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A Diarsagermylene and a Diarsastannylene Stabilised by Arene…Ge/Sn Interactions†

Keith Izod,* Peter Evans, Paul G. Waddell

ORCID K. Izod: 0000-0003-3882-9343

ORCID P. Evans: 0000-0002-5916-8786

SUPPORTING INFORMATION

Contents:

Experimental

General details: All manipulations were carried out using standard Schlenk and dry-box techniques under an atmosphere of dry nitrogen or argon. THF, diethyl ether, toluene, *n*-hexane and light petroleum (b.p. 40-60 °C) were dried prior to use by distillation under nitrogen from sodium, potassium, or sodium/potassium alloy, as appropriate. THF was stored over activated 4A molecular sieves; all other solvents were stored over a potassium film. Deuterated toluene was distilled from potassium under nitrogen and $CDCl_3$ was distilled from CaH_2 under nitrogen; both solvents were deoxygenated by three freeze-pump-thaw cycles and were stored over activated 4A molecular sieves. *n*-Butyllithium was purchased from Aldrich as a 2.5 M solution in hexanes. $Dipp_2PLi.OEt_2$ was prepared by a previously published procedure.[S1] All other compounds were used as supplied by the manufacturer.

^1H and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker AvanceIII 500 spectrometer operating at 500.16 and 125.65 MHz, respectively, or a Bruker AvanceIII 300 spectrometer operating at 300.15 and 75.47 MHz, respectively; chemical shifts are quoted in ppm relative to tetramethylsilane. Due to the air-, temperature-, and light-sensitive nature of the compounds satisfactory elemental analyses could not be obtained.

Synthesis of (iPr$_2$N)AsCl$_2$: To a solution of $AsCl_3$ (1.0 mL, 11.9 mmol) in Et_2O (60 mL) was added iPr$_2$NH (3.3 mL, 23.5 mmol) and this mixture was stirred for 2 h. The solid was removed by filtration and washed with Et_2O (20 mL). The solvent was removed under reduced pressure (10 mmHg) from the combined Et_2O solutions to give an orange oil. Yield: 2.77 g, 95%. ^1H NMR [$CDCl_3$]: δ 1.31 (d, J_{HH} = 6.8 Hz, 1H, CH*Me*$_2$), 4.03 (sept, J_{HH} = 6.8 Hz, 6H, C*H*Me$_2$). $^{13}C\{^1H\}$ NMR [$CDCl_3$]: δ 25.10 (CH*Me*$_2$), 49.37 (*C*HMe$_2$).

Synthesis of Dipp$_2$As(NiPr$_2$): To a solution of (iPr$_2$N)AsCl$_2$ (2.77 g, 11.3 mmol) in Et_2O (40 mL) was added, dropwise, a solution of $DippLi.OEt_2$ (5.46 g, 22.5 mmol) in Et_2O (40 mL). The resulting brown solution with pale solids was stirred for 30 mins. The solvent was removed *in vacuo* and the product was extracted into *n*-hexane (50 mL) and filtered. The solvent was removed from the filtrate *in vacuo* to give a pale brown powder. Yield: 5.45 g, 97%. ^1H NMR [d_8-toluene, 213 K]: δ 0.35 (d, J_{HH} = 6.3 Hz, 3H, ArCH*Me*), 0.45 (d, J_{HH} = 6.4 Hz, 3H, ArCH*Me*), 0.71 (d, J_{HH} = 6.2 Hz, 3H, NH*Me*), 1.13 (d, J_{HH} = 6.6 Hz, 3H, ArCH*Me*), 1.17 (d, J_{HH} = 6.6 Hz, 3H, ArCH*Me*), 1.21 (d, J_{HH} = 6.4 Hz, 3H, ArCH*Me*), 1.30 (d, J_{HH} = 6.4 Hz, 3H, NCH*Me*), 1.36 (d, J_{HH} = 6.5 Hz, 3H, ArCH*Me*), 1.41 (m, 6H, ArCH*Me*), 1.55 (d, J_{HH} = 6.5 Hz, 3H, NCH*Me*), 3.25 (sept, J_{HH} = 6.7 Hz, 1H, NC*H*Me), 3.38 (sept, J_{HH} = 6.5 Hz, 1H, ArC*H*Me), 3.65 (sept, J_{HH} = 6.5 Hz, 1H, ArC*H*Me), 3.81 (sept, J_{HH} = 6.7 Hz, 1H, NC*H*Me), 4.57 (sept, J_{HH} = 6.7 Hz, 1H, ArC*H*Me), 5.32 (sept, J_{HH} = 6.6 Hz, 1H, ArC*H*Me), 6.83 (dd, J_{HH} = 6.9 Hz, J_{HH} = 2.0 Hz, 1H, ArH), 6.91 (dd, J_{HH} = 7.7 Hz, J_{HH} = 1.1 Hz, 1H, ArH), 7.06 (dd, J_{HH} = 7.6 Hz, J_{HH} = 1.1 Hz, 1H, ArH), 7.16 (m, 3H, ArH). $^{13}C\{^1H\}$ NMR [d_8-toluene, 213 K]: δ 20.81 (NCH*Me*), 22.34, 22.64 (ArCH*Me*), 23.60 (NCH*Me*), 23.70, 24.75, 24.98, 25.01 (ArCH*Me*), 25.13 (Ar*C*HMe), 25.41 (ArCH*Me*), 25.88 (NCH*Me*), 26.88 (ArCH*Me*), 27.32 (NCH*Me*), 29.90, 32.42, 35.42 (Ar*C*HMe), 46.10, 53.40 (N*C*HMe), 123.92, 124.52, 125.43, 125.83, 130.15 (ArH), 140.70, 141.64, 150.21, 152.58, 152.75, 152.78 (Ar). Remaining aromatic carbon signal is obscured by the solvent peak.

Synthesis of Dipp$_2$AsCl (5): To a solution of Dipp$_2$As(NiPr$_2$) (5.45 g, 11.0 mmol) in Et_2O (60 mL) was added a solution of anhydrous HCl in Et_2O (2.0 M, 10 mL, 20.0 mmol) and this mixture was stirred

for 3 h. The solid was removed by filtration and washed with Et_2O (20 mL). The solvent was removed *in vacuo* from the combined filtrate and washings to give a white microcrystalline solid. Yield: 4.19 g, 96%. ^{1}H NMR [$CDCl_3$]: δ 1.04 (d, J_{HH} = 6.7 Hz, 12H, CH*Me*Me), 1.04 (d, J_{HH} = 6.7 Hz, 12H, CHMe*Me*), 3.57 (sept, J_{HH} = 6.7 Hz, 4H, C*H*MeMe), 7.12 (d, J_{HH} = 7.8 Hz, 4H, ArH), 7.28 (m, 2H, ArH). ^{13}C{^{1}H} NMR [$CDCl_3$]: δ 24.12 (CH*Me*Me), 24.87 (CHMe*Me*), 32.60 (*C*HMeMe), 124.73, 129.96 (ArH), 141.77, 151.91 (Ar).

Synthesis of $Dipp_2AsH$ (6): To a cold (0 °C) solution of $Dipp_2AsCl$ (4.19 g, 9.68 mmol) in Et_2O (50 mL) was added solid $LiAlH_4$ (0.370 g, 9.74 mmol) in portions. The mixture was stirred for 3 h at room temperature then quenched by the careful addition of degassed water (40 mL). The organic phase was separated and the aqueous phase was extracted into light petroleum (3 x 15 mL). The combined organic phases were dried over 4 Å molecular sieves. The solution was filtered and the solvent was removed from the filtrate *in vacuo* to give a white microcrystalline solid. Residual solvent was removed by heating (ca. 80 °C) under vacuum. Yield: 3.53 g, 92%. ^{1}H NMR [$CDCl_3$]: δ 1.03 (d, J_{HH} = 6.8 Hz, 12H, CH*Me*Me), 1.06 (d, J_{HH} = 6.8 Hz, 12H, CHMe*Me*), 3.40 (sept, J_{HH} = 6.8 Hz, 4H, C*H*MeMe), 4.67 (s, 1H, AsH), 7.09 (d, J_{HH} = 7.6 Hz, 4H, ArH), 7.24 (m, 2H, ArH). ^{13}C{^{1}H} NMR [$CDCl_3$]: δ 23.92 (CH*Me*Me), 24.30 (CHMe*Me*), 34.31 (*C*HMeMe), 123.46, 128.54 (ArH), 136.69, 152.50 (Ar).

Synthesis of $(Dipp_2As)Li(THF)_{2.75}(OEt_2)_{0.25}$ (7): To a solution of $Dipp_2AsH$ (0.78 g, 1.96 mmol) in THF (10 mL) was added a solution of *n*BuLi in hexanes (0.85 mL, 2.0 mmol). The resulting red solution was stirred for 1 h. The solvent was removed *in vacuo* and the resulting yellow solid was dissolved in Et_2O (5 mL). On standing at -25 °C overnight yellow crystals of $(Dipp_2As)Li(THF)_{2.75}(OEt_2)_{0.25}$ (**7**) suitable for X-ray crystallography formed. These were washed with cold (-10 °C) light petroleum (2 x 5 mL) and residual solvent was removed *in vacuo* to give **7** as a yellow crystalline powder. Yield: 0.69 g, 60%. ^{1}H NMR [d_8-toluene]: δ 1.08 (t, 1.5H, Et_2O), 1.11 (d, J_{HH} = 6.9 Hz, 24H, CHMe_2), 1.39 (m, 11H, THF), 3.25 (q, 1H, Et_2O), 3.47 (m, 11H, THF), 4.40 (sept, J_{HH} = 6.9 Hz, 4H, C*H*Me_2), 7.08 (m, 4H, ArH), 7.16 (m, 2H, ArH). ^{13}C{^{1}H} NMR [d_8-toluene]: δ 15.49 (Et_2O), 25.03 (CHMe_2), 25.57 (THF), 35.82 (*C*HMe_2), 65.92 (Et_2O), 68.47 (THF), 122.54, 125.17 (ArH), 150.66 (br. s, Ar), 152.93 (Ar). ^{7}Li NMR [d_8-toluene]: δ 1.7 (s).

Synthesis of $\{(Dipp)_2As\}_2Ge.C_7H_8$ (8Ge): To a solution of $(Dipp)_2AsH$ (0.66 g, 1.66 mmol) in THF (10 mL) was added a solution of *n*BuLi in hexanes (2.3 M, 0.7 mL, 1.61 mmol). The resulting red solution was stirred for 30 min and added, dropwise, to a cold (-78 °C) solution of $GeCl_2$(1,4-dioxane) (0.192 g, 0.83 mmol) in THF (10 mL). The resulting red solution was allowed to warm to room temperature and the solvent was removed *in vacuo* to give a sticky red solid. The product was extracted into toluene (15 mL) to give a dark red solution with pale solids. The mixture was filtered and the dark red filtrate was reduced to 5 mL in volume. Storage at -25 °C overnight gave red crystals of $\{(Dipp)_2As\}_2Ge.C_7H_8$. The supernatant solution was removed by filtration and the remaining solid was washed with cold (0 °C) light petroleum (10 mL). Residual solvent was removed under vacuum to give a red crystalline powder. Yield: 0.20 g, 25%. ^{1}H NMR [213 K, d_8-toluene]: δ 0.48 (d, J_{HH} = 5.6 Hz, 6H, ^{B}CH*Me*Me), 0.82 (d, J_{HH} = 4.4 Hz, 6H, ^{A}CH*Me*Me), 0.86 (d, J_{HH} = 5.3 Hz, 6H, ^{C}CH*Me*Me), 1.19 (d, J_{HH} = 5.3 Hz, 6H, ^{A}CHMe*Me*), 1.36 (d, J_{HH} = 5.3 Hz, 6H, ^{D}CH*Me*Me), 1.41 (d, J_{HH} = 6.2 Hz, 6H, ^{D}CHMe*Me*), 1.43 (d, J_{HH} = 6.0 Hz, 6H, ^{C}CHMe*Me*), 1.52 (d, J_{HH} = 5.7 Hz, 6H, ^{B}CHMe*Me*), 2.10 (s, 3H, Ph*Me*), 2.51 (br. m, 2H, ^{A}C*H*MeMe), 3.26 (br. m, 2H, ^{B}C*H*MeMe), 3.98 (br.

m, 2H, ^{C}C*H*MeMe), 4.86 (br. m, 2H, ^{D}C*H*MeMe), 6.70-7.25 (br. m, 17H, ArH + *Ph*Me). $^{13}C\{^{1}H\}$ NMR [213 K, d_8-toluene]: δ 21.37 (Ph*Me*), 21.56 (^{C}CH*Me*Me), 23.88 (^{D}CHMe*Me*), 24.23 (^{B}CH*Me*Me), 25.49 (^{A}CHMe*Me*), 26.04 (^{D}CH*Me*Me), 26.32 (^{C}CHMe*Me*), 26.79 (^{A}CH*Me*Me), 28.23 (^{B}CHMe*Me*), 34.08 (^{B}*C*HMeMe), 34.37 (^{C}*C*HMeMe), 35.03 (^{A}*C*HMeMe, ^{D}*C*HMeMe), 123.13, 124.53 (ArH), 125.59 (*Ph*Me), 126.12, 126.78 (ArH), 128.45, 129.22 (*Ph*Me), 130.78 (Ar), 131.14 (ArH), 140.73, 152.18, 152.59, 157.20, 158.67 (Ar). One ArH peak in the $^{13}C\{^{1}H\}$ spectrum is obscured by the solvent peak.

