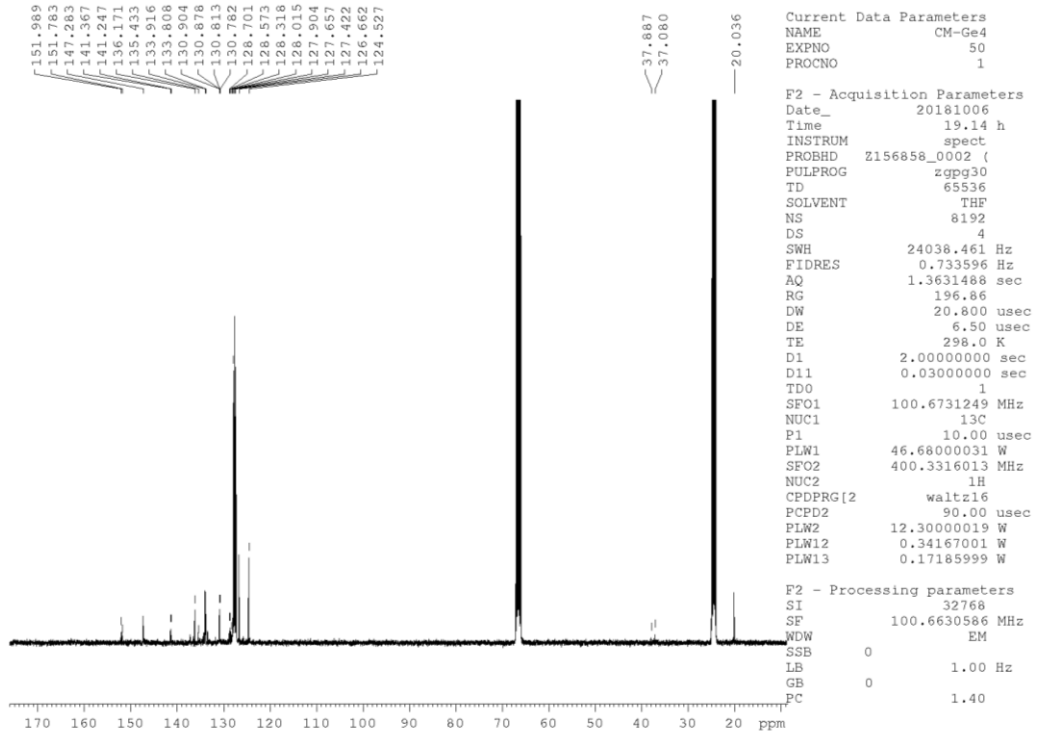


Figure S11. $^{13}C\{^{1}H\}$ spectrum of **4** in THF-d_8.

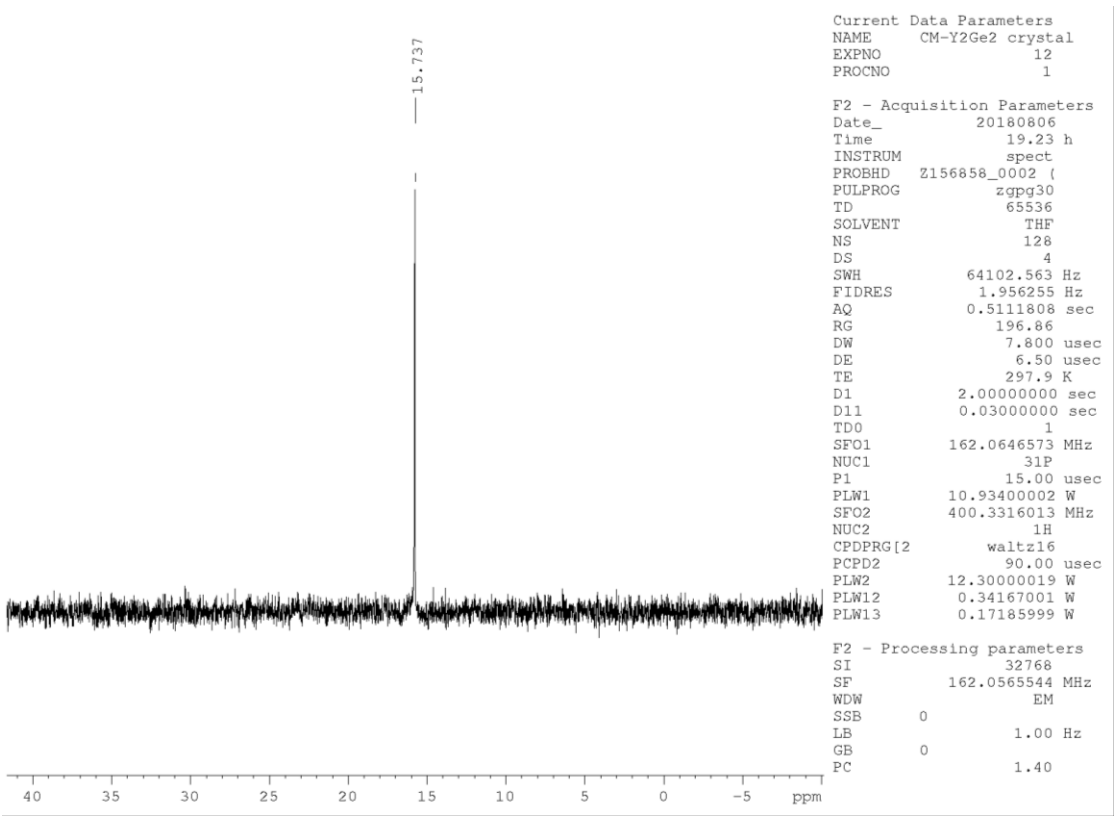
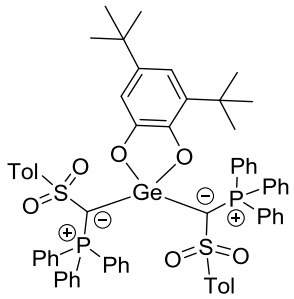


Figure S12. $^{31}P\{^{1}H\}$ spectrum of **4** in THF-d_8.

1.5 Synthesis of Y_2GeBQ (5a)



Y_2GeBQ

A J-Young-NMR tube was filled with **Y_2Ge** (40 mg, 0.043 mmol) and 3,5-Di-*tert*-butyl-*o*-benzoquinone (BQ) (9.5 mg, 0.043 mmol) in 1:1 molar ratio. To this mixture, C_6D_6 and THF-d_8 were added in 4:1 (v/v, total 0.5 mL) and the reaction mixture was shaken for 15 minutes to form a colourless solution. The ^{31}P NMR spectrum of the reaction mixture confirmed the formation of **5a** (~75%) (Figure S13). The reaction mixture was filtered into a glass vial and kept in a further vial with hexane for two days to yield **5a** as pure colorless solid (26 mg, 52%). Single crystals of **5a** were grown by a similar method like in case of **Y_2Ge**.

^{1}H NMR (400.3 MHz, THF-d_8): δ 0.95 (s, 9H; C$H_{3\ BQ,\ t\mathrm{Bu}}$), 1.10 (s, 9H; C$H_{3\ BQ,\ t\mathrm{Bu}}$), 2.27 (s, 12H; C$H_{3\mathrm{STol}}$), 5.61-5.62 (br, d, 1H; C(*t*Bu)C*H*C(*t*Bu)$_{BQ}$), 6.25-6.26 (br, d, 1H; OCC*H*C(*t*Bu)$_{BQ}$), 6.82-6.84 (d, 4H; C$H_{\mathrm{STol,meta}}$), 7.13-7.18 (m, 12H; C$H_{\mathrm{PPh,ortho}}$), 7.33.7.37 (m, 6H; C$H_{\mathrm{PPh,para}}$) 7.44-7.63 (br, m, 4H; C$H_{\mathrm{STol,ortho}}$), 7.69-7.74 (m, 12H; C$H_{\mathrm{STol,ortho}}$ and C$H_{\mathrm{PPh,meta}}$). $^{13}C\{^{1}H\}$ NMR (100.6 MHz, THF-d_8): δ 20.25 (*C*$H_{3\mathrm{STol}}$), 22.52 (*C*(*t*Bu)$_{BQ}$), 29.34 (*C*$H_{3\ BQ,\ t\mathrm{Bu}}$), 31.23 (*C*$H_{3\ BQ,\ t\mathrm{Bu}}$), 31.58 (*C*(*t*Bu)$_{BQ}$), 33.58-33.86 (br, d, $^{1}J_{PC}$ = 27.84 Hz; P*C*S), 108.45 (OC*C*HC(*t*Bu)$_{BQ}$), 111.56 (C(*t*Bu)*C*HC(*t*Bu)$_{BQ}$), 125.53-126.44 (d, $^{1}J_{PC}$ = 92.11 Hz, *C*$_{\mathrm{PPh,ipso}}$), 127.03

($CH_{STol,ortho}$), 127.34-127.46 (d, $^{3}J_{PC}$ = 12.60 Hz; $CH_{PPh,meta}$), 127.54 ($CH_{STol,meta}$), 131.12-131.14 (d, $^{4}J_{PC}$ = 2.79 Hz; $CH_{PPh,para}$), 131.96 ($OCC(tBu)_{BQ}$), 134.92-135.02 (d, $^{2}J_{PC}$ = 10.47 Hz; $CH_{PPh,ortho}$), 138.90 ($OCC(tBu)_{BQ}$), 139.00 ($C_{STol,para}$), 145.65 ($OCCH_{BQ}$), 146.63 ($C_{STol,ipso}$), 149.96 ($CHC(tBu)CH_{BQ}$). $^{31}P\{^{1}H\}$ NMR (162.05 MHz, THF-d_8): 16.53. Anal. Calcd. for $C_{66}H_{64}O_6P_2S_2Ge$: C, 68.82; H 5.60 Found: C, 69.19; H, 5.71.

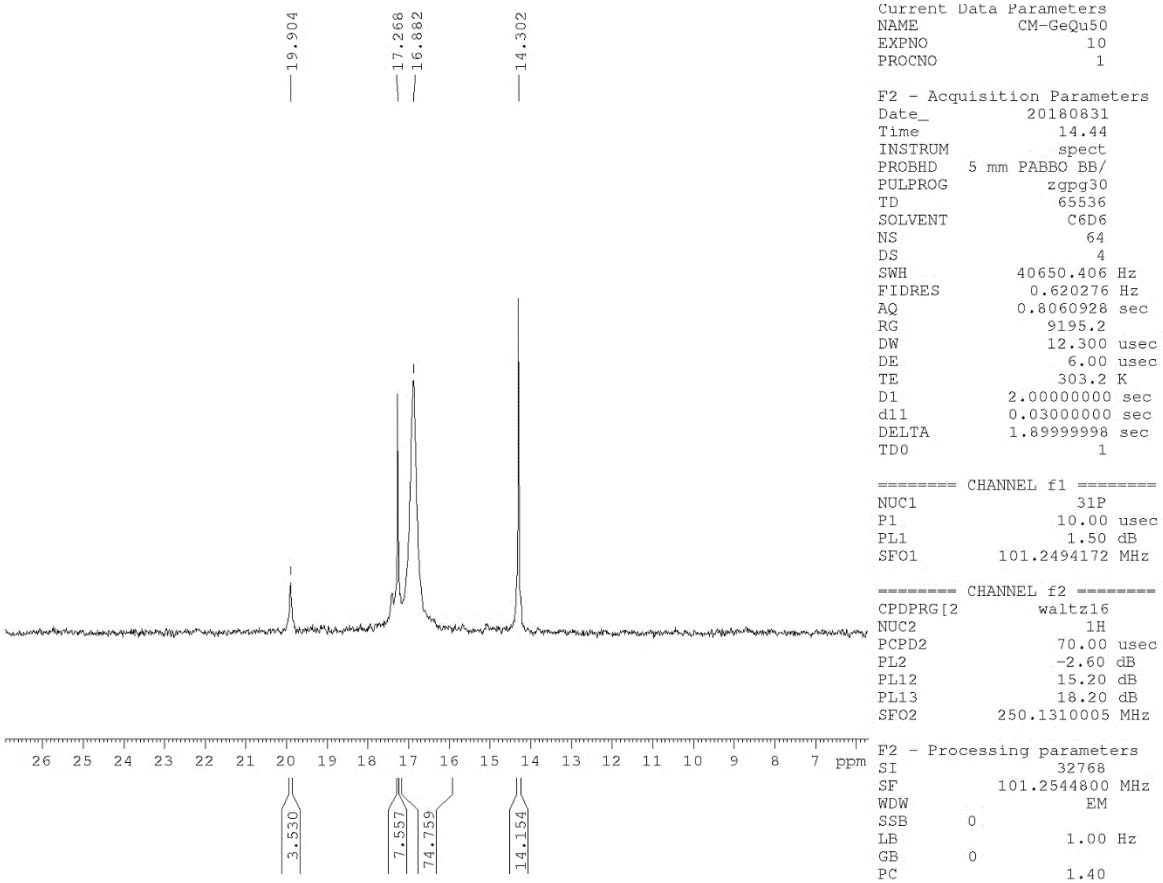


Figure S13. $^{31}P\{^{1}H\}$ spectrum of the reaction mixture of **5a**.

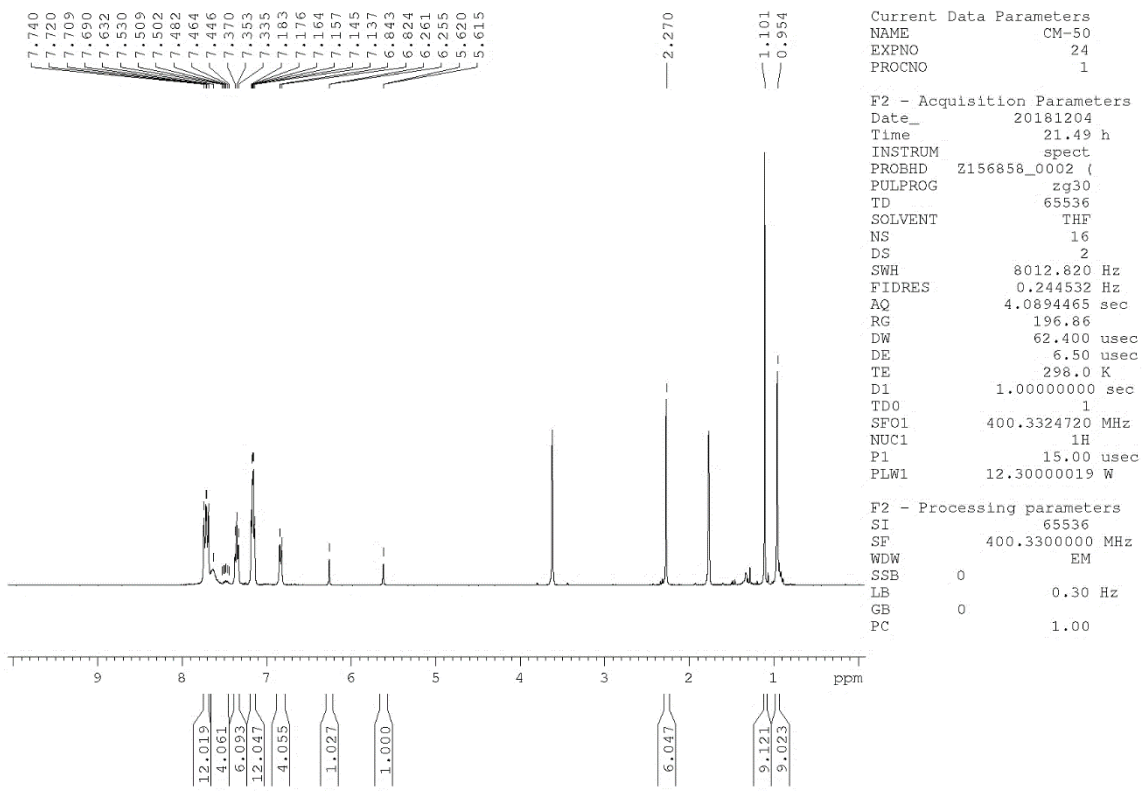


Figure S14. ^{1}H spectra of **5a** in THF-d_8.

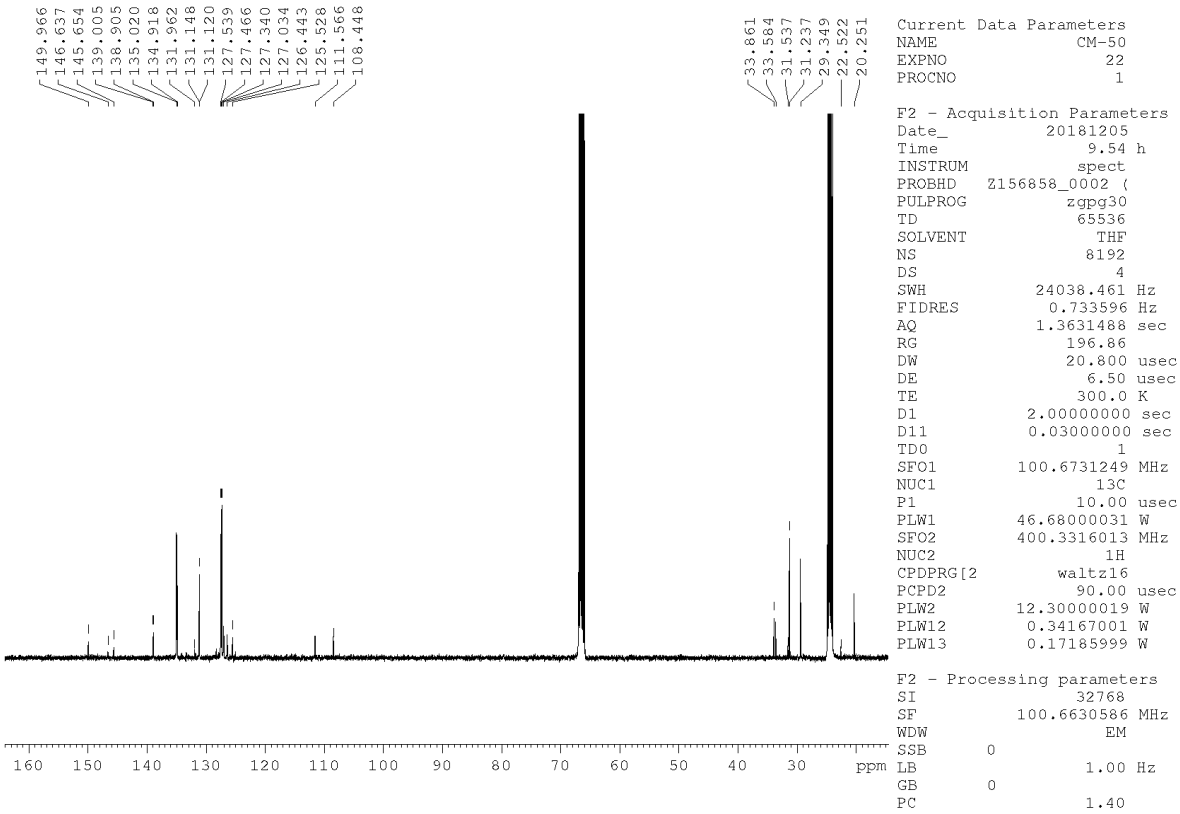


Figure S15. $^{13}C\{^{1}H\}$ spectra of **5a** in THF-d_8.

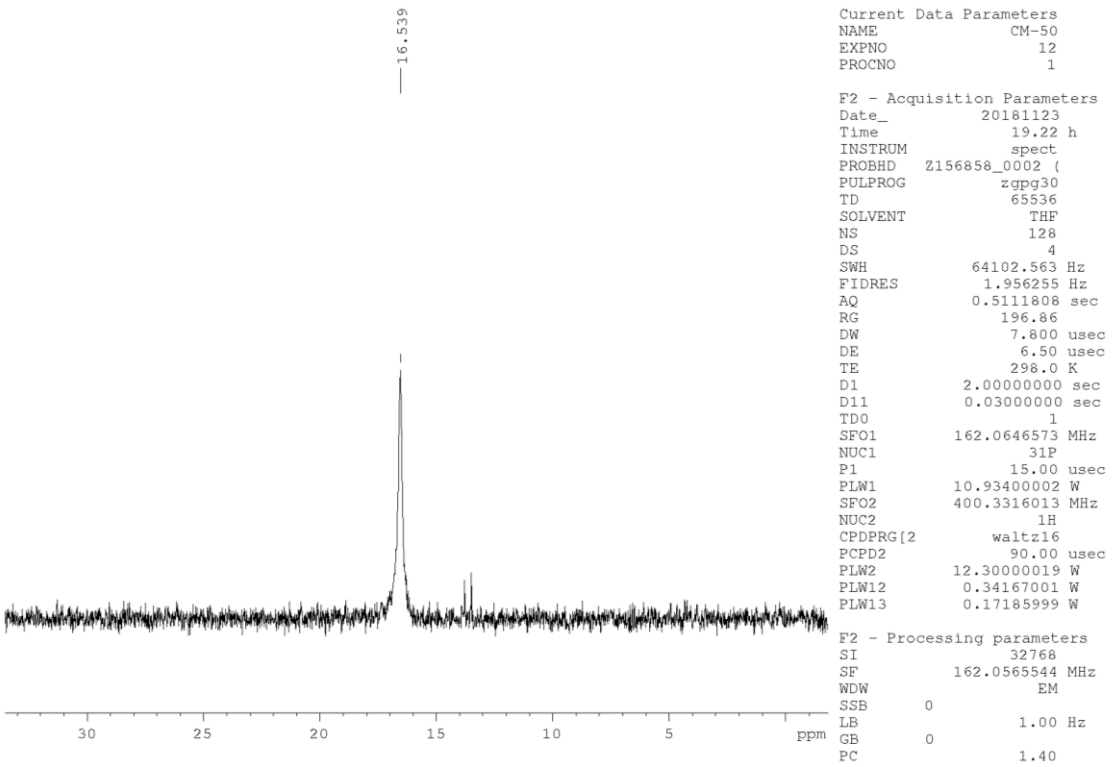
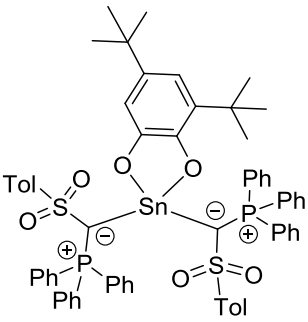


Figure S16. $^{31}P\{^{1}H\}$ spectrum of **5a** in THF-d_8.

1.6 Synthesis of Y_2SnBQ (5b)



Y_2SnBQ

A J-Young-NMR tube was filled with **Y_2Sn** (51 mg, 0.052 mmol) and 3,5-Di-*tert*-butyl-*o*-benzoquinone (BQ) (11.4 mg, 0.052 mmol) in 1:1 molar ratio. To this mixture, C_6D_6 and THF-d_8 were added in 4:1 (v/v, total 0.5 mL) and the reaction mixture was shaken for 15 minutes to form a colourless solution. The ^{31}P NMR spectrum of the reaction mixture confirmed the formation of **5b** (~92%) (Figure S17). The reaction mixture was filtered into a glass vial giving a clear solution, which was kept in further vial filled with hexane overnight to yield **5b** as pure colorless solid (42 mg, 67% yield). Single crystals of **5b** were grown by a similar method like in case of **Y_2Ge**.

^{1}H NMR (400.3 MHz, THF-d_8): δ 0.93 (s, 9H; C*H*$_{3\ BQ,\ t\mathrm{Bu}}$), 1.27 (s, 9H; C*H*$_{3BQ,\ t\mathrm{Bu}}$), 2.31 (s, 12H; C*H*$_{3STol}$), 6.16 (br, s, 1H; C(*t*Bu)C*H*C(*t*Bu)$_{\ BQ}$), 6.33-6.34 (br, d, 1H; OCC*H*C(*t*Bu)$_{\ BQ}$), 6.92-6.94 (d, 4H; C*H*$_{STol,meta}$), 7.15-7.20 (m, 12H; C*H*$_{PPh,ortho}$), 7.37-7.41 (m, 6H; C*H*$_{PPh,para}$) 7.63-7.68 (m, 16H; C*H*$_{STol,ortho}$ and C*H*$_{PPh,meta}$). $^{13}C\{^{1}H\}$ NMR (100.6 MHz, THF-d_8): δ 20.28 (*C*H$_{3STol}$), 26.77 (*C*(*t*Bu)$_{BQ}$), 29.45 (*C*H$_{3\ BQ,\ t\mathrm{Bu}}$), 31.53 (*C*H$_{3\ BQ,\ t\mathrm{Bu}}$), 33.68-34.06 (br, d, $^{1}J_{PC}$ = 38.33 Hz; P*C*S), 34.48 (*C*(*t*Bu)$_{BQ}$), 109.95

(OC*C*HC(*t*Bu) $_{BQ}$), 110.11 (C(*t*Bu)*C*HC(*t*Bu) $_{BQ}$), 125.14 (*C*H$_{STol,ortho}$), 126.06 (*C*H$_{STol,meta}$), 127.16-127.93 (d, $^{1}J_{PC}$ = 78.11 Hz, *C*$_{PPh,ipso}$), 127.78-127.91 (d, $^{3}J_{PC}$ = 12.75 Hz; *C*H$_{PPh,meta}$), 131.48-131.51 (d, $^{4}J_{PC}$ = 2.84 Hz; *C*H$_{PPh,para}$), 132.78 (O*C*C(tBu)$_{BQ}$), 134.40-134.50 (d, $^{2}J_{PC}$ = 10.47 Hz; *C*H$_{PPh,ortho}$), 137.05 (OC*C*(tBu)$_{BQ}$), 139.53 (*C*$_{STol,para}$), 145.66 (O*C*CH$_{BQ}$), 148.53 (*C*$_{STol,ipso}$), 151.97 (CH*C*(tBu)CH$_{BQ}$). $^{31}P\{^{1}H\}$ NMR (162.05 MHz, THF-d$_8$): 12.55. ^{119}Sn NMR (149.3 MHz, THF-d$_8$): -241.35 (br). Anal. Calcd. for $C_{66}H_{64}O_6P_2S_2Sn$: C, 66.17; H, 5.38 Found: C, 65.93; H, 4.97.

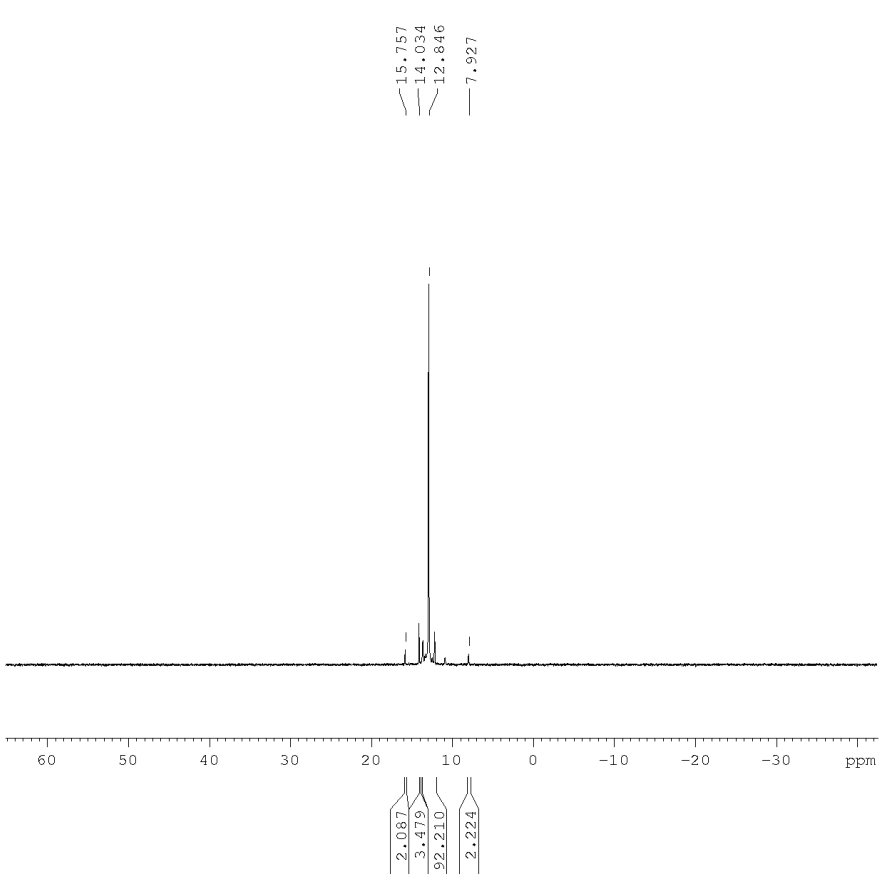


Figure S17. $^{31}P\{^{1}H\}$ spectrum of the reaction mixture of **5b**.

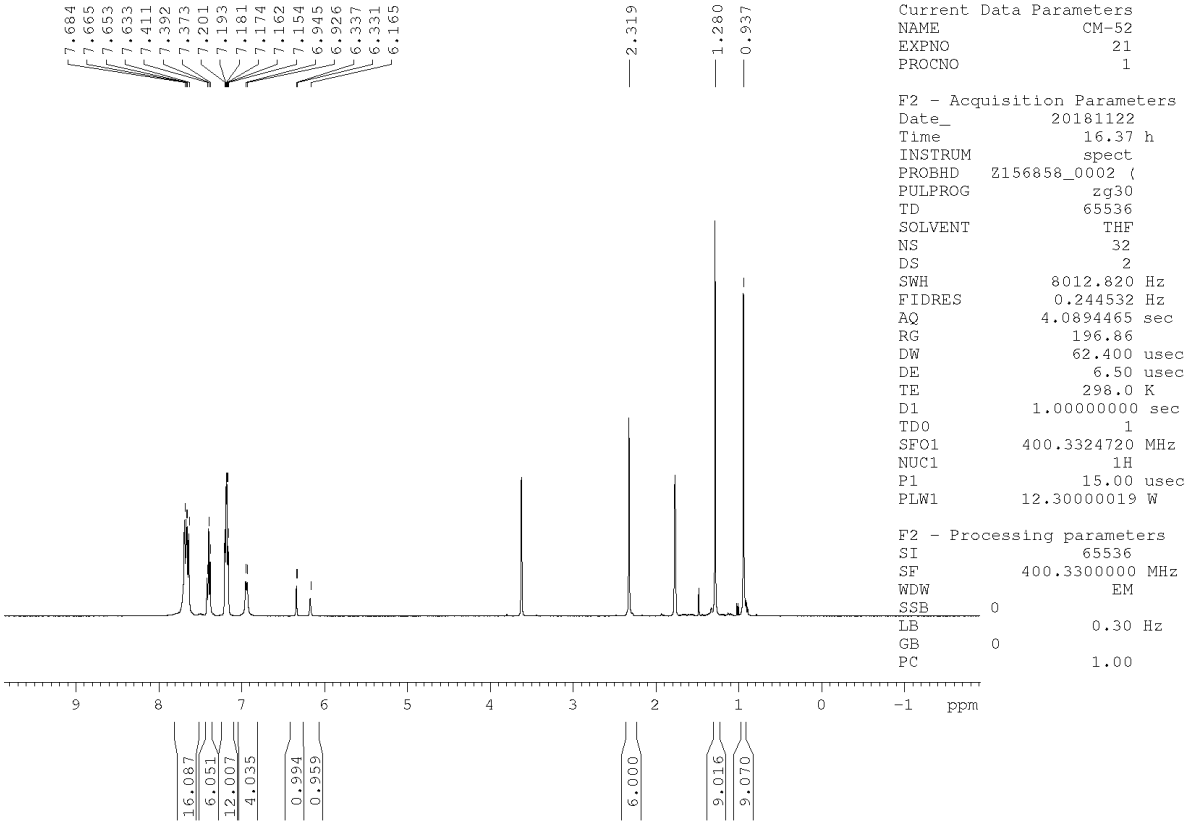


Figure S18. ^{1}H spectrum of **5b** in THF-d_8.

