Supporting Information

for

Kinetic stabilization of low-oxidation state and terminal hydrido main group metal complexes with a sterically demanding N,N'-bis(2,6-terphenyl)triazenide

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Experimental

General Synthetic Procedures

All manipulations were performed using conventional Schlenk or glovebox techniques under an atmosphere of high purity argon in flame-dried glassware. Diethyl ether, THF, toluene, *n*-pentane and *n*-hexane were dried over sodium wire and purged with nitrogen prior to distillation from sodium benzophenone ketyl. Benzene-d_6 (C_6D_6) was dried over sodium and freeze-thaw degassed prior to use. Infrared spectra were recorded as Nujol mulls using sodium chloride plates on a Nicolet Avatar 320 FTIR spectrophotometer. ^{1}H and ^{13}C{^{1}H} NMR spectroscopic characterizations were recorded on Bruker spectrometers (see below for MHz) at 298 K unless otherwise stated, with chemical shifts referenced to the residual ^{1}H and ^{13}C{^{1}H} resonances of benzene-d_6 (δ 7.16 and δ 128.06 respectively).[1] Melting points were determined in sealed glass capillaries under argon and are uncorrected. Microanalyses were conducted at the Microanalytical unit of the Australian National University, Canberra, Australia or the Campbell Microanalytical Lab of the University of Otago, P.O. Box 56, Dunedin, New Zealand.

Starting Materials

Dmp_2N_3H,[2] $[Li(N_3Dmp_2)]$,[3] $[K(N_3Dmp_2)]$[3] and Me_2TlCl[4] were prepared according to literature procedures. $[Li(N_3Dmp_2)(OEt_2)]$,[2] $LiGaH_4$,[5] $LiInH_4$,[6] $[InH_3(NMe_3)]$[7] and 'GaI'[8] were prepared according to literature procedures and used *in situ*. All other reagents were purchased from commercial sources and used as received.

Synthesis of $[GeCl(N_3Dmp_2)]$ (1)

An *in situ* prepared solution of $[Li(N_3Dmp_2)(OEt_2)]$ (*ca*. 0.32 mmol) in diethyl ether (10 mL) was added to solid $GeCl_2$·dioxane (74 mg, 0.32 mmol) at -10 °C and stirred for 20 mins, resulting in a cloudy bright yellow solution. Insoluble material was removed by filtration. The filtrate was concentrated *in vacuo* (5 mL) and allowed to stand at -20 °C overnight, affording large bright yellow blocks of the titled compound (142 mg, 57% over 2 crops). ^{1}H NMR (400 MHz, C_6D_6) δ 1.95 (s, 12H, *o*-CH_3), 2.00 (s, 12H, *o*-CH_3), 2.17 (s, 12H, *p*-CH_3), 6.72-6.87 (m, 14H, ArC*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H$_3$), 21.6, 21.7 (*o*-*C*H$_3$), 126.3, 129.1, 129.2, 130.5 (Ar*C*H), 134.2, 136.2, 136.6,

136.7, 137.0, 139.5 (Ar*C*). Anal. Cal. for $C_{48}H_{50}ClGeN_3$: C, 74.20; H, 6.49; N, 5.41. Found: C, 74.24; H, 6.95; N, 4.90%.

Synthesis of [SnCl(N_3Dmp$_2$)] (2)

A solution of *in situ* prepared [Li(N_3Dmp$_2$)(OEt_2)] (*ca*. 0.21 mmol) in diethyl ether (10 mL) was added to solid $SnCl_2$ (40 mg, 0.21 mmol) at -10 °C and stirred for 20 mins, resulting in a cloudy pale orange solution. The mixture was filtered and quickly concentrated to incipient crystallization to minimize precipitation of decomposition material. The filtrate was allowed to stand at -20 °C overnight, resulting in a yellow precipitate of the titled compound which contained a few yellow crystals (126 mg, 73%). ^{1}H NMR (400 MHz, C_6D_6) δ 2.01 (s, 12H, *o*-CH_3), 2.03 (s, 12H, *o*-CH_3), 2.16 (s, 12H, *p*-CH_3), 6.72-6.87 (m, 14H, ArC*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H_3), 21.8, 21.8 (*o*-*C*H_3), 125.3, 129.2, 129.7, 130.5 (Ar*C*H), 133.4, 136.0, 136.6, 137.1, 137.1, 140.7 (Ar*C*). Anal. Cal. for $C_{48}H_{50}ClSnN_3$: C, 70.04; H, 6.12; N, 5.11. Found: C, 69.25; H, 6.33; N, 5.19%.

Synthesis of [GeH(N_3Dmp$_2$)] (3)

A solution of *in situ* prepared **1** (*ca*. 0.30 mmol) in diethyl ether (10 mL) was added to solid Li[BEt_3H] (35 mg, 0.33 mmol) at -30 °C and stirred for 30 mins while warming to room temperature, resulting in a bright yellow suspension. The mixture was filtered, concentrated *in vacuo* (8 mL) and allowed to stand at -20 °C overnight, resulting in large yellow blocks of the titled compound (70 mg, 31%). Crystals suitable for X-ray diffraction structure determination were grown by slowly cooling a toluene solution of the complex to -20 °C overnight. m.p. 190 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ 1.97 (s, 24H, *o*-CH_3), 2.15 (s, 12H, *p*-CH_3), 6.75-6.86 (m, 14H, ArC*H*), 8.95 (s, 1H, Ge-*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H_3), 21.3, 21.3 (*o*-*C*H_3), 125.6, 128.8, 128.9, 130.2 (Ar*C*H), 133.3, 136.2, 136.6, 136.6, 140.2 (Ar*C*). IR (Nujol, cm^{-1}): 1807 (m, Ge-H), 1820 (m, Ge-H). Anal. Cal. for $C_{48}H_{51}GeN_3 \cdot OC_4H_{10}$: C, 76.47; H, 7.53; N, 5.15. Found: C, 76.52; H, 7.18; N, 5.18%.

Synthesis of [SnH(N_3Dmp$_2$)] (4)

A solution of *in situ* prepared **2** (*ca*. 0.21 mmol) in diethyl ether (10 mL) was added to solid Li[BEt_3H] (22 mg, 0.21 mmol) at -30 °C and stirred for 30 mins while warming to 0 °C, during which time LiCl slowly precipitated. The solution was cooled to -10 °C and

filtered. The filtrate was concentrated *in vacuo* (6 mL) and allowed to stand at -20 °C overnight, affording yellow blocks of the titled compound (94 mg, 57% over 2 crops). m.p. 180-185 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ 2.00 (s, 12H, *o*-C*H*$_3$), 2.01 (s, 12H, *o*-C*H*$_3$), 2.15 (s, 12H, *p*-C*H*$_3$), 6.73-6.88 (m, 14H, ArC*H*), 16.42 (s, ^{1}J(^{119}Sn-^{1}H) = 60 Hz, 1H, Sn-*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6): δ 21.2 (*p*-*C*H$_3$), 21.5, 21.6 (*o*-*C*H$_3$), 124.8, 129.1, 130.2 (Ar*C*H), 132.9, 136.1, 136.5, 136.7, 137.1, 141.6 (Ar*C*). Crystalline samples repeatedly gave microanalyses low in carbon which presumably emanates from the high thermal, oxygen and moisture sensitivity of this complex. Representative example Anal. Cal. for $C_{48}H_{51}N_3Sn$: C, 73.10; H, 6.52; N, 5.33. Found: C, 70.83; H, 6.85; N, 4.24%.

Synthesis of [AlH$_2$(N$_3$Dmp$_2$)] (5)

A pale yellow solution of Dmp$_2$N$_3$H (461 mg, 0.69 mmol) in diethyl ether (40 mL) was added dropwise to a cooled (0 °C) solution of LiAlH$_4$ (39 mg, 1.03 mmol) in diethyl ether (20 mL). The resultant solution was stirred for a further 2 h at 0 °C, over this period the color changed from pale yellow to radiant yellow. The solution was stirred at ambient temperature overnight. The volatiles were removed *in vacuo* and the yellow solid was extracted with hexane (60 mL), concentrated (*ca.* 20 mL) and slow cooled to -25 °C to afford large yellow prisms suitable for X-ray diffraction structure determination (240 mg, 50%). m.p. > 360 °C. ^{1}H NMR (500 MHz, C_6D_6) δ 1.96 (s, 24H, *o*-C*H*$_3$), 2.15 (s, 12H, *p*-C*H*$_3$), 6.77-6.79 (m, 4H, *m*-Ar*H*), 6.84 (s, 8H, *m*-Ar'*H*), 6.84-6.86 (m, 2H, *p*-Ar*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H$_3$), 21.3 (*o*-*C*H$_3$), 126.0, 129.2, 130.3 (Ar*C*H), 133.7, 136.0, 36.5, 136.9, 139.4 (Ar*C*). IR (Nujol, cm^{-1}) 1873 (br m, Al-H). Anal. Calc. for $C_{48}H_{52}AlN_3$: C, 82.60; H, 7.51; N, 6.02. Found: C, 81.50; H, 7.64; N, 5.83%.

Synthesis of [GaH$_2$(N$_3$Dmp$_2$)] (6)

A pale yellow solution of Dmp$_2$N$_3$H (117 mg, 0.175 mmol) in diethyl ether (20 mL) was added dropwise to a cooled (-78 °C) solution of LiGaH$_4$ (0.18 mmol) in diethyl ether (40 mL). The resultant pale yellow mixture was allowed to warm to ambient temperature overnight, with a noticeable color change to bright yellow. The solution was isolated by filtration and removal of volatiles *in vacuo* afforded a yellow solid that was washed with cold (0 °C) hexane (3×3 mL), then extracted with toluene (30 mL), concentrated (10 mL) and slow cooled to -25 °C to afford large yellow prisms suitable

for X-ray diffraction structure determination (100 mg, 70%). m.p. 270-272 °C (dec.). ^{1}H NMR (500 MHz, C_6D_6) δ 1.95 (s, 24H, *o*-C*H*$_3$), 2.15 (s, 12H, *p*-C*H*$_3$), 4.46 (br s, 2H, Ga-*H*), 6.75-6.79 (m, 4H, *m*-Ar*H*), 6.83 (s, 8H, *m*-Ar'H), 6.83-6.85 (m, 2H, *p*-Ar*H*). ^{13}C{^{1}H} (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H$_3$), 21.3 (*o*-*C*H$_3$), 125.5, 129.0, 130.2 (Ar*C*H), 133.6, 136.0, 136.6, 136.9, 140.0 (Ar*C*). IR (Nujol, cm^{-1}) 1940 (br m, Ga-H). Anal. Calc. for $C_{48}H_{52}GaN_3 \cdot 0.5(C_7H_8)$: C, 78.62; H, 7.17; N, 5.34. Found: C, 78.17; H, 7.71; N, 5.09%.

Synthesis of [Tl(N$_3$Dmp$_2$)] (7)

TlOEt (24 µL, 0.34 mmol) was added dropwise to a solution of Dmp_2N_3H (221 mg, 0.33 mmol) in toluene (30 mL) at -20 °C with immediate color change from pale yellow to deep red. With the exclusion of light, the mixture was allowed to warm to ambient temperature and stirred for a further 24 h, during which a small amount of metal deposition was observed. The solvent was removed *in vacuo* and the red residue was extracted into hexane (60 mL). Concentration of the solution *in vacuo* (*ca.* 10 mL) and standing at ambient temperature after light warming to dissolve precipitated solids afforded large red blocks suitable for X-ray diffraction structure determination (175 mg, 58%). m.p. 243-250 °C (dec.). ^{1}H NMR (500 MHz, C_6D_6) δ 1.97 (s, 24H, *o*-C*H*$_3$), 2.13 (s, 12H, *p*-C*H*$_3$), 6.78 (t, $^{AAB}J_{HH}$ = 7.4 Hz, 2H, *p*-Ar*H*), 6.84 (m, 12H, *m*-Ar*H* and *m*-Ar'*H*). ^{13}C NMR (100 MHz, C_6D_6) δ 21.1 (*p*-*C*H$_3$), 23.1 (*o*-*C*H$_3$), 122.9, 128.7, 129.9 (Ar*C*H), 133.1, 135.6, 136.1, 139.6 (Ar*C*). IR (Nujol, cm^{-1}) 1610 (w), 1278 (w), 1262 (m), 1230 (w), 1077 (br w), 1030 (br w), 854 (w), 845 (w), 801 (w), 784 (w), 764 (w), 756 (w), 737 (w). Anal. Calc. for $C_{48}H_{50}TlN_3 \cdot 0.5(C_6H_{14})$: C, 66.84; H, 6.27; N, 4.58. Found: C, 66.78; H, 6.35; N, 4.38%.