Synthesis of $\{(Dipp)_2As\}_2Sn.C_7H_8$ (8Sn): To a solution of $(Dipp)_2AsH$ (0.67 g, 1.68 mmol) in THF (10 mL) was added a solution of *n*BuLi in hexanes (2.3 M, 0.7 mL, 1.61 mmol). The resulting red solution was stirred for 30 min and added, dropwise, to a cold (-78 °C) solution of $SnCl_2$ (0.159 g, 0.84 mmol) in THF (10 mL). The resulting orange solution was allowed to warm to room temperature and the solvent was removed *in vacuo* to give a sticky orange solid. The product was extracted into toluene (10 mL) to give a very dark purple solution with pale solids. The mixture was filtered and the dark purple filtrate was reduced to 5 mL in volume. Storage at -25 °C overnight gave purple crystals of $\{(Dipp)_2As\}_2Sn.C_7H_8$. The supernatant solution was removed by filtration and the remaining solid was washed with cold (-10 °C) light petroleum (10 mL). Residual solvent was removed under vacuum to give purple crystalline material. Yield: 0.25 g, 30%. ^{1}H NMR [213 K, d_8-toluene]: δ 0.51 (d, J_{HH} = 4.5 Hz, 6H, ^{B}CH*Me*Me), 0.93 (d, J_{HH} = 3.0 Hz, 6H, ^{A}CH*Me*Me), 0.98 (d, J_{HH} = 4.1 Hz, 6H, ^{C}CH*Me*Me), 1.18 (d, J_{HH} = 3.9 Hz, 6H, ^{A}CHMe*Me*), 1.40 (br. m, 6H, ^{D}CH*Me*Me), 1.42 (d, J_{HH} = 5.8 Hz, 6H, ^{B}CHMe*Me*), 1.45 (br. m, 6H, ^{D}CHMe*Me*), 1.52 (br. m, 6H, ^{C}CHMe*Me*), 2.11 (s, 3H, Ph*Me*), 2.80 (br. m, 2H, ^{A}C*H*MeMe), 3.08 (br. m, 2H, ^{B}C*H*MeMe), 4.01 (br. m, 2H, ^{C}C*H*MeMe), 4.93 (br. m, 2H, ^{D}C*H*MeMe), 6.78 (d, J_{HH} = 7.1 Hz, 2H, ArH), 6.88 (d, J_{HH} = 7.3 Hz, 2H, ArH), 6.74-7.04 (m, 8H, ArH and *Ph*Me), 7.08 (m, 1H, *Ph*Me), 7.16 (m, 4H, ArH). $^{13}C\{^{1}H\}$ NMR [213 K, d_8-toluene]: δ 21.34 (Ph*Me*), 21.43 (^{C}CH*Me*Me), 23.61 (^{D}CHMe*Me*), 24.89 (^{B}CH*Me*Me), 25.30 (^{A}CHMe*Me*), 26.30 (^{D}CH*Me*Me), 26.33 (^{A}CH*Me*Me), 26.62 (^{C}CHMe*Me*), 28.33 (^{B}CHMe*Me*), 33.73 (^{B}*C*MeMe), 34.96 (^{C}*C*MeMe and ^{D}*C*MeMe), 35.04 (^{A}*C*MeMe), 122.79, 124.45 (ArH), 125.58 (*Ph*Me), 126.29, 126.76 (ArH), 128.43, 129.21 (*Ph*Me), 129.69 (ArH), 133.33 (Ar), 137.66 (*Ph*Me), 139.92, 151.90, 153.18, 155.11, 157.22 (Ar). $^{119}Sn\{^{1}H\}$ NMR [213 K, d_8-toluene]: δ 547 (FWHM 500 Hz). One ArH peak in the $^{13}C\{^{1}H\}$ spectrum is obscured by the solvent peak.

X-ray crystallography: Data for all compounds were collected on an Xcalibur, Atlas, Gemini ultra diffractometer using an Enhance Ultra X-ray Source ($\lambda_{CuK\alpha}$ = 1.54184 Å) for **8Ge** and a fine-focus sealed X-ray tube ($\lambda_{MoK\alpha}$ = 0.71073 Å) for **7** and **8Sn**. Using an Oxford Cryosystems CryostreamPlus open-flow N_2 cooling device, data for all structures were collected at 150 K. Cell refinement, data collection and data reduction were undertaken using CrysAlisPro. For all compounds an analytical numeric absorption correction was applied using a multifaceted crystal model based on expressions derived by R. C. Clark and J. S. Reid,[S2] with the exception of **7**, for which the intensities were corrected for absorption empirically using spherical harmonics. The structures were solved using XT[S3] and refined by XL[S4] through the Olex2 interface.[S5] Hydrogen atoms were positioned with idealised geometry and their displacement parameters were constrained using a riding model. Disorder in the structures was modelled using restraints and constraints where appropriate to maintain a physically meaningful refinement.

Table S1. Crystallographic details for **7**, **8Ge** and **8Sn**.

Compound	**7**	**8Ge**	**8Sn**
formula	$C_{72.10}H_{116.97}As_2Li_2O_6$	$C_{55}H_{76}As_2Ge$	$C_{55}H_{76}As_2Sn$
M_w	1242.46	959.58	1005.68
cryst. size (mm)	0.39x0.26x0.19	0.20x0.12x0.07	0.35x0.18x0.09
cryst. syst.	Triclinic	Triclinic	Triclinic
space group	*P*-1	*P*-1	*P*-1
a (Å)	11.4059(2)	12.6717(3)	12.7953(4)
b (Å)	17.5174(3)	12.8423(3)	12.9297(3)
c (Å)	19.3810(5)	16.8971(3)	16.8382(6)
α (deg)	68.376(2)	77.0882(17)	75.874(3)
β (deg)	80.7734(18)	78.4162(17)	77.693(3)
γ (deg)	89.4407(16)	71.263(2)	69.763(3)
V (Å^3)	3548.14(14)	2513.24(10)	2509.21(15)
Z	2	2	2
μ (mm^{-1})	0.989	2.528	1.852
reflns. measd.	71162	53120	40464
unique reflns.	16256	8893	11268
R_{int}	0.043	0.032	0.042
refined parameters	805	624	604
R (on *F*, $F^2>2\sigma$)[a]	0.040	0.037	0.036
R_w (on F^2, all data)[a]	0.093	0.101	0.078
goodness of fit[a]	1.020	1.024	1.025
max, min electron density (e Å^{-3})	0.47,-0.37	1.87,-0.43	0.69,-0.83

[a] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $R_w = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; $S = [\Sigma w(F_o^2-F_c^2)^2/(\text{no. data - no. params})]^{1/2}$ for all data.

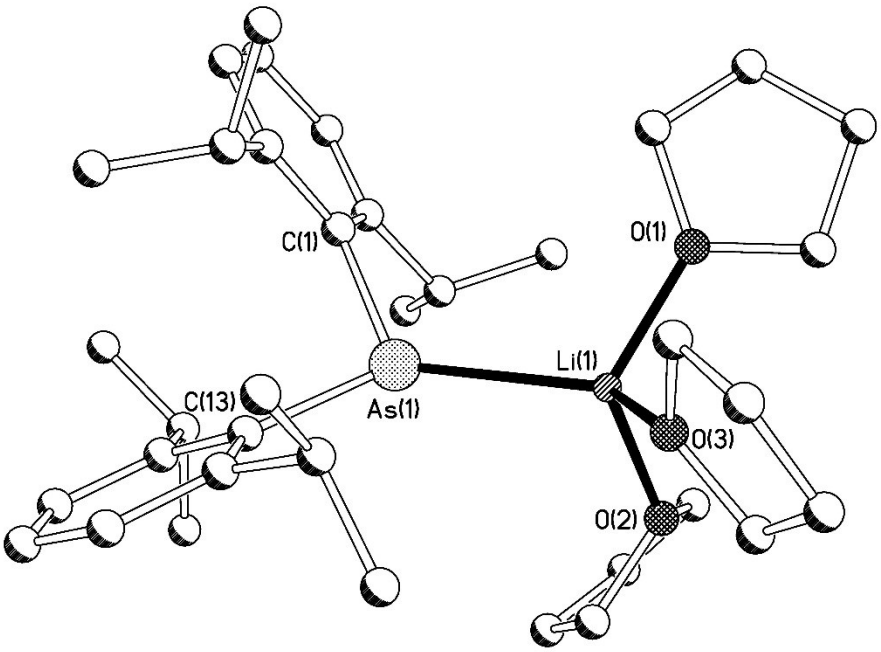
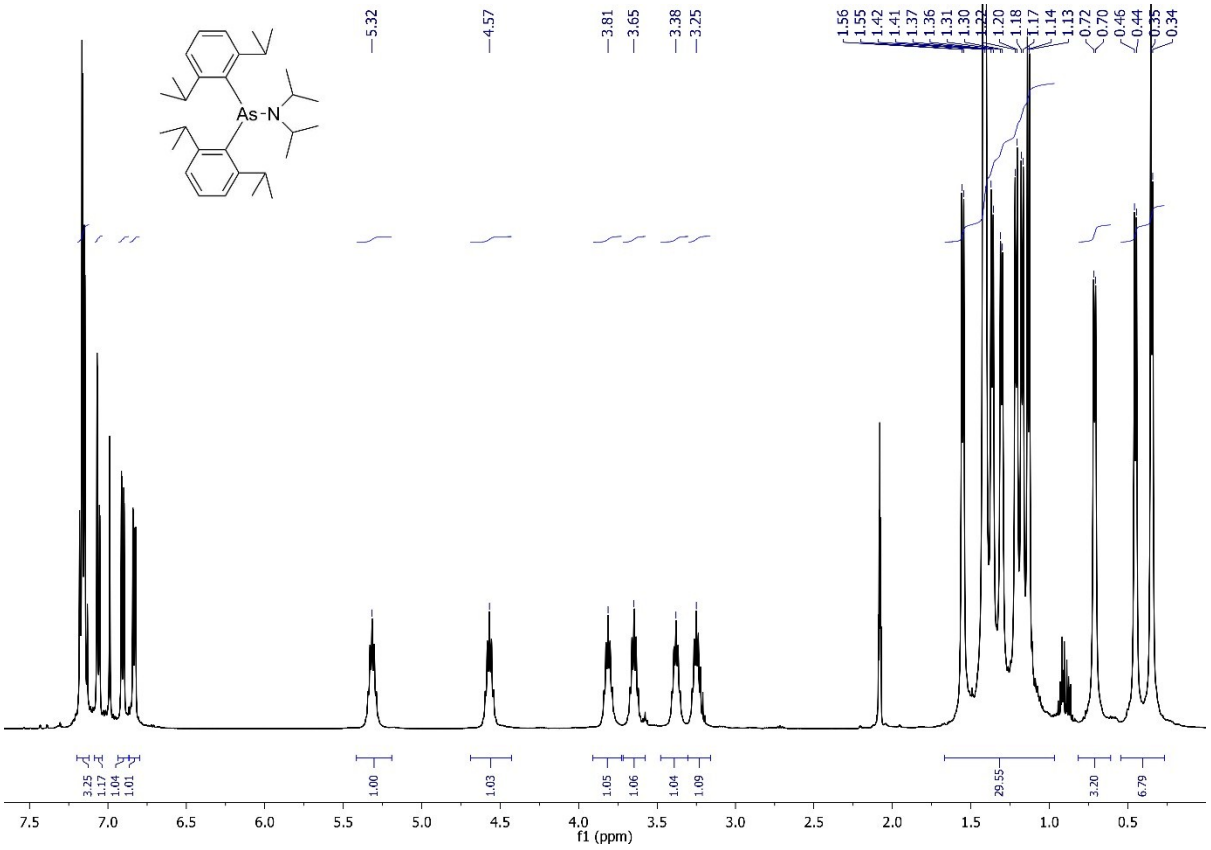
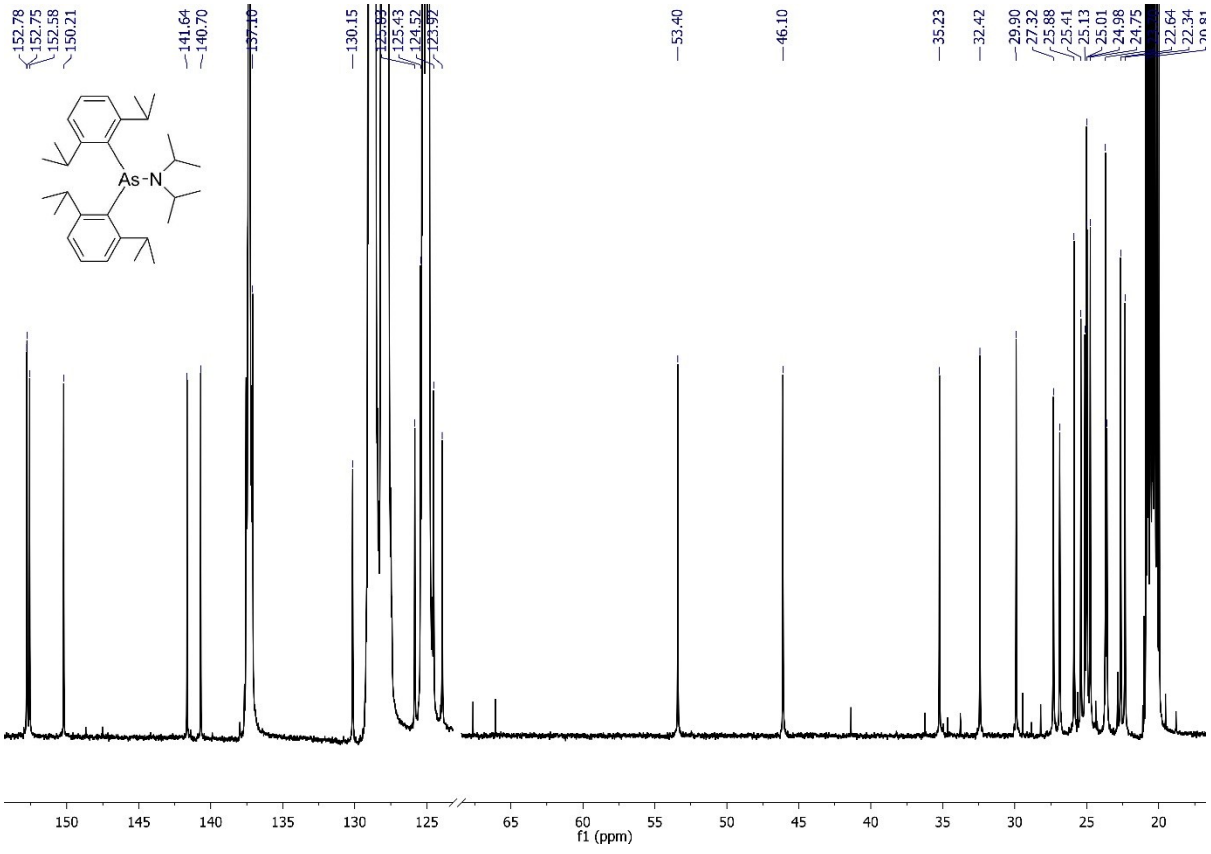