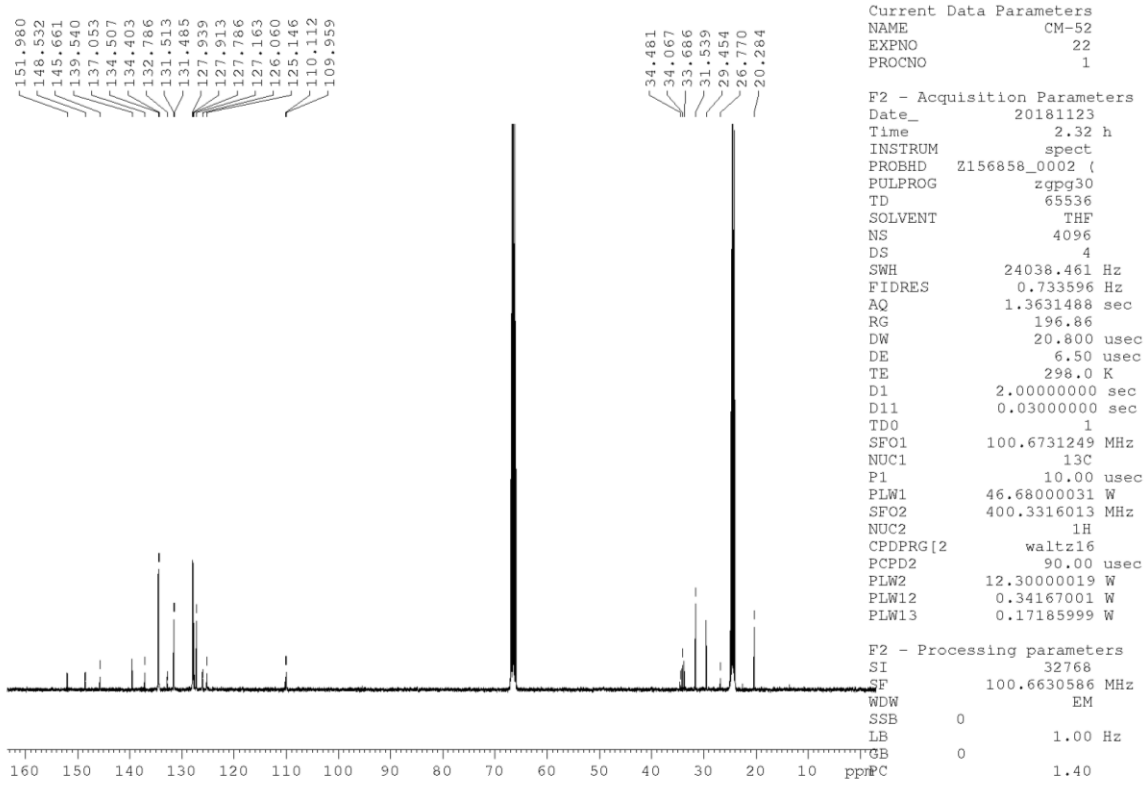


Figure S19. $^{13}C\{^{1}H\}$ spectrum of **5b** in THF-d_8.

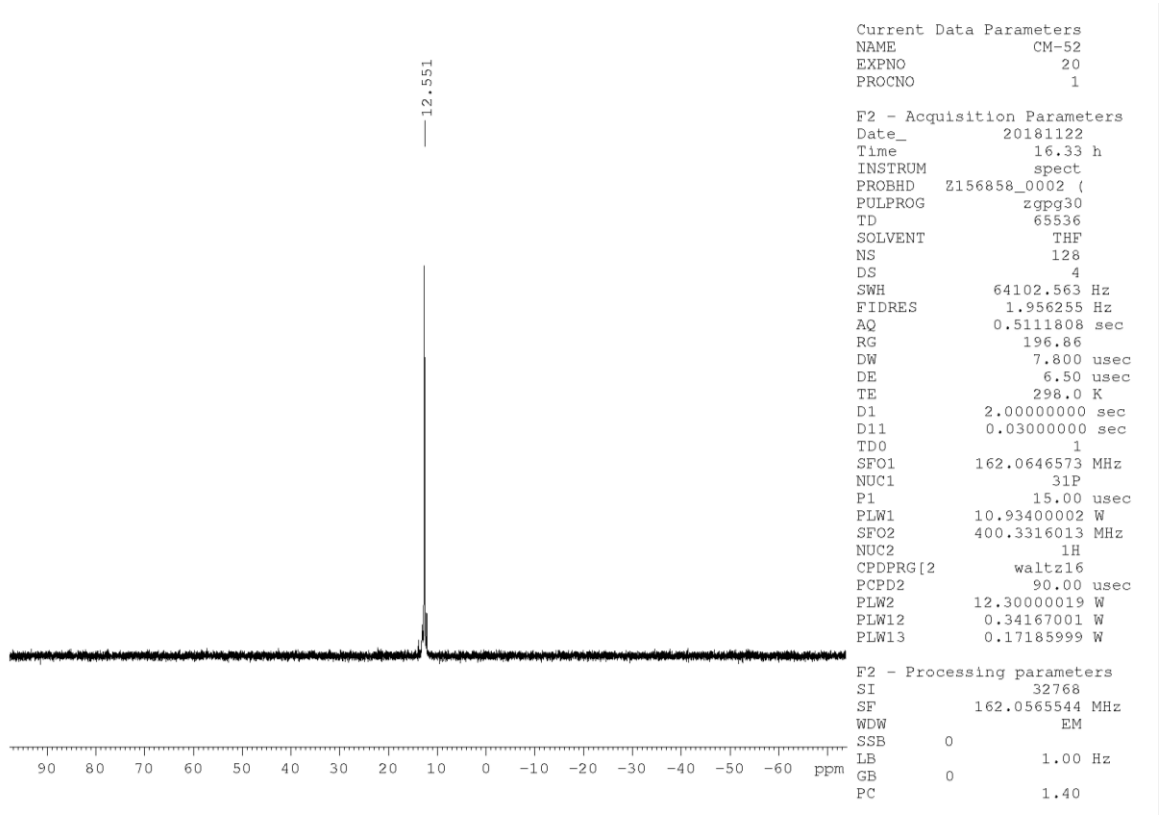


Figure S20. $^{31}P\{^{1}H\}$ spectrum of **5b** in THF-d_8.

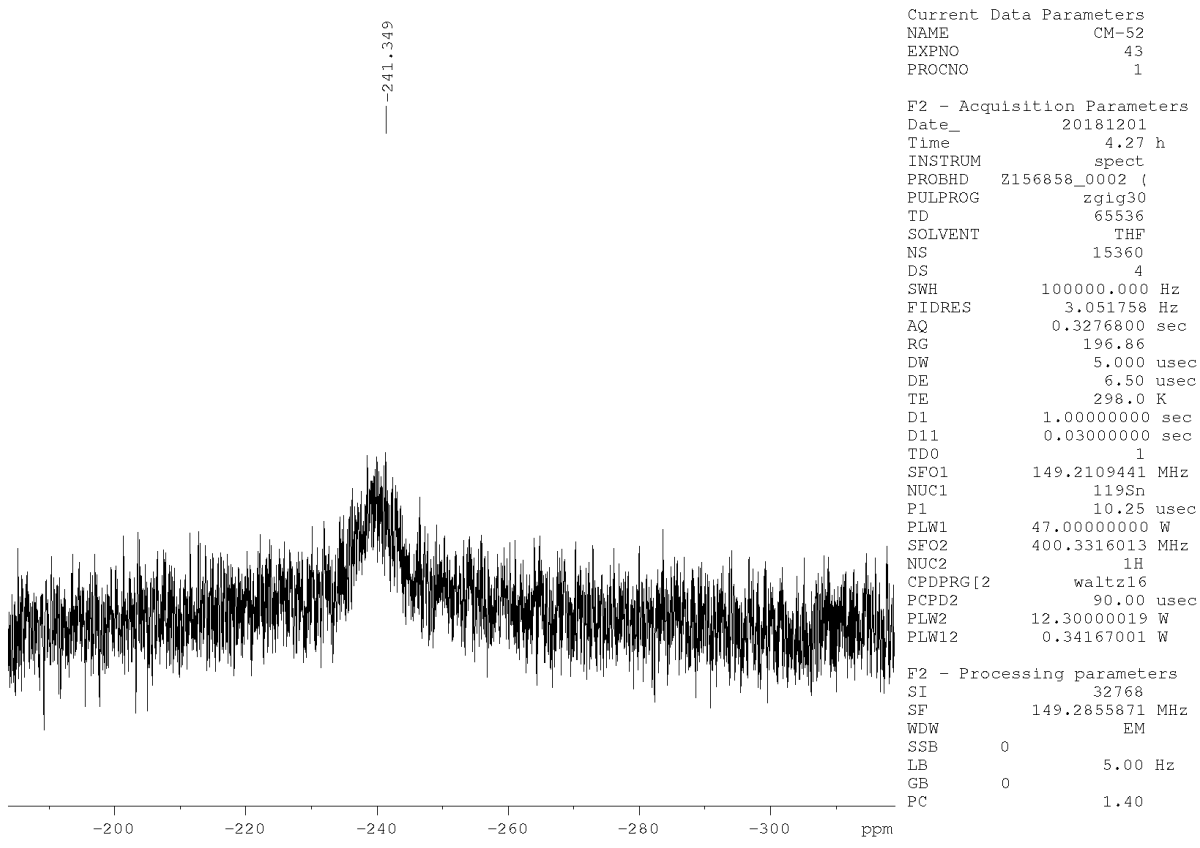
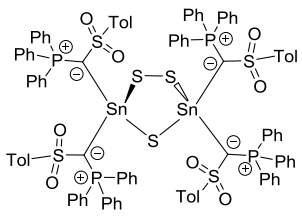


Figure S21. ^{119}Sn spectrum of **5b** in THF-d_8.

1.7 Synthesis of $Y_4Sn_2S_3$ (6)



$Y_4Sn_2S_3$

A glass vial was filled with elemental sulfur (2.4 mg, 0.075 mmol). A solution of **Y_2Sn** (51 mg, 0.052 mmol) in a mixture C_6D_6 and THF in 4:1 (v/v, total 0.5 mL) was added to the vial and the reaction mixture was shaken for 15 minutes to completely dissolve all solids. The reaction mixture was filtered into another vial giving a clear solution, which was kept in further vial filled with hexane to form **6** as pure pale-yellow solid (37 mg, 69.4% yield). Single crystals of **6** were grown from its solution in THF by vapour diffusion technique with hexane.

^{1}H NMR (400.3 MHz, CD_2Cl_2): *δ* 2.28-2.38 (br, m, 12H; C*H*$_{3STol}$), 6.36-7.87 (br, m, 72H; C*H*$_{PPh,STol}$). ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): *δ* 20.87-20.97 (br, *C*H$_{3STol}$), 124.28- 124.66 (C*H*$_{STol,ortho}$), 125.19-125.56 (C*H*$_{STol,meta}$), 126.24-127.15 (d, $^1J_{PC}$ = 90.75 Hz, *C*$_{PPh,ipso}$), 126.86-128.09 (d, $^1J_{PC}$ = 123.55 Hz, *C*$_{PPh,ipso}$), 127.69-128.39 (d, $^1J_{PC}$ = 69.62 Hz, *C*$_{PPh,ipso}$), 127.44-127.57 (d, $^3J_{PC}$ = 13.04 Hz; *C*H$_{PPh,meta}$), 127.89-128.02 (d, $^3J_{PC}$ = 12.58 Hz; *C*H$_{PPh,meta}$), 128.57-128.69 (d, $^3J_{PC}$ = 12.50 Hz; *C*H$_{PPh,meta}$), 131.12 (br, s, *C*H$_{PPh,para}$), 131.53-131.56 (d, $^4J_{PC}$ = 3.31 Hz; *C*H$_{PPh,para}$), 131.82-131.85 (d, $^4J_{PC}$ = 3.07 Hz; *C*H$_{PPh,para}$), 132.47-132.50 (d, $^4J_{PC}$ = 3.12 Hz; *C*H$_{PPh,para}$), 134.23-134.33 (d, $^2J_{PC}$ = 10.27 Hz; *C*H$_{PPh,ortho}$), 135.18-135.28 (d, $^2J_{PC}$ = 10.29 Hz; *C*H$_{PPh,ortho}$), 135.37-135.47 (d, $^2J_{PC}$ = 10.13 Hz; *C*H$_{PPh,ortho}$), 135.58-135.68 (d, $^2J_{PC}$ = 10.37 Hz; *C*H$_{PPh,ortho}$), 138.71-140.30 (*C*$_{STol,para}$), 145.18-145.64 (*C*$_{STol,ipso}$). ^{31}P{^{1}H} NMR (162.05 MHz, CD_2Cl_2): 13.29-15.24 (br). Anal. Calcd. for $C_{104}H_{88}O_8P_4S_7Sn_2$: C, 60.89; H, 4.32; S, 10.94. Found: C, 60.77; H, 4.47; S, 10.96.

Due to the low solubility and fluxional behaviour of **6** in solution, ^{13}C NMR signals of the quaternary carbon atoms as well as ^{119}Sn NMR signals could not be detected. The fluxional behaviour of **6** in solution results in broad signals for the aromatic protons, hence they were not able to be assigned in detail.

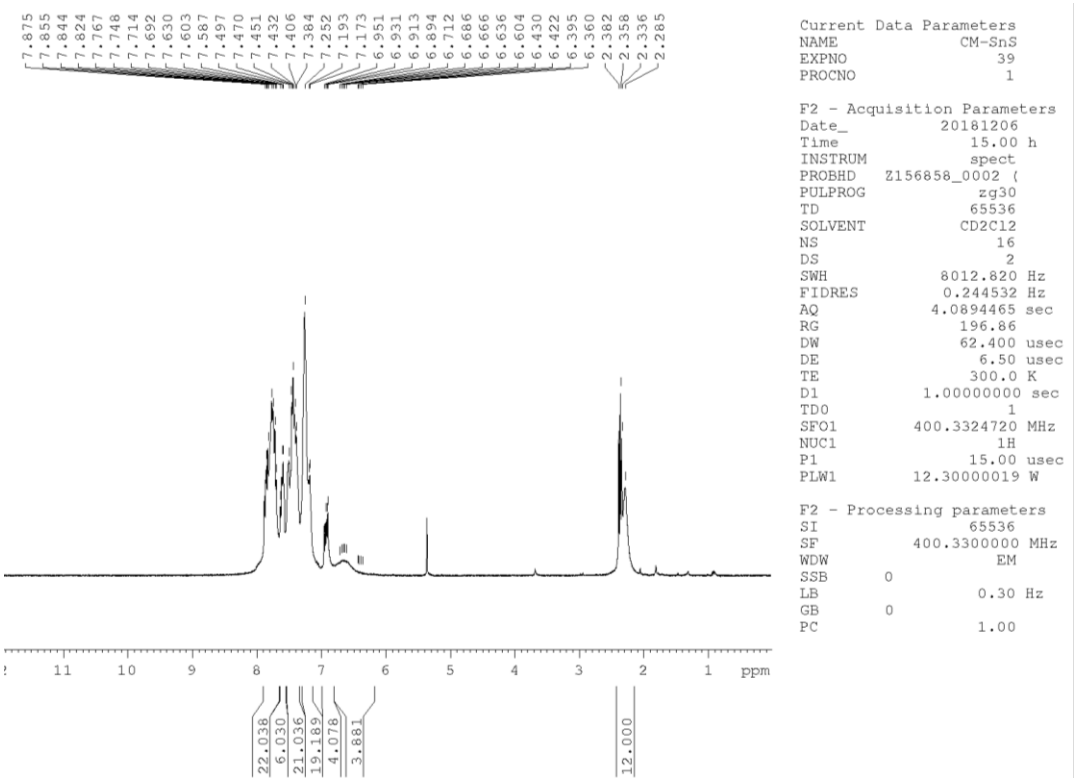


Figure S22. ^{1}H spectrum of **6** in DCM-d_2.

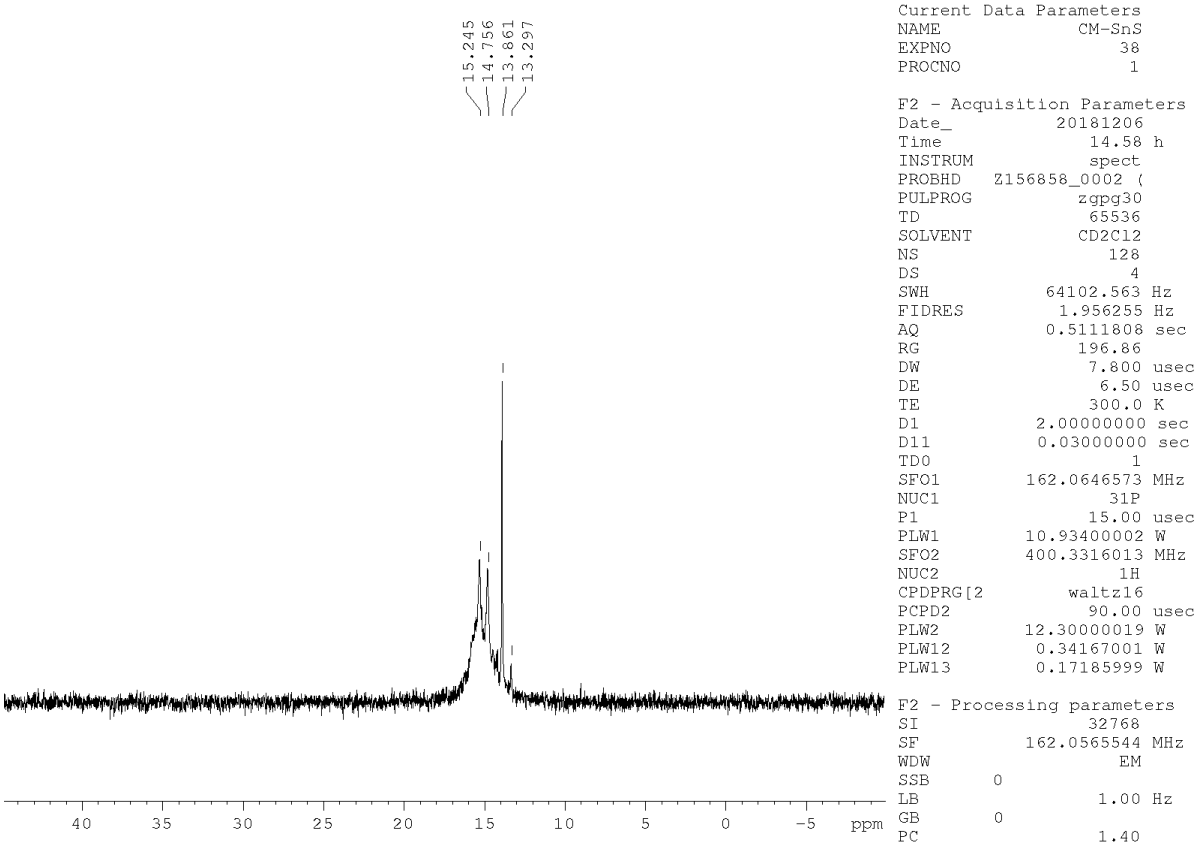


Figure S23. $^{31}P\{^{1}H\}$ spectrum of **6** in DCM-d_2.

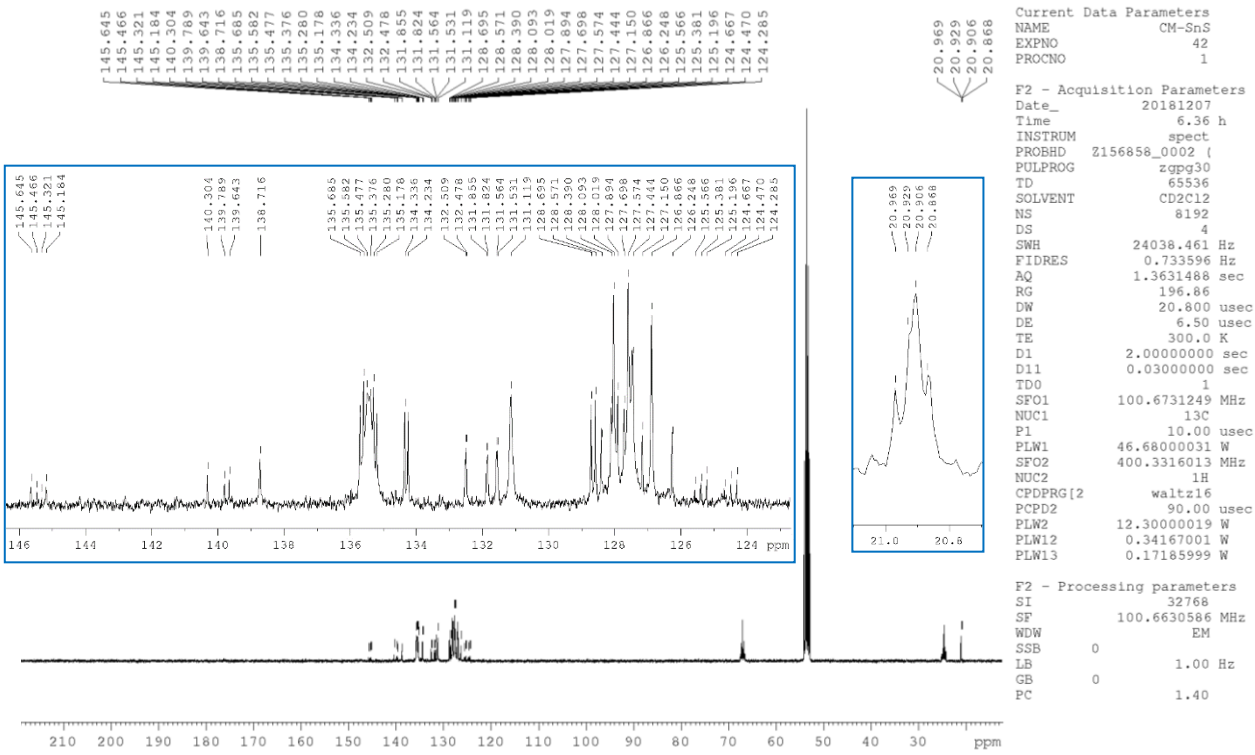


Figure S24. $^{13}C\{^{1}H\}$ spectrum of **6** in DCM-d_2.

2. Crystal Structure Determination

2.1 General information

Data collection of all compounds was conducted either with Oxford SuperNova (**Y_2Ge**, **Y_2Sn**, **4**, **5a**, **6**) or Oxford Synergy (**5b**). The structures were solved using direct methods, refined with the Shelx software package[2] 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-1901204-1901209. 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].

Table S1. Data collection and structure refinement details for compounds **Y_2Ge, Y_2Sn** and **4**.

Compound	**Y_2Ge**	**Y_2Sn**	**4**
CCDC No.	CCDC 1901208	CCDC 1901204	CCDC 1901207
Empirical formula	$C_{58}H_{50}O_4P_2S_2Ge$	$C_{52}H_{44}O_4P_2S_2Sn$	$C_{146}H_{132}Ge_4O_8P_4S_4$
Formula weight	1009.63	977.62	2556.99
Temperature (K)	100.4(3)	100.2(14)	100.6(8)
Wavelength	1.54184 Å	1.54184 Å	1.54184 Å
Crystal system	Monoclinic	triclinic	triclinic
Space group	$P2_1/c$	P-1	P-1
a (Å)	23.2312(2)	11.0750(3)	18.2582(8)
b (Å)	10.71684(11)	13.9752(5)	18.5515(8)
c (Å)	20.2615(2)	17.0539(7)	22.6058(8)
α (°)	90	68.027(3)	73.148(4)
β (°)	102.2324(11)	82.329(3)	68.776(4)
γ (°)	90	66.789(3)	60.938(5)
Volume ($Å^3$)	4929.88(9)	2249.36(15)	6177.5(5)
Z	4	2	2
Density (calculated)	1.360 Mg/m^3	1.443 Mg/m^3	1.375 Mg/m^3
Absorption coefficient	2.625 mm^{-1}	6.421 mm^{-1}	2.713 mm^{-1}
F(000)	2096.0	1000.0	2648.0
Crystal dimensions (mm^3)	0.263 × 0.192 × 0.116	0.239 × 0.207 × 0.175	0.606 × 0.196 × 0.141
Theta range (°)	3.894 to 74.413	3.678 to 74.34	3.23 to 75.516
Index ranges	-29 ≤ h ≤ 23, -13 ≤ k ≤ 13, -25 ≤ l ≤ 24	-13 ≤ h ≤ 13, -17 ≤ k ≤ 17, -21 ≤ l ≤ 21	-22 ≤ h ≤ 22, -23 ≤ k ≤ 23, -27 ≤ l ≤ 27
Reflections collected	35925	16336	112522
Independent reflections	9932 [*R*(int)= 0.0367]	8884 [*R*(int) = 0.0206]	24767 [*R*(int) = 0.0551]
Data / restraints / parameters	9932/0/606	8884/0/552	24767/0/1499
Goodness-of-fit on F^2	1.042	1.055	1.038
Final R indices [I>2sigma(I)]	R_1 = 0.0341, wR_2 = 0.0888	R_1 = 0.0252, wR_2 = 0.0657	R_1 = 0.0446, wR_2 = 0.1099
R indices (all data)	R_1 = 0.0388, wR_2 = 0.0933	R_1 = 0.0261, wR_2 = 0.0664	R_1 = 0.0613, wR_2 = 0.1212
Largest diff. peak and hole	0.49 and -0.40 e.$Å^{-3}$	0.35 and -0.68 e.$Å^{-3}$	1.05and -0.82 e.$Å^{-3}$

Table S2. Data collection and structure refinement details for compounds **5a, 5b** and **6**.

Compound	**5a**	**5b**	**6**
CCDC No.	CCDC 1901205	1901209	1901206
Empirical formula	$C_{75}H_{73}O_6P_2S_2Ge$	$C_{75}H_{73}O_6P_2S_2Sn$	$C_{112}H_{104}O_{10}P_4S_7Sn_2$
Formula weight	1268.98	1315.08	2195.63
Temperature	100(2) K	100(2) K	101.2(10)
Wavelength	1.54184 Å	1.54184 Å	1.54184 Å
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	*P*-1	*P* -1	*C*2/c
a (Å)	10.8073(5)	10.6912(3)	30.8747(7)
b (Å)	15.0932(9)	15.2028(3)	11.0570(2)
c (Å)	21.9324(13)	22.2336(4)	29.3124(6)
α (°)	86.787(5)	87.354(2)	90
β (°)	77.816(5)	78.738(2)	93.451(2)
γ (°)	77.593(5)	78.000(2)	90
Volume ($Å^3$)	3415.1(3)	3466.67(14)	9988.6(4)
Z	2	2	4
Density (calculated)	1.234 Mg/m^3	1.260 Mg/m^3	1.460 Mg/m^3
Absorption coefficient	2.021 mm^{-1}	4.322 mm^{-1}	6.435 mm^{-1}
F(000)	1330	1366	4512.0
Crystal dimensions (mm^3)	0.448 × 0.097 × 0.056	0.245× 0.053 × 0.013	0.169 × 0.107 × 0.037
Theta range (°)	3.620 to 69.997	2.972 to 67.071	8.08 to 135.992
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 18, -24 ≤ l ≤ 26	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -26 ≤ l ≤ 20	-36 ≤ h ≤ 37, -13 ≤ k ≤ 13, -35 ≤ l ≤ 34
Reflections collected	23890	36156	37966
Independent reflections	12887 [*R*(int) = 0.0625]	12115 [*R*(int) = 0.0523]	9108 [*R*(int) = 0.0668]
Data / restraints / parameters	12887 / 0 / 784	12115 / 0 / 786	9108/16/597
Goodness-of-fit on F^2	1.002	1.043	1.250
Final R indices [I>2sigma(I)]	R_1 = 0.0543, wR_2 =0.1302	R_1= 0.0520, wR_2 = 0.1334	R_1=0.0819, wR_2=0.2189
R indices (all data)	R_1 = 0.0773, wR_2 =0.1472	R_1= 0.0577, wR_2 = 0.1375	R_1=0.0879, wR_2 = 0.2217
Largest diff. peak and hole	0.909 and -0.719 e.$Å^{-3}$	2.138 and -1.717 e.$Å^{-3}$	3.44 and -1.15 e.$Å^{-3}$

2.2 Crystal Structure of Y_2Ge

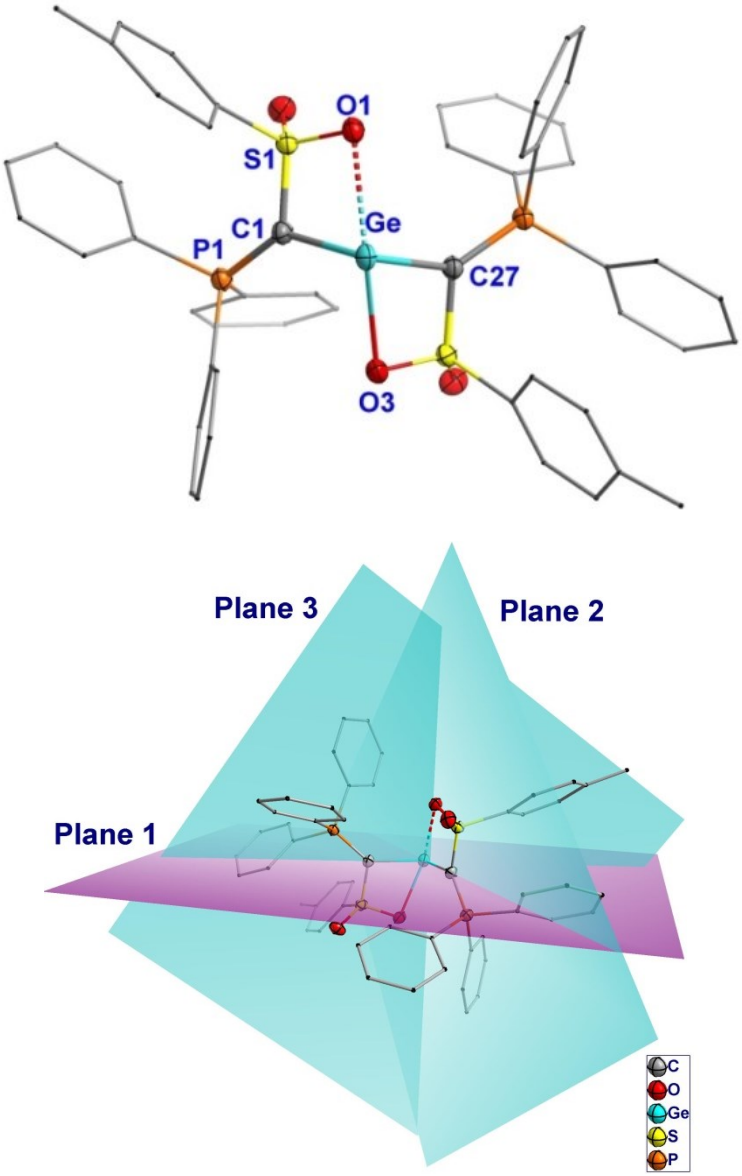


Figure S25. (top) X-Ray structure of **Y_2Ge**. (Bottom) Plane passing through C1-Ge-C27 (Plane 1) and planes passing through S1-C1-P1 (Plane 2) and S2-C27-P2 (Plane 3). Dihedral angles (˚): Plane 1-Plane 2, 89.64(9); Plane 1-Plane 3, 88.94(8).