Attempted Synthesis of [In(N$_3$Dmp$_2$)] (8)

A cool (-78 °C) solution of [Li(N$_3$Dmp$_2$)] (330 mg, 0.44 mmol) in toluene (15 mL) was added dropwise to a stirred slurry of InCl (75 mg, 0.50 mmol) in toluene (10 mL) at -78 °C. The resultant slurry was stirred at -78 °C for 1 h, then allowed to warm to ambient temperature overnight, which afforded a red solution and dark grey precipitate. Filtration and followed by concentration *in vacuo* (*ca*. 5 mL) and standing at ambient temperature after light warming to dissolve precipitated solids afforded a crop of dark orange prisms suitable for X-ray diffraction structure determination. The supernatant was decanted and slowly cooled to -25 °C overnight to afford a second

crop of orange prisms (203 mg, 59% over 2 crops). m.p. 223-229 °C (dec.). ^{1}H NMR (250 MHz, C_6D_6, selected resonances) δ 1.97 (s, 24H, *o*-C*H*$_3$), 2.13 (s, 12H, *p*-C*H*$_3$), 6.78-6.83 (m, 6H, *m*- and *p*-Ar*H*), 6.86 (s, 8H, *m*-Ar'*H*). ^{13}C{^{1}H} NMR (50 MHz, C_6D_6, selected resonances) δ 21.1 (*p*-*C*H$_3$), 21.6 (*o*-*C*H$_3$), 122.9, 129.0, 130.0 (Ar*C*H), 133.1, 135.9, 136.0, 139.0 (Ar*C*).

Attempted Synthesis of [Ga(N$_3$Dmp$_2$)] (9)

A cool (-78 °C) solution of [K(N$_3$Dmp$_2$)] (204 mg, 0.44 mmol) in toluene (15 mL) was added dropwise to a stirred slurry of "GaI" (120 mg, 0.61 mmol) in toluene (10 mL) at -78 °C. The resultant slurry was stirred at -78 °C for 1 h followed by warming to ambient temperature overnight, which afforded a red solution and dark grey precipitate. Filtration and followed by concentration *in vacuo* (*ca*. 5 mL) and standing at ambient temperature after light warming to dissolve precipitated solids afforded a crop of dark orange prisms suitable for X-ray diffraction structure determination. The supernant was decanted and slowly cooled to -25 °C overnight to afford a second crop of orange prisms. Yield of combined crops (203 mg, 62%).

Synthesis of [GaCl$_2$(N$_3$Dmp$_2$)] (10)

An *in situ* prepared solution of [Li(N$_3$Dmp$_2$)(OEt$_2$)] (*ca*. 1.00 mmol) in diethyl ether (50 mL) was added dropwise to a solution of GaCl$_3$ (180 mg, 1.00 mmol) in diethyl ether (30 mL) at ambient temperature. The resultant bright yellow solution was stirred for a further 12 h, followed by the removal of volatiles *in vacuo*. Extraction with pentane (60 mL), concentration (*ca*. 25 mL) and cooling to -25 °C afforded yellow crystals (615 mg, 72%). m.p. 162-164 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ 1.96 (s, 24H, *o*-C*H*$_3$), 2.20 (s, 12H, *p*-C*H*$_3$), 6.69 (d, $^{AAB}J_{HH}$ = 7.6 Hz, 4H, *m*-Ar*H*), 6.83 (t, $^{AAB}J_{HH}$ = 7.6 Hz, 2H, *p*-Ar*H*), 6.87 (s, 8H, *m*-Ar'*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.2 (*p*-*C*H$_3$), 21.6 (*o*-*C*H$_3$), 127.2, 129.5, 130.9 (Ar*C*H), 135.1, 135.6, 136.1, 137.6 (Ar*C*). IR (Nujol, cm^{-1}) 2732 (w), 1941 (w), 1727 (w), 1613 (s), 1573 (w), 1485 (w), 1414 (m), 1290 (s), 1270 (s), 1246 (w), 1236 (w), 1192 (w), 1171 (s), 1104 (w), 1032 (m), 882 (w), 848 (s), 803 (s), 782 (s), 763 (s), 744 (w), 685 (m), 665 (w), 607 (w), 587 (w). Anal. Cal. for $C_{48}H_{50}GaCl_2N_3$: C, 71.21; H, 6.23; N, 5.19. Found: C, 70.93; H, 6.60; N, 4.41%.

Synthesis of [$InBr_2(N_3Dmp_2)$] (11)

An *in situ* prepared solution of [$Li(N_3Dmp_2)(OEt_2)$] (*ca*. 0.29 mmol) in diethyl ether (30 mL) was added dropwise to a solution of $InBr_3$ (102 mg, 0.29 mmol) in diethyl ether (30 mL) at ambient temperature. The resultant bright yellow solution was stirred for a further 2 h, followed by the removal of volatiles *in vacuo*. Extraction with diethyl ether (40 mL), concentration (*ca*. 20 mL) and cooling to -25 °C afforded yellow prisms suitable for X-ray diffraction structure determination (190 mg, 69%). m.p. 145-146 °C (dec.). ^{1}H NMR (500 MHz, C_6D_6) δ 1.97 (s, 24H, *o*-CH_3), 2.20 (s, 12H, *p*-CH_3), 6.69 (d, $^{AAB}J_{HH}$ = 7.6 Hz, 4H, *m*-Ar*H*), 6.82 (t, $^{AAB}J_{HH}$ = 7.6 Hz, 2H, *p*-Ar*H*), 6.87 (s, 8H, *m*-Ar'*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.3 (*o*-*C*H_3), 22.1 (*o*-*C*H_3), 126.6, 129.9, 130.8 (Ar*C*H), 134.7, 135.6, 136.0, 138.0, 138.2 (Ar*C*). IR (Nujol, cm^{-1}) 2732 (w), 1941 (w), 1728 (w), 1612 (s), 1572 (w), 1486 (w), 1411 (m), 1294 (s), 1271 (s), 1248 (w), 1236 (w), 1192 (m), 1177 (m), 1104 (w), 1032 (m), 852 (s), 804 (s), 782 (s), 764 (s), 742 (w), 677 (m), 608 (w), 585 (w). Anal. Calc. for $C_{48}H_{50}InBr_2N_3 \cdot 0.5(OC_4H_{10})$: C, 61.24; H, 5.65; N, 4.29. Found: C, 60.49; H, 5.72; N, 3.84%.

Synthesis of [$AlCl_2(N_3Dmp_2)$] (12)

A solution of $MeAlCl_2$ (1.0 M hexane solution, 0.60 mL, 0.60 mmol) was added to a solution of Dmp_2N_3H (374 mg, 0.56 mmol) in hexane (50 mL) at ambient temperature. Gas evolution was immediately observed and the color changed from pale yellow to bright yellow. The resultant solution was stirred for a further 12 h, followed by the removal of volatiles *in vacuo*. Extraction with hexane (50 mL), concentration (*ca*. 15 mL) and cooling to -25 °C afforded yellow prisms suitable for X-ray diffraction structure determination (152 mg, 35%). m.p. 184-185 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6, selected resonances) δ 1.99 (s, 24H, *o*-CH_3), 2.19 (s, 12H, *p*-CH_3), 6.82 (d, $^{AAB}J_{HH}$ = 7.6 Hz, 4H, *m*-Ar*H*), 6.89 (s, 8H, *m*-Ar'*H*), 6.94 (t, $^{AAB}J_{HH}$ = 7.6 Hz, 2H, *p*-Ar*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, selected resonances) δ 20.6 (*p*-*C*H_3), 21.1 (*o*-*C*H_3), 126.3, 130.1, 130.4 (Ar*C*H), 132.5, 133.0, 133.8, 136.1, 138.9 (Ar*C*). IR (Nujol, cm^{-1}) 2731 (m), 1612 (s), 1570 (w), 1285 (m), 1264 (s), 1191 (m), 1168 (s), 1093 (w), 1031 (m), 1013 (m), 849 (s), 803 (s), 780 (s), 763 (s), 742 (s), 723 (w), 676 (br s), 567 (w), 528 (w). Anal. Calc. for $C_{48.5}H_{51.5}AlCl_{1.5}N_3$: C, 76.99; H, 6.86; N, 5.55. Found: C, 76.46; H, 7.87; N, 5.91%.

Synthesis of [$AlMe_2(N_3Dmp_2)$] (13)

To a pale yellow solution of Dmp_2N_3H (409 mg, 0.61 mmol) in toluene (10 mL) was added dropwise a solution of $AlMe_3$ (0.70 mL, 1.4 mmol, 2.0 M in toluene). Gas evolution was immediately observed and the color changed from pale yellow to bright yellow. The resultant solution was stirred for a further 12 h, volatiles were removed *in vacuo*, which afforded a bright yellow powder (428 mg, 97%). Extraction with pentane, concentration and cooling to -25 °C afforded yellow prisms suitable for X-ray diffraction structure determination. m.p. 202-203 °C. ^{1}H NMR (250 MHz, C_6D_6) δ -1.27 (s, 6H, Al-C*H*$_3$), 1.95 (s, 24H, *o*-C*H*$_3$), 2.19 (s, 12H, *p*-C*H*$_3$), 6.72 (d, $^3J_{HH}$ = 7.3 Hz, 4H, *m*-Ar*H*), 6.84 (t, $^3J_{HH}$ = 7.3 Hz, 2H, *p*-Ar*H*), 6.84 (s, 8H, *m*-Ar'*H*). ^{13}C{^{1}H} NMR (50 MHz, C_6D_6) δ -10.1 (Al-C), 21.2, 21.7 (CH_3), 125.9, 129.0, 131.0 (ArCH), 134.3, 136.2, 136.7, 137.2, 140.3 (ArC). IR (Nujol, cm^{-1}) 2731 (m), 1936 (w), 1875 (w), 1759 (w), 1727 (w), 1611 (s), 1573 (w), 1487 (m), 1291 (w), 1262 (s), 1231 (m), 1179 (s), 1093 (w), 1032 (m), 880 (w), 848 (s), 804 (w), 780 (m), 766 (m), 759 (m), 743 (w), 720 (w), 695 (s), 682 (w), 660 (w), 610 (m), 590 (w). Anal. Calc. for $C_{50}H_{56}AlN_3$: C, 82.72; H, 7.77; N, 5.79. Found: C, 82.03, H, 7.80, N, 5.89%.

Synthesis of [$GaMe_2(N_3Dmp_2)$] (14)

A solution of MeLi (1.0 M in diethyl ether, 0.45 mL, 0.45 mmol) was added dropwise to a pale yellow solution of **10** (170 mg, 0.21 mmol) in diethyl ether (20 mL) at ambient temperature. Gas evolution was immediately observed and the color changed from pale yellow to bright yellow. The resultant solution was stirred for a further 12 h followed by removal of volatiles *in vacuo* to yield the title compound as a bright yellow powder. Extraction with hexane (40 mL), concentration (*ca*. 10 mL) and cooling to -25 °C afforded yellow plates suitable for X-ray diffraction structure determination (138 mg, 85%). m.p. 172-174 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ -0.82 (s, 6H, Ga-C*H*$_3$), 1.94 (s, 24H, *o*-C*H*$_3$), 2.20 (s, 12H, *p*-C*H*$_3$), 6.72 (d, $^{AAB}J_{HH}$ = 7.4 Hz, 4H, *m*-Ar*H*), 6.80-6.84 (m, 10H, *p*-Ar*H* and *m*-Ar'*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ -4.5 (Ga-*C*), 21.2 (*p*-*C*H$_3$), 21.7 (*o*-*C*H$_3$), 125.2, 128.9, 130.9 (Ar*C*H), 134.1, 136.1, 136.4, 137.7, 141.1 (Ar*C*). IR (Nujol, cm^{-1}) 1262 (s), 1231 (m), 1194 (m), 1154 (w), 1093 (w), 1030 (m), 965 (w), 849 (s), 802 (s), 765 (m), 754 (w), 741 (w), 723 (w), 666 (s). Anal. Calc. for $C_{50}H_{56}GaN_3$: C, 78.12; H, 7.34; N, 5.46. Found: C, 78.22; H, 7.57; N, 5.50%.

Synthesis of [$InMe_2(N_3Dmp_2)$] (15)

A solution of MeLi (1.0 M in diethyl ether, 0.38 mL, 0.38 mmol) was added dropwise to a pale yellow solution of **11** (170 mg, 0.18 mmol) in diethyl ether (10 mL) at ambient temperature. Gas evolution was immediately observed and the color changed from pale yellow to bright yellow. The resultant solution was stirred for a further 12 h followed by removal of volatiles *in vacuo* to yield the title compound as a bright yellow powder. Extraction with hexane (40 mL), concentration (*ca*. 10 mL) and cooling to -25 °C afforded yellow prisms suitable for X-ray diffraction structure determination (95 mg, 65%). m.p. 172-174 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ -0.63 (s, 6H, In-CH_3), 1.95 (s, 24H, *o*-CH_3), 2.19 (s, 12H, *p*-CH_3), 6.73 (d, $^{AAB}J_{HH}$ = 7.6 Hz, 4H, *m*-Ar*H*), 6.80-6.84 (m, 10H, *p*-Ar*H* and *m*-Ar'*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ -3.1 (In-*C*), 21.2 (*p*-*C*H_3), 21.7 (*o*-*C*H_3), 124.5, 129.0, 130.7 (Ar*C*H), 133.5, 135.8, 136.4, 137.8, 138.2 (Ar*C*). IR (Nujol, cm^{-1}) 2730 (w), 1610 (m), 1410 (m), 1280 (m), 1265 (s), 1246 (w), 1231 (m), 1195 (w), 1181 (w), 1092 (w), 1029 (m), 849 (s), 803 (m), 782 (w), 763 (m), 742 (w), 722 (w), 675 (w). Anal. Calc. for $C_{50}H_{56}InN_3$: C, 73.79; H, 6.94; N, 5.16. Found: C, 73.13; H, 6.98; N, 5.15%.