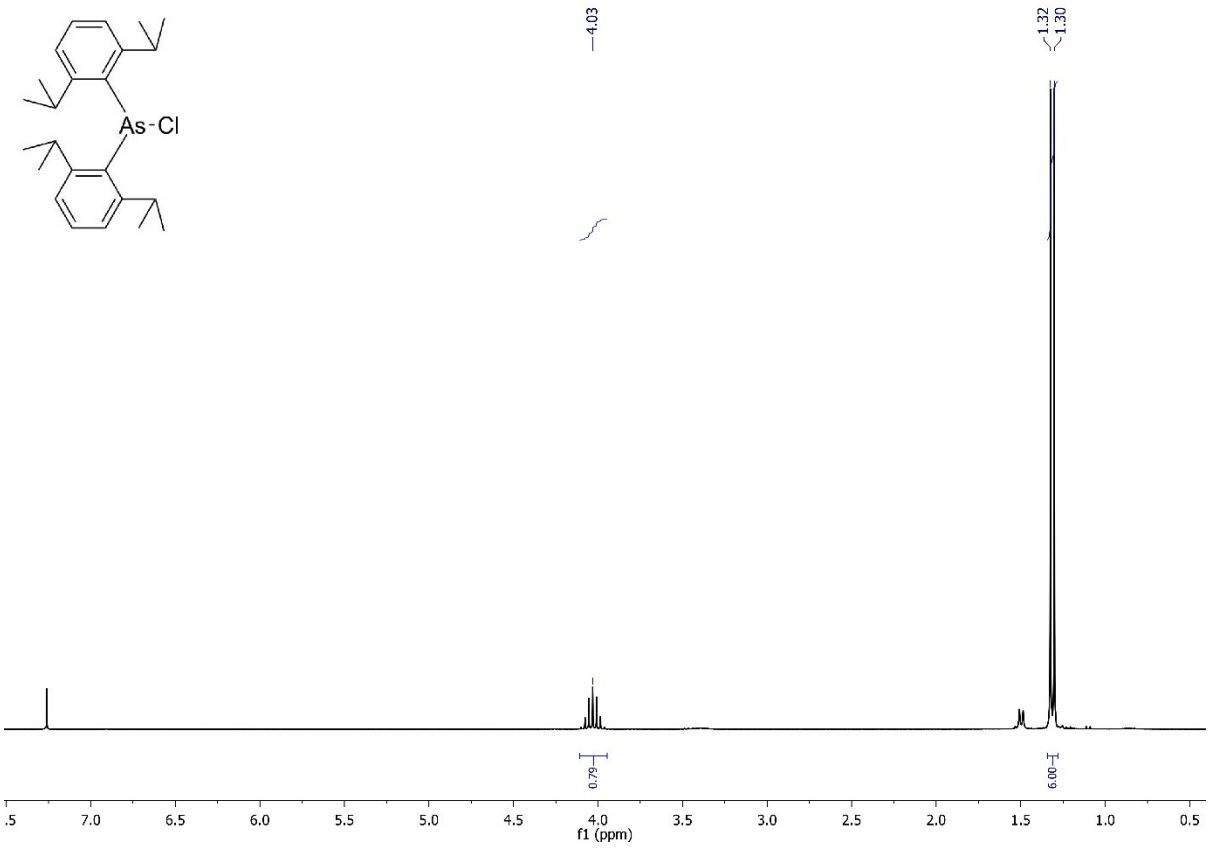
Figure S1. Molecular structure of one of the two independent molecules of **7** with H atoms and minor disorder components omitted for clarity. Selected bond lengths (Å) and angles (°): molecule 1, Li(1)-As(1) 2.568(3), Li(1)-O(1) 1.921(4), Li(1)-O(2) 1.974(4), Li(1)-O(3) 1.940(4), As(1)-C(1) 1.9752(18), As(1)-C(13) 1.9712(19), Li(1)-As(1)-C(1) 123.65(9), Li(1)-As(1)-C(13) 131.74(10), C(1)-As(1)-C(13) 99.84(8); molecule 2, Li(2)-As(2) 2.584(4), Li(2)-O(4A) 1.953(10), Li(2)-O(5) 1.919(4), Li(2)-O(6A) 1.947(11), As(2)-C37 1.9779(18), As(2)-C(49) 1.9795(18), Li(2)-As(2)-C(37) 129.18(10), Li(2)-As(2)-C(49) 123.16(9), C(37)-As(2)-C(49) 99.68(7).



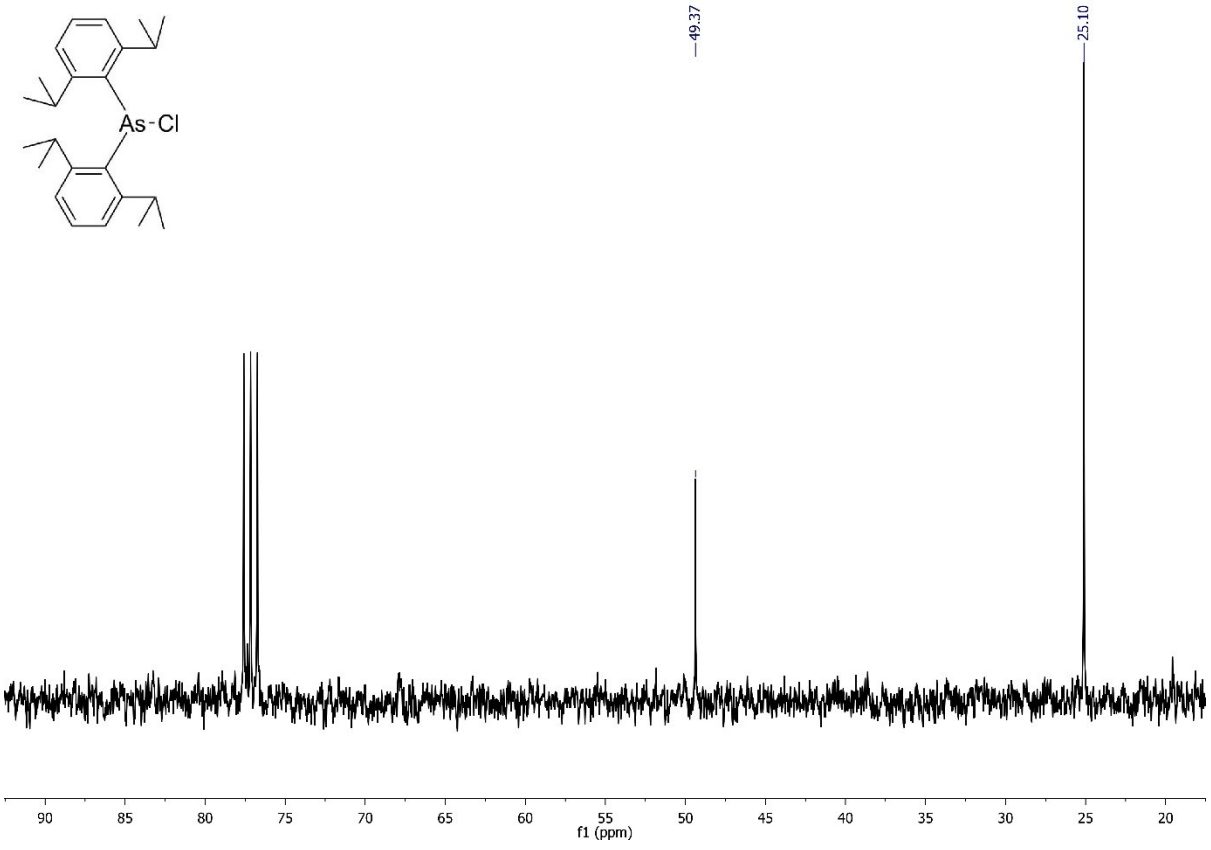
^{1}H NMR spectrum of $(Dipp)_2As(N{i}Pr_2)$ in $CDCl_3$ at 213 K.



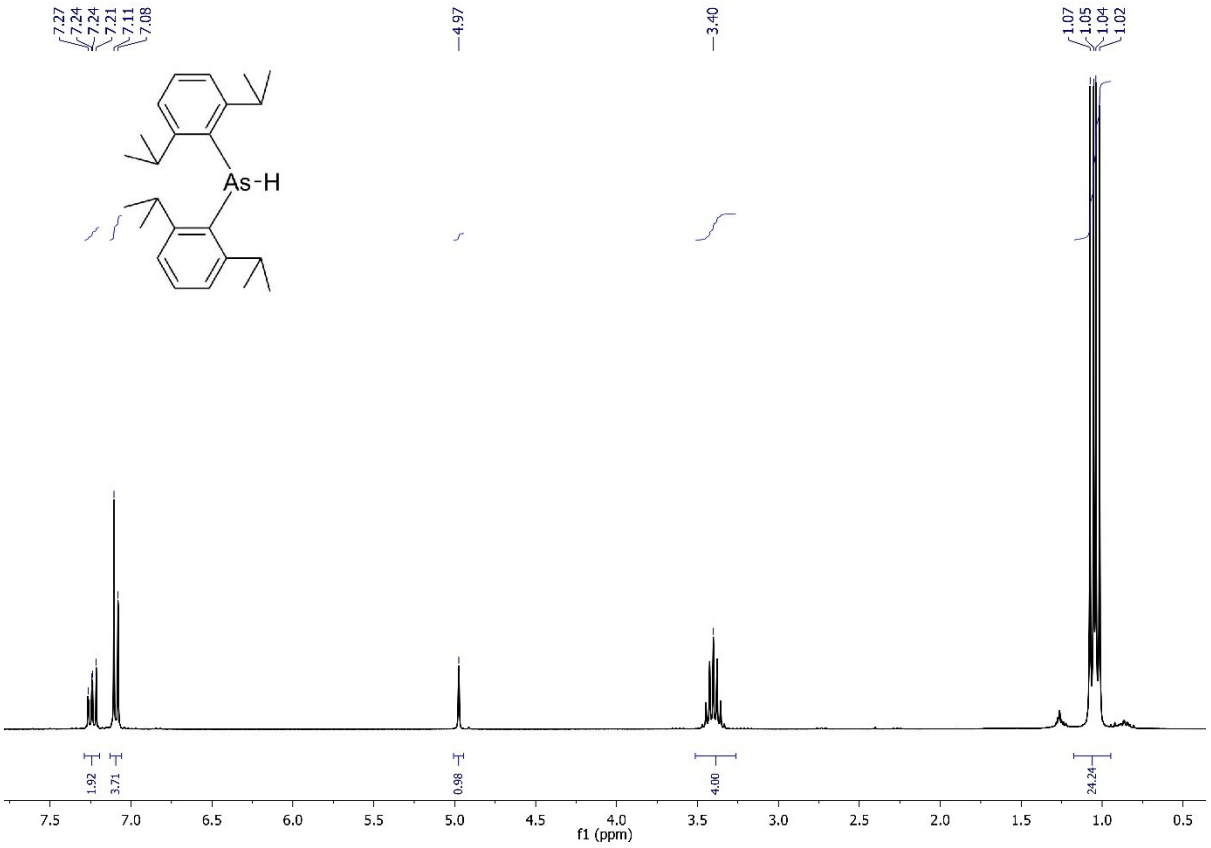
^{13}C{^{1}H} NMR spectrum of $(Dipp)_2As(N{i}Pr_2)$ in $CDCl_3$ at 213 K.



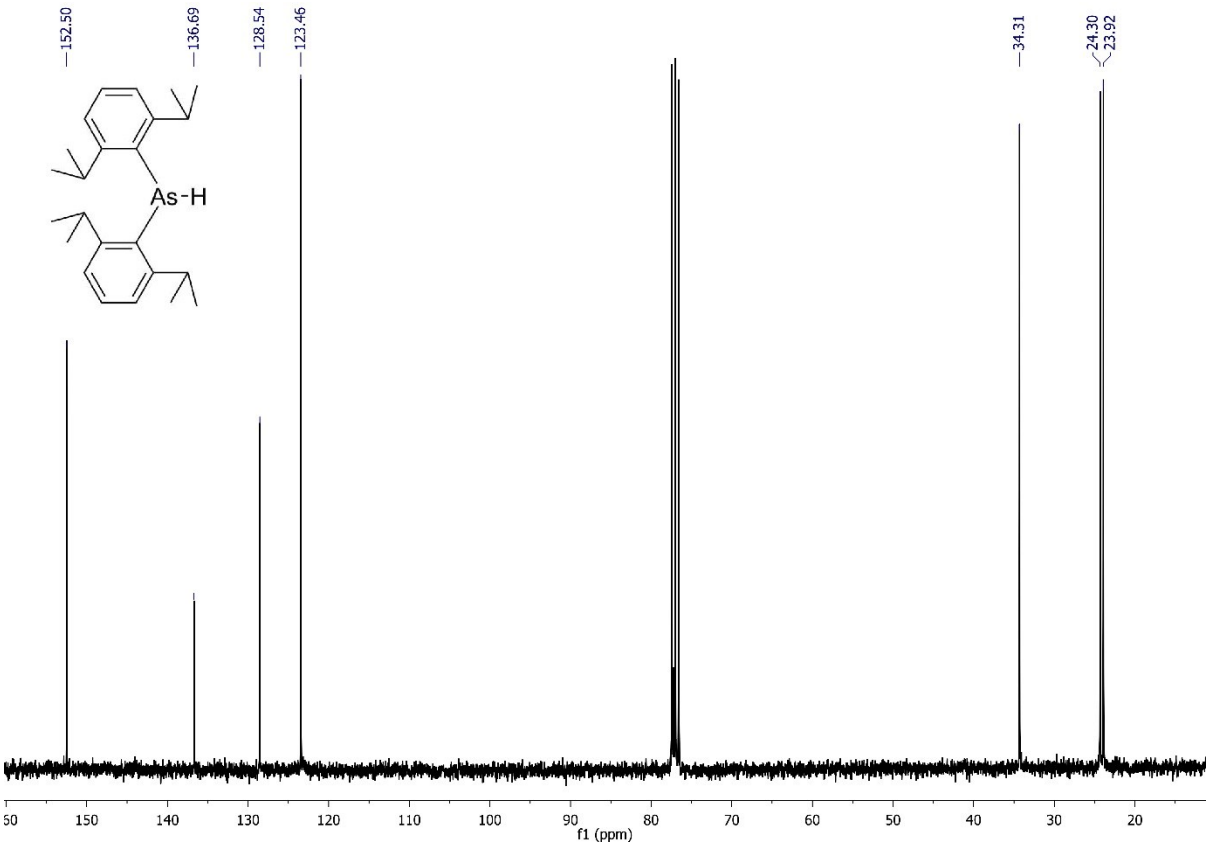
^{1}H NMR spectrum of **5** in $CDCl_3$.