Table S3. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Y_2Ge**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor**.**

Atom	*x*	*y*	*z*	U(eq)
C41	2588.5(8)	5913.9(16)	5072.5(9)	23.6(3)
C40	2532.5(7)	5308.3(16)	4458.2(8)	20.3(3)
C10	3052.8(7)	4632.2(16)	774.0(9)	21.6(3)
O3	3259.8(5)	5629.1(12)	3647.8(6)	24.8(3)
C11	3279.9(8)	3463.5(17)	992.6(9)	26.0(4)
C60	774.8(8)	8040.1(17)	2472.7(9)	25.6(3)

C42	2455.9(8)	5274.5(17)	5618.3(9)	25.0(3)
C31	5036.3(9)	6671(2)	3924.0(11)	41.8(5)
C30	4632.6(8)	7093(2)	3359(1)	32.4(4)
C54	1351.2(8)	3463.3(16)	2465.7(9)	23.5(3)
C53	1126.8(7)	4671.8(16)	2374.9(8)	20.8(3)
C52	885.6(8)	5046.8(17)	3816.0(9)	25.2(3)
C51	642.7(8)	5137.0(19)	4386.7(10)	28.8(4)
C32	5101.9(9)	5411(2)	4056.3(10)	40.4(5)
C1	3188.0(7)	5754.5(16)	2070.4(8)	20.3(3)
Ge1	2824.5(2)	4608.4(2)	2671.5(2)	19.33(7)
O2	2518.8(6)	6675.9(11)	951.9(6)	25.7(3)
S1	2726.4(2)	5555.0(4)	1330.2(2)	18.66(9)
P1	3766.1(2)	6743.8(4)	2186.1(2)	19.40(9)
C12	3507.8(8)	2712.5(18)	556.9(10)	29.1(4)
C18	3916.3(8)	7470(2)	912.8(9)	30.6(4)
C24	3099.3(8)	8613.5(17)	2577.0(9)	26.9(4)
C49	1008.8(9)	7229.0(18)	4572.4(10)	29.6(4)
C48	1253.5(8)	7144.2(17)	4006.1(9)	26.2(4)
C34	4367.2(8)	4962.6(19)	3060.7(10)	28.1(4)
C59	1256.9(7)	7331.1(15)	2382.5(8)	20.3(3)
C46	2349.9(8)	4071.6(16)	4387.9(9)	24.5(3)
C58	593.3(8)	4884.1(17)	1924.9(9)	24.5(3)
C47	1182.7(7)	6056.5(16)	3617.9(8)	21.2(3)
C0AA	3818.1(11)	10565.7(19)	2343.4(12)	38.6(5)
C23	3597.7(8)	8365.7(16)	2326.7(9)	23.6(3)
C28	3960.0(9)	9345.3(18)	2208.7(11)	31.8(4)
C29	4296.4(7)	6238.0(17)	2926.1(9)	22.8(3)
C33	4769.2(9)	4551(2)	3626.9(11)	34.2(4)
C44	2046.4(10)	3395.8(18)	6118.9(10)	32.9(4)
C26	3323.2(11)	10815.1(19)	2596.7(11)	38.0(5)
C13	3530.7(8)	3115.0(19)	-94.4(10)	28.9(4)
C50	696.2(8)	6229.5(19)	4754.5(9)	28.7(4)
C21	4851.7(11)	5856(2)	913.8(13)	43.2(5)
C27	2237.1(7)	5683.4(15)	3044.4(8)	19.8(3)
P2	1504.3(2)	5943.4(4)	2875.9(2)	18.04(9)
O4	2694.1(6)	7440.7(11)	3936.7(6)	27.0(3)
S2	2688.6(2)	6134.8(4)	3754.2(2)	19.39(9)
O1	2265.2(5)	4753.7(11)	1514.7(6)	23.0(2)
C43	2246.3(8)	4050.4(17)	5550.4(9)	24.6(3)
C45	2200.8(8)	3457.8(16)	4928.7(9)	25.5(3)
C55	1040.8(8)	2478.6(17)	2112.6(9)	25.5(3)
C56	505.5(8)	2691.6(17)	1668.1(9)	27.0(4)
C57	283.0(8)	3895.4(17)	1572.1(9)	27.3(4)
C22	4609.7(9)	5941.6(18)	1483.1(11)	32.4(4)
C25	2963.9(10)	9834.4(19)	2716.0(11)	34.3(4)
C17	4137.7(8)	6748.7(17)	1482.6(9)	25.0(3)
C20	4621.6(11)	6554(2)	346.0(11)	43.2(5)
C15	3313.2(8)	4292.8(19)	-294.6(9)	29.5(4)

C19	4157.1(10)	7364(2)	341.3(10)	37.8(5)
C62	867.5(8)	9324.0(17)	1530.8(10)	27.2(4)
C61	587.2(8)	9044.7(17)	2051.5(10)	28.1(4)
C16	3069.5(8)	5051.3(17)	131.1(9)	25.2(3)
C14	3779.0(9)	2277(2)	-564.5(11)	37.2(5)
C63	1341.3(8)	8613.5(18)	1434.2(9)	28.0(4)
C70	1087.5(12)	4272(2)	111.0(13)	46.9(6)
C71	587.8(12)	3592(2)	-127.9(12)	44.9(5)
C72	437.2(11)	3248(2)	-792.6(12)	41.9(5)
C73	783.6(12)	3575(2)	-1235.7(12)	46.4(6)
C74	1289.3(13)	4266(3)	-1007.6(17)	59.3(8)
C75	1440.8(11)	4620(2)	-318.8(17)	55.4(7)
C64	1541.0(8)	7624.1(17)	1864.5(9)	24.7(3)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **Y_2Ge**. 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^{23}	U^{13}	U^{12}
C41	22.1(8)	23.5(8)	25.2(8)	-1.2(6)	5.0(6)	-3.0(6)
C40	18.7(7)	22.2(8)	20.7(8)	0.8(6)	5.8(6)	0.1(6)
C10	18.0(8)	24.5(8)	22.6(8)	-3.9(6)	4.4(6)	-2.7(6)
O3	17.6(6)	33.8(7)	23.4(6)	2.1(5)	4.9(5)	-0.8(5)
C11	24.8(8)	29.0(9)	25.2(8)	-0.7(7)	7.6(7)	0.4(7)
C60	24.6(8)	25.5(8)	28.1(8)	-0.8(7)	8.9(7)	2.5(7)
C42	27.8(9)	26.6(9)	22.0(8)	-1.2(6)	8.2(7)	0.9(7)
C31	28.1(10)	56.3(14)	35.7(11)	-18(1)	-5.3(8)	11.8(9)
C30	24.8(9)	35.6(10)	34.7(10)	-10.3(8)	1.5(7)	5.1(8)
C54	21.4(8)	23.8(8)	26.0(8)	-1.8(6)	6.8(6)	0.1(7)
C53	20.5(8)	22.5(8)	21.1(8)	-2.4(6)	8.3(6)	-4.1(6)
C52	24.0(8)	25.1(8)	27.7(9)	-1.0(7)	8.1(7)	-0.9(7)
C51	25.3(9)	32.0(9)	30.6(9)	4.2(7)	9.4(7)	-2.4(7)
C32	28.4(10)	64.5(15)	26.3(10)	0.2(9)	1.4(8)	18.1(10)
C1	20.4(8)	21.2(7)	20.0(7)	-0.4(6)	6.2(6)	-4.1(6)
Ge1	18.78(11)	17.32(10)	23.15(11)	1.11(7)	7.28(8)	0.82(7)
O2	28.2(6)	23.0(6)	25.9(6)	3.1(5)	5.9(5)	4.7(5)
S1	17.70(18)	19.24(18)	19.54(18)	-0.41(13)	5.03(14)	-0.33(14)
P1	17.17(19)	20.4(2)	21.25(19)	-0.74(14)	5.47(15)	-1.82(14)
C12	23.9(8)	28.1(9)	35.9(10)	-5.3(7)	7.5(7)	1.9(7)
C18	27.2(9)	38.2(10)	26.5(9)	-0.1(7)	6.2(7)	-10.7(8)
C24	29.9(9)	24.5(8)	26.6(8)	1.8(7)	6.6(7)	0.4(7)
C49	32.5(9)	30.0(9)	27.2(9)	-4.8(7)	8.6(7)	1.6(8)
C48	27.9(9)	24.2(8)	27.8(9)	-1.3(7)	8.8(7)	-1.2(7)
C34	20.0(8)	33.5(9)	31.8(9)	4.5(8)	8.0(7)	-0.2(7)
C59	18.5(7)	18.5(7)	22.8(8)	-0.4(6)	2.0(6)	-1.4(6)
C46	27.3(9)	23.3(8)	22.4(8)	-2.1(6)	4.7(7)	0.4(7)
C58	21.4(8)	24.6(8)	27.5(8)	-2.4(7)	4.8(7)	-1.0(7)

C47	18.3(7)	24.3(8)	21.3(8)	1.3(6)	4.8(6)	2.2(6)
C0AA	47.5(12)	23.4(9)	43.2(12)	0.8(8)	6.2(9)	-8.1(8)
C23	25.1(8)	21.3(8)	23.7(8)	0.7(6)	3.7(6)	-0.9(7)
C28	30.8(10)	26.9(9)	38(1)	-1.4(8)	8.5(8)	-5.7(8)
C29	17.1(7)	29.5(9)	23.1(8)	-0.4(6)	7.4(6)	0.9(6)
C33	23.8(9)	45.3(12)	36(1)	12.6(8)	12.0(8)	9.8(8)
C44	40.9(11)	28.2(9)	33.3(10)	5.4(8)	16.1(8)	1.0(8)
C26	52.0(13)	23.1(9)	36.5(10)	-3.1(8)	4.2(9)	5.9(9)
C13	20.4(8)	35.9(10)	31.9(9)	-12.8(8)	9.0(7)	-4.8(7)
C50	25.2(9)	40(1)	22.8(8)	2.3(7)	9.3(7)	5.6(7)
C21	49.8(13)	38.0(11)	51.6(13)	-7.4(10)	33.0(11)	-3.1(10)
C27	17.8(7)	21.4(7)	21.3(7)	-1.2(6)	6.5(6)	-0.1(6)
P2	16.69(19)	17.56(19)	20.53(19)	-0.88(14)	5.42(15)	-0.31(14)
O4	35.5(7)	20.0(6)	26.1(6)	-1.8(5)	8.1(5)	-6.9(5)
S2	18.70(18)	20.21(19)	19.51(18)	-0.24(13)	4.61(14)	-2.69(14)
O1	19.8(6)	23.8(6)	26.7(6)	-2.6(5)	7.6(5)	-2.6(5)
C43	23.1(8)	25.2(8)	26.8(8)	3.7(7)	8.6(7)	4.4(7)
C45	27.8(9)	19.4(8)	29.9(9)	2.0(7)	7.5(7)	-1.0(7)
C55	27.3(9)	21.0(8)	30.4(9)	-3.7(7)	11.1(7)	-1.5(7)
C56	26.1(9)	27.4(9)	28.8(9)	-7.7(7)	8.5(7)	-7.7(7)
C57	21.3(8)	30.8(9)	28.9(9)	-4.0(7)	3.3(7)	-3.8(7)
C22	35.5(10)	28.3(9)	38.5(10)	-1.2(8)	19.1(8)	-1.5(8)
C25	40.5(11)	29.7(10)	34.4(10)	-0.4(8)	11.7(8)	6.8(8)
C17	24.4(8)	27.0(8)	25.5(8)	-3.4(7)	9.8(7)	-7.9(7)
C20	54.8(14)	45.6(12)	37.4(11)	-14.3(9)	28.3(10)	-22.2(11)
C15	28.1(9)	38.6(10)	23.5(8)	-4.9(7)	9.4(7)	-6.7(8)
C19	41.7(11)	47.4(12)	24.9(9)	-1.5(8)	8.1(8)	-21.6(10)
C62	29.0(9)	20.6(8)	29.4(9)	2.4(7)	0.7(7)	0.4(7)
C61	28.2(9)	24.3(9)	31.5(9)	-2.0(7)	5.5(7)	6.8(7)
C16	24.6(8)	27.4(9)	23.9(8)	-1.0(7)	5.6(7)	-3.1(7)
C14	28.7(10)	46.8(12)	38.0(11)	-16.0(9)	11.7(8)	-1.1(9)
C63	28.3(9)	28.4(9)	27.7(9)	6.1(7)	6.7(7)	-0.1(7)
C70	53.4(14)	37.5(11)	43.0(12)	-2.4(9)	-4.9(11)	8.8(10)
C71	55.6(14)	41.3(12)	36.1(11)	4.2(9)	6(1)	0.5(10)
C72	53.2(13)	28.5(10)	38.9(11)	3.5(8)	-1.8(10)	0.1(9)
C73	60.4(15)	39.5(12)	38.8(12)	1.0(9)	9.6(10)	19.7(11)
C74	51.0(15)	52.0(15)	82(2)	23.9(14)	31.4(14)	27.3(13)
C75	34.4(12)	37.6(12)	87(2)	4.9(12)	-4.4(13)	10.2(9)
C64	21.3(8)	25.8(8)	27.8(8)	0.4(7)	7.0(7)	2.3(7)

2.3 Crystal Structure of Y_2Sn

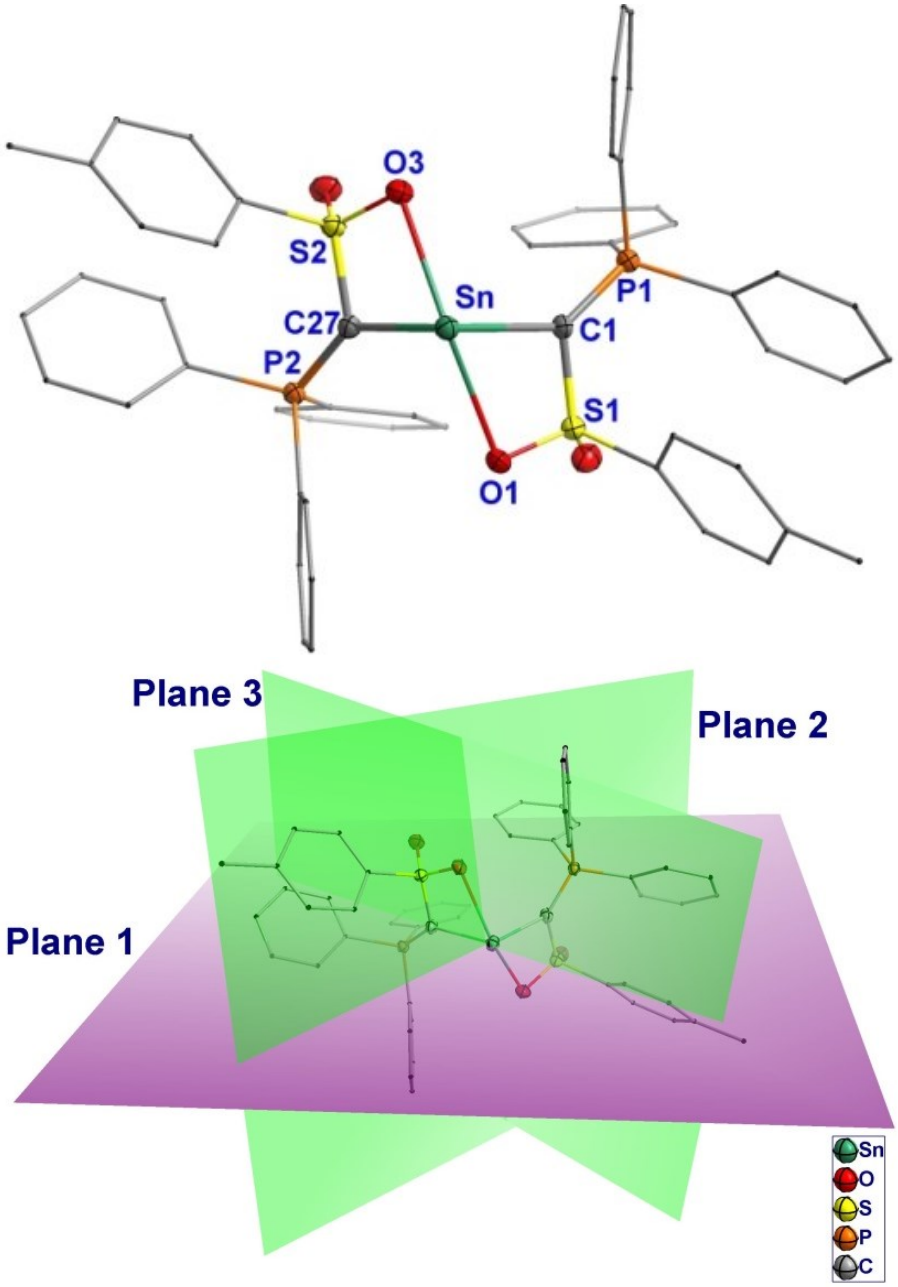


Figure S26. (top) X-Ray structure of **Y_2Sn**. (bottom) Plane passing through C1-Sn-C27 (Plane 1) and planes passing through S1-C1-P1 (Plane 2) and S2-C27-P2 (Plane 3). Dihedral angles (˚): Plane 1-Plane 2, 88.92(6); Plane 1-Plane 3, 86.20(7).

Table S5. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Y_2Sn**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sn1	8913.7(2)	-0.7(2)	1528.0(2)	17.17(5)
O1	6634.9(14)	1105.5(12)	1083.2(9)	23.6(3)
S1	6841.5(4)	2175.2(4)	652.6(3)	18.00(9)

P1	9113.6(4)	2777.8(4)	550.0(3)	15.71(9)
C1	8429.2(18)	1808.8(15)	832.8(12)	17.9(4)
C41	10491(2)	-2618.8(18)	3636.1(14)	26.0(4)
C40	10753.0(19)	-1825.3(16)	3809.2(13)	19.7(4)
C12	5055(2)	3678.0(18)	-1648.5(14)	27.0(4)
C11	5325(2)	3404.8(18)	-802.5(14)	26.4(4)
C10	6491.0(19)	2545.4(16)	-435.8(12)	18.4(4)
O4	10114.5(14)	214.6(12)	3682.1(10)	24.8(3)
C13	5934(2)	3119.9(17)	-2136.8(13)	23.3(4)
C42	11036(2)	-3733.4(18)	4147.4(14)	28.2(5)
C43	11852(2)	-4070.6(18)	4833.9(13)	25.1(4)
C27	8492.0(18)	-104.0(16)	2871.6(12)	17.5(4)
P2	7225.9(4)	-31.1(4)	3560.3(3)	15.67(9)
S2	9989.1(4)	-379.3(4)	3177.8(3)	17.74(9)
O3	10732.7(13)	-240.2(12)	2375.9(9)	22.2(3)
O2	5925.4(14)	3102.0(13)	885.6(9)	25.6(3)
C16	7371.8(19)	1968.3(16)	-911.3(13)	21.1(4)
C15	7093(2)	2252.9(18)	-1756.3(14)	24.3(4)
C14	5663(3)	3451(2)	-3065.5(15)	34.3(5)
C17	8572.4(19)	3790.2(16)	-498.1(12)	18.3(4)
C18	7408(2)	4723.8(18)	-612.6(14)	25.5(4)
C20	7595(2)	5212(2)	-2117.3(14)	29.8(5)
C19	6931(2)	5438.7(19)	-1423.5(15)	30.1(5)
C21	8734(2)	4275(2)	-2007.9(14)	29.4(5)
C22	9224(2)	3566.5(17)	-1202.3(13)	23.0(4)
C23	10886.0(18)	2120.6(16)	526.2(12)	18.2(4)
C24	11698(2)	2520.3(17)	768.5(13)	22.3(4)
C25	13053(2)	2067.9(19)	674.1(15)	28.7(5)
C26	13594(2)	1228(2)	340.6(17)	32.6(5)
C0AA	12789(2)	821(2)	105.3(17)	32.1(5)
C33	8546(2)	5198(2)	1525.6(18)	37.1(6)
C32	8442(2)	4643(2)	2381.1(18)	41.1(6)
C31	8514(2)	3554(2)	2667.1(15)	36.7(6)
C30	8688(2)	3009.5(19)	2104.0(13)	25.9(4)
C29	8806.4(19)	3561.1(17)	1245.8(13)	21.0(4)
C28	11441(2)	1261.7(18)	207.0(14)	24.7(4)
C34	8743(2)	4658.1(19)	956.8(15)	27.4(4)
C44	12420(3)	-5277.6(19)	5397.7(15)	35.1(5)
C45	12122(2)	-3266.0(19)	4985.0(14)	27.2(4)
C46	11578(2)	-2148.3(18)	4483.0(14)	25.5(4)
C47	5954.9(19)	-226.5(16)	3143.6(12)	18.4(4)
C48	4629(2)	313.5(18)	3287.4(13)	23.1(4)
C49	3666(2)	150.7(19)	2963.1(15)	28.7(5)
C51	5328(2)	-1074(2)	2350.4(15)	29.1(5)
C50	4014(2)	-532(2)	2490.9(15)	29.6(5)
C52	6295(2)	-927.1(17)	2680.0(14)	23.9(4)
C53	6418.9(18)	1291.3(16)	3721.0(12)	18.2(4)
C54	6061(2)	1380.5(17)	4516.1(14)	24.0(4)

C55	5466(2)	2425.3(19)	4586.2(16)	29.9(5)
C59	7692.2(19)	-1071.6(16)	4608.5(12)	17.9(4)
C58	6147(2)	2252.1(17)	3004.6(13)	23.5(4)
C57	5527(2)	3291.8(18)	3081.9(15)	28.8(5)
C56	5196(2)	3375.1(18)	3873.7(16)	30.0(5)
C64	8425.9(19)	-959.0(16)	5152.1(13)	20.8(4)
C63	8849(2)	-1783.6(17)	5935.7(13)	22.9(4)
C62	8562(2)	-2736.6(18)	6181.5(14)	26.1(4)
C61	7844(2)	-2854.1(19)	5642.5(14)	31.0(5)
C60	7414(2)	-2029.7(18)	4857.8(13)	25.5(4)

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **Y_2Sn**. 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^{23}	U^{13}	U^{12}
Sn1	18.52(7)	15.51(7)	17.33(7)	-4.12(5)	-1.37(5)	-7.28(5)
O1	20.5(7)	26.5(7)	22.2(7)	0.0(6)	-2.2(5)	-14.6(6)
S1	15.2(2)	19.4(2)	17.0(2)	-2.54(17)	-1.22(16)	-7.15(17)
P1	15.2(2)	15.9(2)	15.2(2)	-2.98(17)	-0.56(16)	-7.17(17)
C1	17.7(9)	14.9(8)	18.4(9)	-0.1(7)	-2.8(7)	-7.8(7)
C41	29.4(11)	22.5(10)	24.5(10)	-4.4(8)	-11.1(8)	-8.2(8)
C40	17.7(9)	18.7(9)	20.7(9)	-4.5(8)	-3.5(7)	-5.7(7)
C12	19.5(10)	25.3(10)	27.5(11)	-0.2(9)	-8.2(8)	-5.6(8)
C11	18.0(9)	26(1)	26.2(11)	-5.2(9)	-1.3(8)	-2.4(8)
C10	17.9(9)	17.5(9)	19.4(9)	-2.0(7)	-2.2(7)	-9.6(7)
O4	26.8(7)	22.6(7)	30.4(8)	-10.3(6)	-5.0(6)	-12.0(6)
C13	26.6(10)	24(1)	22(1)	-1.7(8)	-5.5(8)	-16.3(8)
C42	34.0(11)	21.1(10)	28.0(11)	-5.1(9)	-9.8(9)	-8.9(9)
C43	24.9(10)	23.7(10)	19.6(10)	-4.7(8)	-2.6(8)	-3.8(8)
C27	19.1(9)	18.9(9)	14.6(8)	-2.4(7)	-2.2(7)	-9.7(7)
P2	16.8(2)	14.9(2)	15.1(2)	-2.09(17)	-2.00(17)	-8.09(17)
S2	17.1(2)	16.7(2)	20.1(2)	-4.19(17)	-3.45(16)	-8.02(17)
O3	17.6(6)	23.2(7)	24.7(7)	-5.1(6)	-0.1(5)	-9.6(6)
O2	21.4(7)	28.8(8)	22.7(7)	-9.3(6)	1.5(6)	-5.5(6)
C16	17.8(9)	18.8(9)	23.7(10)	-5.2(8)	-6.0(7)	-4.0(7)
C15	25.6(10)	25.3(10)	24.8(10)	-10.0(8)	-1.9(8)	-10.7(8)
C14	44.2(13)	36.4(12)	23.1(11)	-3.4(9)	-8.6(10)	-19.7(11)
C17	20.0(9)	17.6(9)	18.3(9)	-2.6(7)	-0.7(7)	-11.3(7)
C18	23(1)	25(1)	21.6(10)	-3.4(8)	1.5(8)	-6.9(8)
C20	29.0(11)	33.0(12)	20.2(10)	4.4(9)	-4.2(8)	-15.9(9)
C19	25.0(11)	24.2(10)	27.9(11)	1.7(9)	-3.2(9)	-5.0(9)
C21	30.2(11)	40.4(13)	18.7(10)	-8.9(9)	2.6(8)	-16.4(10)
C22	23.8(10)	22.7(10)	21.9(10)	-7.1(8)	0.1(8)	-8.8(8)
C23	15.1(8)	17.6(9)	19.0(9)	-1.5(7)	-1.5(7)	-7.4(7)
C24	21.2(10)	21.0(9)	24.5(10)	-5.7(8)	-2.1(8)	-9.1(8)
C25	20(1)	28.7(11)	38.0(12)	-9(1)	-3.4(9)	-11.2(9)
C26	16.6(10)	31.3(12)	46.8(14)	-13.4(11)	2.0(9)	-6.7(9)
C0AA	21.6(10)	28.1(11)	47.9(14)	-18(1)	3.5(9)	-7.2(9)

C33	27.1(11)	41.2(13)	58.8(17)	-32.8(13)	6.0(11)	-16.2(10)
C32	24.6(11)	61.8(17)	52.7(16)	-43.8(15)	-2.4(10)	-9.0(11)
C31	25.4(11)	57.3(16)	25.0(11)	-20.8(11)	-5.4(9)	-5.4(11)
C30	19.4(9)	33.9(11)	21.3(10)	-8.5(9)	-4.6(8)	-6.5(8)
C29	15.7(9)	25.8(10)	23.4(10)	-9.5(8)	-0.7(7)	-8.4(8)
C28	20.2(10)	23.6(10)	31.9(11)	-9.4(9)	0.0(8)	-10.1(8)
C34	24.2(10)	29.7(11)	35.8(12)	-16.2(10)	6.3(9)	-15.3(9)
C44	42.8(13)	25.2(11)	25.5(11)	-2.8(9)	-7.6(10)	-4.1(10)
C45	27(1)	30.1(11)	20.1(10)	-8.1(9)	-8.4(8)	-4.2(9)
C46	24.2(10)	25.7(10)	27.6(11)	-10.4(9)	-7.6(8)	-7.0(8)
C47	21.6(9)	18.0(9)	14.4(8)	0.3(7)	-2.3(7)	-11.0(7)
C48	23.2(10)	24.9(10)	22.7(10)	-6.2(8)	-1.1(8)	-12.2(8)
C49	20.5(10)	33.4(12)	31.5(11)	-7.3(9)	-3.9(8)	-11.8(9)
C51	33.6(12)	34.8(12)	30.7(11)	-15(1)	1.5(9)	-21.8(10)
C50	29.2(11)	35.6(12)	30.8(11)	-8.5(10)	-5.4(9)	-20.2(10)
C52	25.2(10)	23.6(10)	25.9(10)	-7.1(8)	0.7(8)	-13.8(8)
C53	16.1(9)	17.7(9)	20.9(9)	-4.6(7)	-2.0(7)	-7.7(7)
C54	23.9(10)	21.5(10)	23.7(10)	-5.8(8)	-1.7(8)	-7.1(8)
C55	27.7(11)	29.4(11)	35.0(12)	-17.4(10)	1.3(9)	-7.6(9)
C59	20.0(9)	17.0(9)	15.7(9)	-2.1(7)	-1.5(7)	-8.9(7)
C58	24.5(10)	21.6(10)	22.1(10)	-3.4(8)	-2.6(8)	-9.4(8)
C57	27.3(11)	17.8(10)	33.9(12)	0.5(9)	-6.6(9)	-7.8(8)
C56	24.4(10)	20.5(10)	45.7(14)	-14.5(10)	-2.6(9)	-5.4(8)
C64	22.5(9)	18.1(9)	23(1)	-5.3(8)	-2.5(8)	-9.7(8)
C63	24(1)	23.5(10)	21.9(10)	-4.5(8)	-5.6(8)	-11.0(8)
C62	29.9(11)	24.8(10)	20.2(10)	1.2(8)	-6.7(8)	-13.1(9)
C61	44.8(13)	25.1(11)	25.3(11)	3.6(9)	-9.2(10)	-24.1(10)
C60	33.0(11)	25.3(10)	21(1)	-0.2(8)	-6.9(8)	-18.8(9)

2.4 Crystal Structure of 4

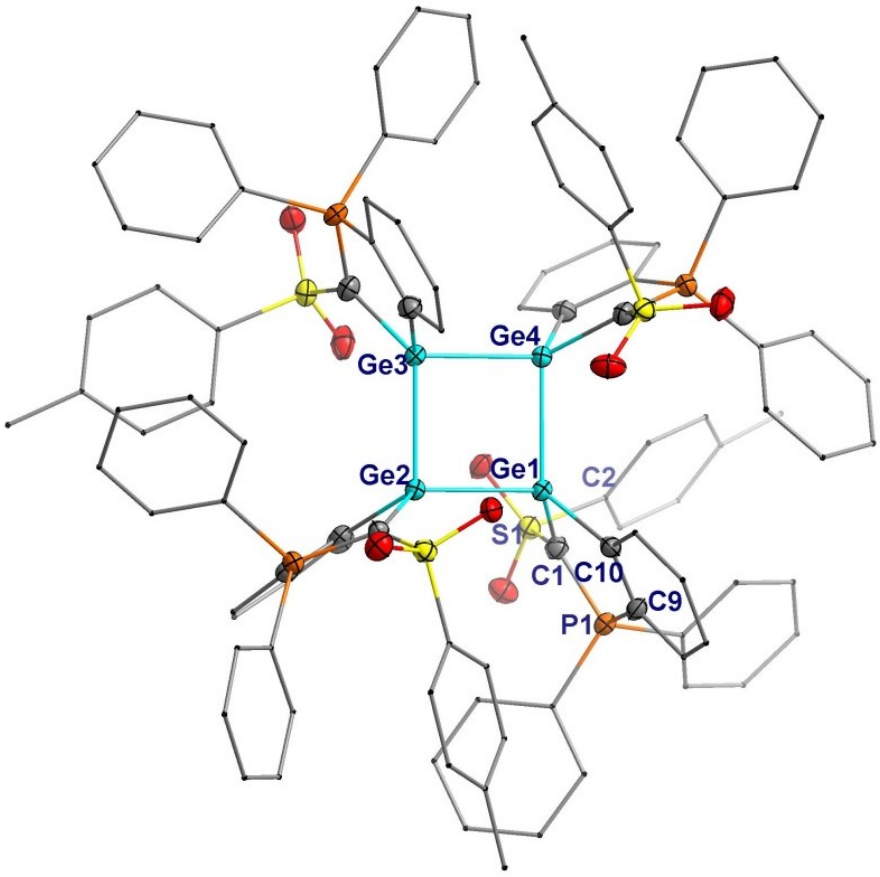


Figure S27. X-Ray structure of **4**. Selected bond lengths [Å] and angles [°]: **4**: Ge1-Ge2 2.492(4), Ge1-Ge4 2.480(5), Ge3-Ge2 2.489(4), Ge3-Ge4 2.486(5), Ge1-C1 1.933(3), Ge1-C10 1.964(3), C1-P1 1.706(3), C1-S1 1.671(3), C1-Ge1-C10 93.18(1), S1-C1-P1 121.73(2), Ge1-Ge2-Ge3 90.42(1), Ge2-Ge3-Ge4 89.38(1), Ge3-Ge4-Ge1 90.78(1), Ge4-Ge1-Ge2 89.42(1).