Synthesis of [$TlMe_2(N_3Dmp_2)$] (16)

A solution of **7** (200 mg, 0.24 mmol) in THF (20 mL) was added to a stirred slurry of Me_2TlCl (100 mg, 0.37 mmol) in THF (10 mL) at ambient temperature. A colorless precipitate formed immediately. After stirring for 1 h, the volatiles were removed *in vacuo* to yield a yellow solid. Extraction with hexane (50 mL), concentration (*ca*. 10 mL) and cooling to -25 °C afforded yellow prisms suitable for X-ray diffraction structure determination (195 mg, 89%). m.p. 192-193 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6) δ 0.13 (br d, $^2J_{TlH}$ = 364 Hz, 6H, Tl-CH_3), 1.96 (s, 24H, *o*-CH_3), 2.20 (s, 12H, *p*-CH_3), 6.75 (d, $^{AAB}J_{HH}$ = 7.4 Hz, 4H, *m*-Ar*H*), 6.81 (s, 8H, *m*-Ar'*H*), 6.83 (t, $^{AAB}J_{HH}$ = 7.4 Hz, 2H, *p*-Ar*H*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6) δ 21.1 (*p*-*C*H_3), 21.8 (*o*-*C*H_3), 23.2 (d, $^1J_{TlC}$ = 1771 Hz, Tl-*C*), 123.4, 128.8, 130.6 (Ar*C*H), 133.2, 135.8, 139.0 (Ar*C*). IR (ATR, cm^{-1}) 2924 (w), 2891 (w), 2830 (w), 2708 (w), 1597 (m), 1565 (w), 1473 (w), 1428 (m), 1392 (m), 1365 (m), 1269 (w), 1249 (s), 1234 (w), 1216 (m), 1185 (w), 1073 (w), 1019 (m), 940 (w), 841 (m), 794 (m), 775 (m), 756 (m), 736 (s), 662 (w), 607 (w), 580 (w), 555 (w), 528 (w), 503 (m), 459 (w), 429 (w). Anal. Calc. for $C_{50}H_{56}TlN_3$: C, 66.48; H, 6.25; N, 4.65. Found: C, 66.11; H, 6.25; N, 4.63%.

NMR Spectra

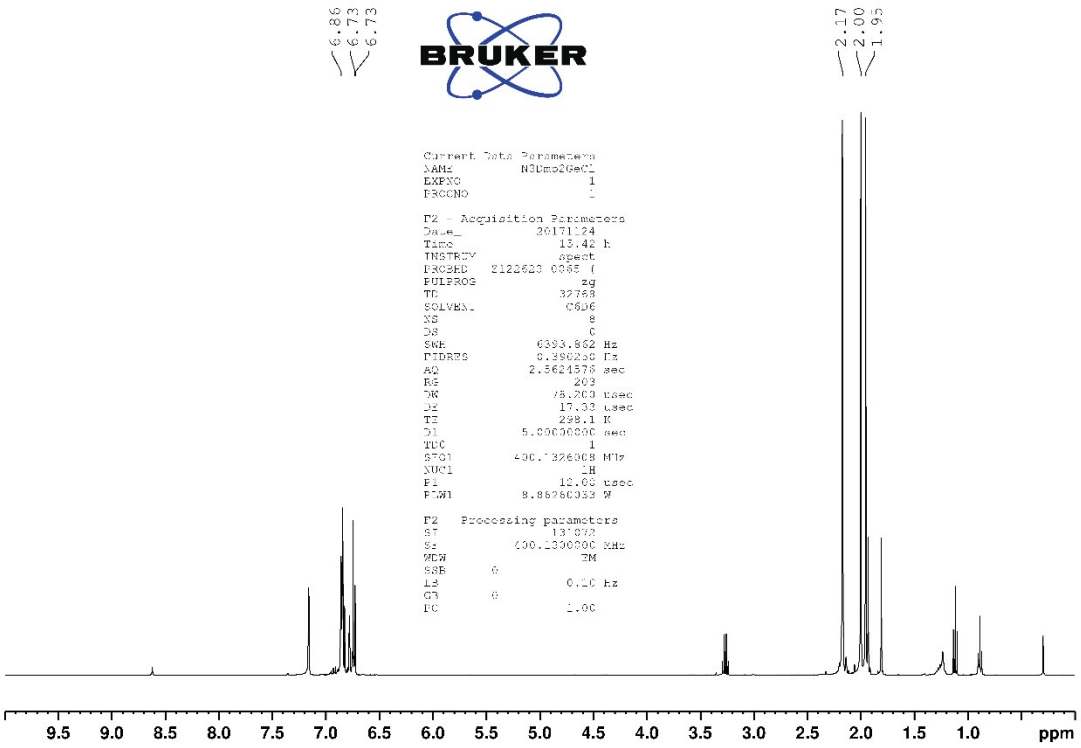

Figure S1. ^{1}H NMR spectrum of complex **1** (C_6D_6).

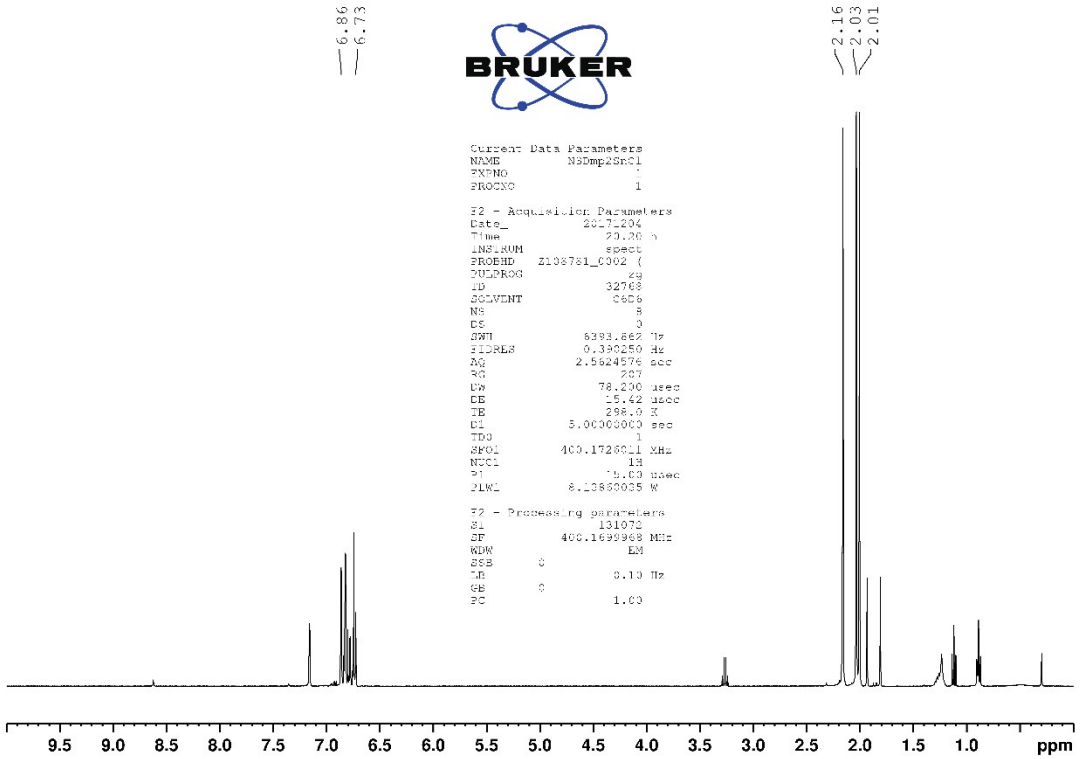

Figure S2. ^{1}H NMR spectrum of complex **2** (C_6D_6).

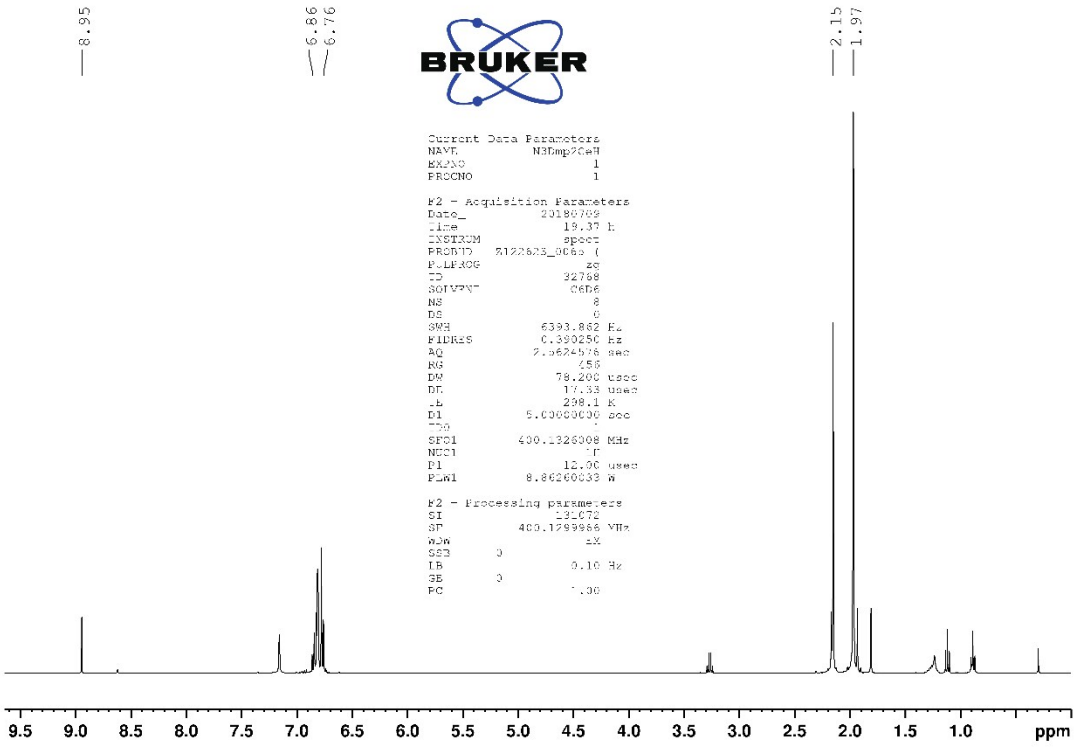

Figure S3. ^{1}H NMR spectrum of complex **3** (C_6D_6).

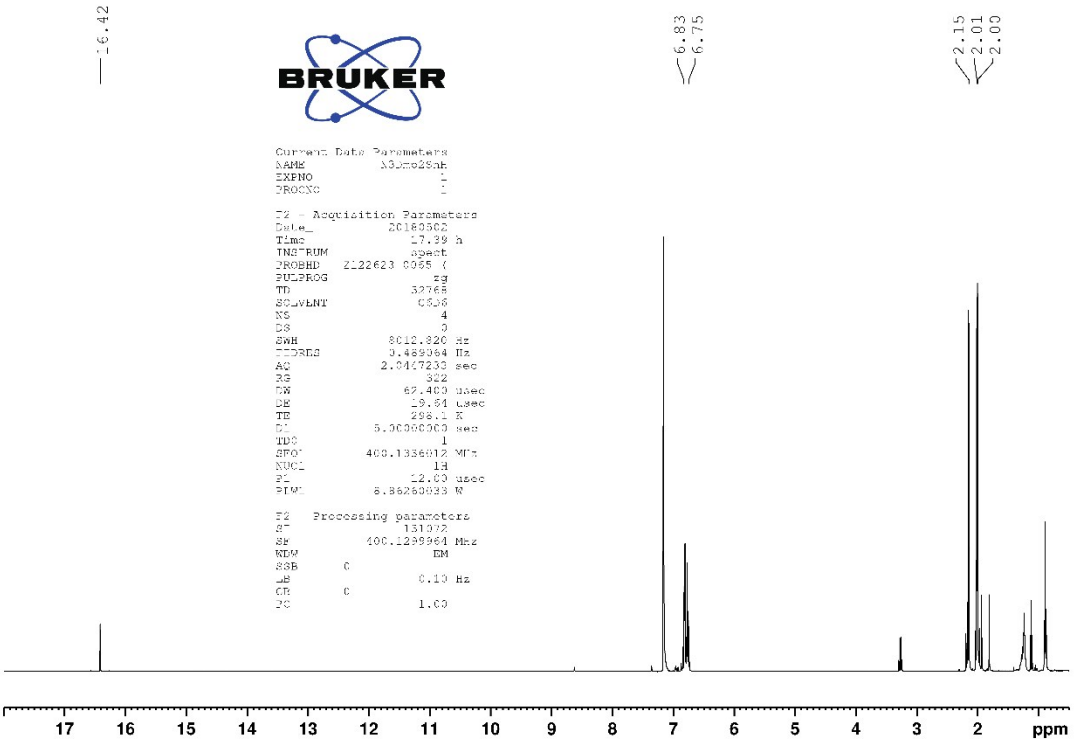

Figure S4. ^{1}H NMR spectrum of complex **4** (C_6D_6).