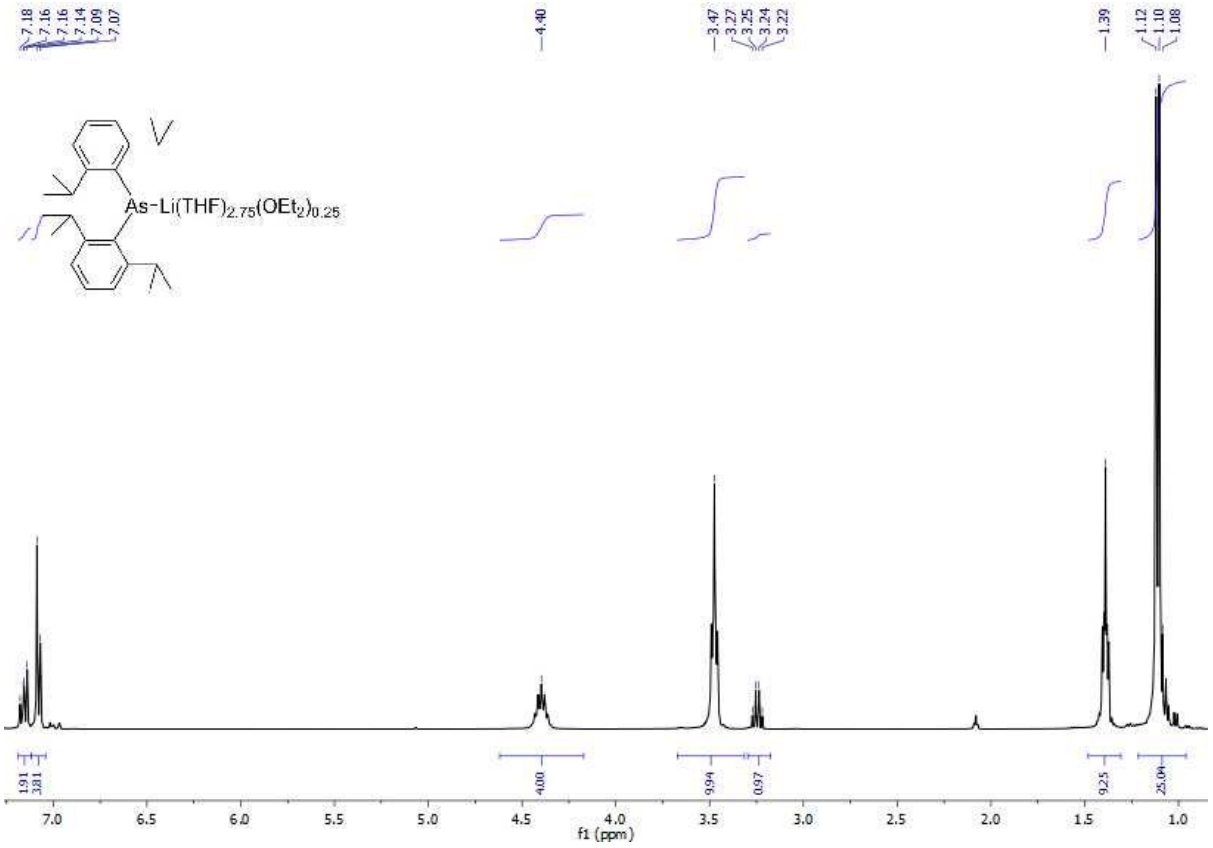
$^{13}C\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$.



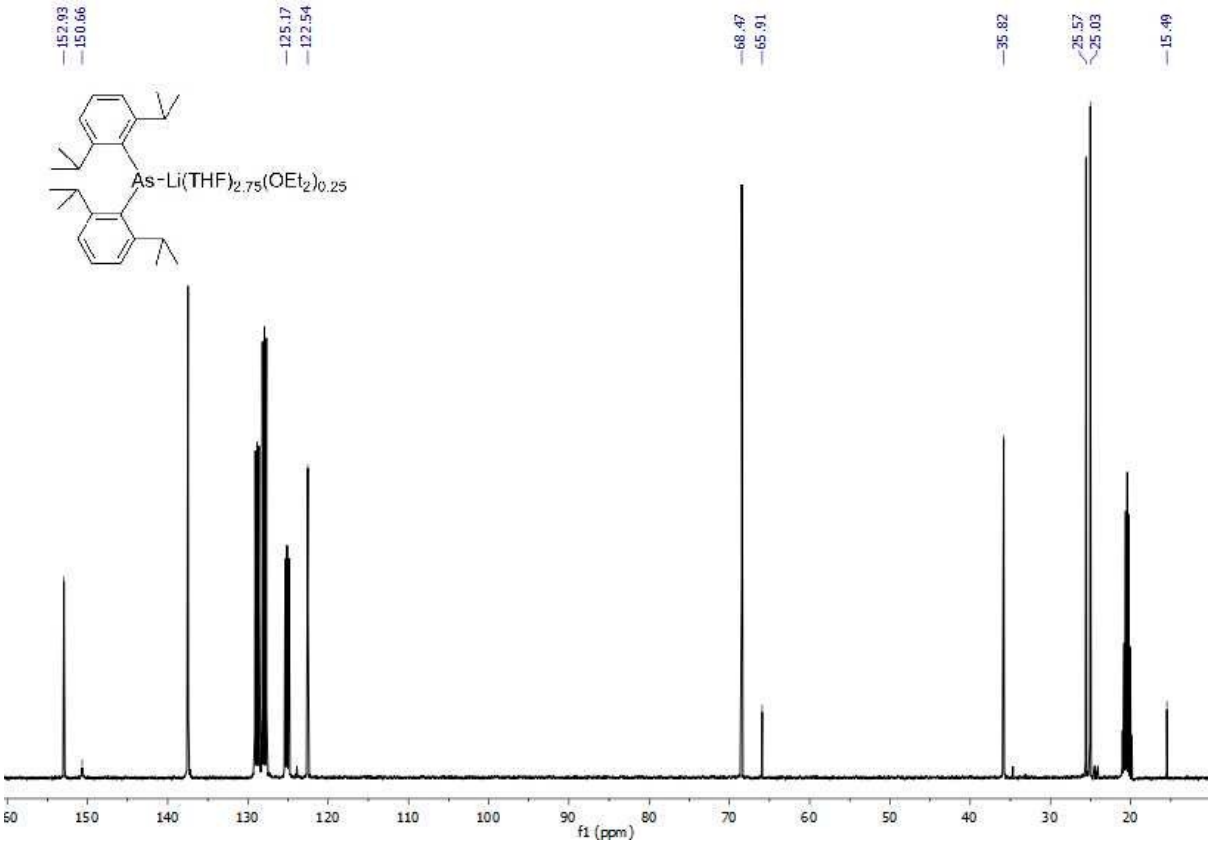
^{1}H NMR spectrum of **6** in $CDCl_3$.



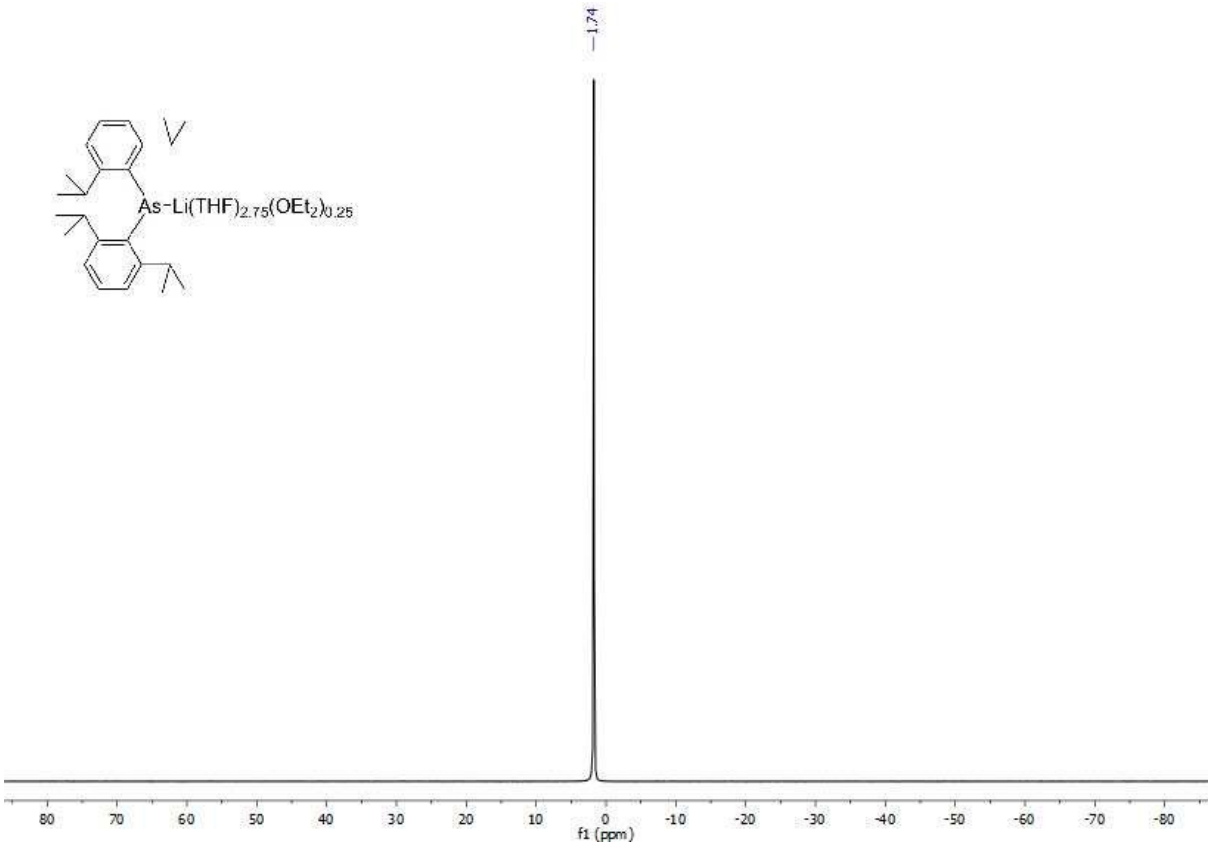
^{13}C{^{1}H} NMR spectrum of **6** in $CDCl_3$.



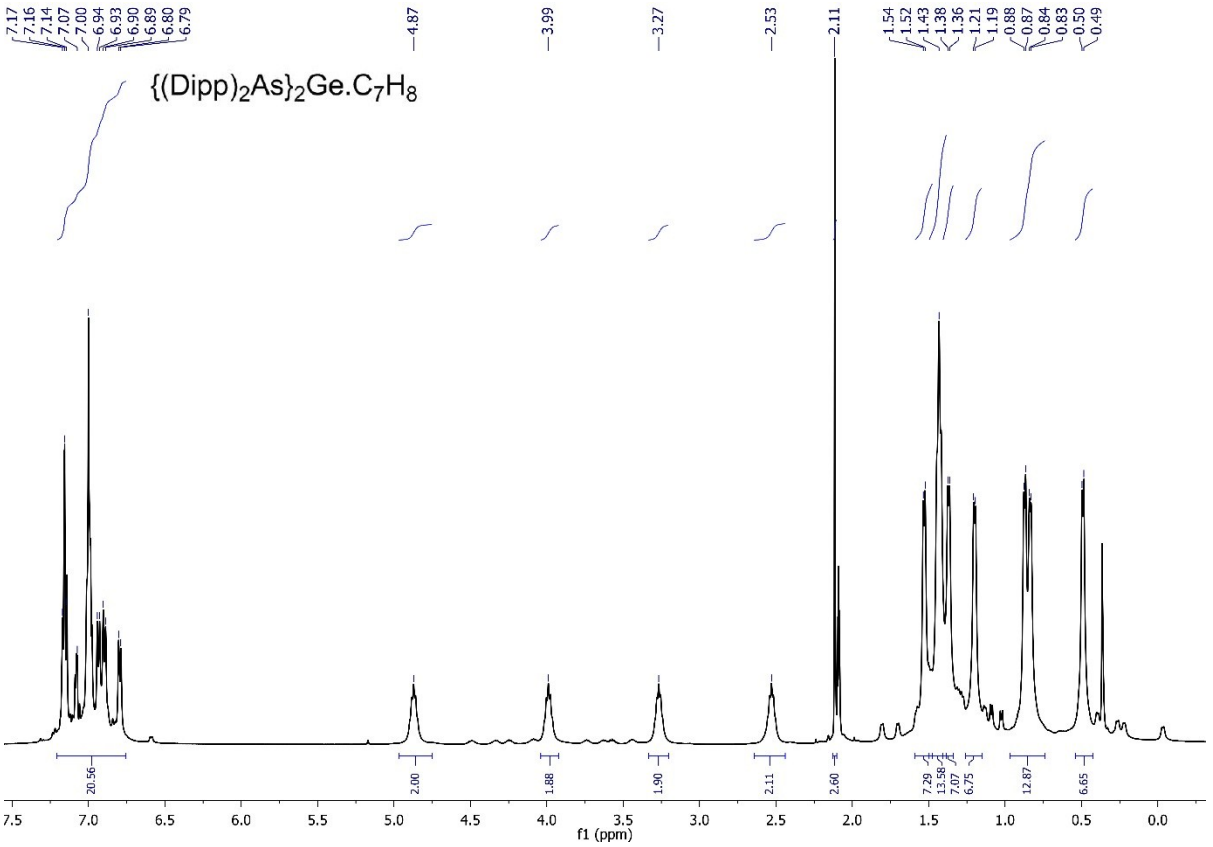
^{1}H NMR spectrum of **7** in d_8-toluene.