Table S7. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
C10	8662.6(18)	4901.0(18)	6630.7(15)	19.3(6)
C9	9107.2(19)	4028.6(18)	6666.0(15)	20.4(6)
O8	5845.5(17)	7191.4(15)	5991.6(12)	32.6(5)
C42	5599(2)	8475(2)	6388.7(16)	24.9(7)
C32	7621.4(19)	7570.5(18)	9612.5(15)	21.4(6)
O7	7110.9(14)	7262.1(14)	6100.9(12)	30.4(5)
Ge2	8850.4(2)	6079.0(2)	7646.3(2)	16.28(8)
C2	7250.4(19)	3642.2(19)	8860.1(15)	22.1(6)
P2	10415.1(5)	6359.4(5)	7425.6(4)	18.45(15)
S2	10004.4(4)	6507.2(4)	6240.3(4)	20.01(15)
C21	9748.2(18)	6390.8(18)	7042.6(15)	18.9(6)

O2	7633.7(14)	4737.2(13)	9011.3(11)	24.2(5)
Ge3	7408.5(2)	7283.2(2)	7906.3(2)	17.09(8)
Ge4	6729.5(2)	6515.8(2)	7720.5(2)	17.22(8)
C40	5837.0(18)	6255.8(19)	8424.9(15)	20.7(6)
C41	6060.9(19)	6880.6(19)	7108.3(15)	20.7(6)
C30	7220.1(19)	8322.7(18)	7303.0(15)	21.7(6)
C31	6827.3(19)	7859.9(19)	8653.2(15)	21.2(6)
C20	9480.3(19)	5565.6(18)	8318.2(15)	19.7(6)
C22	10870.8(19)	5543.6(19)	6009.8(15)	21.2(6)
C101	8635.2(19)	5367.9(19)	6025.9(15)	21.3(6)
C102	9048(2)	4973(2)	5481.4(16)	26.7(7)
C103	9502(2)	4112(2)	5527.1(16)	28.4(7)
C104	9526(2)	3637(2)	6119.9(16)	27.3(7)
C106	6564(2)	4135(2)	8581.4(18)	29.5(7)
C108	5919(2)	3168(2)	9110.3(18)	31.8(8)
C107	5907(2)	3895(2)	8710.5(19)	33.3(8)
C109	5174(3)	2938(3)	9273(2)	45.3(10)
C111	7285(2)	2903(2)	9251.2(17)	28.2(7)
C110	6616(2)	2677(2)	9374.6(18)	32.7(8)
C112	8704(2)	2694.0(19)	7561.6(16)	22.9(6)
C113	7927(2)	2992(2)	7401(2)	35.0(8)
C114	7516(3)	2478(2)	7543(2)	41.4(9)
C115	7873(2)	1670(2)	7836.9(19)	33.5(8)
C116	8635(2)	1380(2)	8001.6(18)	31.5(7)
C117	9052(2)	1889.2(19)	7865.7(17)	26.2(7)
C118	10221.2(19)	2907.5(18)	7517.4(15)	21.6(6)
C119	10457(2)	3212(2)	7880.2(16)	25.1(7)
C120	11311(2)	2855(2)	7910.7(18)	32.7(8)
C121	11931(2)	2201(2)	7571.8(19)	36.3(8)
C122	11706(2)	1894(2)	7209.9(18)	32.1(8)
C123	10850(2)	2245(2)	7176.9(16)	25.7(7)
C209	12928(2)	4778(2)	6720.7(19)	37.3(9)
C208	12058(2)	5085(2)	7058.4(17)	28.4(7)
C207	11566.5(19)	5947(2)	7023.0(16)	22.7(6)
C201	10761(2)	4814.2(19)	6278.3(16)	24.2(6)
C202	11433(2)	4053(2)	6125.4(17)	28.3(7)
C203	12228(2)	4002(2)	5702.2(17)	29.4(7)
C204	12958(3)	3164(2)	5545(2)	44(1)
C205	12326(2)	4734(2)	5436.6(17)	31.4(7)
C206	11656(2)	5503(2)	5584.0(16)	26.9(7)
C219	9576(2)	8080(2)	7305.3(18)	31.7(7)
C218	10149.1(19)	7369.2(19)	7595.4(16)	22.8(6)
C217	9282(2)	5064.2(19)	8888.6(15)	23.4(6)
C210	13302(2)	5312(3)	6355(2)	41.4(9)
C211	12815(2)	6160(3)	6309.2(18)	36.8(8)
C212	11941(2)	6483(2)	6650.2(17)	28.4(7)
C29	10224.7(18)	5699.7(18)	8170.3(15)	20.1(6)
C214	10770(2)	5326(2)	8578.5(16)	26.1(7)

C215	10577(2)	4813(2)	9134.6(17)	30.9(7)
C216	9833(2)	4689(2)	9285.6(17)	29.9(7)
C220	9410(3)	8854(2)	7409(2)	42.1(9)
C221	9802(2)	8917(2)	7800(2)	40.0(9)
C222	10351(3)	8212(3)	8097(2)	44.9(10)
C223	10533(2)	7434(2)	7996(2)	38.4(9)
C301	7537(2)	8403(2)	6638.8(16)	27.2(7)
C302	7316(2)	9181(2)	6275.1(17)	34.7(8)
C303	6766(3)	9899(2)	6574.9(19)	38.1(9)
C304	6449(2)	9832(2)	7233.8(17)	32.1(8)
C39	6676(2)	9047.6(19)	7596.2(16)	25.3(7)
C306	5092(2)	9248(2)	8627.8(16)	25.3(7)
C307	4766(2)	8656(2)	8830.1(17)	28.3(7)
C308	3882(2)	8892(3)	8935.7(19)	38.4(9)
C309	3329(2)	9721(3)	8836(2)	44.9(10)
C310	3643(2)	10325(3)	8633(2)	42.1(9)
C311	4523(2)	10092(2)	8524.8(18)	32.5(8)
C312	6431(2)	9559.3(19)	8792.3(16)	23.7(6)
C313	7277(2)	9490(2)	8609.9(18)	29.6(7)
C314	7481(2)	9918(2)	8889(2)	36.3(8)
C315	6842(2)	10423(2)	9342(2)	36.9(8)
C316	5999(2)	10501(2)	9525.1(18)	31.8(7)
C317	5797(2)	10064(2)	9247.3(16)	25.3(7)
C318	7415(2)	8155(2)	9978.9(19)	32.7(8)
C319	8070(2)	8195(2)	10125(2)	37.2(9)
C320	8934(2)	7659(2)	9908.9(17)	29.8(7)
C321	9125(2)	7088(2)	9535.0(19)	34.8(8)
C322	9643(3)	7694(3)	10074(2)	42.1(9)
C323	8479(2)	7036(2)	9388.1(19)	33.5(8)
C401	5542(3)	8994(2)	5815(2)	40.1(9)
C402	5110(3)	9846(2)	5809(2)	44.1(10)
C403	4718(2)	10196(2)	6370(2)	39.2(9)
C404	4262(3)	11131(3)	6353(2)	53.9(12)
C405	4793(3)	9673(2)	6934(2)	40.9(9)
C406	5234(3)	8811(2)	6953.0(19)	37.9(8)
C407	4217(2)	7247(2)	7283.4(17)	25.9(7)
C408	3760(2)	7899(2)	7645(2)	39.7(9)
C409	2943(3)	8494(3)	7587(3)	54.4(12)
C410	2586(2)	8438(3)	7168(2)	48.9(11)
C411	3042(2)	7805(2)	6798(2)	38.9(9)
C412	3862(2)	7203(2)	6857.4(17)	30.2(7)
C414	6359(2)	5261(2)	6606.8(17)	29.9(7)
C415	6586(3)	4540(2)	6380.4(19)	39.1(9)
C416	6045(3)	4138(2)	6612(2)	43.8(10)
C417	5270(3)	4451(2)	7074(2)	42.5(9)
C418	5031(2)	5175(2)	7299.1(19)	32.6(8)
C419	5571(2)	5586(2)	7069.7(16)	25.1(7)
C49	5186.7(19)	6261.2(19)	8231.2(15)	21.8(6)

C421	4503(2)	6093(2)	8677.6(17)	27.2(7)
C422	4470(2)	5920(2)	9320.9(17)	30.0(7)
C423	5111(2)	5919(2)	9519.5(16)	26.3(7)
C424	5789.0(19)	6080.5(19)	9076.9(16)	23.0(6)
C500	7934(4)	2841(5)	724(3)	84.3(14)
C501	7652(2)	3615(3)	991(2)	45.4(10)
C502	7529(3)	4367(4)	589(2)	58.6(14)
C503	7208(3)	5101(4)	847(3)	66.1(16)
C504	7022(3)	5075(3)	1499(3)	54.9(12)
C505	7168(2)	4330(3)	1883(2)	45.1(10)
C506	7465(2)	3617(3)	1644(2)	41.3(10)
C510	9185(6)	1184(5)	4234(4)	108(3)
C511	8918(4)	1093(5)	4958(3)	80.5(18)
C512	8763(4)	1743(4)	5240(4)	86(2)
C513	8466(4)	1721(5)	5929(4)	92(2)
C514	8350(4)	1024(4)	6267(3)	73.0(16)
C515	8531(4)	373(5)	5960(3)	78.2(18)
C516	8842(4)	371(5)	5281(4)	96(2)
C520	1337(2)	9402(3)	150(2)	41.3(9)
C521	479(2)	9493(2)	627.4(18)	31.6(7)
C522	181(2)	8885(2)	759.9(18)	30.3(7)
C523	-598(2)	8958(2)	1213.1(18)	31.2(7)
C524	-1087(2)	9639(2)	1540.0(19)	35.3(8)
C525	-795(3)	10248(2)	1413(2)	39.0(9)
C526	-24(2)	10179(2)	959.7(19)	35.1(8)
C530	3747(4)	8694(5)	5184(3)	84.3(14)
C531	3958(4)	7858(4)	5041(2)	69.4(16)
C532	4694(4)	7146(6)	5143(3)	86(2)
C533	4867(3)	6395(5)	4995(3)	81(2)
C534	4319(3)	6338(4)	4753(2)	64.0(14)
C535	3584(3)	7033(4)	4664(2)	58.2(13)
C536	3408(3)	7785(3)	4801(2)	56.9(12)
C540	640(4)	390(4)	6661(3)	70.6(15)
C541	2000(3)	601(3)	6116(2)	46.8(10)
C542	2480(4)	977(3)	5674(3)	64.1(13)
C543	2145(4)	1581(3)	5242(3)	64.7(14)
C544	1319(4)	1834(3)	5216(2)	59.6(15)
C545	789(4)	1432(3)	5689(3)	67.0(15)
C546	1162(3)	799(2)	6156(2)	42.6(9)
C550	3096(4)	2812(4)	8372(4)	91(2)
C551	3990(4)	2522(3)	7989(3)	66.1(15)
C552	4216(5)	2565(3)	7319(3)	76.5(19)
C553	5058(6)	2325(4)	6957(4)	87(2)
C554	5719(5)	2015(3)	7240(4)	88(2)
C555	5506(4)	1937(3)	7911(4)	74.4(17)
C556	4663(4)	2185(3)	8269(3)	66.0(15)
C1	8441.9(19)	4208.0(18)	7940.6(15)	20.4(6)
Ge1	8164.5(2)	5313.6(2)	7460.8(2)	16.15(8)

P1	9109.4(5)	3452.1(4)	7456.9(4)	18.78(15)
O1	8734.5(14)	3270.6(14)	9002.7(11)	27.0(5)
S1	8068.2(4)	3975.7(4)	8729.7(4)	19.57(14)
O5	5986.6(14)	8028.1(15)	9822.8(11)	27.8(5)
O6	7024.0(16)	6605.5(14)	9535.6(12)	30.5(5)
O3	10356.3(15)	7118.5(14)	5956.0(11)	27.0(5)
O4	9272.5(14)	6623.6(13)	6048.6(11)	24.0(5)
P4	5285.2(5)	6513.1(5)	7381.5(4)	20.48(16)
P3	6259.0(5)	8901.0(5)	8450.1(4)	20.24(15)
S4	6217.0(5)	7383.4(4)	6363.0(4)	21.43(15)
S3	6798.6(5)	7484.9(5)	9427.6(4)	20.67(15)

Table S8. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4**. 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^{23}	U^{13}	U^{12}
C10	15.6(13)	22.7(14)	20.5(16)	-5.2(12)	-6.1(11)	-6.6(11)
C9	21.5(14)	19.5(14)	21.4(16)	-8.0(12)	-3.5(12)	-8.5(11)
O8	45.0(14)	29.9(12)	29.9(14)	-5.6(10)	-19.8(11)	-13.6(11)
C42	19.7(14)	25.4(15)	28.3(18)	-9.5(13)	-7.0(13)	-5.1(12)
C32	22.6(14)	21.6(14)	21.4(16)	-4.0(12)	-7.0(12)	-8.9(12)
O7	20.9(11)	28.7(12)	30.0(13)	-3.4(10)	-1.8(10)	-5.9(9)
Ge2	14.61(15)	16.46(15)	18.79(18)	-5.55(12)	-4.50(13)	-5.66(12)
C2	20.0(14)	22.3(14)	21.7(16)	-8.1(12)	0.4(12)	-8.8(12)
P2	14.6(3)	20.6(3)	21.5(4)	-5.9(3)	-4.9(3)	-6.8(3)
S2	18.8(3)	20.8(3)	19.9(4)	-3.1(3)	-5.8(3)	-7.5(3)
C21	15.4(13)	23.7(14)	19.2(15)	-5.6(12)	-4.6(11)	-8.0(11)
O2	23.3(10)	27.6(11)	23.0(12)	-13.5(9)	-0.5(9)	-10.4(9)
Ge3	15.96(15)	15.84(15)	19.60(18)	-6.13(13)	-4.86(13)	-4.78(12)
Ge4	14.62(15)	18.83(16)	19.13(18)	-6.52(13)	-4.76(13)	-5.51(12)
C40	15.4(13)	23.9(14)	22.8(16)	-6.3(12)	-4.3(12)	-7.3(11)
C41	19.8(14)	23.2(14)	20.2(16)	-6.6(12)	-5.4(12)	-8.0(12)
C30	22.6(14)	18.3(14)	23.6(17)	-4.9(12)	-7.1(12)	-6.6(12)
C31	22.1(14)	22.5(14)	20.0(16)	-7.7(12)	-4.9(12)	-8.1(12)
C20	19.0(13)	18.2(13)	23.0(16)	-9.3(11)	-6.3(12)	-4.7(11)
C22	20.9(14)	24.9(15)	17.4(15)	-4.7(12)	-6.7(12)	-7.3(12)
C101	19.0(14)	23.6(15)	22.6(16)	-7.3(12)	-5.3(12)	-7.9(12)
C102	27.6(16)	32.0(17)	21.1(17)	-5.9(13)	-9.1(13)	-10.2(13)
C103	30.6(17)	32.2(17)	20.3(17)	-15.1(13)	-4.0(13)	-7.6(14)
C104	29.1(16)	23.6(15)	27.2(18)	-8.2(13)	-8.8(14)	-6.4(13)
C106	26.8(16)	23.8(16)	39(2)	-2.2(14)	-11.4(15)	-11.2(13)
C108	28.4(17)	30.6(17)	38(2)	-19.3(15)	4.2(15)	-15.2(14)
C107	26.4(16)	28.9(17)	47(2)	-10.4(16)	-10.6(16)	-10.6(14)
C109	39(2)	50(2)	56(3)	-26(2)	8.0(19)	-30.2(19)
C111	30.3(16)	22.7(15)	29.2(19)	-3.0(13)	-6.7(14)	-10.8(13)
C110	39.7(19)	26.8(17)	31(2)	-5.6(14)	-0.4(15)	-19.6(15)

C112	22.8(15)	22.1(15)	23.4(17)	-7.7(12)	-4.4(12)	-8.0(12)
C113	37.9(19)	24.2(16)	51(2)	-1.2(15)	-22.6(18)	-13.6(15)
C114	36.7(19)	33.0(19)	67(3)	-2.6(18)	-28(2)	-16.0(16)
C115	34.8(18)	29.3(17)	45(2)	-9.0(15)	-12.2(16)	-17.3(15)
C116	33.6(18)	24.2(16)	38(2)	-4.0(14)	-11.5(15)	-12.3(14)
C117	25.9(15)	21.6(15)	32.6(19)	-5.6(13)	-9.3(14)	-9.2(13)
C118	19.1(14)	20.6(14)	22.8(16)	-3.9(12)	-4.3(12)	-7.2(11)
C119	22.2(15)	26.0(15)	27.0(18)	-10.6(13)	-3.2(13)	-8.7(12)
C120	25.4(16)	40.8(19)	38(2)	-10.6(16)	-9.7(15)	-14.5(15)
C121	20.3(16)	41(2)	44(2)	-6.1(17)	-8.2(15)	-10.4(14)
C122	20.8(15)	32.3(18)	34(2)	-11.7(15)	1.4(14)	-6.5(13)
C123	23.1(15)	24.0(15)	27.0(18)	-9.4(13)	-2.7(13)	-7.3(12)
C209	23.3(16)	36.7(19)	36(2)	-11.5(16)	-6.5(15)	1.4(14)
C208	23.6(15)	30.3(17)	27.4(18)	-6.7(14)	-7.7(14)	-6.4(13)
C207	16.5(13)	29.9(16)	23.6(17)	-7.4(13)	-5.6(12)	-9.2(12)
C201	22.0(15)	26.2(16)	23.4(17)	-7.0(13)	-4.0(13)	-8.9(12)
C202	28.3(16)	23.3(15)	29.0(19)	-3.4(13)	-8.3(14)	-7.3(13)
C203	25.6(16)	29.6(17)	22.8(18)	-7.7(13)	-7.2(13)	-1.3(13)
C204	33.2(19)	34(2)	41(2)	-8.8(17)	-4.3(17)	1.6(16)
C205	20.3(15)	38.6(19)	25.8(18)	-8.5(15)	0.5(13)	-7.9(14)
C206	23.8(15)	31.9(17)	23.1(17)	-3.0(13)	-4.9(13)	-11.9(13)
C219	32.5(17)	29.0(17)	33(2)	-9.7(14)	-9.4(15)	-9.1(14)
C218	17.5(13)	24.5(15)	27.3(17)	-7.1(13)	-1.4(12)	-11.0(12)
C217	23.3(15)	23.0(15)	22.9(17)	-6.5(12)	-3.4(12)	-9.2(12)
C210	17.6(16)	59(3)	40(2)	-19.5(19)	-3.2(15)	-7.1(16)
C211	27.2(17)	56(2)	30(2)	-11.2(17)	0.8(15)	-23.3(17)
C212	21.9(15)	35.0(18)	29.8(19)	-9.8(14)	-4.6(13)	-12.0(14)
C29	16.9(13)	22.2(14)	19.8(16)	-9.4(12)	-3.1(12)	-5.0(11)
C214	23.8(15)	33.0(17)	24.0(17)	-7.4(13)	-8.4(13)	-10.7(13)
C215	29.3(17)	37.7(19)	25.1(18)	-2.3(14)	-13.9(14)	-10.3(14)
C216	34.0(17)	31.8(17)	24.9(18)	-3.0(14)	-10.0(14)	-13.9(14)
C220	45(2)	24.2(17)	51(3)	-10.9(16)	-9.9(19)	-9.2(16)
C221	40(2)	33.8(19)	53(3)	-21.9(18)	2.0(18)	-21.5(16)
C222	43(2)	42(2)	65(3)	-25(2)	-17(2)	-18.0(18)
C223	33.0(18)	35.5(19)	55(3)	-13.3(17)	-19.4(18)	-12.0(15)
C301	30.8(16)	26.2(16)	22.4(17)	-7.6(13)	-5.3(14)	-9.3(13)
C302	45(2)	30.5(18)	20.5(18)	-5.8(14)	-5.7(15)	-10.8(16)
C303	49(2)	20.3(16)	31(2)	1.3(14)	-9.9(17)	-7.0(15)
C304	36.7(18)	20.4(15)	27.5(19)	-7.9(13)	-3.4(15)	-4.5(14)
C39	23.1(15)	21.7(15)	27.6(18)	-7.7(13)	-5.7(13)	-5.2(12)
C306	21.2(15)	28.1(16)	24.8(17)	-9.4(13)	-7.7(13)	-4.9(12)
C307	25.7(16)	34.2(17)	26.8(18)	-14.1(14)	-4.5(13)	-10.6(14)
C308	32.0(18)	57(2)	35(2)	-16.8(18)	-6.3(16)	-22.0(18)
C309	21.9(17)	69(3)	42(2)	-21(2)	-8.6(16)	-10.8(18)
C310	25.8(17)	45(2)	40(2)	-16.5(18)	-10.2(16)	3.0(16)
C311	29.4(17)	29.0(17)	33(2)	-8.5(15)	-10.9(15)	-4.1(14)
C312	25.1(15)	19.7(14)	25.9(17)	-5.9(12)	-5.3(13)	-8.9(12)
C313	28.7(16)	27.9(16)	33(2)	-11.1(14)	1.1(14)	-15.4(14)

C314	31.7(18)	37.0(19)	47(2)	-17.3(17)	-1.1(16)	-19.9(15)
C315	42(2)	36.2(19)	45(2)	-15.3(17)	-8.4(17)	-23.1(17)
C316	36.2(18)	27.6(17)	33(2)	-13.4(14)	-1.8(15)	-14.9(14)
C317	24.5(15)	25.8(15)	25.6(18)	-7.8(13)	-2.0(13)	-11.8(13)
C318	24.5(16)	35.6(18)	40(2)	-23.5(16)	-4.1(15)	-7.8(14)
C319	34.9(19)	41(2)	47(2)	-24.4(17)	-11.6(17)	-13.9(16)
C320	29.3(17)	35.4(18)	29.6(19)	-4.0(14)	-9.4(14)	-16.5(14)
C321	20.2(15)	44(2)	38(2)	-21.3(17)	-7.9(15)	-3.7(14)
C322	36(2)	54(2)	50(3)	-13.0(19)	-15.1(18)	-23.2(18)
C323	27.6(17)	34.0(18)	40(2)	-23.7(16)	-10.4(15)	-3.0(14)
C401	49(2)	31.1(19)	34(2)	-5.9(16)	-14.8(18)	-8.2(16)
C402	55(2)	31.9(19)	39(2)	-2.7(17)	-20.3(19)	-9.7(18)
C403	33.6(19)	25.6(18)	52(3)	-8.9(16)	-13.3(18)	-4.5(15)
C404	54(3)	29(2)	63(3)	-15(2)	-12(2)	-3.4(18)
C405	40(2)	34.1(19)	45(2)	-18.8(17)	-14.7(18)	-3.5(16)
C406	44(2)	33.9(19)	33(2)	-8.7(16)	-15.9(17)	-7.9(16)
C407	17.9(14)	29.0(16)	30.2(18)	-5.4(13)	-8.6(13)	-7.3(12)
C408	28.4(18)	40(2)	53(3)	-23.4(18)	-16.4(17)	-2.8(15)
C409	32(2)	39(2)	83(4)	-29(2)	-20(2)	6.7(17)
C410	25.4(18)	39(2)	72(3)	-3(2)	-24(2)	-0.1(16)
C411	31.5(18)	45(2)	44(2)	3.0(17)	-23.5(17)	-14.8(16)
C412	27.4(16)	35.1(18)	30.2(19)	-2.7(14)	-12.2(14)	-12.8(14)
C414	28.0(16)	28.6(17)	29.8(19)	-9.1(14)	-8.8(14)	-6.0(13)
C415	48(2)	30.6(18)	32(2)	-13.7(15)	-14.1(17)	-3.7(16)
C416	65(3)	28.2(18)	45(2)	-9.1(17)	-27(2)	-13.3(18)
C417	54(2)	39(2)	50(3)	-7.5(18)	-22(2)	-25.1(19)
C418	33.7(18)	33.3(18)	37(2)	-9.5(15)	-11.3(16)	-15.3(15)
C419	25.9(15)	26.8(16)	25.8(17)	-3.5(13)	-13.6(13)	-8.9(13)
C49	17.1(13)	24.1(15)	22.7(17)	-9.6(12)	-2.2(12)	-6.3(12)
C421	18.9(14)	34.1(17)	29.5(19)	-8.4(14)	-5.5(13)	-10.5(13)
C422	19.4(15)	38.6(19)	30.8(19)	-11.3(15)	0.8(13)	-13.2(14)
C423	26.1(16)	31.7(17)	19.6(17)	-9.4(13)	-0.6(13)	-11.8(13)
C424	20.2(14)	23.8(15)	26.5(17)	-6.7(12)	-8.7(13)	-7.1(12)
C500	87(3)	119(4)	68(3)	-37(3)	2(2)	-63(3)
C501	24.2(17)	78(3)	39(2)	-10(2)	-7.0(16)	-25.6(19)
C502	43(2)	116(5)	25(2)	9(2)	-13.9(18)	-47(3)
C503	53(3)	80(4)	75(4)	35(3)	-41(3)	-44(3)
C504	40(2)	64(3)	72(3)	0(2)	-28(2)	-27(2)
C505	29.8(19)	75(3)	40(2)	-4(2)	-15.1(17)	-27(2)
C506	29.8(18)	62(3)	36(2)	7.3(19)	-14.9(16)	-26.0(18)
C510	133(7)	107(6)	81(5)	-22(4)	-6(5)	-60(5)
C511	68(4)	95(5)	79(5)	-7(4)	-30(3)	-31(3)
C512	58(3)	74(4)	126(6)	26(4)	-37(4)	-41(3)
C513	61(4)	102(5)	100(6)	15(4)	-27(4)	-37(4)
C514	56(3)	98(5)	67(4)	-1(3)	-16(3)	-40(3)
C515	66(3)	116(5)	66(4)	1(4)	-21(3)	-55(4)
C516	84(4)	107(5)	108(6)	30(4)	-48(4)	-58(4)
C520	32.0(19)	43(2)	47(2)	-1.4(18)	-15.5(18)	-13.8(16)