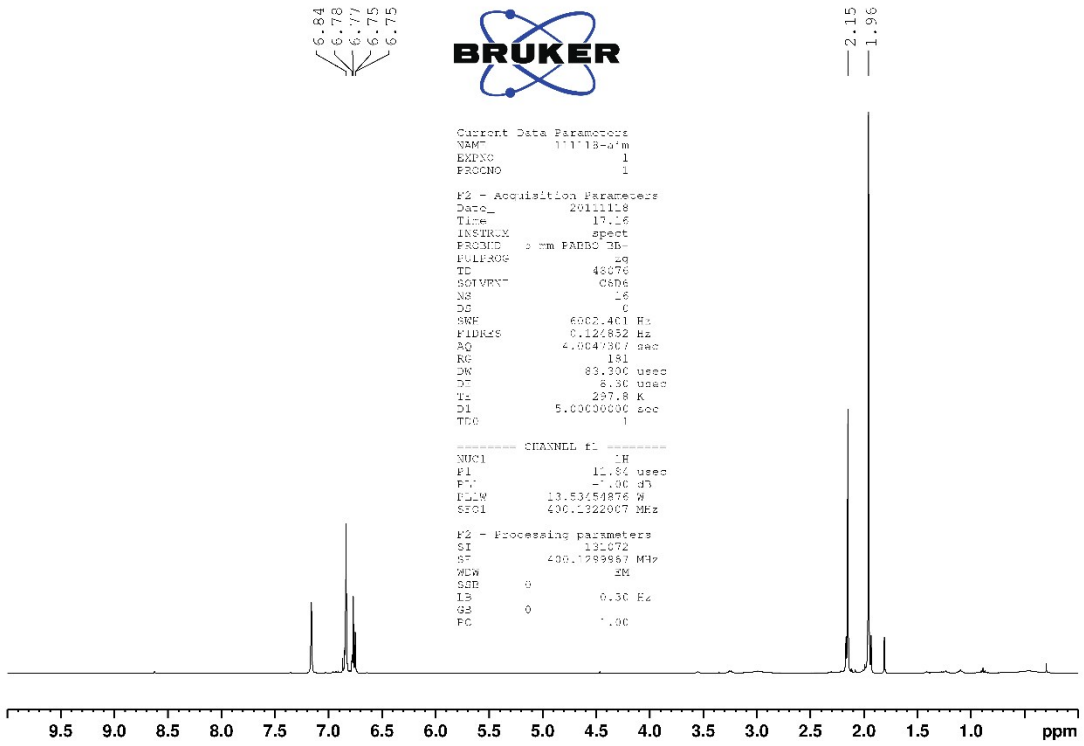

Figure S5. ^{1}H NMR spectrum of complex **5** (C_6D_6).

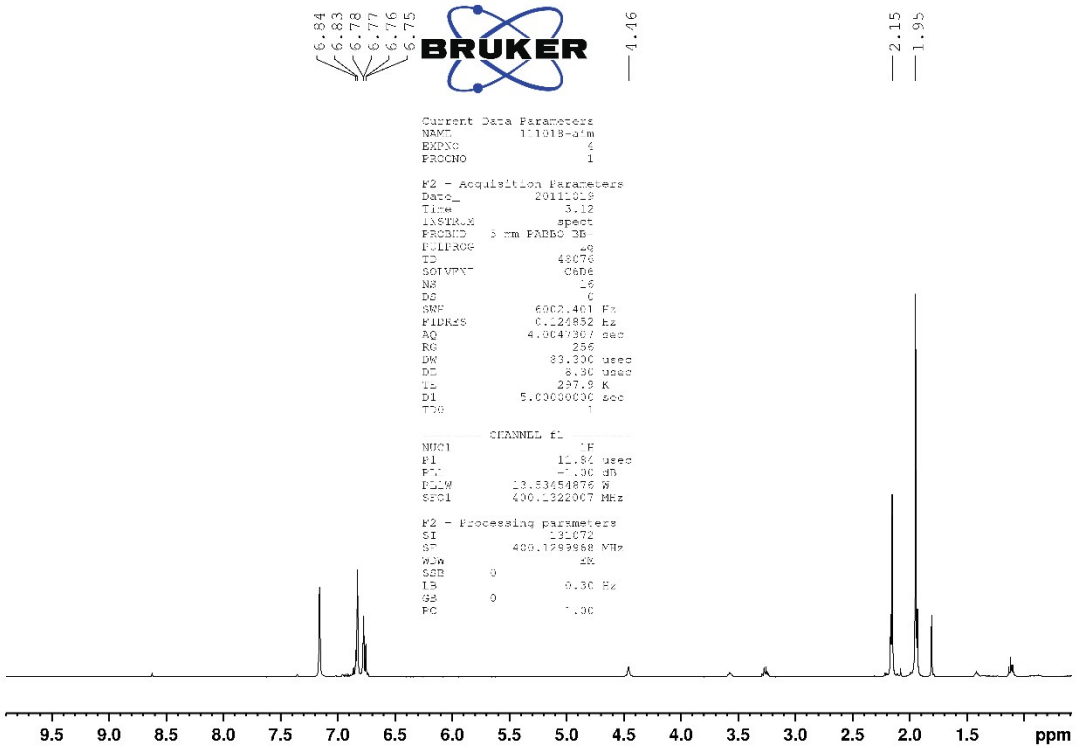

Figure S6. ^{1}H NMR spectrum of complex **6** (C_6D_6).

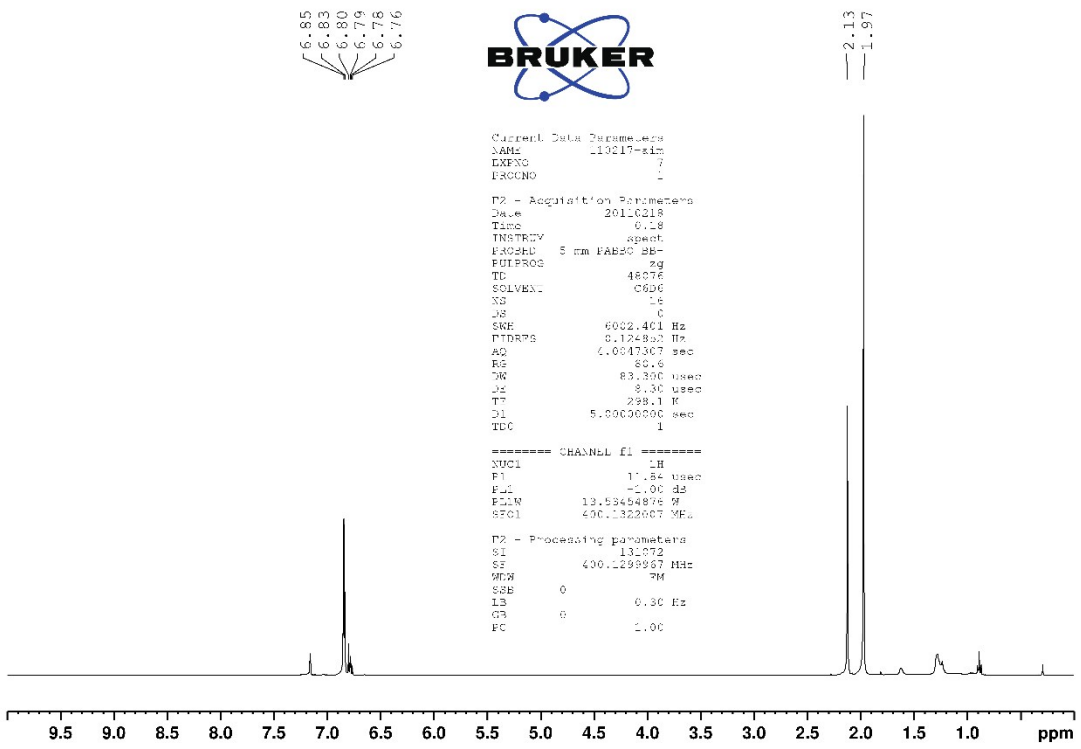

Figure S7. ^{1}H NMR spectrum of complex **7** (C_6D_6).

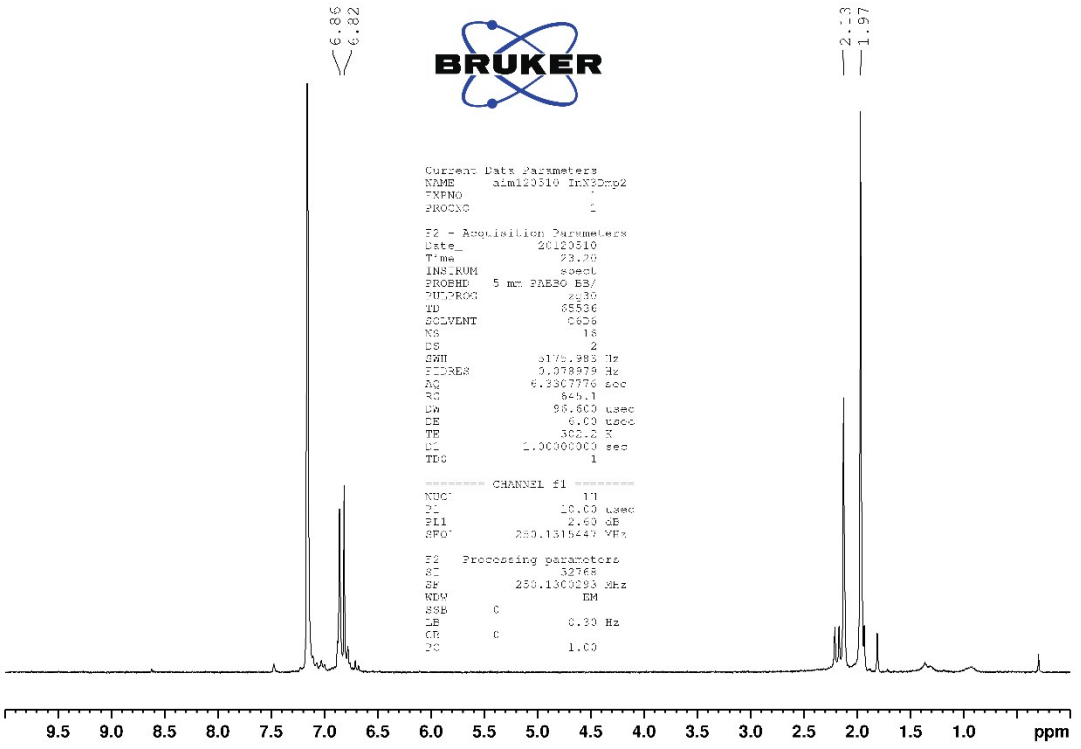

Figure S8. ^{1}H NMR spectrum of complex **8** (C_6D_6).

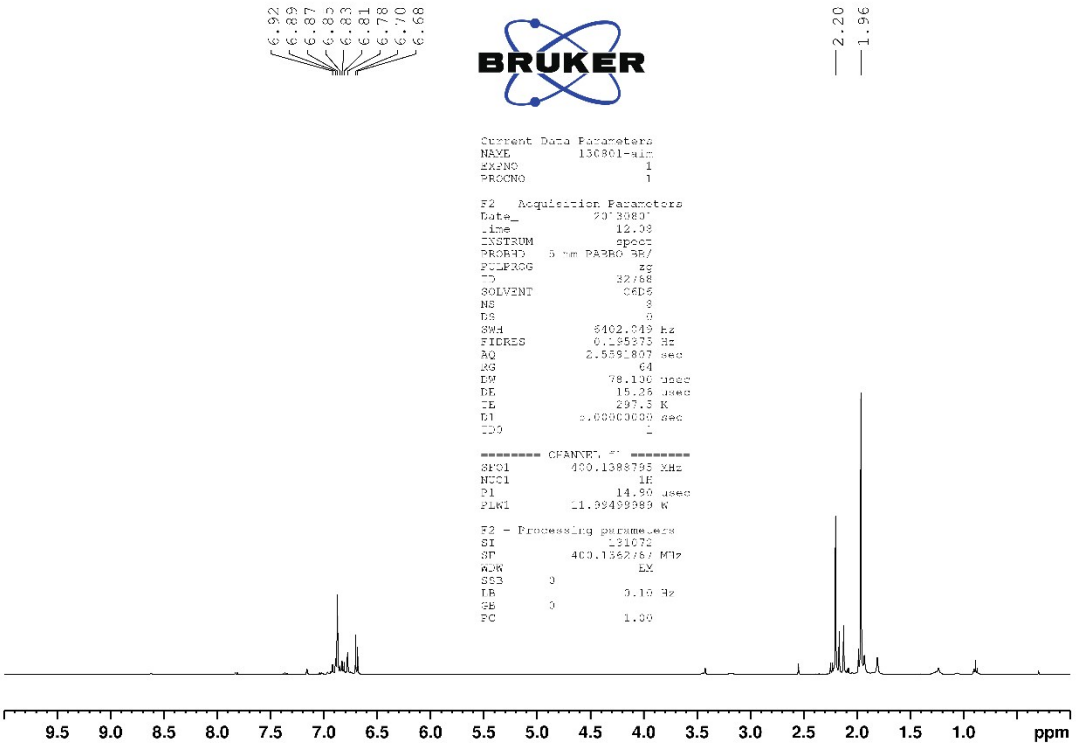

Figure S10. ^{1}H NMR spectrum of complex **10** (C_6D_6).