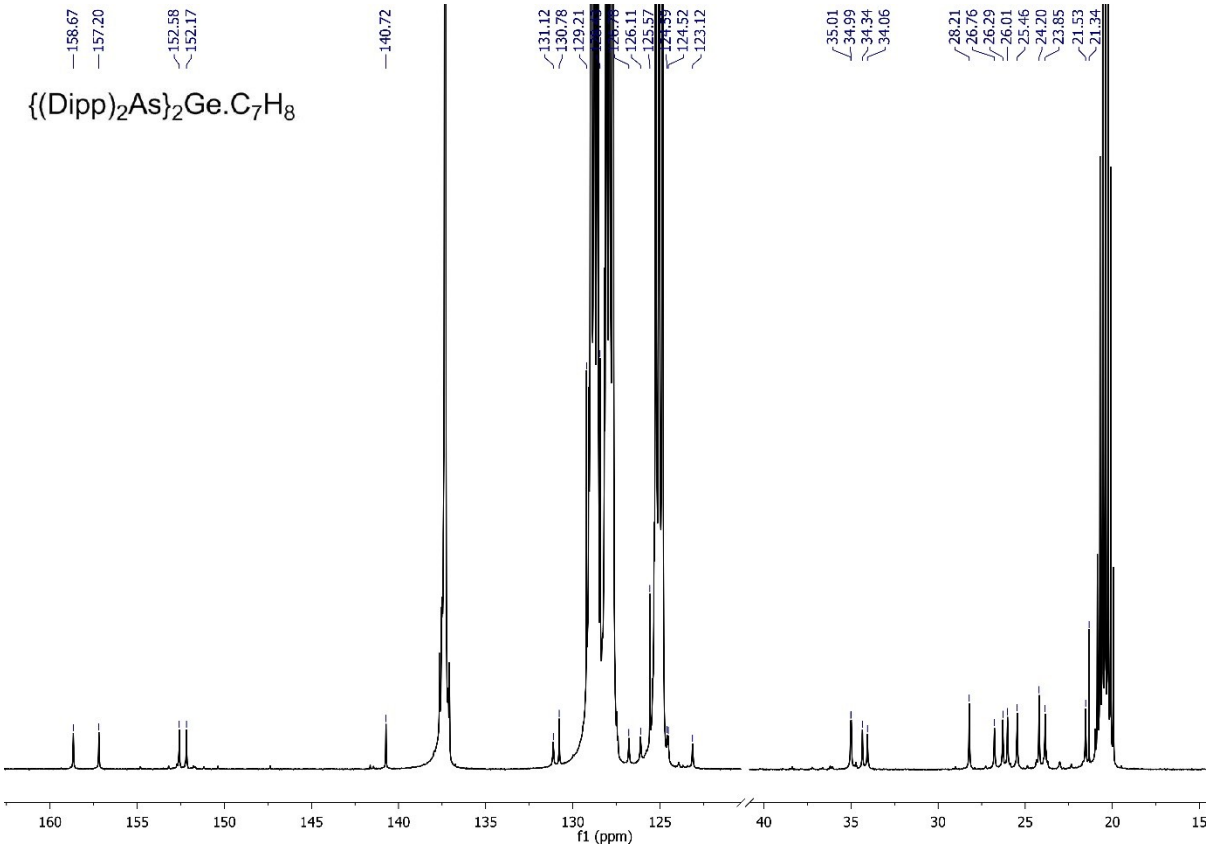
^{13}C{^{1}H} NMR spectrum of **7** in d_8-toluene.



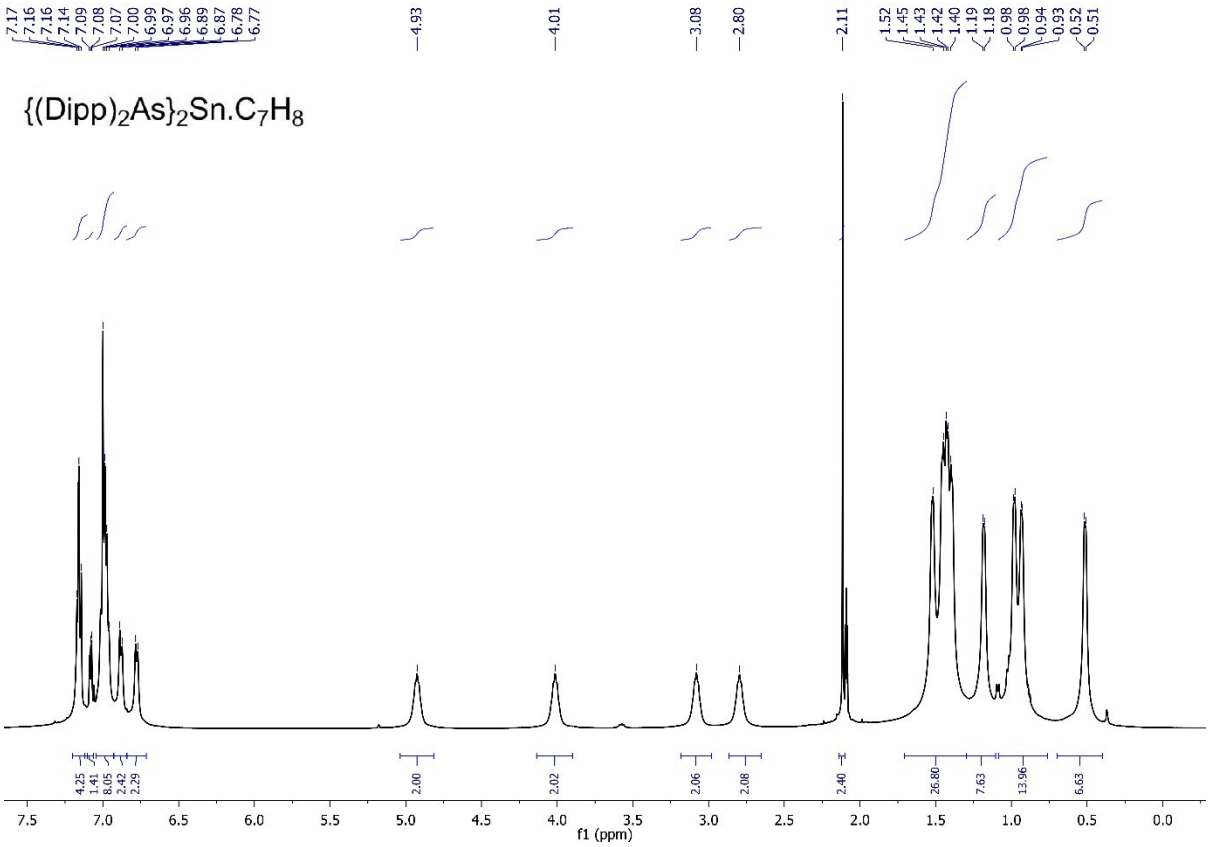
^{7}Li NMR spectrum of **7** in d_8-toluene.



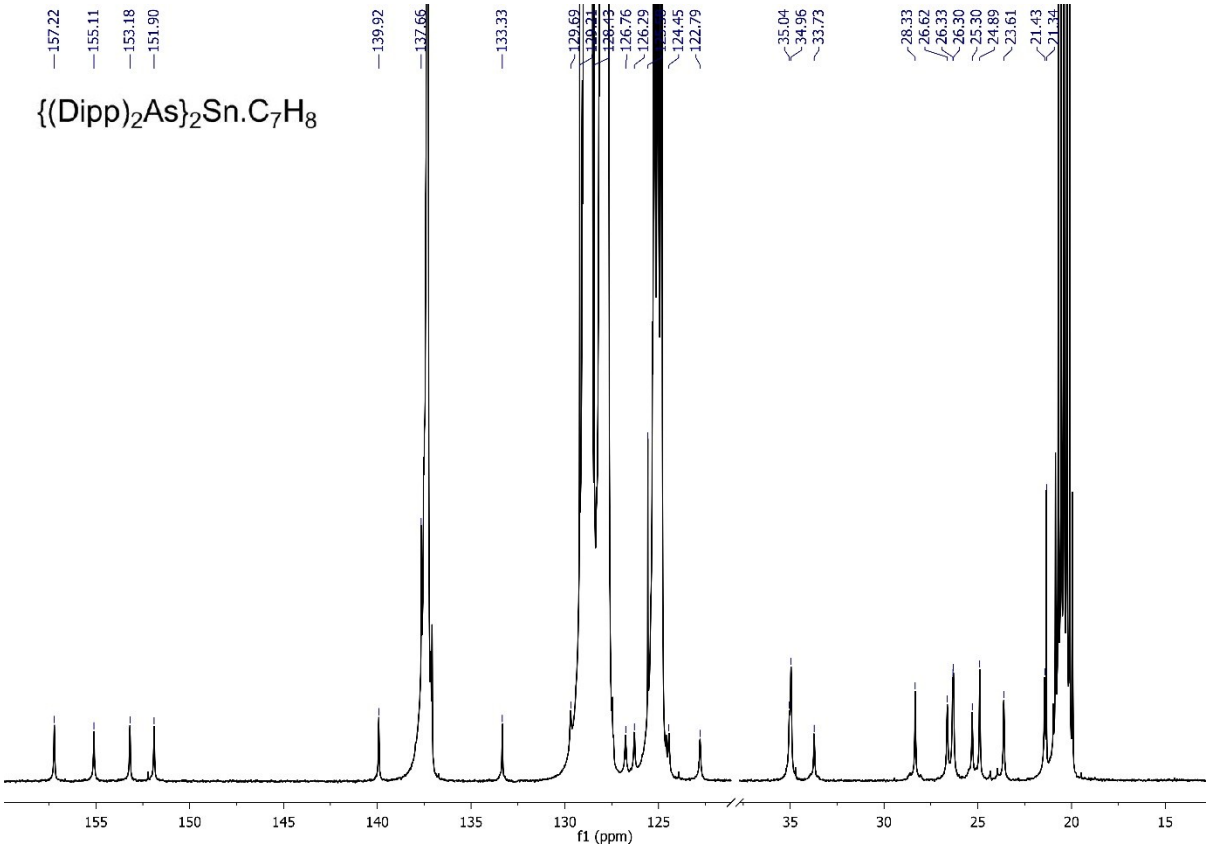
^{1}H NMR spectrum of **8Ge** in d_8-toluene at 213 K.



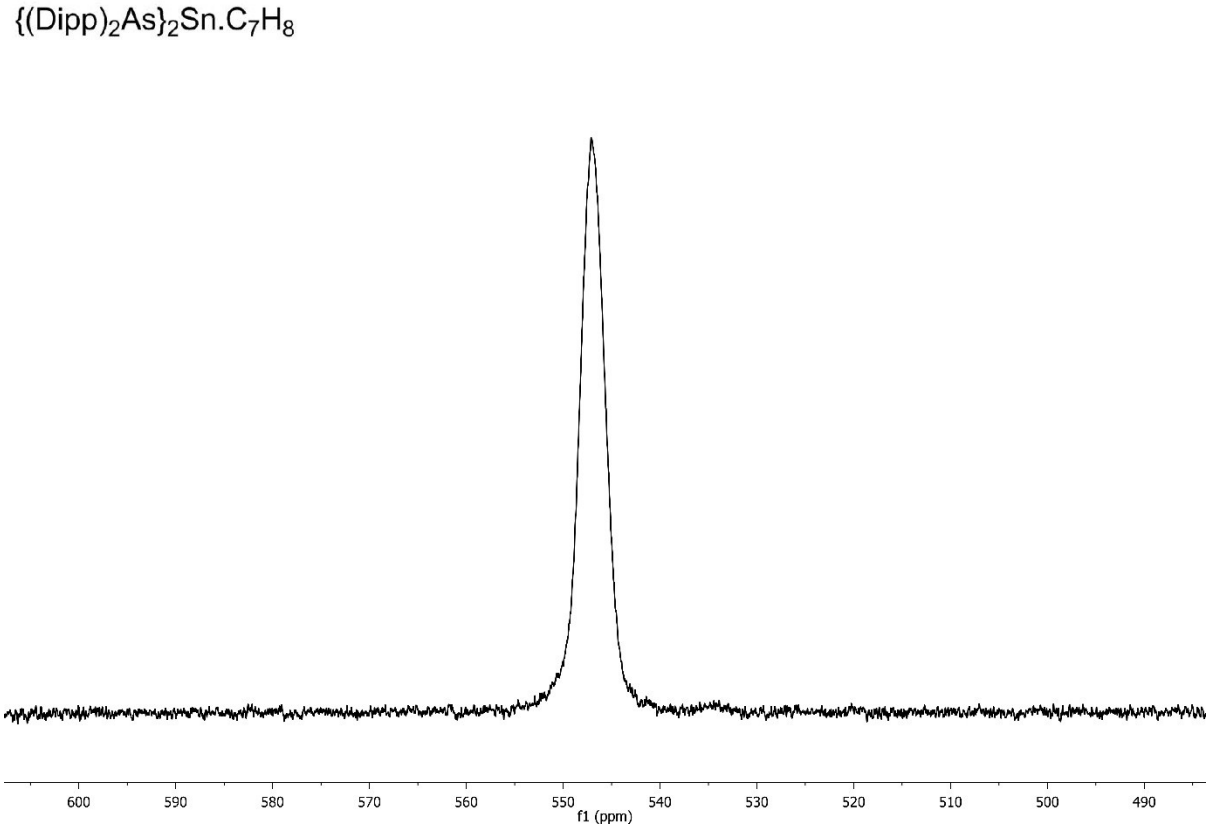
$^{13}C\{^{1}H\}$ NMR spectrum of **8Ge** in d_8-toluene at 213 K.



^{1}H NMR spectrum of **8Sn** in d_8-toluene at 213 K.



$^{13}C\{^{1}H\}$ NMR spectrum of **8Sn** in d_8-toluene at 213 K.



^{119}Sn NMR spectrum of **8Sn** in d_8-toluene at 213 K.