C521	29.6(17)	33.4(18)	33(2)	-1.3(15)	-15.5(15)	-11.4(14)
C522	30.0(17)	28.1(17)	36(2)	-7.9(14)	-16.4(15)	-7.2(14)
C523	34.5(18)	25.4(16)	36(2)	-3.0(14)	-15.1(16)	-11.6(14)
C524	32.6(18)	34.2(19)	35(2)	-7.0(15)	-7.1(16)	-11.2(15)
C525	43(2)	31.9(19)	43(2)	-12.8(16)	-10.6(18)	-13.2(16)
C526	42(2)	30.2(18)	41(2)	-4.2(15)	-16.3(17)	-17.4(16)
C530	87(3)	119(4)	68(3)	-37(3)	2(2)	-63(3)
C531	78(4)	118(5)	35(3)	-30(3)	14(2)	-69(4)
C532	62(3)	183(8)	45(3)	-40(4)	2(3)	-74(5)
C533	40(3)	134(6)	50(3)	-25(4)	-5(2)	-21(3)
C534	45(3)	87(4)	50(3)	-30(3)	-2(2)	-16(3)
C535	46(2)	89(4)	45(3)	-29(3)	-7(2)	-25(2)
C536	55(3)	75(3)	37(3)	-17(2)	-4(2)	-27(2)
C540	58(3)	65(3)	88(4)	-15(3)	-13(3)	-29(3)
C541	50(2)	44(2)	47(3)	-10.6(19)	-7(2)	-20.8(19)
C542	75(3)	66(3)	54(3)	-13(3)	-8(3)	-36(3)
C543	74(4)	62(3)	51(3)	-23(3)	2(3)	-28(3)
C544	99(4)	30(2)	23(2)	-8.3(16)	-21(2)	-2(2)
C545	63(3)	61(3)	70(4)	-40(3)	-26(3)	2(2)
C546	46(2)	33.4(19)	48(3)	-15.1(17)	-12.8(19)	-11.6(17)
C550	94(5)	78(4)	135(7)	2(4)	-53(5)	-56(4)
C551	79(4)	42(2)	95(5)	-2(3)	-43(3)	-29(2)
C552	136(6)	44(3)	84(4)	16(3)	-74(4)	-47(3)
C553	137(7)	59(3)	81(5)	-12(3)	-20(5)	-59(4)
C554	121(6)	37(3)	126(6)	-11(3)	-50(5)	-36(3)
C555	88(4)	45(3)	102(5)	-8(3)	-48(4)	-23(3)
C556	93(4)	48(3)	85(4)	3(3)	-55(4)	-36(3)
C1	19.7(14)	17.6(13)	24.5(17)	-5.1(12)	-4.5(12)	-8.2(11)
Ge1	15.26(15)	15.83(15)	17.81(18)	-5.75(12)	-3.88(13)	-5.47(12)
P1	18.9(3)	16.3(3)	21.7(4)	-6.3(3)	-5.4(3)	-6.0(3)
O1	23.1(11)	29.1(12)	25.5(12)	-0.3(9)	-7.4(9)	-9.9(9)
S1	19.1(3)	20.5(3)	19.5(4)	-4.7(3)	-4.2(3)	-8.3(3)
O5	21.1(11)	40.6(13)	23.2(12)	-11(1)	-1.6(9)	-13.7(10)
O6	43.1(14)	26.0(12)	34.1(14)	1.9(10)	-19.2(11)	-20.5(10)
O3	29.6(11)	25.3(11)	25.5(12)	-2.6(9)	-5.2(10)	-13.3(9)
O4	22.5(10)	25.3(11)	25.4(12)	-6.9(9)	-10.9(9)	-6.1(9)
P4	15.7(3)	23.7(4)	23.1(4)	-7.8(3)	-6.3(3)	-6.0(3)
P3	19.7(3)	17.1(3)	22.5(4)	-8.6(3)	-4.2(3)	-4.7(3)
S4	20.2(3)	21.7(3)	20.1(4)	-5.8(3)	-6.4(3)	-4.9(3)
S3	22.5(3)	23.5(3)	19.9(4)	-4.4(3)	-5.7(3)	-11.9(3)

2.5 Crystal Structure of 5a

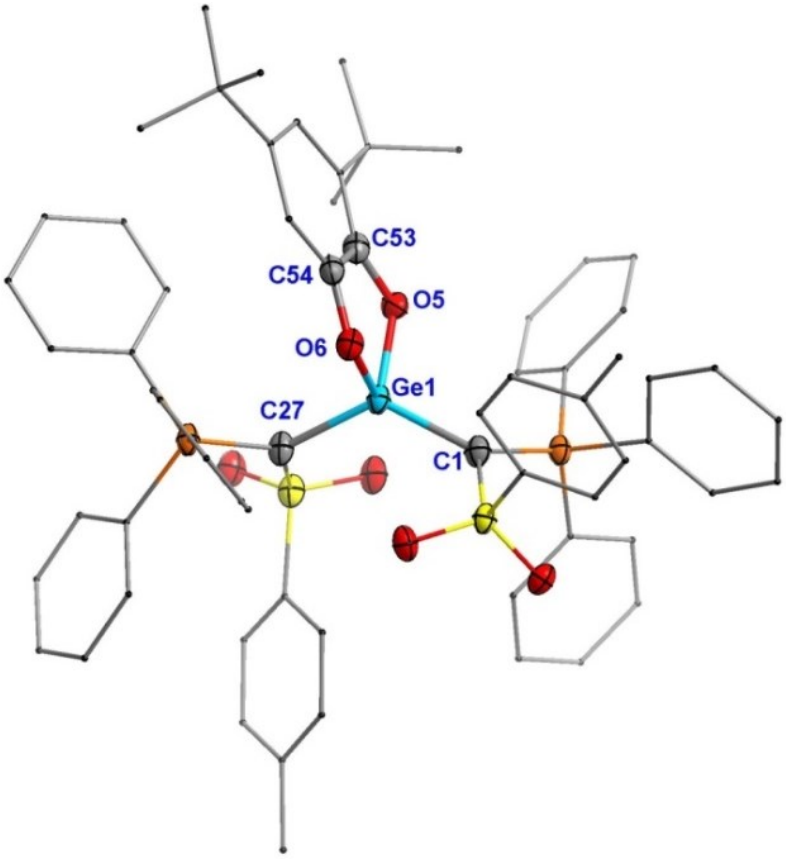


Figure S28. X-Ray structure of **5a**. Selected bond lengths [Å] and angles [°]: **5a**: Ge1-C1 1.899(3), Ge1-C27 1.919(3), Ge1-O6 1.845(2), Ge1-O5 1.842(2), C53-O5 1.373(3), C54-O6 1.344(4), C1-Ge1-C27 126.21(1), O5-Ge1-O6 90.23(1).

Table S9. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ge1	4643(1)	3624(1)	7641(1)	19(1)
S1	4262(1)	4634(1)	6417(1)	20(1)
S2	5435(1)	4877(1)	8399(1)	22(1)
P1	6870(1)	3637(1)	6367(1)	20(1)
P2	2781(1)	4635(1)	8906(1)	21(1)
O1	4997(2)	5130(1)	5942(1)	24(1)
O2	3241(2)	5147(2)	6882(1)	26(1)
O3	6480(2)	4455(2)	7898(1)	27(1)
O4	5698(2)	4802(2)	9018(1)	28(1)
O5	5606(2)	2531(1)	7851(1)	24(1)
O6	3214(2)	3109(2)	7725(1)	26(1)
C1	5294(3)	3903(2)	6795(2)	22(1)
C2	3460(3)	4018(2)	6008(2)	21(1)
C3	2626(3)	3497(2)	6342(2)	28(1)

C4	2027(3)	3011(2)	6018(2)	30(1)
C5	2240(3)	3037(2)	5371(2)	28(1)
C6	3054(3)	3591(2)	5047(2)	29(1)
C7	3662(3)	4080(2)	5366(2)	26(1)
C8	1619(4)	2482(3)	5019(2)	40(1)
C9	6839(3)	3274(2)	5594(2)	27(1)
C10	6167(3)	2591(2)	5572(2)	32(1)
C11	6089(4)	2288(3)	4997(2)	44(1)
C12	6675(5)	2669(3)	4453(2)	53(1)
C13	7337(4)	3347(3)	4474(2)	47(1)
C14	7422(3)	3659(2)	5046(2)	32(1)
C15	7750(3)	4549(2)	6287(2)	24(1)
C16	7178(3)	5372(2)	6577(2)	26(1)
C17	7891(4)	6046(2)	6550(2)	32(1)
C18	9176(4)	5895(3)	6239(2)	37(1)
C19	9754(3)	5076(3)	5949(2)	40(1)
C20	9048(3)	4398(2)	5979(2)	32(1)
C21	7974(3)	2715(2)	6676(2)	25(1)
C22	8460(3)	1892(2)	6360(2)	32(1)
C23	9445(4)	1266(3)	6548(2)	37(1)
C24	9937(3)	1437(2)	7054(2)	35(1)
C25	9450(3)	2247(3)	7366(2)	33(1)
C26	8476(3)	2887(2)	7182(2)	31(1)
C27	4158(3)	4451(2)	8326(2)	22(1)
C28	5119(3)	6062(2)	8210(2)	26(1)
C29	4560(3)	6359(2)	7707(2)	26(1)
C30	4390(4)	7271(2)	7532(2)	32(1)
C31	4771(4)	7884(3)	7872(2)	38(1)
C32	5282(4)	7576(3)	8384(2)	41(1)
C33	5482(4)	6659(3)	8561(2)	35(1)
C34	4606(6)	8873(3)	7669(2)	57(1)
C35	2579(3)	5726(2)	9264(2)	21(1)
C36	1973(3)	6521(2)	9001(2)	29(1)
C37	1892(4)	7355(2)	9259(2)	34(1)
C38	2429(4)	7396(2)	9776(2)	33(1)
C39	3025(3)	6613(2)	10040(2)	29(1)
C40	3106(3)	5780(2)	9789(2)	25(1)
C41	2731(3)	3833(2)	9552(2)	24(1)
C42	1730(3)	4034(2)	10084(2)	29(1)
C43	1641(4)	3410(2)	10570(2)	33(1)
C44	2537(4)	2591(2)	10532(2)	35(1)
C45	3537(4)	2407(2)	10015(2)	35(1)
C46	3644(3)	3035(2)	9528(2)	29(1)
C47	1367(3)	4661(2)	8577(2)	27(1)
C48	378(3)	4212(2)	8849(2)	30(1)
C49	-695(4)	4305(3)	8568(2)	42(1)
C50	-772(4)	4818(3)	8038(2)	41(1)
C51	219(4)	5253(3)	7763(2)	38(1)

C52	1279(3)	5175(3)	8036(2)	30(1)
C53	4738(3)	2013(2)	8132(2)	24(1)
C54	3449(3)	2343(2)	8062(2)	25(1)
C55	2467(3)	1905(2)	8352(2)	26(1)
C56	2768(3)	1127(2)	8705(2)	28(1)
C57	4055(3)	798(2)	8757(2)	27(1)
C58	5065(3)	1229(2)	8471(2)	26(1)
C59	1672(3)	673(2)	9049(2)	36(1)
C60	698(5)	1353(3)	9493(3)	61(1)
C61	970(5)	387(3)	8584(3)	56(1)
C62	2159(4)	-173(3)	9413(3)	57(1)
C63	6464(3)	842(2)	8538(2)	28(1)
C64	6977(3)	1548(2)	8839(2)	34(1)
C65	7307(3)	608(2)	7888(2)	33(1)
C66	6595(4)	-23(2)	8942(2)	38(1)
C11	791(5)	501(4)	4636(4)	78(2)
C21	1310(5)	-296(4)	4886(3)	76(2)
C31	541(6)	-811(4)	5251(4)	80(2)
C12	4483(6)	272(5)	4079(3)	81(2)
C22	5751(6)	84(4)	4133(3)	77(2)
C32	6634(6)	-551(4)	3776(3)	66(1)
C42	6249(6)	-1004(3)	3340(3)	65(1)
C52	4998(5)	-835(3)	3292(2)	54(1)
C62	4109(6)	-215(4)	3650(3)	64(1)

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **5a**. 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^{23}	U^{13}	U^{12}
Ge1	17(1)	23(1)	18(1)	-1(1)	-2(1)	-7(1)
S1	17(1)	26(1)	18(1)	-1(1)	-2(1)	-6(1)
S2	16(1)	31(1)	21(1)	-4(1)	-3(1)	-9(1)
P1	17(1)	24(1)	19(1)	-2(1)	0(1)	-6(1)
P2	17(1)	28(1)	18(1)	-4(1)	0(1)	-8(1)
O1	22(1)	29(1)	21(1)	3(1)	-3(1)	-9(1)
O2	20(1)	32(1)	23(1)	-6(1)	-3(1)	-2(1)
O3	14(1)	39(1)	27(1)	-4(1)	0(1)	-9(1)
O4	26(1)	36(1)	23(1)	-3(1)	-6(1)	-9(1)
O5	19(1)	23(1)	28(1)	-1(1)	0(1)	-7(1)
O6	25(1)	31(1)	21(1)	-1(1)	-2(1)	-7(1)
C1	18(1)	27(1)	23(2)	-2(1)	-2(1)	-6(1)
C2	15(1)	28(1)	20(2)	0(1)	-4(1)	-5(1)
C3	26(2)	39(2)	22(2)	5(1)	-4(1)	-12(1)
C4	25(2)	34(2)	33(2)	5(1)	-8(1)	-13(1)
C5	23(2)	33(2)	32(2)	-4(1)	-9(1)	-9(1)
C6	30(2)	39(2)	21(2)	-2(1)	-7(1)	-12(1)

C7	23(2)	33(2)	24(2)	3(1)	-3(1)	-10(1)
C8	41(2)	49(2)	39(2)	-7(2)	-11(2)	-21(2)
C9	26(2)	27(2)	25(2)	-7(1)	-3(1)	1(1)
C10	30(2)	33(2)	33(2)	-8(1)	-6(2)	-1(1)
C11	48(2)	38(2)	50(3)	-21(2)	-20(2)	2(2)
C12	60(3)	58(3)	34(2)	-23(2)	-16(2)	12(2)
C13	48(2)	56(2)	25(2)	-9(2)	-1(2)	12(2)
C14	32(2)	36(2)	23(2)	0(1)	-1(2)	2(1)
C15	20(1)	31(2)	24(2)	4(1)	-7(1)	-8(1)
C16	24(2)	33(2)	23(2)	-1(1)	-4(1)	-9(1)
C17	36(2)	33(2)	31(2)	0(1)	-12(2)	-15(1)
C18	34(2)	42(2)	45(2)	12(2)	-20(2)	-22(2)
C19	22(2)	47(2)	52(3)	10(2)	-5(2)	-16(2)
C20	21(2)	34(2)	39(2)	1(1)	1(2)	-8(1)
C21	19(1)	28(2)	25(2)	0(1)	1(1)	-5(1)
C22	29(2)	29(2)	36(2)	-2(1)	-9(2)	-2(1)
C23	31(2)	35(2)	42(2)	-6(2)	-3(2)	-1(1)
C24	24(2)	38(2)	40(2)	5(2)	-5(2)	0(1)
C25	25(2)	45(2)	28(2)	1(1)	-6(1)	-6(1)
C26	22(2)	36(2)	33(2)	-3(1)	-3(1)	-4(1)
C27	16(1)	32(2)	20(2)	-5(1)	-2(1)	-11(1)
C28	22(1)	30(2)	25(2)	-4(1)	1(1)	-10(1)
C29	24(2)	29(2)	26(2)	-7(1)	2(1)	-10(1)
C30	36(2)	37(2)	25(2)	-1(1)	-2(2)	-12(1)
C31	45(2)	36(2)	36(2)	-1(2)	-3(2)	-17(2)
C32	53(2)	37(2)	42(2)	-6(2)	-12(2)	-24(2)
C33	38(2)	43(2)	32(2)	-2(2)	-9(2)	-21(2)
C34	83(4)	39(2)	55(3)	1(2)	-14(3)	-26(2)
C35	17(1)	26(1)	20(2)	-5(1)	0(1)	-7(1)
C36	26(2)	40(2)	23(2)	-2(1)	-6(1)	-10(1)
C37	35(2)	29(2)	39(2)	0(1)	-11(2)	-4(1)
C38	39(2)	28(2)	34(2)	-6(1)	-6(2)	-8(1)
C39	30(2)	36(2)	24(2)	-6(1)	-4(1)	-12(1)
C40	23(2)	27(2)	27(2)	-2(1)	-3(1)	-7(1)
C41	24(2)	32(2)	17(2)	-3(1)	-1(1)	-13(1)
C42	25(2)	33(2)	29(2)	-4(1)	1(1)	-10(1)
C43	30(2)	43(2)	25(2)	-1(1)	4(2)	-13(1)
C44	43(2)	38(2)	28(2)	7(1)	-10(2)	-17(2)
C45	40(2)	33(2)	32(2)	-4(1)	-9(2)	-6(1)
C46	27(2)	35(2)	24(2)	-8(1)	-1(1)	-8(1)
C47	16(1)	37(2)	26(2)	-14(1)	4(1)	-9(1)
C48	21(2)	42(2)	28(2)	-13(1)	4(1)	-13(1)
C49	24(2)	55(2)	49(3)	-18(2)	4(2)	-20(2)
C50	21(2)	69(3)	40(2)	-15(2)	-8(2)	-17(2)
C51	24(2)	62(2)	30(2)	-7(2)	-7(2)	-10(2)
C52	16(1)	53(2)	23(2)	-9(1)	-2(1)	-11(1)
C53	23(2)	30(2)	22(2)	-6(1)	-1(1)	-12(1)
C54	25(2)	28(2)	22(2)	-7(1)	1(1)	-9(1)

C55	20(1)	32(2)	30(2)	-2(1)	-6(1)	-11(1)
C56	26(2)	30(2)	31(2)	0(1)	-2(1)	-14(1)
C57	30(2)	23(1)	29(2)	0(1)	-4(1)	-8(1)
C58	25(2)	26(2)	28(2)	-7(1)	-4(1)	-7(1)
C59	28(2)	38(2)	44(2)	7(2)	-4(2)	-16(1)
C60	48(3)	62(3)	64(3)	-1(2)	20(2)	-24(2)
C61	47(2)	58(3)	73(3)	16(2)	-20(2)	-32(2)
C62	40(2)	64(3)	70(3)	29(2)	-7(2)	-26(2)
C63	26(2)	29(2)	30(2)	-2(1)	-6(1)	-8(1)
C64	29(2)	36(2)	39(2)	-3(2)	-13(2)	-7(1)
C65	27(2)	34(2)	37(2)	-2(1)	-2(2)	-6(1)
C66	33(2)	37(2)	46(2)	6(2)	-13(2)	-7(1)
C11	49(3)	64(3)	120(6)	-46(3)	-6(3)	-12(2)
C21	45(3)	62(3)	123(6)	-46(3)	-22(3)	0(2)
C31	55(3)	60(3)	120(6)	-41(3)	-11(3)	0(2)
C12	66(4)	85(4)	83(5)	-38(3)	5(3)	-6(3)
C22	66(4)	83(4)	84(4)	-45(3)	-9(3)	-14(3)
C32	53(3)	74(3)	66(4)	-23(3)	-11(3)	1(2)
C42	84(4)	53(3)	55(3)	-15(2)	-25(3)	4(3)
C52	76(3)	47(2)	43(3)	1(2)	-14(2)	-22(2)
C62	56(3)	76(3)	61(3)	-8(3)	-6(3)	-19(3)

2.6 Crystal Structure of 5b

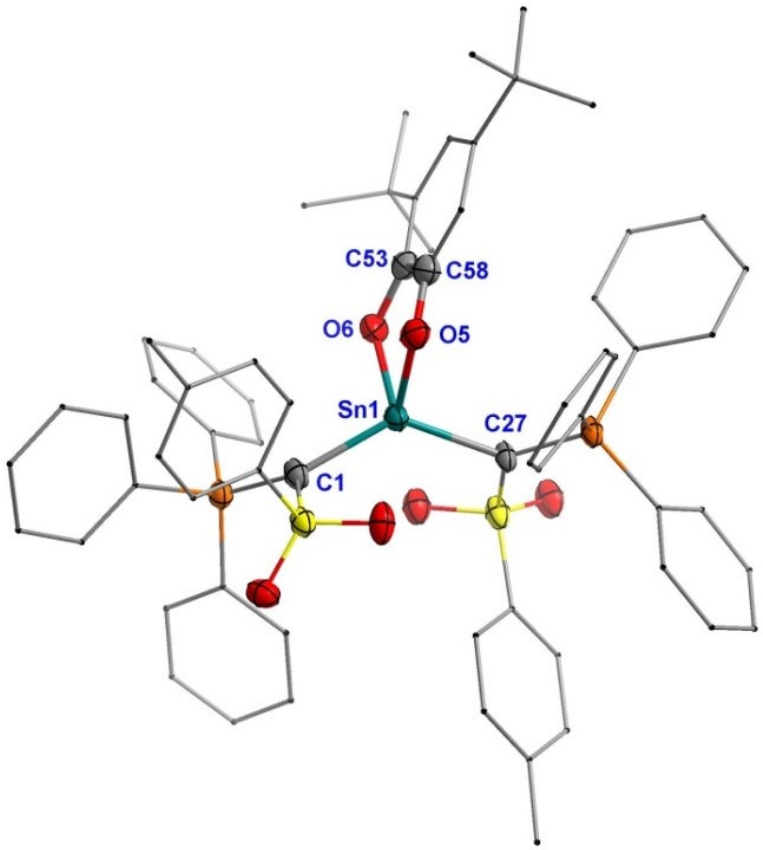


Figure S29. X-Ray structure of **5b**. Selected bond lengths [Å] and angles [°]: **5b**: Sn1-C1 2.082(3), Sn1-C27 2.091(3), Sn1-O6 2.041(3), Sn1-O5 2.064(3), C53-O6 1.387(4), C58-O5 1.340(4), C1-Sn1-C27 131.71(1), O5-Sn1-O6 83.72(1).

Table S11. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **5b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sn1	5282(1)	6407(1)	2381(1)	25(1)
P1	3024(1)	6408(1)	3720(1)	25(1)
S1	5710(1)	5448(1)	3616(1)	26(1)
O1	5099(3)	4854(2)	4052(1)	33(1)
C1	4577(3)	6175(2)	3302(1)	26(1)
O3	3603(2)	5595(2)	2099(1)	32(1)
C3	6332(4)	5961(2)	4669(2)	30(1)
O4	4191(2)	5194(2)	997(1)	35(1)
C4	6945(4)	6441(3)	4990(2)	36(1)
O5	6820(3)	7060(2)	2291(1)	32(1)
C5	7735(4)	7014(2)	4692(2)	36(1)
C6	7920(4)	7074(3)	4053(2)	38(1)
O6	4307(3)	7623(2)	2122(1)	35(1)
C7	7322(4)	6594(3)	3723(2)	35(1)
C8	8370(5)	7556(3)	5042(2)	50(1)

C9	2154(3)	5493(2)	3782(2)	29(1)
C10	2732(4)	4697(2)	3464(2)	34(1)
C11	2020(4)	4030(3)	3464(2)	40(1)
C12	747(4)	4149(3)	3779(2)	45(1)
C14	871(4)	5612(3)	4090(2)	37(1)
C13	173(4)	4931(3)	4090(2)	46(1)
C15	1943(3)	7295(2)	3392(2)	29(1)
C16	1460(4)	7103(3)	2884(2)	38(1)
C17	535(4)	7732(3)	2662(2)	46(1)
C18	64(4)	8552(3)	2938(2)	47(1)
C19	523(5)	8751(3)	3443(2)	51(1)
C21	3078(4)	6764(2)	4479(2)	31(1)
C20	1467(4)	8132(3)	3670(2)	43(1)
C22	3747(4)	7457(3)	4512(2)	40(1)
C23	3849(5)	7748(3)	5075(2)	55(1)
C24	3296(5)	7350(4)	5601(2)	61(1)
C25	2650(5)	6673(3)	5580(2)	53(1)
C26	2534(4)	6366(3)	5014(2)	40(1)
C27	5894(3)	5545(2)	1626(1)	23(1)
C28	4854(4)	3971(3)	1790(2)	32(1)
C29	4526(4)	3360(3)	1439(2)	43(1)
C2	6520(3)	6048(2)	4036(2)	26(1)
O2	6702(3)	5048(2)	3108(1)	38(1)
S2	4573(1)	5136(1)	1587(1)	27(1)
P2	7259(1)	5361(1)	1060(1)	25(1)
C30	4725(5)	2455(3)	1613(2)	53(1)
C31	5210(5)	2166(3)	2139(2)	48(1)
C32	5535(4)	2798(3)	2479(2)	42(1)
C33	5379(4)	3698(2)	2304(2)	33(1)
C34	5390(7)	1184(3)	2342(3)	70(2)
C35	7448(3)	4277(2)	710(2)	27(1)
C36	6871(4)	4211(2)	204(2)	30(1)
C37	6946(4)	3377(3)	-37(2)	36(1)
C38	7585(4)	2607(3)	218(2)	42(1)
C39	8150(5)	2667(3)	720(2)	45(1)
C40	8078(4)	3499(3)	971(2)	36(1)
C41	7304(4)	6155(2)	428(2)	29(1)
C42	8243(4)	5948(3)	-106(2)	36(1)
C43	8338(4)	6572(3)	-579(2)	40(1)
C44	7490(4)	7407(3)	-519(2)	41(1)
C45	6555(4)	7608(3)	2(2)	41(1)
C46	6444(4)	6982(3)	481(2)	35(1)
C47	8659(3)	5356(3)	1404(2)	31(1)
C48	8716(4)	4884(3)	1955(2)	39(1)
C49	9774(4)	4821(4)	2235(2)	49(1)
C50	10792(4)	5225(4)	1964(2)	49(1)
C51	10741(4)	5705(3)	1427(2)	50(1)
C52	9675(4)	5780(3)	1136(2)	39(1)

C53	5251(4)	8101(2)	1860(2)	31(1)
C54	4925(4)	8875(2)	1506(2)	33(1)
C55	5947(4)	9290(2)	1229(2)	37(1)
C56	7234(4)	8976(3)	1294(2)	38(1)
C57	7507(4)	8221(3)	1661(2)	36(1)
C58	6531(4)	7791(2)	1945(2)	33(1)
C59	3522(4)	9235(2)	1426(2)	37(1)
C60	2646(4)	9469(3)	2055(2)	45(1)
C61	3387(5)	10087(3)	1025(2)	50(1)
C62	3028(4)	8525(3)	1114(2)	44(1)
C63	8352(4)	9414(3)	964(2)	49(1)
C64	9299(6)	8737(4)	539(3)	76(2)
C65	7866(6)	10236(4)	595(3)	79(2)
C66	9043(6)	9707(4)	1433(3)	73(2)
C11	5084(4)	840(3)	6724(2)	67(2)
C21	5987(3)	202(3)	6351(2)	86(2)
C31	5585(4)	-269(3)	5927(2)	116(3)
C41	4282(5)	-102(3)	5877(2)	110(3)
C51	3379(4)	536(3)	6250(2)	92(2)
C61	3780(4)	1008(3)	6673(2)	79(2)
C12	10614(13)	9254(11)	5319(8)	170(20)
C22	9265(13)	9516(10)	5431(7)	220(30)
C32	8671(10)	10260(7)	5128(6)	76(9)
C42	9428(11)	10742(7)	4714(5)	68(6)
C52	10777(10)	10480(8)	4602(6)	61(5)
C62	11370(10)	9736(11)	4905(8)	150(18)

Table S12. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **5b**. 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^{23}	U^{13}	U^{12}
Sn1	30(1)	27(1)	17(1)	-1(1)	-2(1)	-10(1)
P1	28(1)	28(1)	19(1)	-3(1)	-2(1)	-7(1)
S1	29(1)	30(1)	18(1)	-1(1)	-4(1)	-7(1)
O1	40(1)	35(1)	28(1)	5(1)	-11(1)	-16(1)
C1	29(2)	35(2)	17(2)	-2(1)	-4(1)	-11(1)
O3	29(1)	43(1)	27(1)	-6(1)	-4(1)	-12(1)
C3	35(2)	36(2)	20(2)	1(1)	-2(1)	-10(2)
O4	34(1)	51(2)	24(1)	-5(1)	-8(1)	-15(1)
C4	42(2)	43(2)	24(2)	-2(2)	-8(2)	-9(2)
O5	43(1)	29(1)	25(1)	-2(1)	-12(1)	-6(1)
C5	39(2)	34(2)	38(2)	-5(2)	-13(2)	-7(2)
C6	40(2)	38(2)	42(2)	7(2)	-12(2)	-17(2)
O6	39(1)	32(1)	33(1)	-4(1)	6(1)	-13(1)
C7	39(2)	45(2)	24(2)	5(2)	-6(2)	-15(2)
C8	58(3)	46(2)	52(3)	-8(2)	-16(2)	-19(2)
C9	32(2)	34(2)	24(2)	2(1)	-6(1)	-10(1)
C10	39(2)	38(2)	27(2)	-3(1)	-8(2)	-14(2)