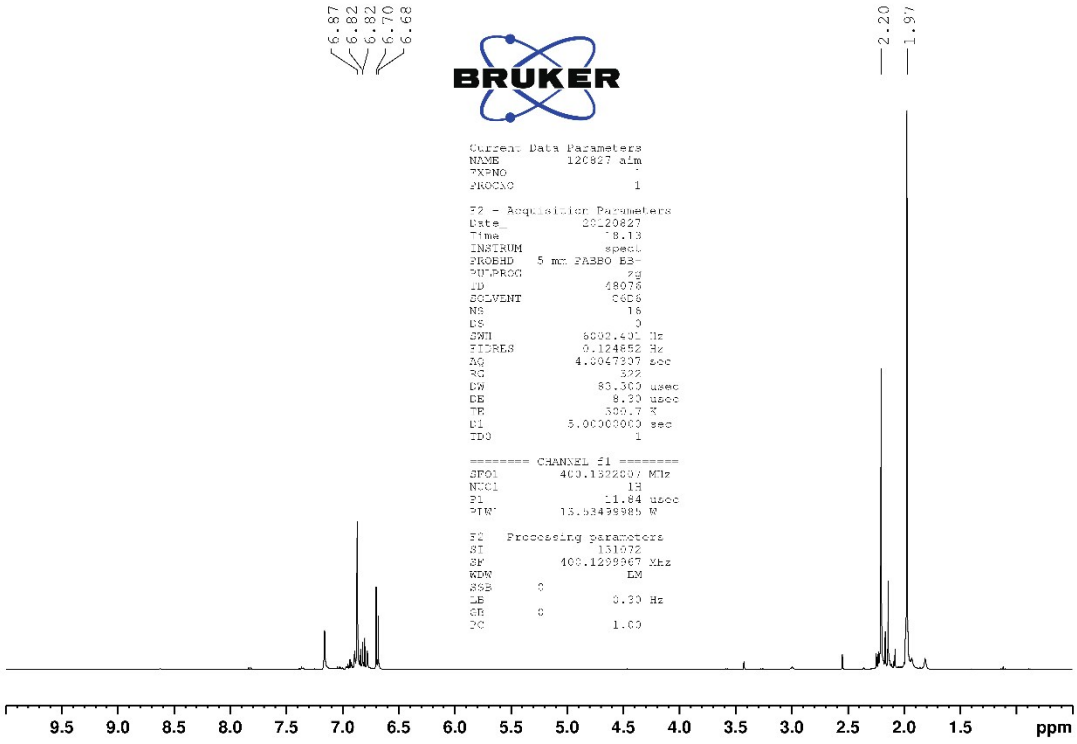

Figure S11. ^{1}H NMR spectrum of complex **11** (C_6D_6).

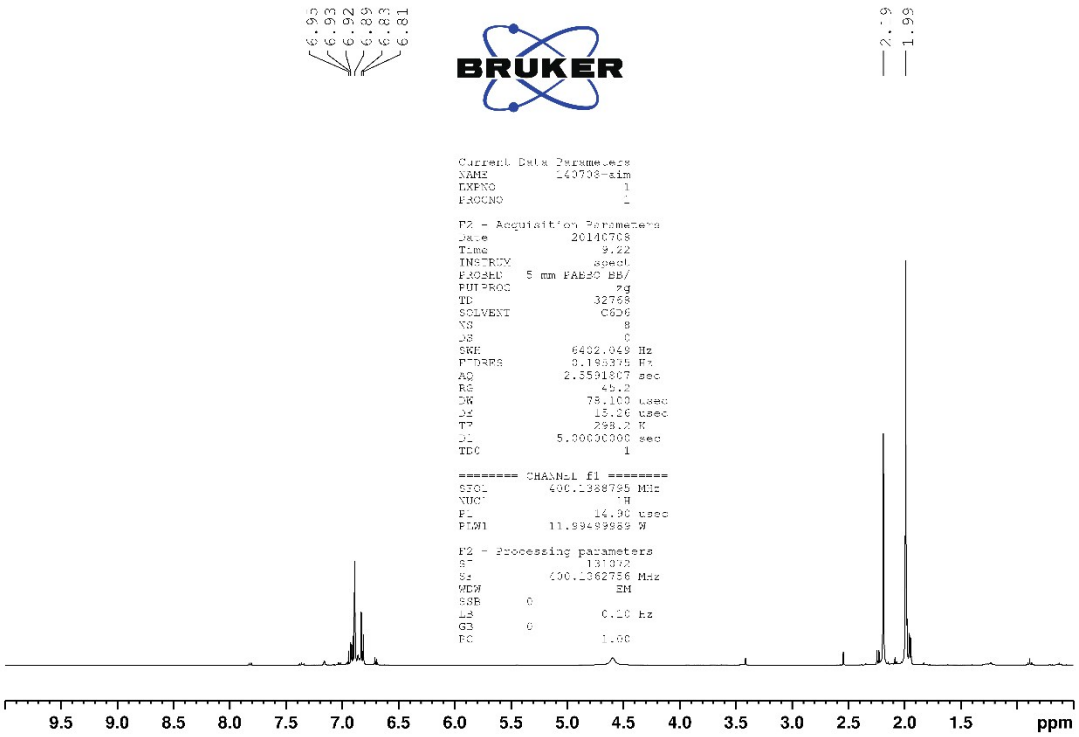

Figure S12. ^{1}H NMR spectrum of complex **12** (C_6D_6).

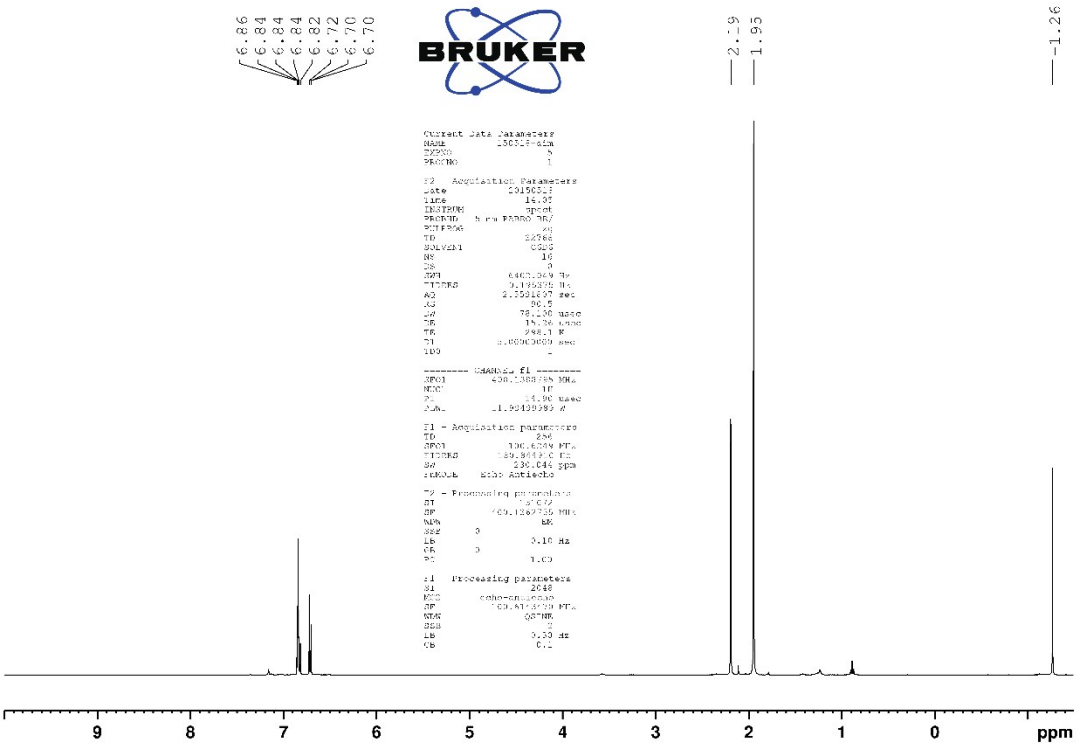

Figure S13. ^{1}H NMR spectrum of complex **13** (C_6D_6).

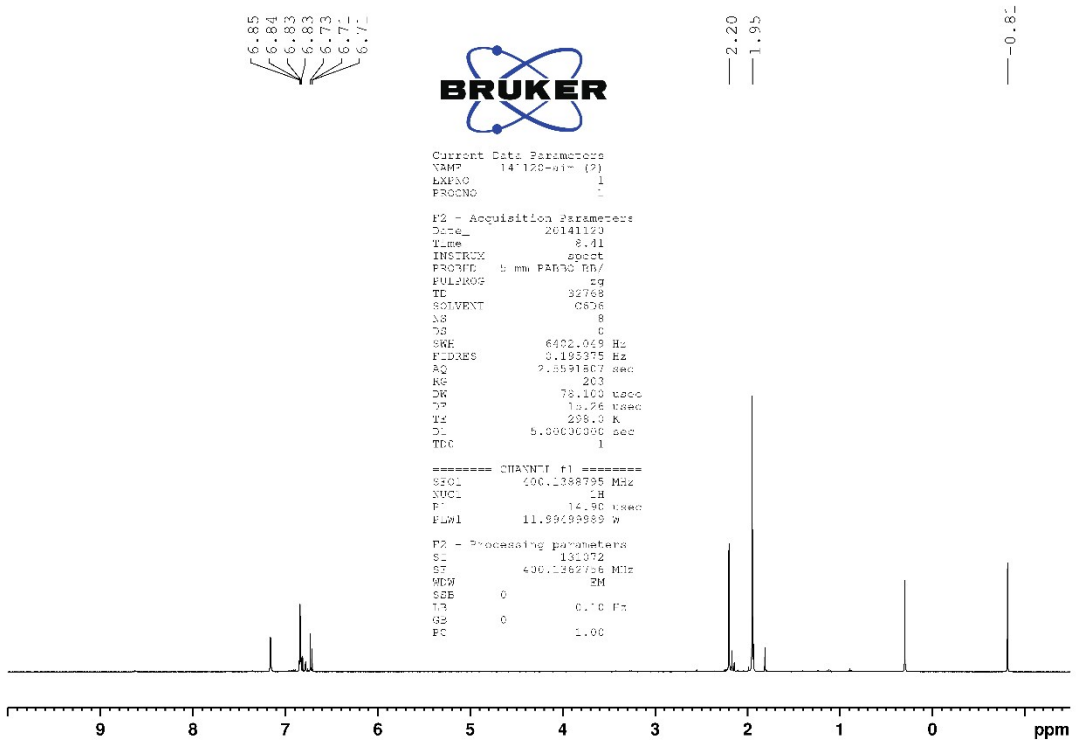

Figure S14. ^{1}H NMR spectrum of complex **14** (C_6D_6).