DFT Calculations: Geometry optimisations were performed with the Gaussian09 suite of programs (revision D.01).[S6] The pure B97D functional,[S7] which includes a correction for dispersion effects, was employed throughout; the 6-311G(2d,p) all-electron basis set[S8] was used on all atoms except Sn, where the LANL2DZ effective core potential basis set was used.[S9] The identity of minima was confirmed by the absence of imaginary vibrational frequencies in each case. Automatic density fitting was employed for all geometry optimisations and frequency calculations. The singlet-triplet free energy gap was calculated by subtracting the free energy of the optimised singlet ground state from the free energy of the optimised triplet state geometry. Natural Bond Orbital analyses were performed using the NBO 3.1 module of Gaussian09.[S10]

Final atomic coordinates, energies, geometries and HOMOs, LUMOs or SOMOs:

8Ge (pyramidal):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	33	0	-1.820280	0.159509	0.898667
2	33	0	1.756238	-0.178179	0.902585
3	32	0	-0.037135	-0.079165	-0.871279
4	6	0	-3.443510	1.037873	0.105402
5	6	0	-3.345783	2.233147	-0.651584
6	6	0	-4.524605	2.845779	-1.107420
7	1	0	-4.451498	3.746569	-1.713684
8	6	0	-5.776968	2.327382	-0.798420
9	1	0	-6.679471	2.816134	-1.162810
10	6	0	-5.869751	1.185582	-0.004505
11	1	0	-6.852570	0.798138	0.252206
12	6	0	-4.724200	0.526960	0.461678
13	6	0	-2.023722	2.893686	-1.041368
14	1	0	-1.217893	2.453477	-0.446084
15	6	0	-1.999903	4.406097	-0.741633
16	1	0	-2.695283	4.956103	-1.389452
17	1	0	-0.988754	4.792515	-0.918966
18	1	0	-2.272408	4.606281	0.301693
19	6	0	-1.701675	2.643456	-2.528630
20	1	0	-1.663100	1.570758	-2.752375
21	1	0	-0.730393	3.085967	-2.786300
22	1	0	-2.474241	3.099221	-3.163792
23	6	0	-4.894078	-0.675249	1.395451
24	1	0	-4.065877	-1.369461	1.216019
25	6	0	-6.189652	-1.481499	1.188229

26	1	0	-7.074525	-0.915192	1.509057
27	1	0	-6.146328	-2.395227	1.795155
28	1	0	-6.328687	-1.770476	0.139215
29	6	0	-4.811004	-0.204250	2.865099
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31	1	0	-4.891862	-1.062305	3.547395
32	1	0	-5.635267	0.489679	3.080776
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34	6	0	-2.359329	-2.116232	-1.149042
35	6	0	-2.367352	-3.475729	-1.505251
36	1	0	-2.784719	-3.759417	-2.469352
37	6	0	-1.850021	-4.452779	-0.665952
38	1	0	-1.868524	-5.499977	-0.964545
39	6	0	-1.289871	-4.081998	0.556761
40	1	0	-0.871635	-4.847452	1.205779
41	6	0	-1.261282	-2.746795	0.969209
42	6	0	-2.921505	-1.142663	-2.181864
43	1	0	-2.767899	-0.124591	-1.822162
44	6	0	-4.437893	-1.343272	-2.369536
45	1	0	-4.646569	-2.346068	-2.767600
46	1	0	-4.829379	-0.600293	-3.076709
47	1	0	-4.969933	-1.225325	-1.422281
48	6	0	-2.201828	-1.262077	-3.542103
49	1	0	-1.119237	-1.126187	-3.427124
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51	1	0	-2.380957	-2.241226	-4.005934
52	6	0	-0.688163	-2.437799	2.349847
53	1	0	-0.435839	-1.374076	2.387176
54	6	0	0.609101	-3.202470	2.667374
55	1	0	0.431821	-4.279145	2.791585
56	1	0	1.032992	-2.823176	3.606049
57	1	0	1.353976	-3.066165	1.874697
58	6	0	-1.765066	-2.689276	3.424643
59	1	0	-2.652774	-2.074760	3.232069
60	1	0	-1.376518	-2.437190	4.421203
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63	6	0	3.394146	-2.211545	-0.606303
64	6	0	4.609563	-2.743238	-1.063164
65	1	0	4.595706	-3.642123	-1.676965
66	6	0	5.828629	-2.150709	-0.741218
67	1	0	6.760506	-2.576503	-1.110500
68	6	0	5.845315	-1.025293	0.078165
69	1	0	6.796476	-0.578496	0.364193
70	6	0	4.656376	-0.449296	0.548388
71	6	0	2.112622	-2.955563	-0.979442
72	1	0	1.281388	-2.535382	-0.404472
73	6	0	2.179047	-4.451140	-0.609817
74	1	0	2.933349	-4.978260	-1.208868
75	1	0	1.204341	-4.918161	-0.798604
76	1	0	2.430088	-4.583857	0.449994
77	6	0	1.775828	-2.790780	-2.475000
78	1	0	1.674821	-1.733749	-2.747937
79	1	0	0.828538	-3.296552	-2.705975
80	1	0	2.569677	-3.231196	-3.094590
81	6	0	4.783181	0.743463	1.499143

82	1	0	3.779203	1.072837	1.782897
83	6	0	1.837426	1.697685	0.092934
84	6	0	2.375764	2.021774	-1.191207
85	6	0	2.480433	3.374977	-1.556530
86	1	0	2.908123	3.620811	-2.526819
87	6	0	2.045012	4.394763	-0.720028
88	1	0	2.142933	5.435658	-1.025041
89	6	0	1.460455	4.073329	0.504603
90	1	0	1.099114	4.869652	1.151637
91	6	0	1.332202	2.744831	0.921741
92	6	0	2.825552	1.005088	-2.241308
93	1	0	2.633420	0.002493	-1.858998
94	6	0	4.334009	1.096464	-2.544339
95	1	0	4.593186	2.096114	-2.919926
96	1	0	4.599057	0.361246	-3.315703
97	1	0	4.933637	0.887851	-1.656067
98	6	0	2.029931	1.161640	-3.555760
99	1	0	0.950574	1.089960	-3.378979
100	1	0	2.322431	0.368702	-4.257584
101	1	0	2.238754	2.128679	-4.032743
102	6	0	0.713564	2.489182	2.294838
103	1	0	0.459648	1.426930	2.365036
104	6	0	-0.594616	3.266161	2.530576
105	1	0	-0.424248	4.349927	2.578057
106	1	0	-1.036057	2.953540	3.485880
107	1	0	-1.322427	3.068346	1.735776
108	6	0	1.743206	2.788538	3.402846
109	1	0	2.637558	2.164794	3.281556
110	1	0	1.309905	2.586218	4.392163
111	1	0	2.049995	3.843060	3.366563
112	6	0	5.479288	1.956648	0.855450
113	1	0	5.576385	2.764654	1.593552
114	1	0	4.900125	2.334434	0.006316
115	1	0	6.486563	1.694896	0.502906
116	6	0	5.497633	0.319856	2.798911
117	1	0	4.971357	-0.515806	3.278242
118	1	0	5.533724	1.163174	3.502739
119	1	0	6.528348	0.001075	2.593467

Final SCF energy (Hartrees): -8421.2614315

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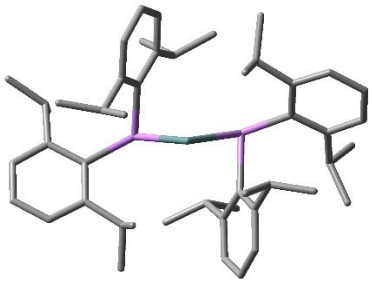	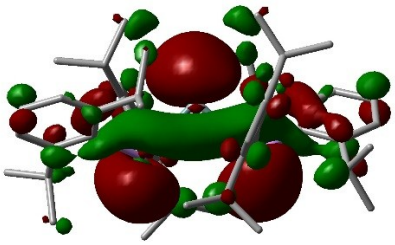	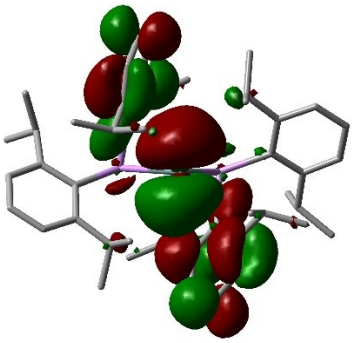
8Ge (pyramidal)	HOMO	LUMO

8Ge (planar):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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5	6	0	-5.959389	-1.186022	-2.282075
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7	6	0	-5.684117	0.162266	-2.068944
8	1	0	-6.429291	0.913606	-2.323739
9	6	0	-4.456624	0.576200	-1.533999
10	6	0	-4.233545	2.069627	-1.325795
11	1	0	-3.183110	2.213878	-1.047829
12	6	0	-5.096390	2.604400	-0.166959
13	1	0	-4.866849	2.079183	0.766464
14	1	0	-6.163999	2.471632	-0.391421
15	1	0	-4.906276	3.675783	-0.017162
16	6	0	-4.463947	2.880098	-2.615054
17	1	0	-3.833782	2.505280	-3.431824
18	1	0	-4.219113	3.936555	-2.439327
19	1	0	-5.512383	2.827541	-2.937994
20	6	0	-2.806708	-2.910621	-1.022996
21	1	0	-2.001439	-2.481491	-0.417994
22	6	0	-3.466619	-4.014648	-0.173787
23	1	0	-3.942184	-3.594267	0.720060
24	1	0	-2.704877	-4.739002	0.144865
25	1	0	-4.229714	-4.562021	-0.742735
26	6	0	-2.159877	-3.509281	-2.286935
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29	1	0	-1.433342	-4.286735	-2.010988
30	6	0	-2.331595	1.049141	1.336286
31	6	0	-1.893619	2.366636	1.621886
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41	6	0	0.328703	3.580924	1.636013
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43	1	0	0.018422	4.258857	2.442397
44	1	0	1.052604	4.111819	1.005992
45	6	0	-1.536866	4.374056	0.120787
46	1	0	-2.389589	4.087366	-0.504908
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53	1	0	-5.830511	-0.662109	2.433778
54	1	0	-5.541118	-2.124368	1.462997
55	6	0	-3.488765	-1.894504	3.279512
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57	1	0	-3.722303	-2.947021	3.068672
58	1	0	-4.136671	-1.565850	4.102622
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61	6	0	4.681626	2.063017	-2.433739
62	1	0	5.026976	3.066606	-2.670256
63	6	0	5.292420	0.971539	-3.048051
64	1	0	6.109683	1.124736	-3.751477
65	6	0	4.844748	-0.312491	-2.760873
66	1	0	5.311243	-1.166681	-3.248803
67	6	0	3.795588	-0.539568	-1.854447
68	6	0	3.375572	-1.993436	-1.654328
69	1	0	2.526212	-2.023815	-0.971810
70	6	0	4.496695	-2.826526	-1.003135
71	1	0	4.781242	-2.408281	-0.032209
72	1	0	5.383959	-2.852520	-1.650761
73	1	0	4.156027	-3.859260	-0.847945
74	6	0	2.915078	-2.636231	-2.979339
75	1	0	2.103654	-2.056038	-3.437329
76	1	0	2.552501	-3.656854	-2.792823
77	1	0	3.741864	-2.695816	-3.699300
78	6	0	1.727292	3.491678	-1.737440
79	1	0	1.014970	2.657320	-1.777125
80	1	0	2.020411	3.741110	-2.766490
81	1	0	1.217614	4.360278	-1.299598
82	6	0	2.972161	3.117873	-0.906818
83	1	0	2.621226	2.846189	0.096606
84	6	0	3.894997	4.336703	-0.737449
85	1	0	4.816819	4.066087	-0.206333
86	1	0	3.373159	5.111321	-0.159586
87	1	0	4.171599	4.778736	-1.704299
88	6	0	2.202864	-2.320679	1.584286
89	6	0	2.958304	-3.209951	2.361408
90	1	0	2.574910	-4.208498	2.556387
91	6	0	4.194170	-2.839631	2.887713
92	1	0	4.772556	-3.547876	3.479062
93	6	0	4.675159	-1.555911	2.658051
94	1	0	5.634678	-1.255885	3.075657
95	6	0	3.949642	-0.627065	1.895002
96	6	0	4.561619	0.766218	1.744108
97	1	0	3.862125	1.400208	1.191880
98	6	0	5.876041	0.726560	0.941559
99	1	0	5.711646	0.311657	-0.058589
100	1	0	6.625614	0.112068	1.459359
101	1	0	6.281930	1.741545	0.832760
102	6	0	4.765619	1.438659	3.116920
103	1	0	3.819318	1.490697	3.671201
104	1	0	5.148705	2.459517	2.980306
105	1	0	5.489512	0.883887	3.728639

106	6	0	0.832563	-2.759875	1.095833
107	1	0	0.663787	-2.273856	0.117655
108	6	0	0.667615	-4.267497	0.848432
109	1	0	1.470979	-4.657362	0.210418
110	1	0	-0.294946	-4.449133	0.353300
111	1	0	0.667856	-4.833390	1.789856
112	6	0	-0.259438	-2.239721	2.042793
113	1	0	-0.213133	-1.149151	2.145634
114	1	0	-0.132320	-2.688185	3.037725
115	1	0	-1.253492	-2.504109	1.665983
116	33	0	-1.797233	0.194512	-0.382724
117	32	0	0.140619	-0.634234	-1.433741
118	33	0	1.775911	0.381869	0.220620
119	6	0	2.713067	-1.022847	1.324696

Final SCF energy (Hartrees): -8421.2524481

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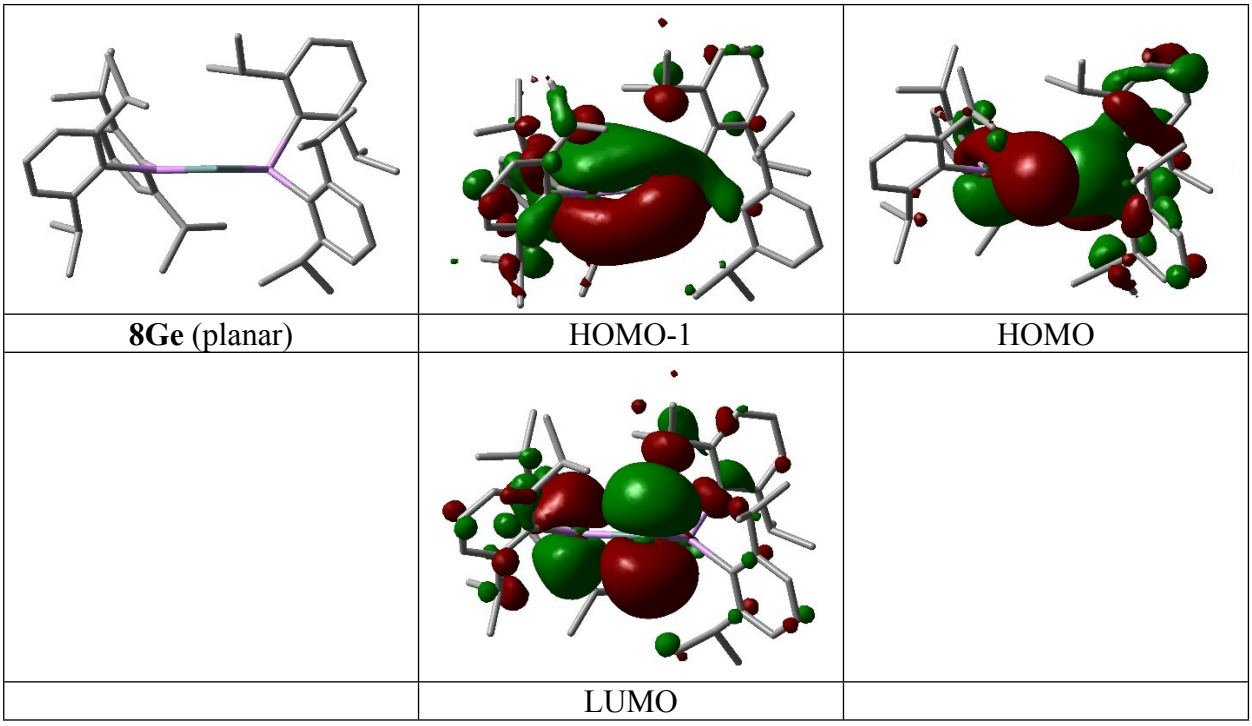