C11	55(3)	38(2)	35(2)	2(2)	-15(2)	-22(2)
C12	49(2)	47(2)	51(2)	15(2)	-24(2)	-27(2)
C14	31(2)	42(2)	36(2)	4(2)	-2(2)	-11(2)
C13	30(2)	59(3)	53(3)	16(2)	-8(2)	-20(2)
C15	23(2)	35(2)	27(2)	2(1)	0(1)	-7(1)
C16	38(2)	42(2)	31(2)	-2(2)	-6(2)	-4(2)
C17	42(2)	60(3)	31(2)	4(2)	-7(2)	-3(2)
C18	39(2)	51(2)	47(2)	10(2)	-6(2)	-1(2)
C19	53(3)	33(2)	62(3)	-2(2)	-10(2)	1(2)
C21	37(2)	34(2)	21(2)	-7(1)	-2(1)	-4(2)
C20	44(2)	37(2)	47(2)	-6(2)	-12(2)	-7(2)
C22	45(2)	37(2)	38(2)	-12(2)	-9(2)	-5(2)
C23	63(3)	50(2)	54(3)	-24(2)	-24(2)	-1(2)
C24	72(3)	68(3)	38(2)	-29(2)	-23(2)	14(3)
C25	61(3)	63(3)	25(2)	-5(2)	-4(2)	12(2)
C26	42(2)	46(2)	24(2)	-2(2)	-3(2)	1(2)
C27	22(2)	34(2)	15(1)	-6(1)	0(1)	-12(1)
C28	33(2)	43(2)	23(2)	-8(1)	1(1)	-18(2)
C29	53(3)	51(2)	33(2)	-4(2)	-10(2)	-29(2)
C2	26(2)	32(2)	23(2)	1(1)	-7(1)	-8(1)
O2	34(1)	52(2)	26(1)	-13(1)	-5(1)	-5(1)
S2	25(1)	39(1)	19(1)	-5(1)	-3(1)	-13(1)
P2	26(1)	34(1)	17(1)	-6(1)	-1(1)	-12(1)
C30	76(3)	47(2)	47(2)	-4(2)	-15(2)	-36(2)
C31	65(3)	43(2)	41(2)	-2(2)	-3(2)	-28(2)
C32	51(2)	47(2)	29(2)	1(2)	-3(2)	-18(2)
C33	39(2)	36(2)	25(2)	-8(1)	-1(2)	-11(2)
C34	106(5)	46(3)	68(3)	7(2)	-21(3)	-33(3)
C35	29(2)	34(2)	20(2)	-6(1)	0(1)	-10(1)
C36	35(2)	35(2)	21(2)	-3(1)	-4(1)	-13(1)
C37	46(2)	39(2)	28(2)	-5(2)	-10(2)	-15(2)
C38	55(3)	34(2)	40(2)	-7(2)	-12(2)	-12(2)
C39	60(3)	34(2)	43(2)	-1(2)	-17(2)	-6(2)
C40	40(2)	39(2)	29(2)	-1(2)	-10(2)	-10(2)
C41	33(2)	35(2)	23(2)	-5(1)	-2(1)	-14(1)
C42	39(2)	39(2)	29(2)	-2(2)	1(2)	-14(2)
C43	46(2)	51(2)	25(2)	-1(2)	2(2)	-23(2)
C44	55(3)	43(2)	31(2)	5(2)	-11(2)	-23(2)
C45	53(2)	37(2)	35(2)	-3(2)	-11(2)	-7(2)
C46	41(2)	41(2)	26(2)	-7(2)	-5(2)	-13(2)
C47	24(2)	44(2)	25(2)	-16(2)	0(1)	-12(2)
C48	31(2)	62(2)	25(2)	-9(2)	-4(2)	-14(2)
C49	37(2)	83(3)	30(2)	-9(2)	-9(2)	-17(2)
C50	33(2)	81(3)	38(2)	-21(2)	-6(2)	-17(2)
C51	31(2)	72(3)	50(3)	-20(2)	-1(2)	-24(2)
C52	35(2)	51(2)	33(2)	-15(2)	4(2)	-21(2)
C53	40(2)	31(2)	24(2)	-6(1)	-4(2)	-15(2)
C54	43(2)	29(2)	29(2)	-4(1)	-10(2)	-10(2)

C55	45(2)	32(2)	36(2)	5(2)	-12(2)	-13(2)
C56	45(2)	38(2)	37(2)	1(2)	-6(2)	-20(2)
C57	38(2)	41(2)	31(2)	1(2)	-9(2)	-14(2)
C58	42(2)	32(2)	26(2)	-2(1)	-6(2)	-11(2)
C59	42(2)	31(2)	39(2)	0(2)	-13(2)	-9(2)
C60	47(2)	36(2)	51(2)	-6(2)	-10(2)	-6(2)
C61	49(3)	42(2)	64(3)	10(2)	-23(2)	-12(2)
C62	45(2)	44(2)	47(2)	-4(2)	-18(2)	-10(2)
C63	46(2)	46(2)	58(3)	18(2)	-9(2)	-22(2)
C64	63(3)	83(4)	77(4)	2(3)	15(3)	-30(3)
C65	61(3)	79(4)	101(5)	50(4)	-14(3)	-35(3)
C66	65(3)	73(3)	95(4)	16(3)	-25(3)	-44(3)
C11	107(5)	55(3)	44(3)	-2(2)	-8(3)	-31(3)
C21	84(5)	92(5)	82(4)	-7(4)	-9(4)	-25(4)
C31	103(6)	121(7)	115(6)	-63(6)	-16(5)	6(5)
C41	101(6)	110(6)	124(7)	-67(5)	-25(5)	-17(5)
C51	89(5)	93(5)	95(5)	-38(4)	-29(4)	3(4)
C61	108(5)	63(3)	67(4)	-24(3)	-39(4)	7(3)
C12	100(30)	130(30)	280(50)	-60(30)	-60(30)	60(20)
C22	120(30)	130(30)	440(60)	-140(30)	-140(30)	10(20)
C32	38(9)	48(9)	150(20)	-67(12)	-43(12)	18(8)
C42	69(14)	55(10)	82(10)	-50(8)	-10(9)	-13(9)
C52	63(11)	42(8)	70(8)	-35(6)	10(7)	-10(7)
C62	120(20)	160(30)	180(30)	-30(20)	20(20)	-90(20)

2.7 Crystal Structure of 6

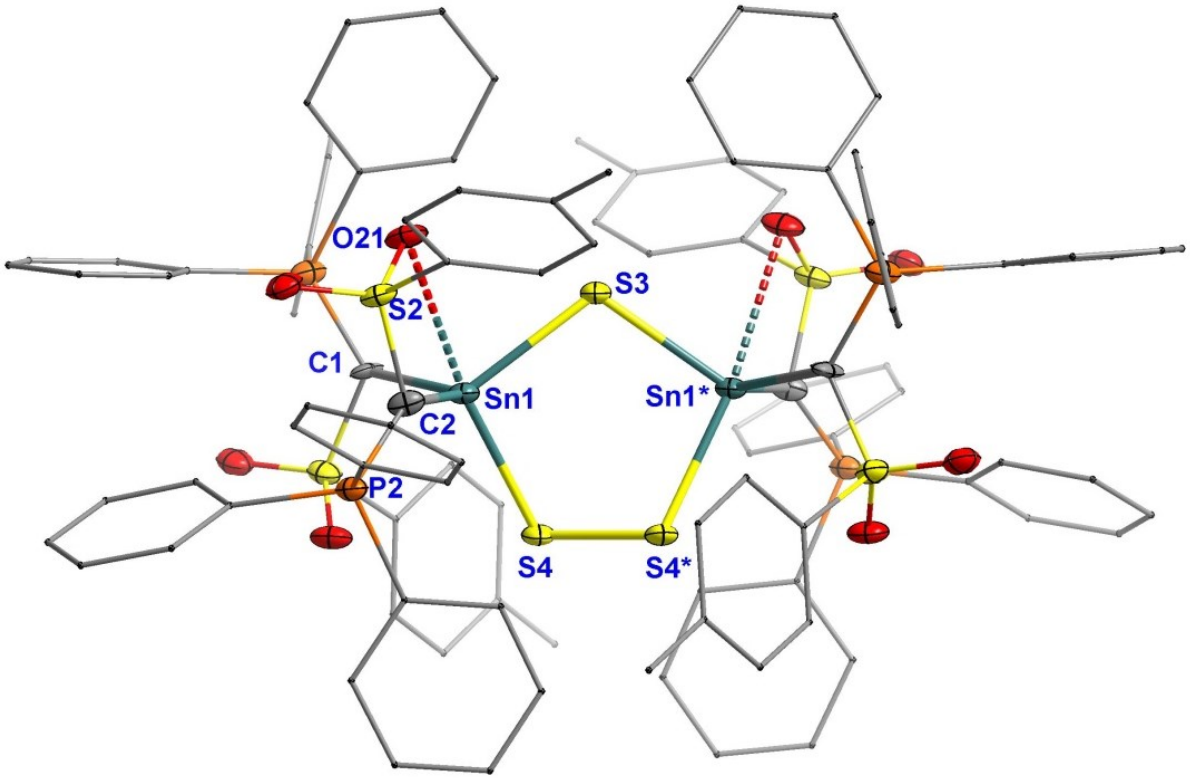


Figure S30. X-ray structure of **6**. Selected bond lengths [Å] and angles [°]: **6**: Sn1-C1 2.144(8), Sn1-C2 2.125(8), Sn1-S3 2.417(2), Sn1-S4 2.432(2), S4-S4* 2.043(5), Sn1-O21 2.761(6), C1-Sn1-C2 115.1(4), S3-Sn1-S4 98.41(8).

Mean plane of Sn_2S_3 core of 6.

	Distance from the mean plane (Å)
Sn1	-0.2155
S4	0.4577
S4*	-0.4577
Sn1*	0.2155
S3	0.0000

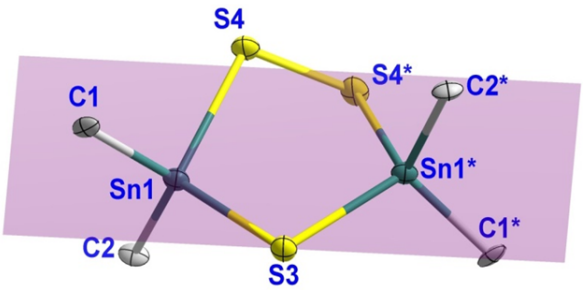


Figure S31. (left) Mean Plane data for 5-membered ring of **6**. (right) The mean plane passing through the Sn_2S_3 core of **6**.

Table S13. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sn1	5394.1(2)	6990.8(5)	3046.1(2)	16.05(17)
P1	6401.6(8)	5431(2)	3169.0(9)	20.4(5)
S1	6336.7(8)	8061(2)	3139.0(8)	20.5(5)
C1	6083(3)	6720(7)	3073(3)	16.9(18)
S2	5095.8(8)	5612.6(19)	3883.4(8)	20.2(5)
P2	5069.8(8)	8142(2)	4111.3(8)	18.8(5)
C2	5116(3)	7053(8)	3691(3)	16.9(18)
C3	6411(3)	8732(9)	2594(3)	25(2)
S3	5000	5700(3)	2500	19.0(6)
C4	6509(3)	8617(10)	1791(4)	30(2)
S4	5314.2(8)	8889.8(19)	2630.7(8)	21.2(5)
C5	6564(3)	9867(10)	1771(4)	31(2)
C6	6639(4)	10500(12)	1324(4)	44(3)
C62A	8149(10)	3410(40)	5781(7)	95(4)
C63A	7842(9)	3570(40)	5381(9)	95(4)
O64A	7421(9)	3400(30)	5569(5)	95(4)
C62B	8154(17)	4380(50)	5897(14)	95(4)
C63B	7881(16)	4120(70)	5482(17)	95(4)
O64B	7445(17)	3920(40)	5629(10)	95(4)
C61	7930(6)	3620(20)	6213(6)	95(4)
C60	7486(6)	3270(20)	6061(6)	95(4)
C7	6539(3)	10538(10)	2169(4)	30(2)
C8	6460(3)	9984(9)	2578(3)	24(2)
C9	6827(3)	5146(9)	2770(3)	23(2)
C10	7103(3)	6045(9)	2630(4)	26(2)
O10	6052(2)	8890(6)	3360(2)	24.5(15)
C11	7408(3)	5799(10)	2315(4)	29(2)
O11	6769(2)	7923(6)	3348(2)	25.7(15)
C12	7449(3)	4640(10)	2140(4)	28(2)
C14	6871(3)	3982(9)	2591(4)	28(2)
C13	7180(3)	3743(9)	2286(4)	30(2)
C16	5818(3)	3953(9)	2704(4)	31(2)
C15	6073(3)	4085(8)	3108(4)	25(2)
C17	5586(4)	2886(11)	2627(5)	43(3)
C18	5615(4)	1972(11)	2951(6)	53(4)
C19	5883(4)	2096(10)	3343(5)	48(4)
C20	6105(4)	3151(10)	3427(4)	36(3)
O20	5295(2)	5459(6)	4341(2)	26.2(15)
C21	6677(4)	5362(10)	3738(4)	32(2)
O21	5275(2)	4879(6)	3525(2)	26.7(15)
C22	7107(4)	5255(16)	3814(5)	55(4)
C23	7285(5)	5210(20)	4255(5)	87(7)
C24	7034(5)	5225(16)	4621(5)	58(4)
C25	6595(4)	5333(10)	4545(4)	41(3)
C26	6412(3)	5386(9)	4107(4)	29(2)

C27	6426(3)	8050(9)	2198(3)	25(2)
C28	4544(3)	5140(8)	3918(3)	22(2)
C29	4253(4)	5308(9)	3548(4)	28(2)
C30	3831(4)	4908(10)	3571(4)	32(2)
C31	3696(4)	4304(10)	3966(4)	33(2)
C32	3240(4)	3901(13)	4003(5)	50(3)
C33	4003(4)	4142(9)	4322(4)	32(2)
C34	4422(4)	4556(9)	4309(4)	30(2)
C35	4609(3)	7778(8)	4451(3)	19.8(19)
C36	4656(3)	7223(9)	4873(3)	25(2)
C37	4293(4)	6924(9)	5108(4)	31(2)
C38	3885(4)	7184(9)	4919(4)	31(2)
C39	3835(4)	7705(10)	4491(4)	33(2)
C40	4195(3)	8002(10)	4259(4)	29(2)
C41	4957(3)	9623(8)	3868(3)	19.7(19)
C42	5126(3)	10673(8)	4084(3)	22(2)
C43	4981(4)	11789(9)	3931(3)	28(2)
C44	4678(4)	11888(9)	3564(3)	29(2)
C45	4529(3)	10855(9)	3341(3)	26(2)
C46	4660(3)	9731(8)	3490(3)	19.9(19)
C47	5538(3)	8342(8)	4512(3)	21(2)
C48	5948(3)	8061(9)	4365(3)	26(2)
C49	6312(4)	8298(9)	4650(4)	30(2)
C50	6273(4)	8806(10)	5078(4)	36(3)
C51	5872(4)	9082(9)	5224(4)	31(2)
C52	5503(3)	8866(9)	4944(3)	25(2)

Table S14. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **6**. 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^{23}	U^{13}	U^{12}
Sn1	19.7(3)	9.3(3)	19.3(3)	0.3(2)	2.4(2)	0.6(2)
P1	16.3(11)	13.3(11)	32.0(13)	2.8(9)	5.0(9)	1.4(9)
S1	26.8(12)	12.5(10)	22.6(11)	0.5(8)	3.5(9)	-4.1(9)
C1	11(4)	6(4)	33(5)	4(3)	1(4)	3(3)
S2	26.4(12)	11.1(10)	23.6(11)	3.6(8)	5.7(9)	4.5(9)
P2	26.3(12)	11.8(10)	18.6(11)	0.4(8)	3.4(9)	1.1(9)
C2	18(4)	14(4)	20(4)	2(3)	11(3)	3(4)
C3	27(5)	19(5)	27(5)	3(4)	4(4)	-7(4)
S3	23.3(16)	10.2(13)	23.2(15)	0	-2.1(12)	0
C4	25(5)	39(6)	24(5)	-1(4)	4(4)	0(5)
S4	27.9(12)	9.9(10)	25.4(11)	1.8(8)	-1.5(9)	-3.1(9)
C5	23(5)	36(6)	35(6)	10(5)	1(4)	-6(5)
C6	47(7)	49(7)	35(6)	14(6)	3(5)	-8(6)
C62A	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C63A	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)

O64A	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C62B	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C63B	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
O64B	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C61	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C60	100(7)	124(10)	62(5)	-6(6)	5(5)	43(8)
C7	28(5)	23(5)	37(6)	7(4)	1(4)	-5(4)
C8	26(5)	16(5)	28(5)	0(4)	0(4)	-3(4)
C9	15(5)	22(5)	31(5)	3(4)	2(4)	5(4)
C10	19(5)	23(5)	36(6)	-3(4)	0(4)	4(4)
O10	33(4)	11(3)	30(4)	-2(3)	9(3)	0(3)
C11	14(5)	31(6)	42(6)	-3(5)	6(4)	-1(4)
O11	35(4)	16(3)	27(4)	1(3)	3(3)	-7(3)
C12	24(5)	28(5)	32(5)	-2(4)	7(4)	1(4)
C14	19(5)	18(5)	48(6)	4(4)	7(4)	6(4)
C13	28(6)	20(5)	43(6)	0(4)	5(5)	12(4)
C16	26(5)	18(5)	50(7)	-6(4)	8(5)	5(4)
C15	16(5)	11(4)	49(6)	1(4)	10(4)	4(4)
C17	31(6)	27(6)	73(9)	-24(6)	13(6)	-4(5)
C18	36(7)	17(6)	110(12)	-21(7)	35(8)	-12(5)
C19	42(7)	13(5)	92(11)	7(6)	31(7)	7(5)
C20	39(6)	22(5)	50(7)	4(5)	19(5)	3(5)
O20	34(4)	16(3)	28(4)	7(3)	1(3)	3(3)
C21	39(6)	25(5)	31(6)	9(4)	1(5)	2(5)
O21	37(4)	13(3)	31(4)	1(3)	9(3)	8(3)
C22	22(6)	101(12)	42(7)	24(7)	6(5)	6(7)
C23	46(9)	180(20)	37(8)	24(11)	-4(7)	13(11)
C24	51(8)	88(12)	35(7)	17(7)	-6(6)	17(8)
C25	63(8)	28(6)	31(6)	7(5)	12(6)	7(6)
C26	26(5)	15(5)	46(6)	3(4)	9(5)	4(4)
C27	26(5)	21(5)	28(5)	-4(4)	3(4)	5(4)
C28	26(5)	10(4)	29(5)	-4(4)	10(4)	2(4)
C29	35(6)	21(5)	30(5)	1(4)	4(4)	-5(4)
C30	30(6)	30(6)	37(6)	-7(5)	4(5)	-1(5)
C31	36(6)	21(5)	44(6)	-12(5)	12(5)	-3(5)
C32	42(7)	45(8)	65(9)	-8(6)	15(6)	-15(6)
C33	46(7)	16(5)	36(6)	-1(4)	19(5)	-6(5)
C34	48(7)	14(5)	28(5)	1(4)	10(5)	9(4)
C35	25(5)	14(4)	21(5)	-3(3)	7(4)	1(4)
C36	29(5)	20(5)	26(5)	3(4)	5(4)	3(4)
C37	51(7)	19(5)	26(5)	4(4)	13(5)	6(5)
C38	36(6)	19(5)	40(6)	3(4)	16(5)	1(4)
C39	24(5)	34(6)	42(6)	7(5)	5(5)	1(5)
C40	30(5)	27(5)	31(5)	4(4)	3(4)	-5(5)
C41	24(5)	16(4)	19(5)	-1(4)	3(4)	2(4)
C42	31(5)	15(4)	19(5)	-4(4)	2(4)	6(4)
C43	42(6)	16(5)	26(5)	-4(4)	4(4)	-3(4)
C44	42(6)	15(5)	30(5)	3(4)	5(4)	7(4)

C45	30(5)	24(5)	24(5)	0(4)	2(4)	2(4)
C46	22(5)	14(4)	24(5)	-5(4)	3(4)	0(4)
C47	32(5)	12(4)	20(5)	2(3)	1(4)	3(4)
C48	34(6)	17(5)	27(5)	-2(4)	2(4)	1(4)
C49	26(5)	26(5)	39(6)	3(4)	-1(4)	2(4)
C50	40(7)	33(6)	33(6)	-6(5)	-10(5)	-7(5)
C51	41(6)	23(5)	28(5)	1(4)	-4(5)	2(5)
C52	27(5)	21(5)	28(5)	-1(4)	4(4)	2(4)

3. VT-NMR studies

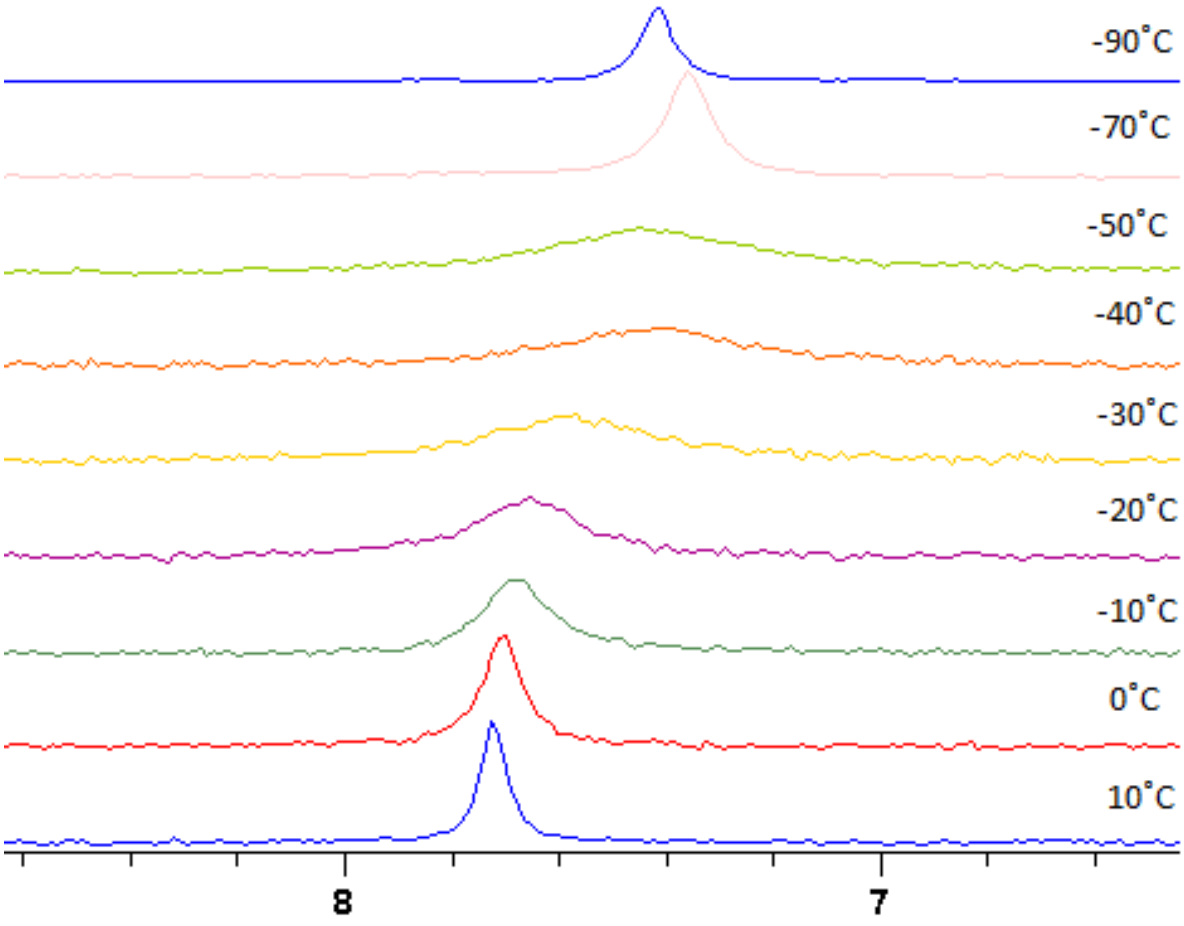


Figure S32. $^{31}P\{^{1}H\}$ NMR spectra of **Y_2Ge** at different temperatures.

4. Computational Studies

General. All calculations were performed without symmetry restrictions. Starting coordinates for were obtained from the crystal structure analyses, via GaussView[3] or from Ref 3. The geometry optimization were done with the Gaussian09 (Revision E.01) program package,[4] using Density-Functional Theory (DFT)[5] with the PBE0 functional[6] and the def2svp basis set[7] with Grimme's D3 dispersion correction with Becke-Johnson damping[8]. For Tin, the LANL2DZdp basis set[9] with the corresponding ECP[10] was used. Single point energies were determined using the def2tzvp basis set[7] and the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM)[11] as implemented in Gaussian09 with the parameters of toluene for the reaction mechanism. The energies for the $GaCl_3$ adducts are reported at the def2svp level. The metrical parameters of the energy-optimized geometry compared well with those determined by X-ray diffraction. Harmonic vibrational frequency analysis was performed on the same levels of theory to determine the nature of the structure.[12] The vibrational frequency analysis showed no imaginary frequencies for the ground states and one imaginary frequency for transition states, corresponding to the expected translational motion of the transition states. The NBO analysis[13] was done with the PBE0 functional and the def2svp basis set.

4.1. Calculations of the electronic structure

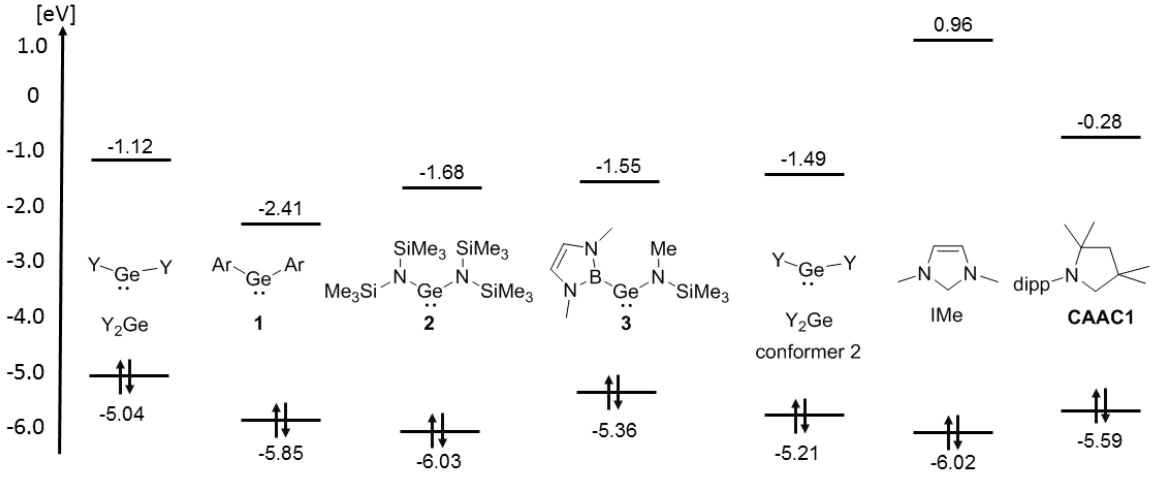


Figure S33. Comparison of the HOMO-LUMO energies of different tetrylenes (Ar = 2,6-dimethyl-phenyl).

Table S15. Comparison of the bonding situations in the tetrylenes depicted in Figure S33. Calculated Wiberg bond indices (WBI) and charges (q).

	Y_2Ge	Y_2Ge (conf. 2)	**1**	**2**	**3**	Y_2Sn	IMe	CAAC
q(E)	0.99991	0.93761	0.99118	1.21711	0.65558	1.23001		
q(X)[a]	–1.47428	–1.45640	–0.51771	–1.74373	–1.25901 (N)	–1.55027		
q(X)[a]	–1.49535	–1.47219	–0.51772	–1.76221	0.40763 (B)	–1.55704		
WBI(Ge–X)	0.5384	0.7441	0.7307	0.6755	0.8662 (N)	0.4471		
WBI(Ge–X)	0.6158	0.8657	0.7307	0.6075	0.9809 (B)	0.4267		
HOMO [E_h]	–0.18538	–0.19139	–0.21509	–0.22144	–0.19712	–0.18748	–0.22113	–0.20541
LUMO [E_h]	–0.04108	–0.05463	–0.08839	–0.06156	–0.05713	–0.03740	0.03528	–0.01025

[a] X corresponds to the atom bond to the central element Sn or Ge, i.e. C for ylides, N for amino, B for boryl groups.

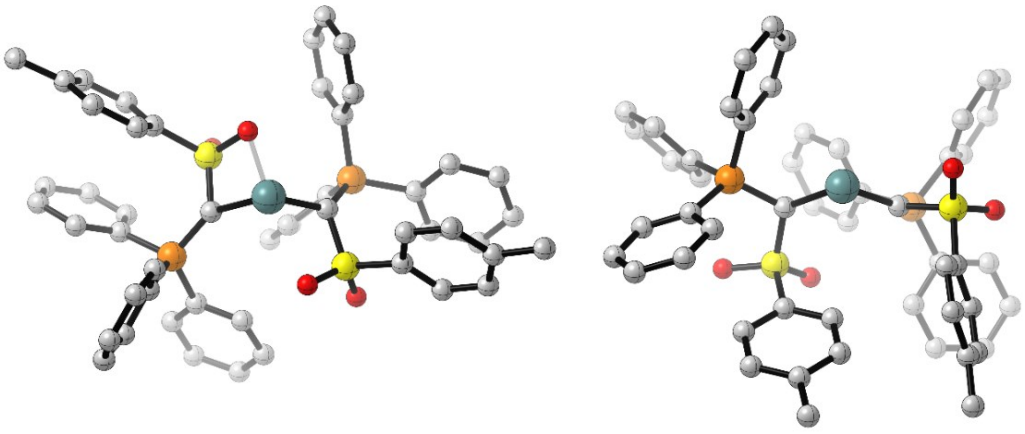


Figure S34. Structures and relative energies of the energy-optimized geometries of **Y_2Ge** and its conformer 2.

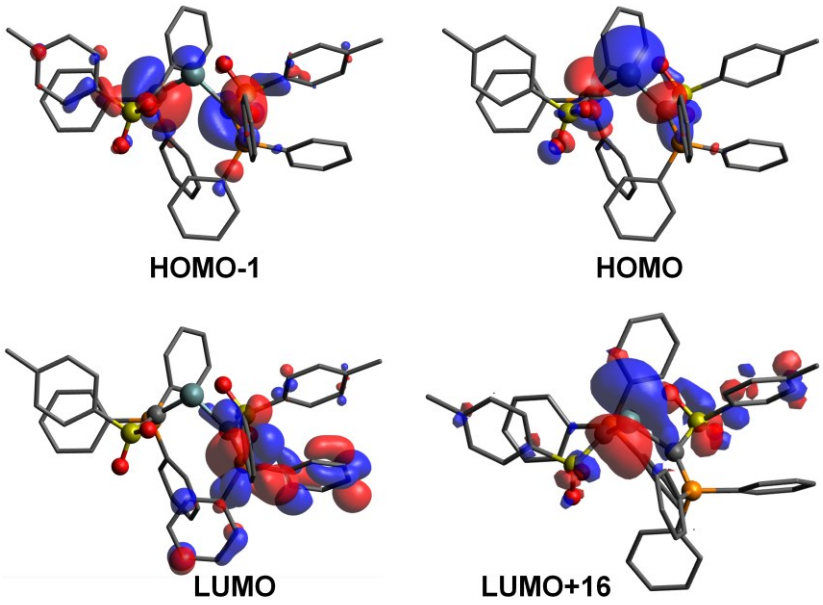


Figure S35. Molecular orbitals of **Y_2Ge**.