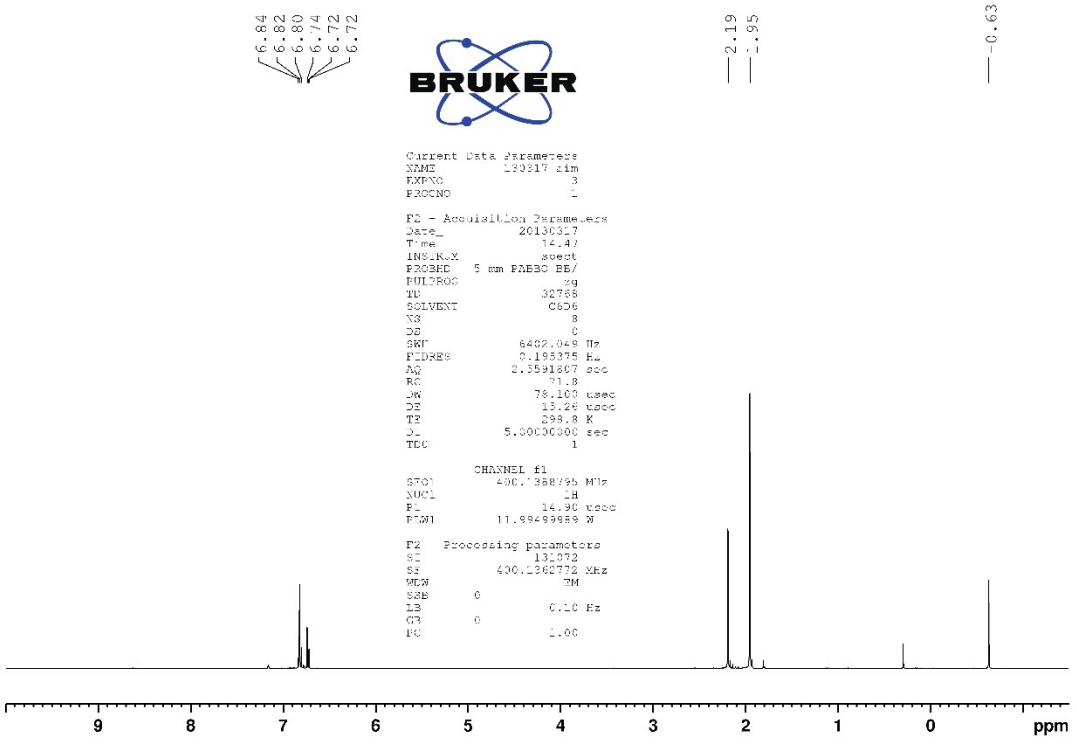

Figure S15. ^{1}H NMR spectrum of complex **15** (C_6D_6).

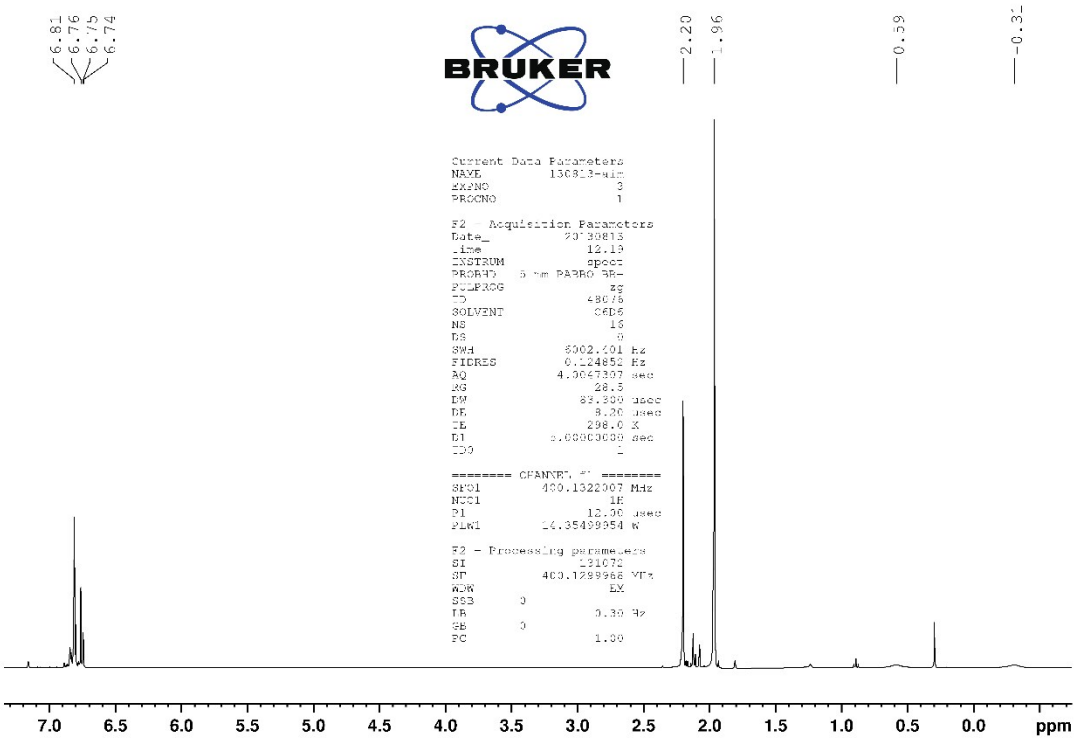

Figure S16. ^{1}H NMR spectrum of complex **16** (C_6D_6).

X-ray Crystallography

General details

Crystalline samples were mounted on MiTeGen micromounts in type NVH immersion oil. Data for **8** was collected on an Oxford Xcalibur^{TM}2 diffractometer with an Enhance (Mo) X-ray Source (λ = 0.71073 Å) and Sapphire2 CCD at 173(2) K. Data for all other complexes were collected on a Bruker Kappa Apex II diffractometer with a Bruker Quazar Multilayer Optics $Mo_{K\alpha}$ X-ray micro source (λ = 0.71073 Å) and a Bruker APEX-II CCD at 150(2) K. Corrections for absorption was carried out using CrysAlisPro[9] or SADABS.[10] The structures were solved with SHELXT[11] and refined with SHELXL[12] using the interface OLEX2.[13] Hydrogen atoms were refined in calculated positions (riding model) for all compounds excepting hydrides in **5** and **6** which were located in the difference map and refined isotropically. Solvent molecules were modelled with the aid of the FragmentDB module in OLEX2.[14,15] A summary of crystallographic data can be found in the tables below.

Variata

The Ge-Cl moiety in **1**, the Ge-H moiety in **3**, the Sn-H moiety in **4**, the Tl atoms in **7** and **7a** were found to be disordered. Each was treated using a split site mode. The hydrides in **3** and **4** were placed in idealized positions.

One of the chloride ligands in **12** was found to be disordered. The other component being a methyl group. Restraints were applied to bond lengths and displacement parameters.

Crystals of **9** were generally of poor quality. The weakness of the data at θ angles greater than 23.256° prompted their exclusion from the structural refinement process. Despite the relatively poor quality of the data, the gross molecular connectivity is unambiguous.

The In atom in **8** and the Ga atom **9** were found to have partial occupancies (75 and 40% respectively). We attribute this to co-crystallization with decomposition product Dmp_2N_3H. Additional partial occupancy hydrogen atoms were added to the molecular formulae.

Data for **11** and **13** contained reflections which were affected by the beamstop, these reflections were omitted from the final refinement.

Table S1: Summary of crystallographic data for compounds

	1·0.5(OC_4H_{10})	**2**·0.5(OC_4H_{10})	**3**·0.5(C_7H_8)	**4**·0.5(OC_4H_{10})	**5**	**6**·0.5(C_7H_8)	**7**·0.5(C_7H_8)	**7**·0.5(C_6H_{14})
empirical formula	$C_{50}H_{55}ClGeO_{0.5}N_3$	$C_{50}H_{55}ClSnO_{0.5}N_3$	$C_{51.5}H_{55}GeN_3$	$C_{50}H_{56}SnO_{0.5}N_3$	$C_{48}H_{52}AlN_3$	$C_{51.5}H_{56}GaN_3$	$C_{51.5}H_{54}TlN_3$	$C_{51}H_{57}TlN_3$
formula weight	814.01	860.11	788.57	825.66	697.90	786.71	919.34	916.36
crystal system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
space group	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P-1
***a* (Å)**	10.637(14)	10.471(3)	10.4270(12)	10.4915(13)	10.440(2)	10.4624(5)	10.558(2)	10.5807(4)
***b* (Å)**	11.483(15)	11.287(3)	11.3856(13)	11.3426(13)	12.331(3)	11.3645(5)	11.470(2)	11.4067(4)
***c* (Å)**	20.41(3)	20.411(6)	20.013(2)	20.245(2)	15.978(3)	20.0930(8)	20.162(7)	20.4425(8)
***α* (deg)**	102.80(4)	94.146(8)	104.001(3)	103.106(3)	89.95(2)	103.836(2)	102.694(7)	98.589(2)
***β* (deg)**	94.73(3)	102.449(9)	93.794(3)	95.487(3)	82.91(2)	94.296(2)	95.730(7)	100.822(2)
***γ* (deg)**	111.41(4)	108.763(8)	110.694(3)	111.383(4)	85.68(2)	110.472(2)	110.677(8)	111.879(2)
***V* (Å^3)**	2226(5)	2204.1(11)	2126.2(4)	2142.3(4)	2035.5(7)	2139.96(17)	2185.9(7)	2182.73(15)
Z	2	2	2	2	2	2	2	2
***ρ*(calcd) (g cm^{-3})**	1.214	1.296	1.232	1.280	1.139	1.221	1.397	1.394
***μ* (mm^{-1})**	0.785	0.678	0.759	0.634	0.086	0.681	3.732	3.737
***F*(000)**	858	894	834	862	748	834	930	930
reflections collected	26484	28929	36335	39235	18050	30979	30536	33432
unique reflections	8105	8392	7829	9102	8589	9324	9447	9662
R_{int}	0.1126	0.0696	0.0710	0.0791	0.0500	0.0415	0.0409	0.0502
R_1 [$I > 2\sigma(I)$]	0.0892	0.0451	0.0580	0.0494	0.0527	0.0415	0.0351	0.0378
wR_2 (all data)	0.2772	0.1153	0.1665	0.1140	0.1451	0.1019	0.1022	0.0836
GooF	1.039	1.043	1.011	1.007	1.014	1.050	1.024	0.993
largest peak and hole (e Å^{-3})	0.56 / -0.94	0.72 / -0.88	0.44 / -0.83	0.42 / -0.71	0.28 / -0.33	0.54 / -0.39	0.54 / -0.85	0.98 / -0.64
CCDC no.	1896479	1896480	1896487	1896488	1896489	1896490	1896491	1896492

	8·0.5(C_7H_8)	**9**·0.5(C_7H_8)	**11**·0.5(OC_4H_{10})	**12**·0.5(C_5H_{12})	**13**·0.5(C_5H_{12})	**14**·0.5(C_6H_{14})	**15**	**16**
empirical formula	$C_{51.5}H_{54.25}In_{0.75}N_3$	$C_{51.5}H_{54.6}Ga_{0.4}N_3$	$C_{50}H_{55}Br_2InO_{0.5}N_3$	$C_{51.5}H_{58.5}Cl_{1.5}AlN_3$	$C_{52.5}H_{62}AlN_3$	$C_{53}H_{63}GaN_3$	$C_{50}H_{56}InN_3$	$C_{50}H_{56}TlN_3$
formula weight	801.34	743.47	980.61	799.66	762.03	811.78	813.79	903.34
crystal system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	monoclinic	monoclinic
space group	P-1	P-1	P-1	P-1	P-1	P-1	$P2_1/n$	$P2_1/n$
***a* (Å)**	10.4601(5)	10.454(5)	11.0858(9)	10.7290(7)	10.7943(5)	10.8007(6)	10.5238(4)	10.5327(8)
***b* (Å)**	11.3940(6)	11.495(6)	11.1952(9)	11.7522(8)	11.7863(6)	11.8461(7)	15.7425(5)	15.7020(12)
***c* (Å)**	19.9439(9)	19.835(11)	19.8902(13)	19.8810(14)	19.6677(9)	19.6602(11)	51.9642(19)	51.888(4)
***α* (deg)**	103.975(4)	103.568(13)	80.214(2)	100.490(3)	98.246(2)	97.282(3)	90	90
***β* (deg)**	95.003(4)	93.883(16)	78.334(3)	95.000(3)	96.521(2)	96.972(3)	93.140(2)	93.222(3)
***γ* (deg)**	110.046(5)	110.470(18)	70.584(2)	111.394(2)	111.357(2)	111.686(2)	90	90
***V* (Å^3)**	2128.86(19)	2141.3(19)	2265.9(3)	2262.5(3)	2268.68(19)	2279.6(2)	8596.0(5)	8567.9(11)
Z	2	2	2	2	2	2	8	8
***ρ*(calcd) (g cm^{-3})**	1.250	1.153	1.437	1.174	1.116	1.183	1.258	1.401
***μ* (mm^{-1})**	0.461	0.311	2.323	0.171	0.082	0.641	0.586	3.807
***F*(000)**	842	794	998	854	822	866	3408	3664
reflections collected	18249	12802	31109	30651	45171	35298	69213	59758
unique reflections	8694	5836	9931	8178	9887	9992	18839	18928
R_{int}	0.0632	0.1366	0.0429	0.0505	0.0431	0.0396	0.0785	0.0918
R_1 [$I > 2\sigma(I)$]	0.0661	0.1043	0.0371	0.0605	0.0520	0.0432	0.0475	0.0551
wR_2 (all data)	0.1420	0.3469	0.0863	0.1789	0.1540	0.1199	0.1038	0.1227
GooF	1.078	0.984	1.009	1.069	1.016	1.043	1.022	1.023
largest peak and hole (e Å^{-3})	1.42 / -1.07	1.19 / -0.36	0.71 / -0.64	0.40 / -0.52	0.69 / -0.35	0.48 / -0.61	0.47 / -0.53	2.11 / -1.22
CCDC no.	1896493	-	1896481	1896482	1896483	1896484	1896485	1896486