8Ge (planar)	HOMO-1	HOMO
	LUMO	

8Ge (triplet):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	32	0	-0.001061	-0.367883	-0.690121
4	6	0	3.414407	-1.574859	0.321683
5	6	0	3.147402	-2.816472	-0.309745
6	6	0	4.225677	-3.587464	-0.769322

7	1	0	4.019797	-4.522401	-1.287402
8	6	0	5.544061	-3.190018	-0.564671
9	1	0	6.366774	-3.799877	-0.934757
10	6	0	5.797875	-2.024330	0.151972
11	1	0	6.824967	-1.733981	0.365865
12	6	0	4.755612	-1.209936	0.617365
13	6	0	1.746966	-3.381635	-0.527533
14	1	0	1.023518	-2.758405	0.009830
15	6	0	1.598318	-4.801090	0.056100
16	1	0	2.236878	-5.522423	-0.470823
17	1	0	0.556531	-5.133215	-0.044746
18	1	0	1.869170	-4.816629	1.119525
19	6	0	1.360997	-3.360923	-2.019175
20	1	0	1.426203	-2.345653	-2.431173
21	1	0	0.331474	-3.719410	-2.154737
22	1	0	2.036740	-4.007237	-2.596499
23	6	0	5.151400	-0.010013	1.477349
24	1	0	4.245936	0.503613	1.808133
25	6	0	6.002380	1.015581	0.706008
26	1	0	6.942573	0.560312	0.365127
27	1	0	6.252215	1.863079	1.358573
28	1	0	5.461683	1.398038	-0.165594
29	6	0	5.876084	-0.475464	2.758614
30	1	0	5.259811	-1.189321	3.320414
31	1	0	6.088891	0.388984	3.402816
32	1	0	6.829823	-0.963682	2.517841
33	6	0	2.676483	1.401130	0.041243
34	6	0	3.033832	1.495658	-1.327370
35	6	0	3.444984	2.741006	-1.828600
36	1	0	3.729696	2.816662	-2.876559
37	6	0	3.496093	3.870966	-1.018550
38	1	0	3.811649	4.828263	-1.430749
39	6	0	3.148248	3.768252	0.327261
40	1	0	3.199404	4.652169	0.958155
41	6	0	2.745973	2.545108	0.880590
42	6	0	3.020930	0.327991	-2.311989
43	1	0	2.620498	-0.553690	-1.809134
44	6	0	4.448380	-0.032945	-2.769345
45	1	0	4.913300	0.813861	-3.292858
46	1	0	4.414692	-0.886820	-3.459483
47	1	0	5.075110	-0.304591	-1.914156
48	6	0	2.116132	0.606149	-3.528659
49	1	0	1.093204	0.842565	-3.212106
50	1	0	2.085874	-0.279375	-4.178449
51	1	0	2.494900	1.448608	-4.122951
52	6	0	2.368456	2.487241	2.362198
53	1	0	2.595435	1.475518	2.725457
54	6	0	0.852180	2.698763	2.545921
55	1	0	0.568628	3.705521	2.216506
56	1	0	0.573164	2.583127	3.602382
57	1	0	0.277397	1.972202	1.958206
58	6	0	3.161628	3.459344	3.253645
59	1	0	4.242549	3.354827	3.093080
60	1	0	2.941740	3.249773	4.308563
61	1	0	2.884347	4.504556	3.061373
62	6	0	-3.062856	1.632508	0.248710

63	6	0	-2.555669	2.755350	-0.453213
64	6	0	-3.458389	3.721444	-0.922608
65	1	0	-3.074046	4.567287	-1.489554
66	6	0	-4.823539	3.627800	-0.667099
67	1	0	-5.507970	4.383972	-1.048681
68	6	0	-5.298708	2.577408	0.112825
69	1	0	-6.356808	2.526445	0.363775
70	6	0	-4.439791	1.578730	0.594222
71	6	0	-1.073519	2.998064	-0.724387
72	1	0	-0.486842	2.270184	-0.154031
73	6	0	-0.621380	4.394508	-0.250860
74	1	0	-1.061325	5.186275	-0.871972
75	1	0	0.471148	4.467172	-0.323823
76	1	0	-0.919415	4.573193	0.789435
77	6	0	-0.722932	2.810473	-2.212164
78	1	0	-0.979567	1.801934	-2.557496
79	1	0	0.353266	2.959534	-2.365839
80	1	0	-1.273059	3.536217	-2.827371
81	6	0	-5.052490	0.533725	1.528795
82	1	0	-4.268720	-0.157441	1.854007
83	6	0	-3.042417	-1.408291	-0.013055
84	6	0	-3.481350	-1.364589	-1.358380
85	6	0	-4.298023	-2.404469	-1.832669
86	1	0	-4.647559	-2.367321	-2.863056
87	6	0	-4.659200	-3.473430	-1.020526
88	1	0	-5.297580	-4.266458	-1.407302
89	6	0	-4.189655	-3.528833	0.291281
90	1	0	-4.462152	-4.374617	0.917402
91	6	0	-3.381128	-2.511682	0.814397
92	6	0	-3.095184	-0.283238	-2.362922
93	1	0	-2.463826	0.451933	-1.863620
94	6	0	-4.318587	0.482027	-2.900421
95	1	0	-5.002590	-0.193523	-3.432536
96	1	0	-3.991052	1.259511	-3.603678
97	1	0	-4.864973	0.964465	-2.083472
98	6	0	-2.265937	-0.880385	-3.518200
99	1	0	-1.376391	-1.398694	-3.134761
100	1	0	-1.938143	-0.081152	-4.197344
101	1	0	-2.857564	-1.602111	-4.097376
102	6	0	-2.828906	-2.644100	2.232590
103	1	0	-2.764506	-1.633939	2.662987
104	6	0	-1.392221	-3.209551	2.175433
105	1	0	-1.406176	-4.224926	1.755766
106	1	0	-0.950742	-3.252020	3.180864
107	1	0	-0.748591	-2.588045	1.538779
108	6	0	-3.698916	-3.477908	3.188172
109	1	0	-4.738927	-3.126266	3.190251
110	1	0	-3.300305	-3.399543	4.207961
111	1	0	-3.695533	-4.541775	2.914362
112	6	0	-6.148187	-0.302756	0.843166
113	1	0	-6.555263	-1.039201	1.549254
114	1	0	-5.750496	-0.838451	-0.024517
115	1	0	-6.974070	0.341047	0.510325
116	6	0	-5.593525	1.208103	2.807871
117	1	0	-4.806559	1.784886	3.310776
118	1	0	-5.970681	0.444879	3.502744

119	1	0	-6.419163	1.891978	2.570768

Final SCF energy (Hartrees): -8421.2277252

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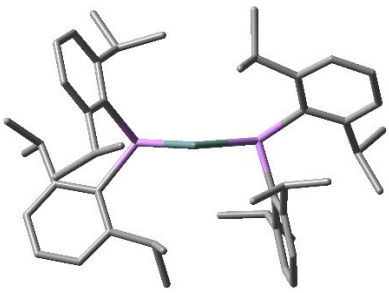
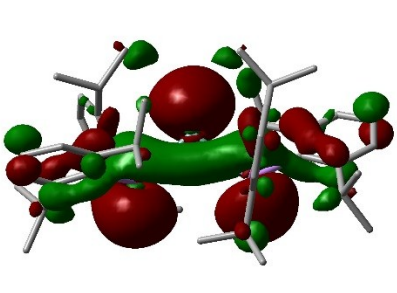
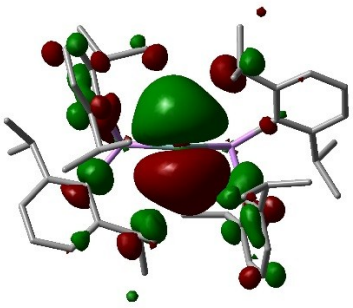


8Ge (triplet)



SOMO1



SOMO2

8Sn (pyramidal):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-0.000162	0.000363	-1.099815
2	33	0	-1.865393	-0.129829	0.871086
3	33	0	1.865254	0.129729	0.870936
4	6	0	-3.566651	-0.955449	0.196031
5	6	0	-3.563537	-2.163523	-0.547687
6	6	0	-4.790380	-2.731782	-0.927496
7	1	0	-4.790172	-3.642439	-1.523438
8	6	0	-6.000861	-2.157753	-0.555165
9	1	0	-6.942146	-2.611865	-0.861616
10	6	0	-6.000027	-1.007400	0.231873
11	1	0	-6.949307	-0.579045	0.544314
12	6	0	-4.803204	-0.394114	0.624549
13	6	0	-2.293572	-2.886311	-0.996747
14	1	0	-1.440128	-2.473376	-0.449815
15	6	0	-2.312594	-4.392759	-0.669719
16	1	0	-2.511238	-4.560619	0.395945
17	1	0	-1.336161	-4.828702	-0.915620
18	1	0	-3.079317	-4.922728	-1.249946
19	6	0	-2.042447	-2.672362	-2.503556
20	1	0	-2.850230	-3.132408	-3.089719
21	1	0	-1.089372	-3.131012	-2.801312
22	1	0	-2.006773	-1.605607	-2.757209
23	6	0	-4.867473	0.804114	1.575298
24	1	0	-4.017156	1.461477	1.362943
25	6	0	-6.132171	1.673705	1.448904
26	1	0	-6.308610	1.994445	0.414780
27	1	0	-6.015140	2.569760	2.072173
28	1	0	-7.026356	1.142326	1.801825
29	6	0	-4.731122	0.301032	3.030294

30	1	0	-5.581818	-0.348213	3.279940
31	1	0	-4.722164	1.147507	3.731400
32	1	0	-3.806101	-0.272252	3.163972
33	6	0	-1.870801	1.771463	0.115952
34	6	0	-2.435132	2.170617	-1.136868
35	6	0	-2.390600	3.526877	-1.503561
36	1	0	-2.843516	3.828328	-2.446141
37	6	0	-1.777390	4.479102	-0.700615
38	1	0	-1.753402	5.524032	-1.006553
39	6	0	-1.178197	4.083827	0.495568
40	1	0	-0.685896	4.829000	1.115264
41	6	0	-1.205837	2.751595	0.919746
42	6	0	-3.101579	1.218289	-2.127278
43	1	0	-2.952437	0.194571	-1.778087
44	6	0	-4.620810	1.465877	-2.199935
45	1	0	-5.084207	1.362306	-1.216429
46	1	0	-5.088785	0.738882	-2.876820
47	1	0	-4.823115	2.476913	-2.580360
48	6	0	-2.495338	1.321723	-3.543336
49	1	0	-2.703098	2.300192	-3.995841
50	1	0	-2.938503	0.551789	-4.189312
51	1	0	-1.407577	1.176623	-3.525126
52	6	0	-0.596793	2.416304	2.279763
53	1	0	-0.351211	1.350045	2.291229
54	6	0	0.713904	3.161601	2.585154
55	1	0	1.442818	3.033240	1.776717
56	1	0	1.151104	2.758385	3.507620
57	1	0	0.551411	4.237294	2.736447
58	6	0	-1.644834	2.658721	3.384958
59	1	0	-1.932660	3.719164	3.411211
60	1	0	-1.235184	2.384572	4.367208
61	1	0	-2.543519	2.057736	3.203853
62	6	0	3.566612	0.955325	0.196142
63	6	0	3.563675	2.163466	-0.547481
64	6	0	4.790611	2.731744	-0.926957
65	1	0	4.790565	3.642478	-1.522780
66	6	0	6.001001	2.157653	-0.554444
67	1	0	6.942357	2.611782	-0.860653
68	6	0	5.999983	1.007191	0.232441
69	1	0	6.949195	0.578758	0.544975
70	6	0	4.803070	0.393864	0.624772
71	6	0	2.293804	2.886220	-0.996851
72	1	0	1.440239	2.473354	-0.450074
73	6	0	2.312720	4.392684	-0.669952
74	1	0	2.510869	4.560525	0.395809
75	1	0	1.336388	4.828621	-0.916257
76	1	0	3.079699	4.922650	-1.249833
77	6	0	2.043015	2.672010	-2.503687
78	1	0	2.850800	3.132099	-3.089820
79	1	0	1.089894	3.130409	-2.801678
80	1	0	2.007606	1.605190	-2.757123
81	6	0	4.867100	-0.804536	1.575324
82	1	0	4.016681	-1.461684	1.362829
83	6	0	6.131566	-1.674436	1.448879
84	1	0	6.307940	-1.995086	0.414719
85	1	0	6.014219	-2.570549	2.071998