4.2. Calculations of the sum of angles in the $GaCl_3$ complexes and correlation with the Tolman electronic parameter

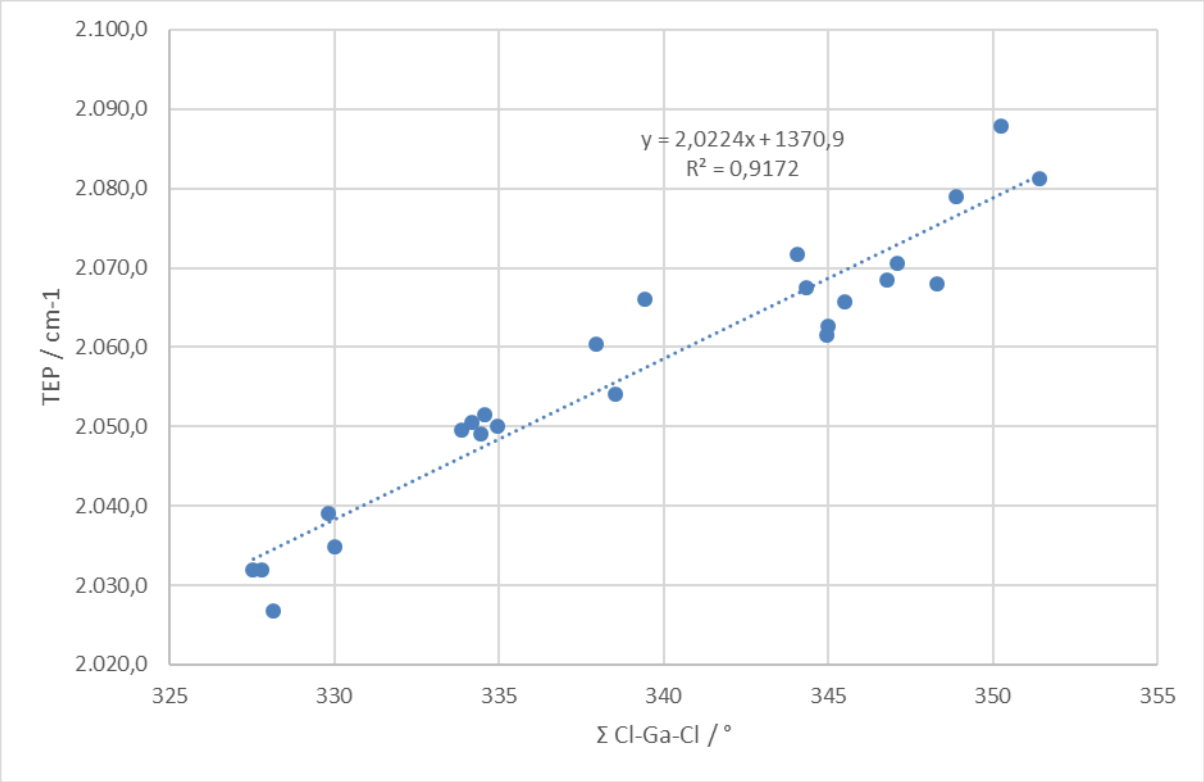


Figure S36. Correlation between the sum of Cl-Ga-Cl angles in L·$GaCl_3$ and its correlation with the TEP value.

Table S16. Calculated sum of Cl-Ga-Cl angles in L·$GaCl_3$ and corresponding TEP values (experimental or calculated). Structures of the compounds are given in Figure S36.

Compound	∑(Cl-Ga-Cl) [°]	TEP [cm^{-1}] [a]
Y_2Ge	327.038	2032.3*
2	339.389	2057.3*
3	338.676	2055.8*
$tBuPCl_2$	350.239	2,087.9
THF	351.404	2,081.2
Me_3PO	344.075	2,071.7
3,5-Me_2Py	346.794	2,068.5
DMAP	345.492	2,065.8
iPr_2NH	339.431	2,066.0
PEt_3	345.017	2,062.7
IMe	338.543	2,054.1
$IPrMe_2$	333.878	2,049.6
Me_3SiN_3	348.891	2,079.0

N_3P_2	347.102	2,070.6
Piperidine	348.306	2,068.0
PPh_3	344.350	2,067.5
PPr_3	344.950	2,061.6
N_2B	337.949	2,060.4
SIPr	334.581	2,051.5
IPr	334.189	2,050.5
CAAC1	334.973	2,050.0
CAAC2	334.463	2,049.0
Bisylide1	329.828	2,039.0
Bisylide2	330.035	2,034.9
Bisylide3	327.807	2,032.0
Bisylide4	327.546	2,031.9
Bisylide5	328.135	2,026.7

a. Taken from Ref 14; *) calculated from correlation.

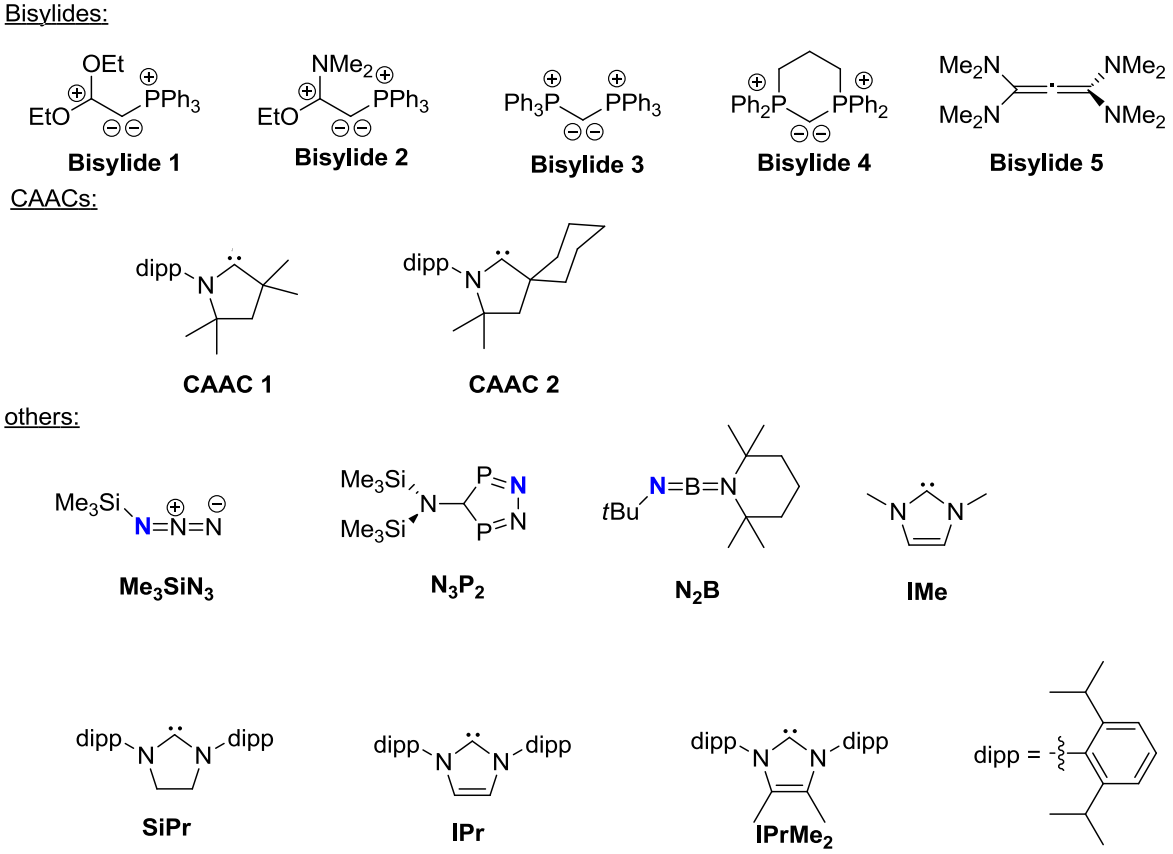


Figure S37. Structures of the compounds used for correlation of the sum of Cl-Ga-Cl angles with the TEP. Coordinating atom is highlighted in blue; central carbon atom for bisylides, CAACs and NHCs.

4.3. Mechanism of the C-H activation to 4

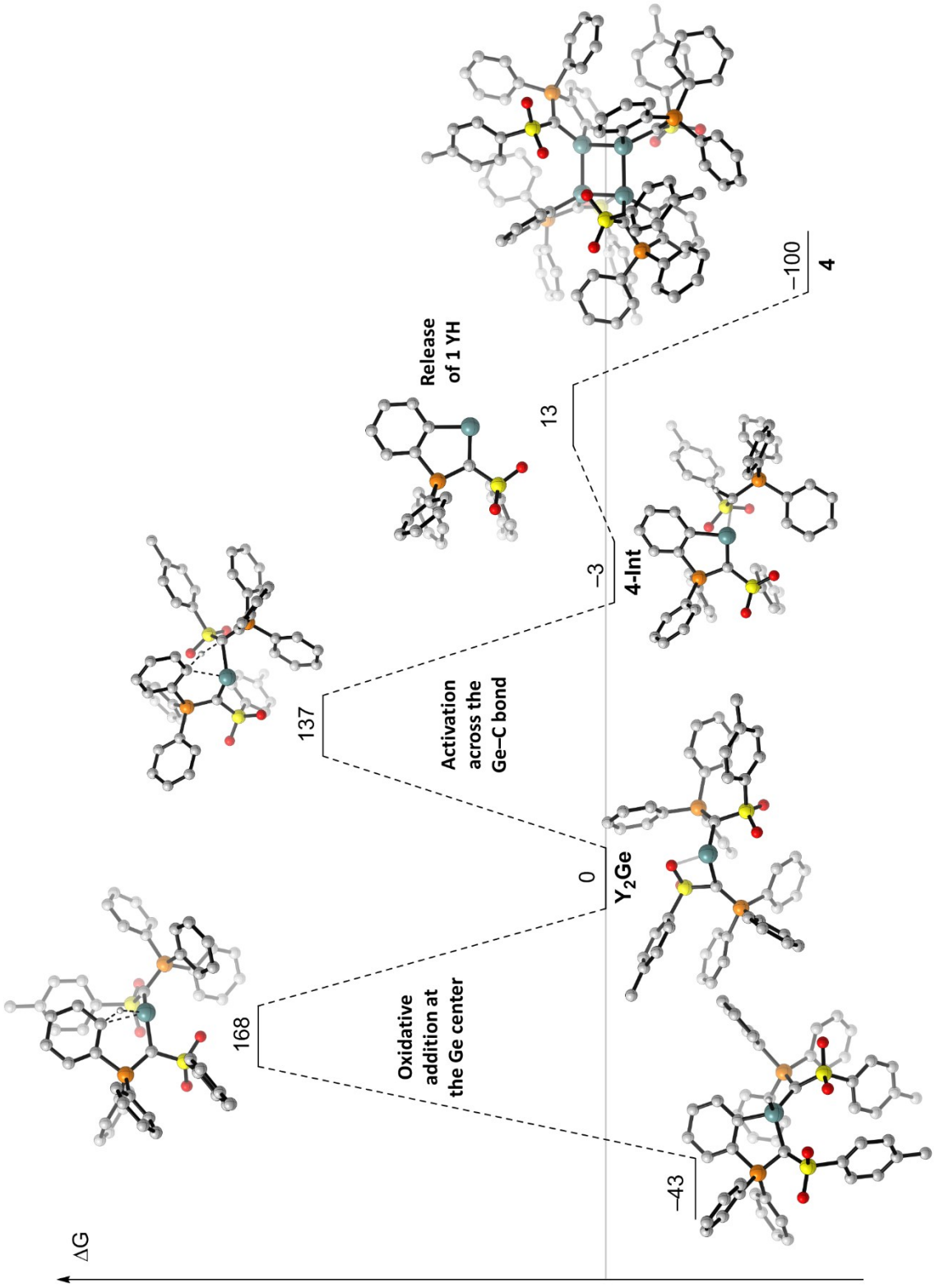


Figure S38. Structures and free energies in toluene [kJ/mol] for the calculated mechanism of the C-H activation in **Y_2Ge** to **4**.

Table S17. Overview of computed energies and vibrations.

	E(SCF(Tol)) / E_h	$E_{corr,ZPE}$ / E_h	$E_{corrΔH}$ / Eh	$E_{corrΔG}$ / Eh	#(im. freq.)	v / cm^{-1}
Y_2Ge	-5862.53686482	0.825638	0.883264	0.726147	0	-
Y_2Ge(conf2)	-5862.51616200[a)]	0.826676	0.883892	0.730073	0	-
Y	-1893.47112149	0.422266	0.450263	0.361257	0	-
TS(OA)	-5862.47220966	0.821066	0.877895	0.725534	1	-1160.2612
OA	-5862.55838736	0.824818	0.881146	0.731219	0	-
TS(Ge–C)	-5862.48254787	0.821019	0.878000	0.723978	1	-1076.9138
4-Int	-5862.53999092	0.825608	0.882839	0.728143	0	-
Rel(Y-H)	-3969.03680298	0.401600	0.430355	0.340843	0	-
4	-15876.4010296	1.612615	1.729042	1.445507	0	-

a) Gas phase.

4.4. Coordinates and Energies

Germylenes and Stannylenes

Energies are given in $E_{hartree}$ (gas phase) and coordinates in Å.

Y_2Ge
E = -5862.52550258
Ge 0.166093 0.013406 -1.722986
S -1.673644 1.395027 -0.141769
S 2.342459 -1.506429 -0.449325
P -2.483901 -1.433578 0.196892
P 2.300594 1.172427 0.717894
O -0.578880 1.948821 -1.047839
O -1.670971 1.916876 1.233280
O 1.371294 -2.254090 -1.309352
O 2.657678 -2.093992 0.869791
C -1.456097 -0.232384 -0.421796
C -4.027146 -0.712669 0.826051
C -4.003321 0.015433 2.023811
H -3.077370 0.106211 2.594797
C -5.156983 0.657840 2.463888
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C -6.327684 0.593433 1.709101
H -7.228703 1.105885 2.054758
C -6.346088 -0.112115 0.507177
H -7.257647 -0.151494 -0.093284
C -5.199780 -0.767487 0.064925
H -5.211943 -1.318347 -0.878060
C -2.937648 -2.629599 -1.091787
C -2.701510 -2.320886 -2.433339
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C -3.077810 -3.222323 -3.427915
H -2.878871 -2.985964 -4.475556
C -3.694987 -4.423300 -3.084521
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C -3.927742 -4.734183 -1.743337
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Y_2Ge(not coordinated)
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P 2.129025 1.698893 -0.341865
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Y_2Sn

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P -2.477026 1.377746 0.582662
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O 2.148637 1.869963 1.226312
O -1.086147 -2.164677 -0.918587
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Ar_2Ge
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H 2.241278 -2.678896 -0.812624
H 2.007435 -1.551684 -2.162941
H 3.651668 -1.997585 -1.643249
C -0.389523 -2.223927 0.918126
H -0.076430 -2.650638 -0.049957
H 0.486211 -1.709123 1.342913
H -0.643622 -3.068034 1.574371
C -2.639914 1.762932 -1.282553
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H -2.007952 1.550390 -2.163864
H -3.651851 1.997153 -1.643802
C 0.389658 2.224491 0.917270
H 0.077197 2.651481 -0.050898
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H 0.643554 3.068389 1.573858

$NTMS_2Ge$
E = -3822.57232294
Ge 0.092987 -0.279977 -1.288509
N 1.504425 0.114987 -0.104581
N -1.431668 -0.184234 -0.163824
Si -1.712696 -1.519941 0.961659
Si -2.748074 0.870743 -0.679463
Si 3.020559 -0.717809 -0.485150
Si 1.405401 1.526146 0.964334
C -0.094932 -2.243183 1.595498
H 0.483576 -2.722706 0.790544
H 0.551855 -1.491716 2.065366
H -0.331699 -3.023088 2.337549
C -2.591643 -2.937769 0.080666
H -2.013829 -3.255239 -0.802458
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H -3.599796 -2.662899 -0.260878
C -2.769546 -0.991705 2.427923
H -2.950153 -1.865982 3.074201
H -2.277887 -0.218281 3.036032
H -3.751951 -0.607351 2.114029
C -3.036730 2.228392 0.592433
H -3.845147 2.899125 0.258586
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C -4.374911 -0.041131 -0.943696
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H 4.239400 -0.575075 1.716794
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C 2.657561 -2.216135 -1.575320
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Boryl-Amino-Germylene
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H 4.660286 -0.817669 -1.624548
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C 3.299121 -1.040420 1.340103
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H 2.626500 -1.188557 0.891561

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C -0.646959 -1.184764 2.329232
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H 4.687291 0.397072 0.038213
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H 3.269918 2.423173 -0.062801
C 1.405707 1.341430 -0.055104
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C 1.006535 -2.775025 -1.778504
H 0.453481 -1.994671 -2.322833
H 0.528441 -3.747091 -1.980116
H 2.034746 -2.811164 -2.172703
C 1.666844 -3.585899 0.529108
H 2.703859 -3.769385 0.207348
H 1.117929 -4.530751 0.395130

H	1.686032	-3.351269	1.604497
C	0.567298	2.581261	-0.294884
H	-0.466847	2.345218	-0.017718
C	0.552812	2.887535	-1.794908
H	1.568225	3.104985	-2.163186
H	-0.082434	3.762627	-2.006615
H	0.156425	2.026169	-2.352999
C	1.003990	3.787978	0.528538
H	1.034147	3.558331	1.604822
H	0.304115	4.624476	0.378784
H	2.002398	4.148523	0.235415
N	-0.596473	-0.081215	0.059300

Mechanism

Ylide YH
E = -1893.46167059
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O 1.272818 -1.981529 -3.123488
O 0.741191 -2.894453 -0.810503
C -0.307688 -0.628955 -1.647665
C -1.047798 -1.142198 1.122105
C -1.478532 -2.450568 0.864066
H -1.730970 -2.744231 -0.155594
C -1.531015 -3.375957 1.901057
H -1.858925 -4.397214 1.696307
C -1.137713 -3.009365 3.188012
H -1.170197 -3.742849 3.997337
C -0.688779 -1.714250 3.441532
H -0.367040 -1.430213 4.445990
C -0.643945 -0.777787 2.410924
H -0.282076 0.232949 2.608191
C -0.335354 1.587901 0.402046
C 0.931307 2.002029 -0.014456
H 1.486224 1.398448 -0.735229
C 1.478974 3.181823 0.488242
H 2.473036 3.494885 0.160629
C 0.760020 3.952980 1.398792
H 1.188659 4.878744 1.790417
C -0.514587 3.550818 1.804569
H -1.084341 4.162353 2.508200
C -1.064208 2.373419 1.306224
H -2.067214 2.065597 1.614953
C -2.745063 0.500771 -0.646274
C -3.843400 -0.179542 -0.114159
H -3.691243 -1.001355 0.588864
C -5.135492 0.196751 -0.478667
H -5.991850 -0.335010 -0.057688
C -5.334321 1.244959 -1.374826
H -6.348166 1.535265 -1.660171
C -4.238597 1.927511 -1.904269
H -4.391456 2.752837 -2.603408
C -2.946779 1.562844 -1.537451
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C 3.233751 -0.167983 -1.829048
H 3.050182 -0.163286 -2.905811
C 4.262746 0.578230 -1.257953
H 4.909429 1.183388 -1.899606
C 4.486318 0.565949 0.124601
C 3.664776 -0.242652 0.923093
H 3.836451 -0.281525 2.002671
C 2.637896 -0.997381 0.367107
H 2.000324 -1.635686 0.983015
C 5.579373 1.386643 0.744632
H 6.298820 0.750308 1.283965
H 5.171331 2.102292 1.476504
H 6.135796 1.956850 -0.012221
H -0.545976 -0.180588 -2.613143

Tetragermane 4

E = -15876.3778431

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H -1.008050 3.335970 4.868852
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C -0.450409 5.313352 2.152335
H -0.368002 6.366768 1.870943
C -0.339021 4.306076 1.190021
C -0.314100 3.119694 -1.277610
C -2.945548 -0.462205 -1.534217
C -2.605717 -0.696212 -2.870562
H -1.557076 -0.786532 -3.165461
C -3.612306 -0.815272 -3.829185
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C -4.958150 -0.693972 -3.476879
H -5.735365 -0.790930 -4.238712
C -5.313598 -0.449845 -2.151918
H -6.366990 -0.367362 -1.870456
C -4.306256 -0.338725 -1.189643
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C -5.187813 1.730703 0.703125
C -6.375967 2.191204 0.122251
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C -7.821652 -2.844634 2.217618
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C	-3.973141	-4.679840	-1.444737
H	-4.661043	-4.018480	-1.977104
C	-2.622631	-4.343169	-1.370116
H	-2.245191	-3.433824	-1.842356
C	1.060715	-5.971188	-1.150855
C	0.595481	-6.961241	-2.019441
H	-0.460279	-6.992808	-2.296633
C	1.492284	-7.889933	-2.546696
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C	2.844767	-7.821019	-2.219303
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C	3.312080	-6.815545	-1.370845
H	4.376119	-6.739772	-1.136318
C	2.424641	-5.888105	-0.839944
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C	2.945516	0.462410	-1.534111
C	2.605655	0.696606	-2.870414
H	1.557003	0.786857	-3.165296
C	3.612227	0.815941	-3.829021
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H	6.366963	0.367969	-1.870379
C	4.306235	0.339006	-1.189564
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H	7.632577	-3.901189	-0.258762
C	5.855511	-4.433734	0.852336
H	6.118912	-5.492887	0.911803
C	4.680166	-3.973306	1.443671
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H	3.434211	-2.245428	1.841805
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C	6.961582	0.595362	2.018379
H	6.993183	-0.460395	2.295577
C	7.890445	1.492135	2.545384
H	8.665425	1.131208	3.225415
C	7.821523	2.844610	2.217963
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C	2.622770	4.343216	-1.368850
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H	-3.102641	2.072934	-1.983457
C	-6.181825	5.007484	-3.917520
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H	-6.794832	4.278606	-4.472565
H	-6.188562	5.949317	-4.484149
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C	-4.619339	-2.394778	4.133761
H	-5.086180	-1.529104	4.606693
C	-5.091401	-3.690994	4.340684
H	-5.950862	-3.850002	4.997880
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H	-2.915035	-5.394242	2.362002
C	-2.919697	-3.271775	2.650415
H	-2.073170	-3.103059	1.983558
C	-5.008119	-6.182041	3.917294
H	-4.278414	-6.795953	4.470232
H	-5.186160	-6.685831	2.953775
H	-5.948820	-6.188856	4.485793
C	2.194212	-3.541195	-3.281148
C	2.395143	-4.618249	-4.134219
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C	3.691496	-5.089956	-4.341088

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C 4.786893 -4.494322 -3.710932
C 4.555146 -3.396646 -2.867643
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Ge 1.712001 0.316107 -0.014317
Ge 0.316195 -1.712088 0.014233
O -3.905259 0.353126 3.672226
O -1.539001 -0.501256 3.287981
O -0.353031 -3.904891 -3.672743
O 0.500805 -1.538493 -3.288107
O 3.905237 -0.353845 3.672208
O 1.538851 0.500195 3.288003
O 0.353490 3.905406 -3.671809
O -0.500715 1.539051 -3.287750
P 0.000904 4.632792 -0.559321
P -4.632856 0.000908 0.559778
P -0.000849 -4.632854 -0.560393
P 4.632875 -0.000914 0.559792
S -2.971883 -0.530938 2.948575
S 0.530796 -2.971422 -2.948921
S 2.971751 0.530213 2.948695
S -0.530559 2.971918 -2.948284

4-Int
E = -5862.52678991
Ge -0.543165 0.019436 -2.103577
S 1.199658 -0.612042 1.061444
S -2.764091 1.960096 -0.810217
P 2.897387 0.857758 -0.796728
P -3.003231 -0.960391 -0.485541
O -0.116472 -1.246132 1.162137
O 1.459930 0.629792 1.812777
O -4.221941 1.959857 -1.055943
O -1.949486 2.939450 -1.548124
C 1.580986 -0.292524 -0.602415
C 4.280609 0.585107 0.350990
C 4.501143 1.429737 1.442051
H 3.854881 2.295105 1.598365
C 5.533180 1.148217 2.335980
H 5.705757 1.811899 3.186245
C 6.336141 0.024647 2.150206
H 7.144443 -0.190977 2.853078
C 6.099162 -0.834780 1.076724
H 6.710832 -1.729262 0.941749
C 5.070481 -0.560780 0.182815
H 4.877942 -1.243087 -0.649042
C 3.607768 0.660937 -2.456673
C 4.972359 0.896836 -2.674576
H 5.633188 1.135110 -1.838693
C 5.494909 0.816434 -3.962684
H 6.559732 0.997859 -4.125350
C 4.663530 0.505217 -5.037915

H	5.077242	0.440809	-6.047159
C	3.304192	0.284258	-4.824187
H	2.643716	0.053712	-5.663159
C	2.771293	0.367109	-3.540103
H	1.694568	0.229330	-3.382906
C	2.374484	2.573643	-0.642721
C	1.025915	2.887315	-0.480648
H	0.277794	2.100279	-0.406399
C	0.624339	4.220975	-0.440821
H	-0.442306	4.435946	-0.361161
C	1.573050	5.233684	-0.545535
H	1.257937	6.279549	-0.514679
C	2.925924	4.921619	-0.708458
H	3.667059	5.718744	-0.801738
C	3.330056	3.593336	-0.768618
H	4.386073	3.351955	-0.916085
C	2.338610	-1.842919	1.668743
C	2.364350	-3.105094	1.072255
H	1.688875	-3.337527	0.243745
C	3.250369	-4.059017	1.554132
H	3.281410	-5.047093	1.086308
C	4.096293	-3.782954	2.641005
C	4.022813	-2.520151	3.235077
H	4.669513	-2.287362	4.085249
C	3.148574	-1.546235	2.756223
H	3.095250	-0.552741	3.204673
C	5.039617	-4.831119	3.153637
H	5.708053	-4.429246	3.927627
H	5.662339	-5.240276	2.342822
H	4.488163	-5.677789	3.593631
C	-2.096619	0.405879	-1.016368
C	-1.934175	-2.341953	-0.941582
C	-2.202123	-3.672640	-0.620617
H	-3.077660	-3.939447	-0.022561
C	-1.331339	-4.665974	-1.066398
H	-1.518725	-5.711311	-0.810056
C	-0.230870	-4.321599	-1.852477
H	0.441050	-5.103656	-2.217218
C	0.005411	-2.985663	-2.185587
H	0.863110	-2.739721	-2.822912
C	-0.829719	-1.963248	-1.722121
H	1.755716	-1.217538	-1.162589
C	-4.561961	-1.231125	-1.389906
C	-5.526268	-2.115542	-0.894244
H	-5.391848	-2.581601	0.085516
C	-6.669562	-2.386727	-1.641936
H	-7.423128	-3.075582	-1.252845
C	-6.853712	-1.771847	-2.880271
H	-7.753849	-1.980333	-3.463863
C	-5.897136	-0.882374	-3.368154
H	-6.048885	-0.386451	-4.329565
C	-4.750898	-0.609867	-2.626002
H	-4.008540	0.107694	-2.980142
C	-3.491646	-0.987169	1.260357
C	-4.515469	-0.106280	1.642032
H	-5.033163	0.486570	0.882545
C	-4.832330	0.042256	2.987985
H	-5.613095	0.746089	3.284087
C	-4.144344	-0.693922	3.952995
H	-4.394036	-0.574089	5.010327

C -3.135059 -1.576253 3.571779
H -2.590965 -2.147481 4.327635
C -2.797575 -1.719949 2.227307
H -1.970641 -2.366554 1.934417
C -2.623491 2.364359 0.931572
C -3.515994 3.294031 1.461893
H -4.275655 3.738152 0.815309
C -3.443855 3.608841 2.815544
H -4.147833 4.332130 3.237282
C -2.495947 3.004637 3.652581
C -1.604397 2.084393 3.089580
H -0.848065 1.595263 3.708771
C -1.666325 1.761708 1.739139
H -0.997598 1.009701 1.325746
C -2.457857 3.302724 5.122841
H -1.424409 3.418234 5.482899
H -2.910306 2.478115 5.699189
H -3.011642 4.220648 5.366406

TS – addition across Ge–C bond
E = -5862.46965222
Ge -0.430909 -0.135972 -1.810139
S 1.014545 -0.247560 1.334672
S -2.706796 1.801030 -0.964094
P 2.593498 0.510297 -1.014756
P -2.910320 -1.034908 -0.111427
O -0.300272 -0.846525 1.637858
O 1.309959 1.075760 1.923278
O -4.181580 1.754718 -0.900894
O -2.081895 2.443802 -2.136506
C 1.212824 -0.300516 -0.364422
C 3.969120 0.638674 0.165019
C 4.175532 1.806298 0.903243
H 3.525266 2.669556 0.752216
C 5.205495 1.856970 1.840516
H 5.364805 2.770546 2.417532
C 6.026433 0.749038 2.041404
H 6.833239 0.794292 2.776967
C 5.815834 -0.420407 1.310332
H 6.447173 -1.295809 1.475988
C 4.786822 -0.479524 0.377507
H 4.614235 -1.400133 -0.184096
C 3.342949 -0.312159 -2.460195
C 4.675075 -0.025793 -2.792796
H 5.263671 0.648530 -2.166523
C 5.258720 -0.608583 -3.914736
H 6.297783 -0.380758 -4.163285
C 4.520967 -1.481449 -4.713884
H 4.981178 -1.940327 -5.592186
C 3.195529 -1.764462 -4.390838
H 2.608032 -2.440603 -5.016057
C 2.607305 -1.180813 -3.270684
H 1.558788 -1.379666 -3.040553
C 2.156642 2.187420 -1.562082
C 1.200931 2.873921 -0.801163
H 0.775594 2.406992 0.091170
C 0.792612 4.146515 -1.189489
H 0.030553 4.662015 -0.602324
C 1.335501 4.735108 -2.329555
H 1.001917 5.727590 -2.641617