Molecular Structures

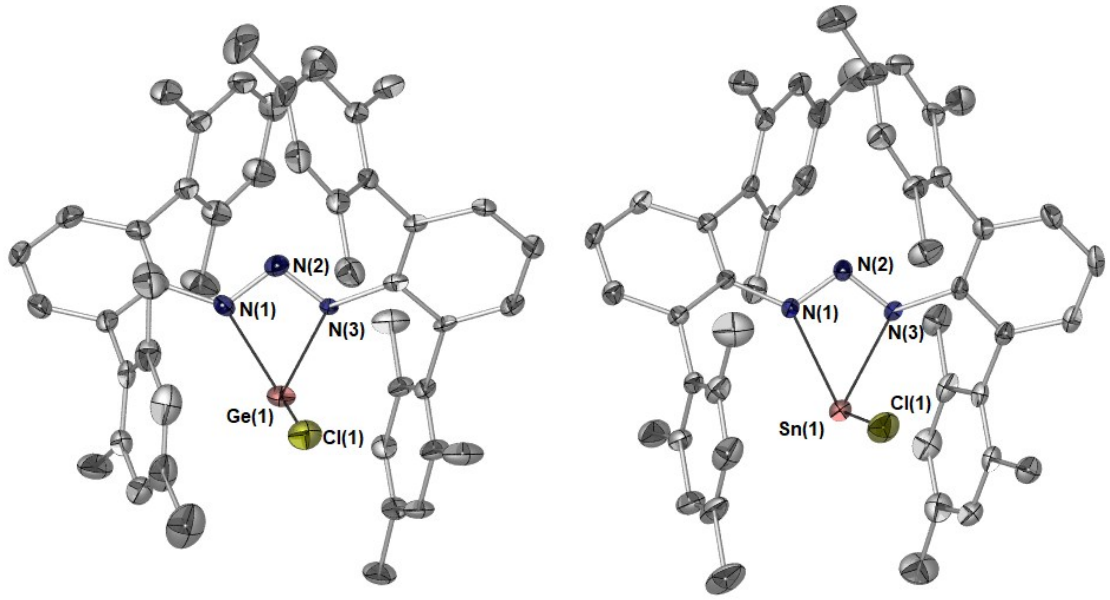

Figure S17. Molecular structures (50% displacement ellipsoids) of **1** (left) and **2** (right). All hydrogen atoms and lowest occupancy disorder components omitted for clarity.

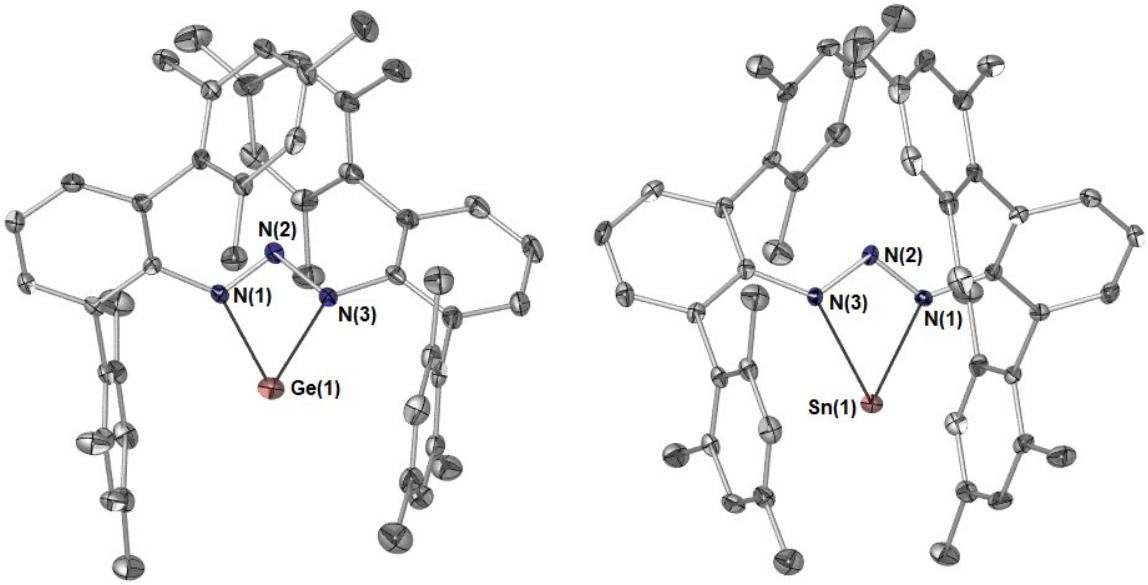

Figure S18. Molecular structures (50% displacement ellipsoids) of **3** (left) and **4** (right). All hydrogen atoms and lowest occupancy disorder components omitted for clarity.

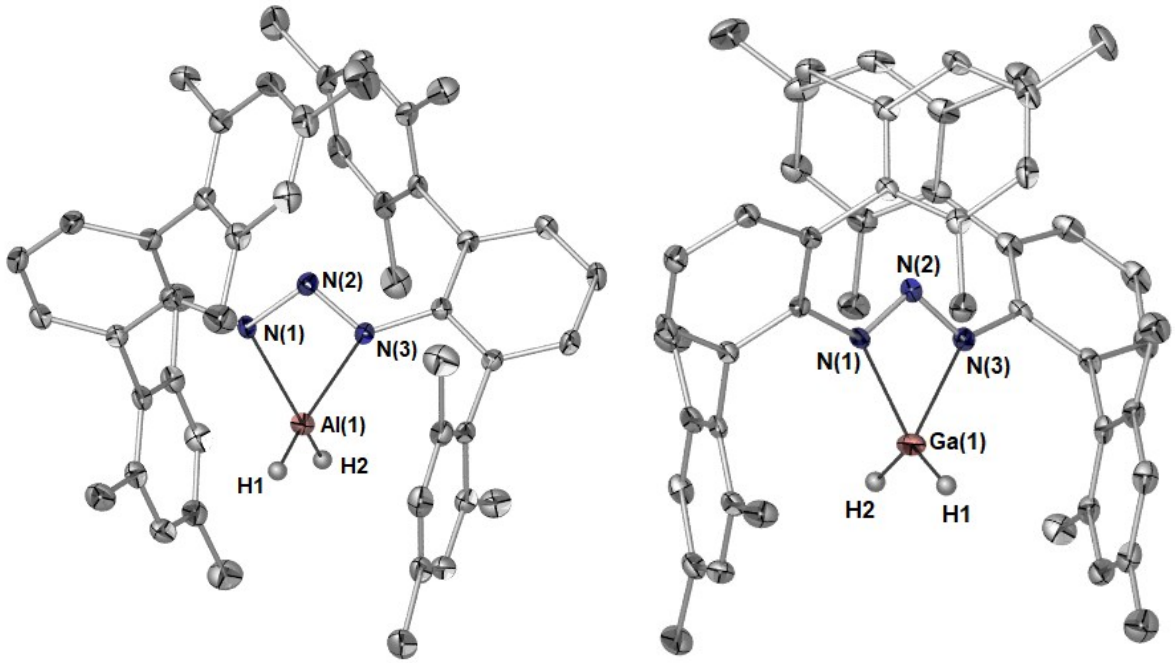

Figure S19. Molecular structures (50% displacement ellipsoids) of **5** (left) and **6** (right). All non-hydride hydrogen atoms omitted for clarity.

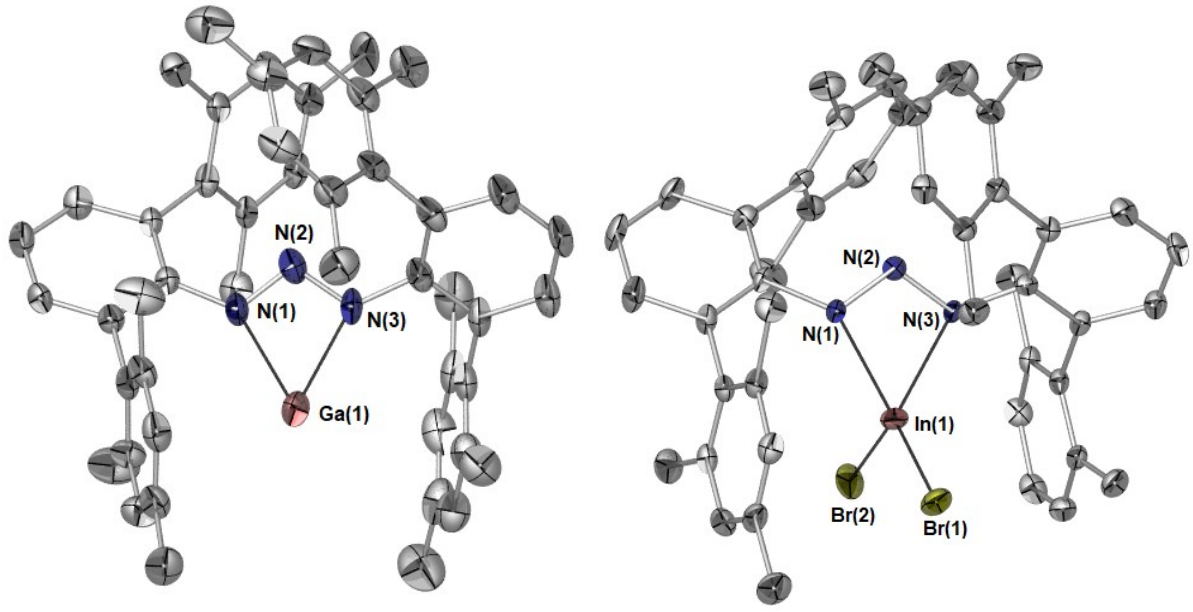

Figure S20. Molecular structures (50% displacement ellipsoids) of **9** (left) and **11** (right). All hydrogen atoms omitted for clarity.

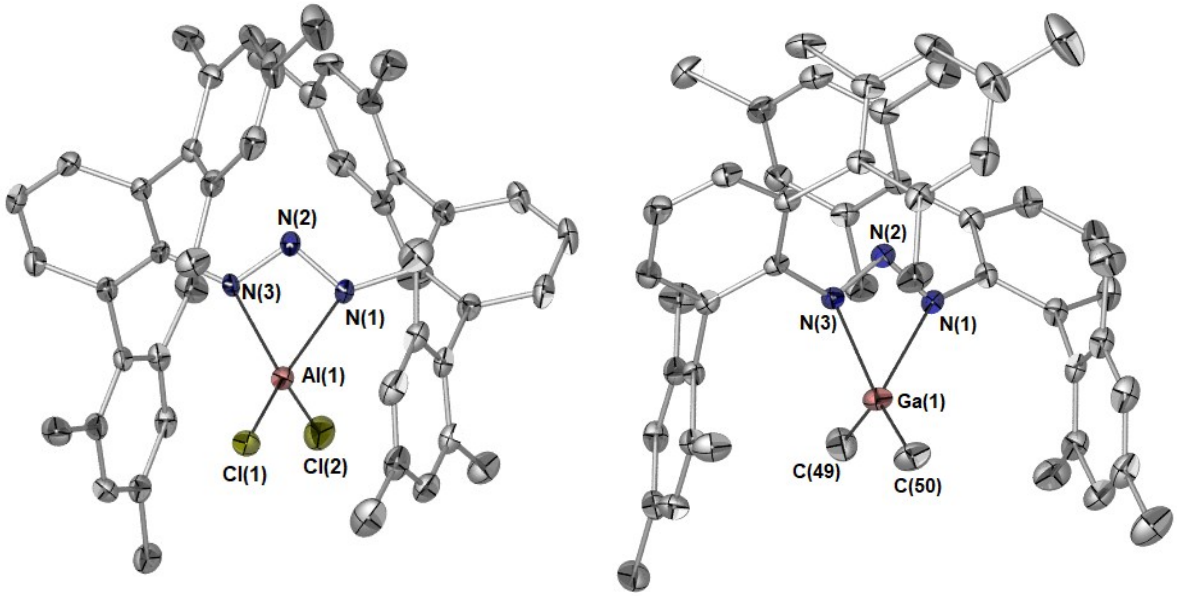

Figure S21. Molecular structures (50% displacement ellipsoids) of **12** (left) and **14** (right). All hydrogen atoms and lowest order disorder components omitted for clarity.