86	1	0	7.025893	-1.143404	1.801959
87	6	0	4.730665	-0.301656	3.030380
88	1	0	5.581546	0.347227	3.280343
89	1	0	4.721203	-1.148245	3.731340
90	1	0	3.805836	0.271967	3.163906
91	6	0	1.870744	-1.771430	0.115471
92	6	0	2.435009	-2.170278	-1.137475
93	6	0	2.390617	-3.526465	-1.504428
94	1	0	2.843385	-3.827686	-2.447151
95	6	0	1.777795	-4.478961	-0.701506
96	1	0	1.753986	-5.523845	-1.007618
97	6	0	1.178782	-4.084012	0.494868
98	1	0	0.686856	-4.829412	1.114596
99	6	0	1.206115	-2.751814	0.919213
100	6	0	3.101310	-1.217651	-2.127689
101	1	0	2.952139	-0.194047	-1.778175
102	6	0	4.620546	-1.465130	-2.200585
103	1	0	5.084031	-1.361802	-1.217086
104	1	0	5.088373	-0.737896	-2.877317
105	1	0	4.822857	-2.476036	-2.581344
106	6	0	2.494940	-1.320690	-3.543721
107	1	0	2.702640	-2.299028	-3.996538
108	1	0	2.938046	-0.550563	-4.189505
109	1	0	1.407187	-1.175602	-3.525337
110	6	0	0.597224	-2.416837	2.279396
111	1	0	0.351347	-1.350633	2.290965
112	6	0	-0.713273	-3.162416	2.584906
113	1	0	-1.442289	-3.034136	1.776556
114	1	0	-1.150407	-2.759267	3.507434
115	1	0	-0.550654	-4.238093	2.736147
116	6	0	1.645554	-2.659053	3.384357
117	1	0	1.933709	-3.719407	3.410462
118	1	0	1.236060	-2.385120	4.366731
119	1	0	2.544033	-2.057803	3.203071

Final SCF energy (Hartrees): -6346.6616614

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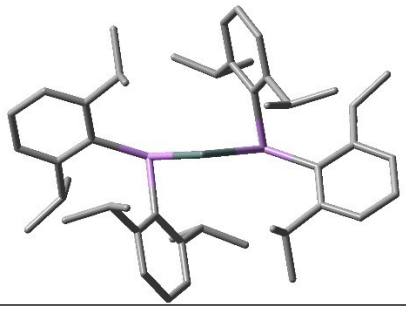	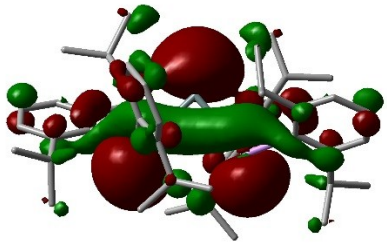	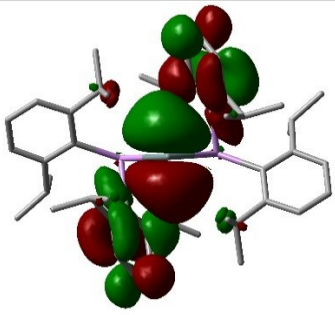
8Sn (pyramidal)	HOMO	LUMO

8Sn (planar):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.637764	-0.372213	-1.086923
2	6	0	-3.938974	-1.748210	-1.265211
3	6	0	-5.199889	-2.098106	-1.770188
4	1	0	-5.436657	-3.150526	-1.915024
5	6	0	-6.155969	-1.132494	-2.072570
6	1	0	-7.133056	-1.428913	-2.451233
7	6	0	-5.855054	0.213992	-1.884506
8	1	0	-6.601412	0.971969	-2.114888
9	6	0	-4.600873	0.618048	-1.406791
10	6	0	-4.351704	2.110746	-1.227187
11	1	0	-3.287456	2.242566	-1.002086
12	6	0	-5.151812	2.670030	-0.035438
13	1	0	-4.885931	2.152468	0.892517
14	1	0	-6.230563	2.549835	-0.208415
15	1	0	-4.940538	3.740367	0.092478
16	6	0	-4.634815	2.909640	-2.513281
17	1	0	-4.051607	2.516643	-3.356063
18	1	0	-4.366716	3.964415	-2.362825
19	1	0	-5.698661	2.869148	-2.783355
20	6	0	-2.974471	-2.884256	-0.935100
21	1	0	-2.134924	-2.458225	-0.375245
22	6	0	-3.606617	-3.968819	-0.041153
23	1	0	-4.032867	-3.530846	0.868711
24	1	0	-2.839809	-4.699733	0.249680
25	1	0	-4.403679	-4.512642	-0.565320
26	6	0	-2.399910	-3.507585	-2.221403
27	1	0	-1.897496	-2.747959	-2.834183
28	1	0	-3.202107	-3.956700	-2.822976
29	1	0	-1.671761	-4.293388	-1.973985
30	6	0	-2.344460	1.082548	1.362424
31	6	0	-1.872179	2.393309	1.628019
32	6	0	-2.367215	3.067978	2.753736
33	1	0	-2.022458	4.081232	2.949543
34	6	0	-3.286800	2.475636	3.613323
35	1	0	-3.667076	3.023354	4.474200
36	6	0	-3.703188	1.170546	3.370406
37	1	0	-4.403190	0.691259	4.051991
38	6	0	-3.238705	0.446115	2.262671
39	6	0	-0.866742	3.144276	0.758098
40	1	0	-0.504694	2.467227	-0.023126
41	6	0	0.357701	3.598588	1.578532
42	1	0	0.857242	2.741427	2.044639
43	1	0	0.064788	4.309583	2.362741
44	1	0	1.077961	4.099723	0.920446
45	6	0	-1.523046	4.359102	0.069963
46	1	0	-2.380745	4.061804	-0.543431
47	1	0	-0.794612	4.866374	-0.576422
48	1	0	-1.873901	5.079575	0.821198
49	6	0	-3.741688	-0.986079	2.115175
50	1	0	-3.197240	-1.457848	1.293272

51	6	0	-5.246957	-1.021463	1.785058
52	1	0	-5.470551	-0.470338	0.867258
53	1	0	-5.820557	-0.576514	2.609959
54	1	0	-5.583580	-2.058638	1.655856
55	6	0	-3.460793	-1.822210	3.381727
56	1	0	-2.407479	-1.760673	3.674914
57	1	0	-3.711390	-2.875288	3.193925
58	1	0	-4.074157	-1.477224	4.224440
59	6	0	3.286925	0.555129	-1.155154
60	6	0	3.710461	1.863335	-1.519235
61	6	0	4.762893	2.014437	-2.431810
62	1	0	5.094256	3.011484	-2.711743
63	6	0	5.404727	0.906663	-2.982336
64	1	0	6.230894	1.041691	-3.679001
65	6	0	4.976532	-0.370479	-2.640002
66	1	0	5.468618	-1.237598	-3.077707
67	6	0	3.915919	-0.573335	-1.741411
68	6	0	3.519949	-2.023723	-1.475238
69	1	0	2.646523	-2.032712	-0.822428
70	6	0	4.631766	-2.792590	-0.735544
71	1	0	4.863023	-2.317398	0.222910
72	1	0	5.546319	-2.826570	-1.343620
73	1	0	4.310386	-3.824817	-0.540905
74	6	0	3.127972	-2.753889	-2.776896
75	1	0	2.341446	-2.210527	-3.317386
76	1	0	2.758455	-3.762342	-2.543821
77	1	0	3.990698	-2.855754	-3.447931
78	6	0	1.743621	3.400590	-1.803276
79	1	0	1.046003	2.553449	-1.775340
80	1	0	2.010225	3.590686	-2.851972
81	1	0	1.222012	4.283183	-1.409739
82	6	0	3.012994	3.107876	-0.976048
83	1	0	2.686045	2.883196	0.047398
84	6	0	3.897645	4.363161	-0.896089
85	1	0	4.837765	4.154850	-0.369272
86	1	0	3.360418	5.152925	-0.354144
87	1	0	4.140267	4.755314	-1.893226
88	6	0	2.233709	-2.227768	1.742945
89	6	0	2.965982	-3.070488	2.591161
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91	6	0	4.180235	-2.665142	3.141182
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93	6	0	4.664019	-1.392762	2.860358
94	1	0	5.607255	-1.065809	3.294738
95	6	0	3.962434	-0.509894	2.024181
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98	6	0	5.913327	0.791142	1.049942
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112	6	0	-0.250630	-2.145509	2.089171
113	1	0	-0.217888	-1.050738	2.132944
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115	1	0	-1.226314	-2.439727	1.684981
116	33	0	-1.890951	0.212124	-0.369212
117	33	0	1.831779	0.404760	0.244170
118	6	0	2.745735	-0.940156	1.434346
119	50	0	0.150733	-0.703937	-1.586401

Final SCF energy (Hartrees): -6346.6491958

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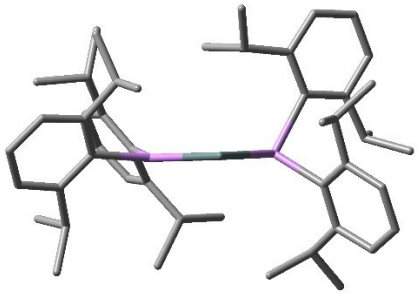	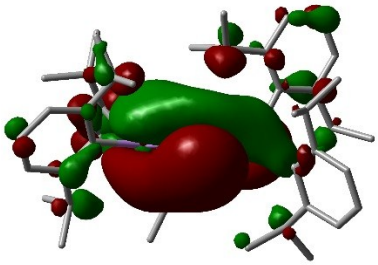	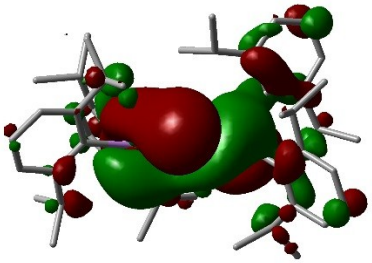
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	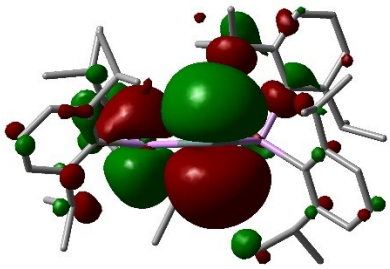	
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8Sn (triplet):

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3	33	0	-2.019314	-0.547343	0.815712
4	6	0	2.971924	1.406638	-0.380315
5	6	0	2.684562	2.179204	-1.533451
6	6	0	3.675963	3.034648	-2.037153
7	1	0	3.465925	3.605615	-2.939600
8	6	0	4.909077	3.171694	-1.407634
9	1	0	5.668001	3.834022	-1.821301

10	6	0	5.149323	2.476868	-0.225354
11	1	0	6.092567	2.613885	0.300386
12	6	0	4.194705	1.605672	0.316887
13	6	0	1.352255	2.155519	-2.274403
14	1	0	0.649159	1.527220	-1.718697
15	6	0	0.720348	3.559659	-2.340162
16	1	0	0.587868	3.974431	-1.334171
17	1	0	-0.266058	3.497161	-2.815095
18	1	0	1.343347	4.249689	-2.925283
19	6	0	1.500210	1.553156	-3.685118
20	1	0	2.229386	2.126774	-4.272829
21	1	0	0.537960	1.577482	-4.212325
22	1	0	1.841073	0.511636	-3.640772
23	6	0	4.530616	0.970830	1.665773
24	1	0	3.684381	0.360096	1.990541
25	6	0	5.761210	0.049213	1.582287
26	1	0	5.604740	-0.750642	0.851552
27	1	0	5.956580	-0.408927	2.561167
28	1	0	6.651914	0.622584	1.290438
29	6	0	4.723368	2.055467	2.746782
30	1	0	5.588484	2.690895	2.516041
31	1	0	4.898331	1.582200	3.722949
32	1	0	3.836603	2.697224	2.820719
33	6	0	2.990352	-1.541090	0.394923
34	6	0	3.719355	-1.936340	-0.750174
35	6	0	4.636939	-2.991703	-0.633300
36	1	0	5.209975	-3.291398	-1.509399
37	6	0	4.818230	-3.660375	0.573314
38	1	0	5.537232	-4.475026	0.646302
39	6	0	4.069198	-3.286514	1.689152
40	1	0	4.208603	-3.820966	2.625719
41	6	0	3.152454	-2.229441	1.624859
42	6	0	3.541308	-1.302853	-2.124271
43	1	0	2.767848	-0.535576	-2.049782
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46	1	0	4.650894	-0.140539	-3.591318
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59	1	0	3.138885	-3.218990	4.385045
60	1	0	2.396579	-1.740321	5.014087
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62	6	0	-3.926019	-0.983667	0.347665
63	6	0	-4.274756	-2.064515	-0.502695
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65	1	0	-5.885404	-3.074049	-1.511426

66	6	0	-6.631198	-1.476813	-0.283226
67	1	0	-7.673167	-1.653220	-0.545777
68	6	0	-6.291395	-0.478890	0.624225
69	1	0	-7.074033	0.116367	1.091411
70	6	0	-4.954580	-0.214987	0.956418
71	6	0	-3.263094	-3.034454	-1.105902
72	1	0	-2.297446	-2.885953	-0.609422
73	6	0	-3.639754	-4.508353	-0.852455
74	1	0	-3.797413	-4.693004	0.217618
75	1	0	-2.831955	-5.162584	-1.207236
76	1	0	-4.557541	-4.786819	-1.386728
77	6	0	-3.074797	-2.775970	-2.614472
78	1	0	-4.023323	-2.934825	-3.145612
79	1	0	-2.323475	-3.459422	-3.033458
80	1	0	-2.750349	-1.745372	-2.807680
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82	1	0	-3.634864	0.979222	2.149857
83	6	0	-5.260442	2.236256	1.607218
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90	1	0	-4.856371	-0.551732	3.683689
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Final SCF energy (Hartrees): -6346.6223082

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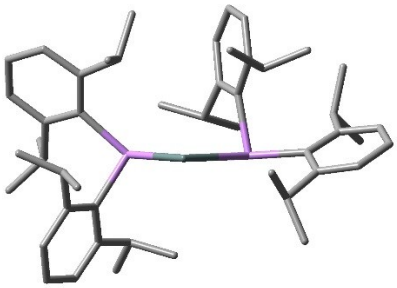	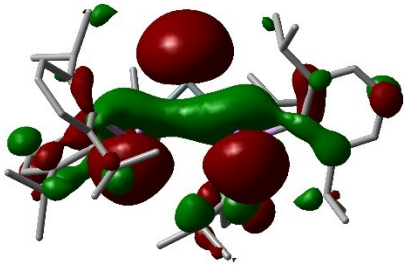	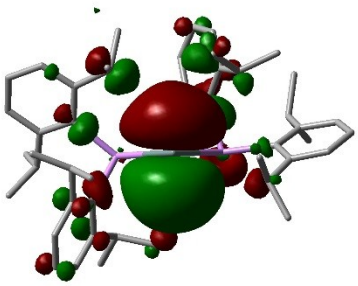
8Sn (triplet)	SOMO1	SOMO2

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