C 2.288577 4.053182 -3.086447
H 2.701904 4.509834 -3.988736
C 2.700336 2.778090 -2.708629
H 3.425094 2.237006 -3.320152
C 2.213119 -1.354147 2.074352
C 2.362766 -2.652687 1.588498
H 1.771730 -2.987074 0.732439
C 3.282413 -3.501512 2.190841
H 3.409063 -4.517322 1.805442
C 4.051415 -3.078639 3.286760
C 3.866164 -1.777530 3.762778
H 4.459433 -1.426897 4.611737
C 2.951410 -0.912993 3.164965
H 2.817661 0.112894 3.512567
C 5.034075 -4.011446 3.932047
H 5.679145 -3.485271 4.649501
H 5.679112 -4.496837 3.183344
H 4.514621 -4.815639 4.478586
C -2.031684 0.259663 -0.787166
C -1.896050 -2.490380 -0.503821
C -2.434330 -3.774214 -0.387117
H -3.433740 -3.914772 0.032515
C -1.706593 -4.879808 -0.821214
H -2.126589 -5.882574 -0.714971
C -0.449772 -4.701165 -1.401282
H 0.119485 -5.566152 -1.750886
C 0.077663 -3.420115 -1.530944
H 1.077722 -3.289387 -1.955807
C -0.625789 -2.289443 -1.083931
H 0.313683 -1.457056 -0.664193
C -4.502231 -1.355580 -0.944071
C -5.532906 -2.047337 -0.299761
H -5.429334 -2.332123 0.750425
C -6.703039 -2.354376 -0.992036
H -7.508789 -2.890871 -0.485404
C -6.847558 -1.965581 -2.322695
H -7.768232 -2.199997 -2.862697
C -5.824188 -1.264330 -2.960929
H -5.943976 -0.941684 -3.997637
C -4.653324 -0.957224 -2.275041
H -3.858272 -0.382315 -2.754783
C -3.352992 -0.970630 1.645284
C -4.236070 0.047900 2.032033
H -4.638552 0.734583 1.280114
C -4.575699 0.187260 3.374364
H -5.255066 0.986434 3.679200
C -4.046242 -0.686682 4.324513
H -4.316056 -0.575152 5.377675
C -3.165939 -1.695553 3.935832
H -2.740123 -2.369906 4.682420
C -2.808912 -1.835519 2.596625
H -2.084435 -2.593088 2.294364
C -2.225435 2.800621 0.437809
C -2.514233 4.166902 0.374819
H -3.002035 4.576117 -0.512638
C -2.158776 4.984155 1.439250
H -2.379473 6.054790 1.392954
C -1.508777 4.461821 2.570854
C -1.236131 3.093181 2.604957
H -0.705943 2.659751 3.456085

C -1.600218 2.256446 1.549611
H -1.369100 1.190379 1.584559
C -1.129443 5.360123 3.712037
H -0.474268 4.843940 4.427539
H -2.022526 5.700951 4.261585
H -0.606038 6.261766 3.357737

4-Int without YH
E = -3969.02771301
Ge -1.292743 -2.409913 -1.283657
S 0.846440 -0.200232 -2.110907
P -0.953557 0.290840 0.221132
O 0.716549 1.247394 -2.369707
O 0.937940 -1.118418 -3.246050
C -0.423493 -0.728394 -1.076190
C -2.229814 -0.724600 0.992889
C -2.970337 -0.331900 2.108191
H -2.796848 0.635437 2.587436
C -3.944888 -1.195792 2.607076
H -4.532805 -0.906737 3.481258
C -4.170665 -2.424168 1.985033
H -4.937919 -3.096289 2.378228
C -3.426788 -2.796355 0.863139
H -3.622276 -3.762057 0.386101
C -2.437865 -1.954391 0.341668
C -1.684102 1.876313 -0.257893
C -1.874629 2.882321 0.697032
H -1.508350 2.749740 1.718589
C -2.514324 4.065006 0.336057
H -2.661375 4.852409 1.078778
C -2.957267 4.244425 -0.974544
H -3.454254 5.175317 -1.258024
C -2.755898 3.245680 -1.926390
H -3.086535 3.394674 -2.956557
C -2.118598 2.059279 -1.573141
H -1.923803 1.284391 -2.316247
C 0.341931 0.669488 1.426869
C 1.285927 1.653039 1.102445
H 1.165902 2.242021 0.189189
C 2.390682 1.844048 1.926424
H 3.135033 2.598834 1.664790
C 2.554252 1.063825 3.070981
H 3.423996 1.217143 3.714501
C 1.613979 0.086371 3.394119
H 1.743232 -0.525213 4.289976
C 0.509816 -0.118811 2.570189
H -0.219566 -0.895943 2.810881
C 2.362648 -0.343811 -1.162205
C 3.360043 0.598427 -1.398514
H 3.181521 1.389571 -2.129479
C 4.547412 0.533599 -0.675194
H 5.329080 1.276210 -0.858099
C 4.751372 -0.454071 0.294779
C 3.738250 -1.399830 0.501124
H 3.877375 -2.181903 1.252537
C 2.553805 -1.355407 -0.224739
H 1.761256 -2.084065 -0.042274
C 6.002876 -0.486374 1.121137
H 6.787947 0.152497 0.693118
H 5.802828 -0.128798 2.145316

H 6.401804 -1.508225 1.208519

TS – oxidative addition at Ge
E = -5862.45930654
Ge 0.090659 0.442143 -0.827647
S -1.917367 1.395424 1.269181
S 2.071876 -1.035407 1.218627
P -2.440530 -1.260488 0.035036
P 2.991028 1.368782 0.001687
O -0.758929 2.307049 1.376014
O -2.568249 0.916119 2.499648
O 0.977168 -1.125999 2.196900
O 3.433325 -0.757105 1.729134
C -1.454043 0.110776 0.269846
C -4.054334 -0.871438 -0.706568
C -5.040149 -0.302931 0.111638
H -4.874947 -0.227785 1.189928
C -6.208714 0.195266 -0.456889
H -6.966581 0.654421 0.181313
C -6.402493 0.123016 -1.836170
H -7.321212 0.515607 -2.278936
C -5.424296 -0.445401 -2.651281
H -5.575653 -0.502631 -3.731793
C -4.247101 -0.935667 -2.090241
H -3.471105 -1.365111 -2.729106
C -1.478509 -2.231351 -1.143214
C -0.297116 -1.646044 -1.632544
H -0.242947 -0.335181 -2.203818
C 0.542614 -2.401553 -2.458356
H 1.461918 -1.950393 -2.844157
C 0.214772 -3.712836 -2.783868
H 0.890941 -4.304030 -3.406065
C -0.975456 -4.278992 -2.315152
H -1.234068 -5.306673 -2.580370
C -1.820695 -3.543548 -1.489862
H -2.732076 -3.999392 -1.092810
C -2.816924 -2.268380 1.493455
C -3.903900 -3.151152 1.513316
H -4.602530 -3.184843 0.672744
C -4.102389 -3.974290 2.618673
H -4.950276 -4.663053 2.640251
C -3.222173 -3.909996 3.700116
H -3.381933 -4.553755 4.568792
C -2.146694 -3.022680 3.679811
H -1.461892 -2.966376 4.528871
C -1.937283 -2.195723 2.578059
H -1.095131 -1.498763 2.548482
C -3.202572 2.324310 0.424345
C -3.177154 2.484026 -0.960206
H -2.363900 2.045298 -1.544410
C -4.212069 3.165920 -1.588149
H -4.201853 3.271154 -2.676608
C -5.277288 3.705335 -0.853171
C -5.265285 3.554918 0.537317
H -6.083994 3.973419 1.129640
C -4.238735 2.865404 1.178673
H -4.241713 2.712796 2.259795
C -6.413571 4.391477 -1.552536
H -7.050514 4.942751 -0.846641
H -7.050575 3.657504 -2.074250

H -6.050714 5.100434 -2.312247
C 1.784037 0.132737 -0.005529
C 2.494550 2.669621 -1.169665
C 1.342739 3.403614 -0.840926
H 0.784733 3.193331 0.078234
C 0.900513 4.410782 -1.693329
H -0.002988 4.968287 -1.436190
C 1.603543 4.701664 -2.862601
H 1.254333 5.495176 -3.527928
C 2.757193 3.987325 -3.177819
H 3.318046 4.221271 -4.085720
C 3.205452 2.971146 -2.333421
H 4.115296 2.422726 -2.583254
C 4.615353 0.741688 -0.520399
C 4.680023 0.082853 -1.754861
H 3.776744 -0.012856 -2.363896
C 5.879845 -0.475264 -2.188260
H 5.925788 -0.983692 -3.154257
C 7.014688 -0.397688 -1.380480
H 7.954797 -0.843089 -1.714647
C 6.943634 0.231729 -0.138795
H 7.823655 0.269183 0.507217
C 5.747325 0.799110 0.294808
H 5.682834 1.257602 1.282776
C 3.178613 2.310556 1.543217
C 4.102586 3.361671 1.607283
H 4.749556 3.581190 0.753382
C 4.184750 4.142277 2.756038
H 4.908390 4.959115 2.808455
C 3.331296 3.888399 3.831149
H 3.390165 4.506783 4.730244
C 2.395166 2.859882 3.753536
H 1.711198 2.672086 4.583755
C 2.314163 2.064967 2.611868
H 1.562865 1.275520 2.547077
C 2.151542 -2.646507 0.455734
C 1.164267 -3.588365 0.727850
H 0.331189 -3.317577 1.378173
C 1.266975 -4.857034 0.167662
H 0.489120 -5.596976 0.374694
C 2.344699 -5.200548 -0.657775
C 3.330560 -4.235874 -0.901565
H 4.188119 -4.490950 -1.530490
C 3.244673 -2.963390 -0.345350
H 4.024140 -2.218462 -0.518453
C 2.420273 -6.564353 -1.278357
H 1.627561 -6.696087 -2.034077
H 2.280084 -7.356048 -0.526458
H 3.386499 -6.732501 -1.774209

Product of Oxidative Addition
E = -5862.54384995
Ge -0.574062 -0.736180 -1.408820
S 2.211065 0.438142 -1.890263
S -2.220172 2.036877 -1.524866
P 2.111669 -1.672714 0.139419
P -3.119928 -0.171638 0.119327
O 1.258189 1.145728 -2.760355
O 3.346188 -0.261187 -2.523158
O -3.505722 2.493445 -0.943557

O	-2.121029	1.924390	-2.984979
C	1.282488	-0.586368	-0.885957
C	3.746205	-1.073749	0.683040
C	4.865438	-1.356406	-0.109943
H	4.751669	-1.929643	-1.030574
C	6.117206	-0.874408	0.261530
H	6.985600	-1.094324	-0.363395
C	6.259288	-0.106934	1.415867
H	7.242833	0.273360	1.702129
C	5.145114	0.181418	2.202061
H	5.249667	0.787336	3.104743
C	3.890874	-0.301159	1.840331
H	3.026448	-0.074209	2.465316
C	1.125583	-1.913097	1.646930
C	0.612097	-0.749320	2.236649
H	0.733549	0.208923	1.726565
C	-0.062533	-0.823954	3.450844
H	-0.450028	0.087541	3.909564
C	-0.270564	-2.061991	4.058564
H	-0.810999	-2.121639	5.006679
C	0.189067	-3.225549	3.444879
H	-0.001494	-4.199321	3.901379
C	0.895476	-3.153779	2.245917
H	1.243605	-4.070306	1.768418
C	2.503645	-3.288542	-0.607354
C	3.151536	-4.307350	0.103995
H	3.439715	-4.155366	1.147276
C	3.455976	-5.508789	-0.529284
H	3.955002	-6.305725	0.027003
C	3.138427	-5.688474	-1.877220
H	3.382879	-6.631125	-2.372749
C	2.533137	-4.660006	-2.596588
H	2.312118	-4.786619	-3.658657
C	2.218463	-3.457763	-1.964631
H	1.777845	-2.625226	-2.519718
C	2.958937	1.644487	-0.795217
C	2.195234	2.247271	0.201230
H	1.130805	2.014979	0.286959
C	2.801786	3.138616	1.077579
H	2.201333	3.607697	1.861249
C	4.161643	3.457400	0.961953
C	4.895908	2.865510	-0.071381
H	5.957010	3.105248	-0.183002
C	4.304513	1.958894	-0.947615
H	4.876183	1.465640	-1.735607
C	4.818322	4.382394	1.944390
H	5.689786	4.888373	1.504427
H	5.175121	3.826435	2.828288
H	4.119492	5.151503	2.305111
C	-1.836939	0.558687	-0.755113
C	-2.573515	-1.901877	0.261982
C	-3.331956	-2.872445	0.925706
H	-4.247903	-2.596814	1.454245
C	-2.925370	-4.203082	0.892945
H	-3.511115	-4.964137	1.413707
C	-1.786440	-4.562769	0.171782
H	-1.477665	-5.610329	0.126619
C	-1.048456	-3.594499	-0.506153
H	-0.170434	-3.901374	-1.078362
C	-1.420614	-2.246761	-0.462405

H	-0.664162	-0.975940	-2.923072
C	-4.729272	-0.278265	-0.728266
C	-5.905176	-0.530730	-0.015253
H	-5.888210	-0.575604	1.076792
C	-7.106920	-0.705761	-0.698491
H	-8.026055	-0.899189	-0.140341
C	-7.135517	-0.622986	-2.089807
H	-8.079415	-0.753703	-2.624635
C	-5.963406	-0.358753	-2.798268
H	-5.986812	-0.273277	-3.886946
C	-4.758552	-0.185998	-2.123024
H	-3.846456	0.058079	-2.674573
C	-3.521745	0.461590	1.781614
C	-4.134696	1.719093	1.899127
H	-4.362977	2.285243	0.992707
C	-4.419874	2.234088	3.160814
H	-4.893795	3.214851	3.246110
C	-4.108623	1.504691	4.309221
H	-4.341194	1.911330	5.296522
C	-3.504552	0.254721	4.193377
H	-3.261429	-0.323747	5.088441
C	-3.208218	-0.265788	2.934010
H	-2.724783	-1.239688	2.851665
C	-1.024983	3.269886	-1.043135
C	-1.099566	3.826066	0.231999
H	-1.855044	3.471514	0.936780
C	-0.214896	4.841972	0.580397
H	-0.271449	5.288308	1.577431
C	0.742093	5.310408	-0.329812
C	0.789045	4.732487	-1.603519
H	1.537138	5.076216	-2.322916
C	-0.090349	3.719174	-1.970895
H	-0.053487	3.254356	-2.955917
C	1.719047	6.382609	0.051284
H	1.697693	7.217586	-0.666150
H	2.746660	5.983701	0.054710
H	1.508385	6.788135	1.051167

$GaCl_3$ adducts (energies at the def2svp level):

Y_2Ge
E = -9163.55674431
S 2.029316 1.040255 1.099365
S -2.013397 0.041703 -1.444572
P 2.524016 0.198363 -1.765612
P -2.391641 1.769474 0.968269
O 0.862034 0.526297 1.946128
O 2.184013 2.498191 0.992865
O -0.818154 -0.867758 -1.717478
O -2.274657 1.098801 -2.434789
C 1.657992 0.191741 -0.296385
C 4.268892 0.543407 -1.410441
C 4.692071 1.874216 -1.307878
H 3.997450 2.688231 -1.525529
C 5.996915 2.154830 -0.910843
H 6.326767 3.193205 -0.832329
C 6.873315 1.115629 -0.603952
H 7.894569 1.339101 -0.286544
C 6.446698 -0.209118 -0.691001
H 7.129252 -1.024091 -0.440812
C 5.146464 -0.499040 -1.093846
H 4.812176 -1.536615 -1.160845
C 2.327368 -1.430410 -2.520567
C 2.335355 -2.548709 -1.676896
H 2.472701 -2.434520 -0.598948
C 2.119130 -3.817443 -2.204458
H 2.089362 -4.674415 -1.529297
C 1.901068 -3.972477 -3.572038
H 1.712933 -4.966876 -3.983360
C 1.894322 -2.859745 -4.412653
H 1.703716 -2.981257 -5.481326
C 2.100341 -1.585144 -3.891692
H 2.055296 -0.712564 -4.546153
C 2.007535 1.444820 -2.973447
C 2.821677 1.804647 -4.056674
H 3.814962 1.362431 -4.171919
C 2.362147 2.738725 -4.980345
H 2.995156 3.025893 -5.823215
C 1.094147 3.306717 -4.830192
H 0.736889 4.035748 -5.561721
C 0.285801 2.946020 -3.754650
H -0.712671 3.369505 -3.630368
C 0.745830 2.020093 -2.821499
H 0.115500 1.736515 -1.979880
C 3.506494 0.448301 1.884761
C 3.619611 -0.908062 2.187574
H 2.805081 -1.606302 1.979463
C 4.793785 -1.370916 2.763591
H 4.879330 -2.434709 3.001261
C 5.859731 -0.501389 3.042347
C 5.707015 0.855646 2.742223
H 6.523037 1.549900 2.959717
C 4.534464 1.340094 2.166600
H 4.406055 2.396282 1.926325
C 7.135371 -1.027543 3.629922
H 7.789063 -0.214538 3.975262

H 7.696282 -1.615113 2.884235
H 6.937681 -1.695835 4.481603
C -1.596203 0.516456 0.111471
C -1.886230 1.710052 2.695654
C -1.546466 2.876269 3.387536
H -1.586141 3.845990 2.886899
C -1.132567 2.788645 4.714404
H -0.856578 3.696605 5.255229
C -1.053828 1.546590 5.343753
H -0.714511 1.483287 6.380540
C -1.392491 0.385535 4.649937
H -1.315783 -0.596309 5.121822
C -1.811281 0.464016 3.326666
H -2.047363 -0.457682 2.789505
C -4.190103 1.550772 0.860288
C -4.919950 1.076445 1.954975
H -4.433431 0.949309 2.924340
C -6.266177 0.752741 1.802111
H -6.831988 0.378681 2.658240
C -6.884334 0.896674 0.561251
H -7.937119 0.630234 0.441494
C -6.159909 1.377785 -0.528647
H -6.639211 1.482794 -1.504183
C -4.815805 1.708271 -0.384975
H -4.243803 2.058104 -1.248313
C -2.023160 3.434595 0.350933
C -2.997574 4.434612 0.264987
H -4.028736 4.224029 0.557345
C -2.648511 5.699765 -0.204260
H -3.410638 6.478674 -0.281162
C -1.331293 5.968793 -0.575241
H -1.062084 6.961417 -0.944598
C -0.357090 4.975526 -0.471078
H 0.679275 5.180531 -0.747715
C -0.699410 3.707633 -0.011503
H 0.074200 2.943054 0.082335
C -3.458070 -0.991918 -1.452680
C -3.758929 -1.777810 -0.342758
H -3.118165 -1.772252 0.541075
C -4.904367 -2.560987 -0.363014
H -5.135587 -3.177621 0.509126
C -5.754757 -2.574908 -1.477047
C -5.420154 -1.782605 -2.581595
H -6.070535 -1.783766 -3.460436
C -4.276894 -0.989213 -2.577913
H -4.021173 -0.352807 -3.426762
C -6.991758 -3.422849 -1.473951
H -7.553539 -3.325607 -2.413235
H -7.660963 -3.141888 -0.645177
H -6.739273 -4.486129 -1.336843
Ge -0.010036 -0.597121 0.296435
Ga -0.285133 -2.933434 1.027227
Cl 1.659154 -3.797566 1.670966
Cl -1.087123 -4.158186 -0.600519
Cl -1.746781 -2.973784 2.702692

$NTMS_2Ge$
E = -7125.55800131
N -1.900373 0.271602 0.025349
N 0.472719 -1.597283 0.128774

Si 0.940664 -2.002116 1.802383
Si 1.053471 -2.458513 -1.314253
Si -2.619881 1.903664 0.329073
Si -2.991352 -1.105669 -0.394803
C -0.084083 -0.878472 2.917927
H   0.201790 0.182115 2.791736
H -1.167834 -0.974545 2.758606
H   0.131429 -1.122379 3.970771
C   2.741778 -1.627915 2.151599
H   2.965699 -0.565719 1.971431
H   2.961439 -1.846336 3.209557
H   3.424564 -2.225954 1.532387
C   0.598442 -3.814937 2.145468
H   0.898305 -4.053773 3.178428
H -0.463668 -4.073409 2.028824
H   1.186438 -4.462695 1.476496
C -0.032032 -3.958769 -1.647821
H   0.350031 -4.499424 -2.529135
H -0.009091 -4.655337 -0.795389
H -1.082067 -3.698299 -1.840826
C   2.813383 -3.065641 -1.111003
H   2.908307 -3.805375 -0.301169
H   3.136836 -3.555085 -2.043911
H   3.493181 -2.225807 -0.907801
C   0.973987 -1.247638 -2.755255
H   0.028298 -0.682808 -2.823455
H   1.801899 -0.525093 -2.686269
H   1.078722 -1.788931 -3.709243
C -2.629053 -2.638052 0.613974
H -1.617057 -3.016208 0.438048
H -2.743599 -2.430526 1.689045
H -3.354732 -3.422187 0.344143
C -4.802091 -0.715193 -0.068683
H -5.173197 0.213274 -0.523133
H -5.369784 -1.548306 -0.515984
H -5.036172 -0.700971 1.005192
C -2.831542 -1.413475 -2.239378
H -1.817188 -1.706130 -2.541191
H -3.517411 -2.216137 -2.554136
H -3.098642 -0.501802 -2.796825
C -3.791117 1.803009 1.795897
H -4.767299 1.355623 1.573721
H -3.324959 1.234115 2.616154
H -3.967464 2.826456 2.164066
C -3.452174 2.496637 -1.244906
H -3.938421 3.470312 -1.073956
H -2.686977 2.638575 -2.024943
H -4.212412 1.804743 -1.634540
C -1.314181 3.152054 0.798542
H -0.691151 2.855361 1.655482
H -0.653993 3.430546 -0.035454
H -1.854280 4.067076 1.094599
Ge -0.100852 0.129255 -0.044034
Ga 1.771319 1.809382 -0.210335
Cl 2.037825 2.434501 1.869768
Cl 3.477756 0.593940 -0.838793
Cl 1.295118 3.324796 -1.699356

Boryl-Amino-Germylene
E = -6175.24854007

N 0.157536 1.933564 -0.307090
Si 1.896265 2.448712 -0.235111
C 1.889202 4.249591 0.301698
H 1.404969 4.917010 -0.426627
H 1.393158 4.379626 1.276662
H 2.932142 4.586668 0.414860
C 2.604990 2.264580 -1.956479
H 3.632876 2.658655 -1.999044
H 2.640653 1.197555 -2.226950
H 2.004748 2.801936 -2.707060
C 2.836530 1.430903 1.012603
H 2.286751 1.287994 1.954630
H 3.108924 0.442173 0.616776
H 3.776095 1.957685 1.247032
C -4.650139 -0.267138 -0.390030
C -4.610420 0.720174 0.547277
H -5.521641 -0.763562 -0.813745
H -5.439333 1.191052 1.073183
B -2.464785 0.241056 -0.040923
N -3.365599 -0.599653 -0.767505
N -3.295124 1.066442 0.787878
C -2.930944 2.054594 1.771013
H -1.837667 2.145874 1.817862
H -3.347654 3.043311 1.518996
H -3.290198 1.772256 2.773135
C -3.099597 -1.597737 -1.777265
H -3.291755 -1.207546 -2.789765
H -2.057240 -1.935797 -1.710157
H -3.735516 -2.481062 -1.617841
C -0.772585 2.981217 -0.716203
H -1.777021 2.571529 -0.900551
H -0.861151 3.770821 0.048140
H -0.436159 3.463611 -1.650210
Ge -0.413072 0.242232 -0.071190
Ga 1.100192 -1.714578 0.201638
Cl -0.246277 -3.349084 -0.384924
Cl 1.637271 -1.790384 2.315036
Cl 2.798635 -1.549127 -1.172732

3,5-Me$_2$Py
E = -3630.62067414
C 1.279081 1.162475 -0.060253
C 2.670237 1.219122 -0.011663
C 3.353012 0.000052 0.014382
C 2.670281 -1.219006 -0.011952
C 1.279102 -1.162367 -0.060678
N 0.619232 0.000027 -0.077602
H 0.661397 2.064252 -0.101967
H 0.661453 -2.064149 -0.102881
Ga -1.418653 0.000083 -0.001886
Cl -1.906460 1.851656 -1.022176
Cl -1.906086 -1.850879 -1.023576
Cl -1.825495 -0.001091 2.122842
H 4.447163 0.000077 0.051744
C 3.390921 -2.531601 0.010026
H 2.690714 -3.374635 -0.058809
H 4.099353 -2.606870 -0.828947
H 3.969312 -2.645858 0.939882
C 3.390932 2.531689 0.010163
H 4.095642 2.608768 -0.831806

H 2.690438 3.374859 -0.053893
H 3.973449 2.643944 0.937661

Bisylide1
E = -4723.48289311
C -0.495856 0.622241 0.077222
C -0.264453 1.902060 0.519877
C -2.289378 2.919483 -0.285734
H -3.095683 2.485042 0.321405
H -2.134009 2.269361 -1.159615
C -2.590768 4.341999 -0.675998
H -2.719161 4.976959 0.212892
H -3.526752 4.367624 -1.252419
H -1.791343 4.770049 -1.299472
C 1.343802 3.590455 1.089915
H 2.238115 3.561503 1.727301
H 0.576384 4.193824 1.595166
C 1.671007 4.133167 -0.281791
H 2.429434 3.513234 -0.780813
H 2.065301 5.156412 -0.190775
H 0.774888 4.173646 -0.917046
C 2.400427 0.440938 -0.686598
C 3.395561 0.881826 0.194054
H 3.290692 0.704379 1.265770
C 4.510576 1.556831 -0.294485
H 5.285550 1.893387 0.398051
C 4.634686 1.808754 -1.661246
H 5.509838 2.340282 -2.042309
C 3.641894 1.378647 -2.539893
H 3.735156 1.570026 -3.611168
C 2.529993 0.691174 -2.056714
H 1.765277 0.339941 -2.752728
C 0.542564 -1.662614 -1.335511
C -0.282753 -1.298018 -2.404903
H -0.743504 -0.308274 -2.432952
C -0.578255 -2.226148 -3.399564
H -1.250048 -1.943686 -4.212586
C -0.046629 -3.511666 -3.335287
H -0.288440 -4.242568 -4.110412
C 0.775183 -3.874446 -2.268201
H 1.174496 -4.889002 -2.203893
C 1.068531 -2.955676 -1.266002
H 1.673484 -3.262568 -0.411834
C 1.388016 -1.209833 1.477865
C 2.587286 -1.928165 1.586688
H 3.271528 -1.995498 0.737029
C 2.920487 -2.542743 2.790049
H 3.854344 -3.103240 2.873353
C 2.063974 -2.437198 3.886706
H 2.326466 -2.921015 4.830542
C 0.878868 -1.712057 3.782494
H 0.207637 -1.625728 4.639386
C 0.536116 -1.096594 2.580865
H -0.393421 -0.527730 2.501799

- -1.094065 2.919188 0.507058
- 0.915104 2.225762 1.046505

P 0.905360 -0.412704 -0.074874
Cl -3.491171 -0.060518 -1.631290
Cl -3.270165 0.528178 1.984793
Cl -1.930087 -2.447669 0.585754

Ga -2.279873 -0.312250 0.194830

Bisylide2
E = -4703.64335090
C -0.356979 -0.696684 -0.298860
C 0.218734 -1.947995 -0.312596
C 2.427040 -2.851496 -0.617834
H 1.919257 -3.666067 -1.154318
H 2.857835 -2.173263 -1.373485
C 3.491454 -3.378356 0.308212
H 3.977280 -2.555419 0.851659
H 4.262070 -3.911429 -0.267619
H 3.067575 -4.073617 1.047944
C -0.230480 -4.322353 0.009723
H 0.535187 -4.207902 0.785453
H 0.051390 -5.152467 -0.659856
H -1.182994 -4.571270 0.507231
C -1.490854 -3.075055 -1.662118
H -2.459272 -3.207995 -1.154174
H -1.351073 -3.897743 -2.383393
H -1.518649 -2.121779 -2.201600
C -0.108678 2.137628 -0.748470
C -0.886879 1.962679 -1.898287
H -1.049644 0.962946 -2.306537
C -1.522519 3.056001 -2.480105
H -2.154714 2.903127 -3.357013
C -1.379593 4.324059 -1.922923
H -1.888208 5.179677 -2.373214
C -0.608871 4.497794 -0.773421
H -0.516376 5.486945 -0.319588
C 0.022427 3.408814 -0.181636
H 0.581471 3.547900 0.744243
C 2.294539 0.533425 -0.904457
C 2.317198 0.664984 -2.297900
H 1.399768 0.903665 -2.840363
C 3.510620 0.499469 -2.996719
H 3.519415 0.603905 -4.083953
C 4.689541 0.210291 -2.309988
H 5.626075 0.086634 -2.858814
C 4.670933 0.081692 -0.921798
H 5.591123 -0.147988 -0.379475
C 3.477633 0.236440 -0.219641
H 3.462101 0.109365 0.864035
C 1.081795 0.966549 1.704507
C 0.429527 0.196381 2.671941
H -0.294058 -0.564070 2.369249
C 0.703261 0.406650 4.021318
H 0.185331 -0.192194 4.773294
C 1.622960 1.379142 4.407953
H 1.831457 1.542797 5.467935
C 2.281817 2.143261 3.444063
H 3.008446 2.901286 3.745113
C 2.015352 1.937893 2.093456
H 2.548449 2.526449 1.342528
N -0.391922 -3.086225 -0.725155
- 1.481675 -2.102700 0.151150

P 0.692400 0.673148 -0.040627
Cl -3.570140 -0.269560 -1.683193
Cl -2.520987 1.368543 1.354722
Cl -2.853143 -2.195539 1.354112

Ga -2.305563 -0.437722 0.115116

Bisylide3
E = -5411.93576887
C   0.070117 -0.463003 -0.132961
P -1.510819 0.198187 -0.120227
P   1.467863 0.509073 0.012573
C -1.606517 1.972556 -0.549597
C -2.381729 0.126209 1.483661
C   2.980843 -0.470643 0.212779
C -2.542074 -0.622223 -1.374652
C   1.407528 1.635188 1.446657
C   1.867999 1.510968 -1.459799
C -1.361073 2.945725 0.426988
C -1.380457 4.296171 0.087923
C -1.654227 4.685956 -1.222086
C -1.922561 3.721938 -2.192873
C -1.921224 -0.734595 2.484194
C -2.576069 -0.787543 3.712478
C -1.903189 2.370694 -1.858606
C -3.691081 0.013571 3.950176
C -4.151560 0.878355 2.957462
C -3.498278 0.937977 1.729296
C   3.410764 -1.226708 -0.883384
C   4.552266 -2.014029 -0.775203
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Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

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