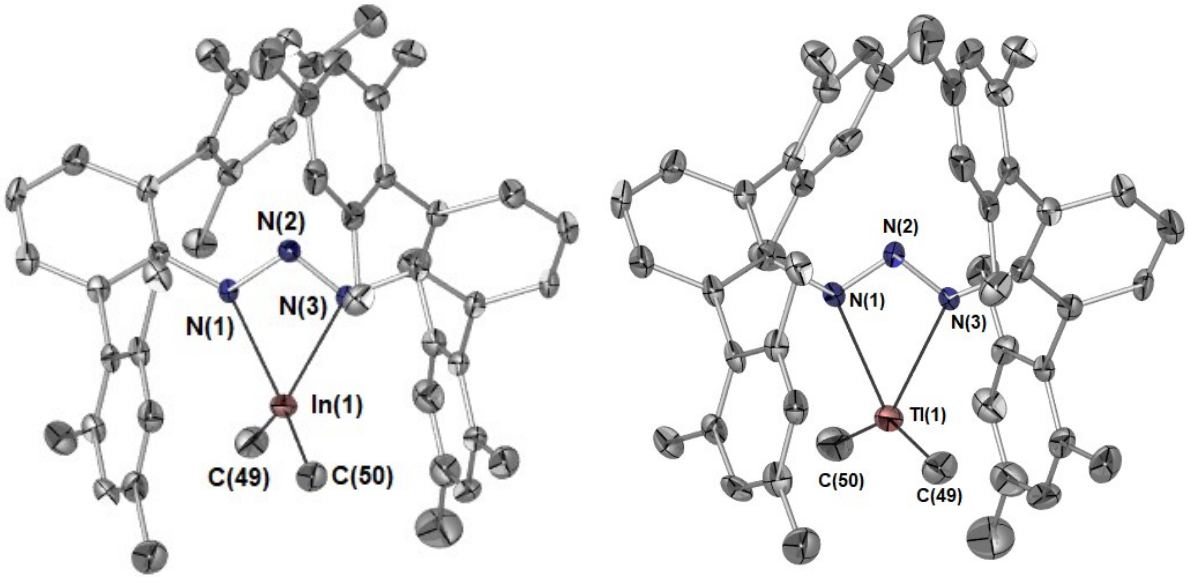

Figure S22. Molecular structures (50% displacement ellipsoids) of **15** (left) and **16** (right). All hydrogen atoms omitted for clarity. Only one molecule for each of the asymmetric units depicted.

Computational Studies

General details

Computations using density functional theory were carried out at the pbe0[16]/def2-tzvp (E and N atoms) + def2-svp[17] (C and H atoms) level of theory using Gaussian16.[18] Basis sets were obtained from the Basis Set Exchange.[19,20] All computations were carried out on the full molecules :EL (E = Ga, In, Tl; L = N_3Dmp_2, ^{Dipp}nacnac, CGiso) and [(Dmp_2N_3)EH] (E = Ge, Sn) with their solid-state structures as starting points. The molecules were optimized in their singlet states. That a local minimum had been obtained was tested using normal mode analysis. Atomic charge and orbital population analyses were carried out using NBO6.[21] Molecular orbitals were analysed using the ChemCraft software package.[22] Results are summarised in Table 2 in the main text and below. All energies are in kJ mol^{-1}.

Table S2: Selected data for the DFT optimized complexes [E(^{Dipp}nacnac)] and [E(CGiso)].

	[Ga(^{Dipp}nacnac)]	[Ga(CGiso)]	[In(^{Dipp}nacnac)]	[In(CGiso)]	[Tl(^{Dipp}nacnac)]
E-N (Å)	2.082	2.115	2.309	2.331	2.415
N-C (Å)	1.327	1.343	1.324	1.342	1.321
C-X (Å)[a]	1.403	1.371	1.407	1.380	1.408
$\Delta E_{HOMO-LUMO}$/kJ mol^{-1}	433	452	460	437	431
$\Delta E_{E(s)-E(p)}$/kJ mol^{-1}	469	452	476	437	508
	HOMO – LUMO+1	HOMO – LUMO	HOMO-1 – LUMO	HOMO – LUMO	HOMO-2 – LUMO
LP hybridization on M	95% s, 7% p	94% s, 6% p	97% s, 3% p	97% s, 3% p	99% s, 1% p
Charge, E	0.719	0.739	0.838	0.833	0.831
Charges, N1/N2	-0.743	-0.816	-0.764	-0.820	-0.727
Charges, C1[a]	0.316	0.663	0.307	0.641	0.301
Charge, X[b]	-0.419	-0.440	-0.426	-0.449	-0.430

[a] For L = ^{Dipp}nacnac, C1 = DippN-*C*(Me)-C; for L = CGiso, C1 = N_3C. [b] For L = ^{Dipp}nacnac, X = C; for L = CGiso, X = N.

Atomic coordinates for optimized geometries

[Ga(^{Dipp}nacnac)]

Ga	-0.94495	9.3748	10.13355
N	0.03723	10.82788	9.01151
C	0.14404	12.13268	9.22609
N	-1.45566	10.91463	11.43888
C	-0.42801	12.78355	10.32974
H	-0.26857	13.85925	10.38936
C	-1.17513	12.2094	11.36953
C	0.91724	12.97253	8.2455
H	1.95434	12.61358	8.16565
H	0.92731	14.02963	8.53812
H	0.48446	12.8843	7.23771
C	-1.67458	13.12348	12.4557
H	-1.28748	12.80442	13.43507
H	-2.77128	13.07176	12.52848
H	-1.37752	14.16413	12.27681
C	0.6588	10.25041	7.86733
C	1.96771	9.73512	7.97738
C	2.52119	9.0837	6.87114
H	3.53155	8.67237	6.94163
C	1.80727	8.94445	5.68589
H	2.25525	8.42872	4.83303
C	0.51983	9.46174	5.59127
H	-0.03839	9.34663	4.65851
C	-0.0765	10.1213	6.67
C	-1.49376	10.65296	6.54918
H	-1.68873	11.27581	7.43567
C	-2.50849	9.5077	6.56684
H	-2.4055	8.89697	7.4777
H	-2.36435	8.83957	5.70249
H	-3.53932	9.89514	6.52923
C	-1.68134	11.54038	5.31872
H	-0.95148	12.36445	5.29819
H	-2.69082	11.98045	5.3116
H	-1.56627	10.97186	4.38237
C	2.75938	9.85011	9.26811
H	2.20642	10.5298	9.93452
C	2.85007	8.49578	9.97448
H	1.849	8.08222	10.1745
H	3.38029	8.58865	10.93592
H	3.39327	7.76319	9.35599
C	4.1461	10.45504	9.04923
H	4.08731	11.42958	8.54032
H	4.78665	9.79973	8.4381
H	4.65733	10.60552	10.01297
C	-2.21294	10.41759	12.53814
C	-1.53946	9.9429	13.68358
C	-2.29589	9.36962	14.71
H	-1.78946	8.99066	15.60155
C	-3.67946	9.26727	14.614
H	-4.25346	8.81264	15.42509
C	-4.32934	9.74314	13.48031
H	-5.41666	9.65689	13.40814
C	-3.61651	10.32464	12.42768
C	-4.34793	10.81135	11.18913
H	-3.62595	11.37839	10.58163
C	-5.50141	11.75619	11.5259
H	-5.16356	12.60592	12.13911
H	-6.30188	11.24321	12.08202
H	-5.9504	12.15944	10.60473
C	-4.82713	9.63124	10.34096
H	-5.31353	9.983	9.41693
H	-5.55435	9.01638	10.89538
H	-3.98795	8.97631	10.05797
C	-0.02736	10.01728	13.80217
H	0.33801	10.64341	12.97372
C	0.60079	8.63194	13.63539
H	0.31344	8.17655	12.67454
H	0.27193	7.95015	14.4362
H	1.70047	8.6921	13.67024
C	0.42362	10.67706	15.10524
H	1.51851	10.79462	15.11876
H	0.14858	10.0748	15.9855
H	-0.02646	11.67387	15.23159

[In(DippnacnacNacnac)]

In	-0.72025	1.12967	10.42759
N	0.14103	2.83803	9.13477
N	-1.4143	2.94202	11.67898
C	0.19734	4.13927	9.37263
C	-0.35184	4.7687	10.50429
H	-0.20083	5.84644	10.55257
C	-1.12946	4.22792	11.54412
C	0.87464	5.03097	8.36238
H	1.90833	4.70015	8.18371
H	0.88621	6.07833	8.68779
H	0.36095	4.96729	7.3912
C	-1.68563	5.20184	12.55236
H	-2.78585	5.1815	12.53668
H	-1.3487	6.22699	12.35598
H	-1.38903	4.91649	13.57238
C	0.65108	2.32032	7.91458
C	-0.21798	2.17632	6.80953
C	0.27067	1.57297	5.64707
H	-0.3931	1.45259	4.78654
C	1.58282	1.11921	5.56688
H	1.94654	0.64788	4.65064
C	2.42821	1.26582	6.66133
H	3.45807	0.90438	6.59666
C	1.98598	1.86361	7.8452
C	-1.66325	2.63925	6.87214
H	-1.79718	3.1718	7.82628
C	-2.62219	1.44712	6.87519
H	-3.66697	1.78245	6.97402
H	-2.40661	0.75904	7.70802
H	-2.53959	0.8675	5.94175
C	-2.00688	3.61886	5.74965
H	-3.03522	3.99568	5.86616
H	-1.94122	3.14238	4.75858
H	-1.32723	4.48466	5.74673
C	2.92879	1.98864	9.02867
H	2.41682	2.59446	9.79224
C	4.22672	2.71011	8.66418
H	4.85074	2.85925	9.55932
H	4.03086	3.69769	8.21922
H	4.82381	2.13342	7.94009
C	3.21761	0.61894	9.6469
H	3.86304	0.71591	10.53455
H	3.72926	-0.04044	8.92739
H	2.28916	0.1117	9.9535
C	-2.28815	2.51654	12.71451
C	-3.67257	2.41374	12.44977
C	-4.50814	1.89633	13.4438
H	-5.58049	1.80786	13.24937
C	-4.00021	1.48802	14.67243
H	-4.6684	1.08369	15.43661
C	-2.63616	1.59457	14.92122
H	-2.23924	1.26941	15.88673
C	-1.76058	2.10635	13.9589
C	-4.25601	2.82846	11.11012
H	-3.44867	3.30468	10.53285
C	-4.72809	1.60912	10.31566
H	-5.10296	1.90669	9.32333
H	-5.54107	1.08247	10.84086
H	-3.91167	0.88474	10.1664
C	-5.37852	3.85569	11.25957
H	-5.72643	4.1951	10.27123
H	-5.04443	4.74015	11.8232
H	-6.24871	3.4349	11.78798
C	-0.27406	2.19044	14.2558
H	0.19657	2.72935	13.41897
C	0.01911	2.97875	15.5328
H	1.10505	3.09385	15.67568
H	-0.37753	2.46983	16.42561
H	-0.42691	3.98455	15.50005
C	0.35378	0.79621	14.3155
H	1.44068	0.86096	14.48385
H	0.18555	0.23852	13.38063
H	-0.08018	0.20105	15.13509

[Tl(Dippnacnac)]

Tl	-2.64032	1.43381	11.18302
N	-4.60824	0.87528	9.90013
N	-2.22962	2.55623	9.08422
C	-5.01668	1.30139	8.7183
C	-4.29869	2.18073	7.88494
H	-4.79974	2.4369	6.95198
C	-3.00639	2.72168	8.02869
C	-6.3413	0.80323	8.19196
H	-6.32032	-0.29158	8.08053
H	-6.59033	1.25138	7.22228
H	-7.14955	1.0227	8.90528
C	-2.47998	3.53023	6.86728
H	-2.17462	4.5335	7.19961
H	-3.22479	3.63065	6.06834
H	-1.57713	3.05752	6.4515
C	-5.36064	-0.08099	10.62028
C	-6.31613	0.34115	11.57271
C	-6.96348	-0.62458	12.34878
H	-7.70189	-0.30804	13.09065
C	-6.68479	-1.97891	12.19737
H	-7.20081	-2.71905	12.81366
C	-5.74204	-2.38395	11.25817
H	-5.52092	-3.44883	11.14361
C	-5.06815	-1.45538	10.4599
C	-6.62402	1.81329	11.77852
H	-6.09879	2.36898	10.98651
C	-6.08196	2.30542	13.12228
H	-6.26033	3.38531	13.2485
H	-4.99867	2.12677	13.21152
H	-6.5679	1.78237	13.96164
C	-8.11586	2.12034	11.64569
H	-8.29641	3.20445	11.7176
H	-8.70414	1.63559	12.44101
H	-8.51542	1.7734	10.68057
C	-4.02532	-1.92679	9.46155
H	-3.7029	-1.04597	8.8854
C	-4.59071	-2.94324	8.46931
H	-3.83543	-3.2083	7.71267
H	-5.47187	-2.54543	7.94336
H	-4.89649	-3.87543	8.97058
C	-2.79175	-2.48406	10.17464
H	-2.01472	-2.7749	9.44978
H	-3.04513	-3.37331	10.77396
H	-2.35199	-1.74344	10.86133
C	-0.90992	3.06372	9.09403
C	-0.64826	4.34549	9.62969
C	0.67853	4.77392	9.72992
H	0.89172	5.76233	10.14634
C	1.73191	3.96683	9.31296
H	2.7626	4.31907	9.3996
C	1.4639	2.7068	8.78818
H	2.29353	2.07172	8.46514
C	0.15392	2.23412	8.66959
C	-1.77466	5.2396	10.11566
H	-2.72076	4.75643	9.82698
C	-1.76473	5.35559	11.6415
H	-2.61265	5.96267	11.99704
H	-0.83633	5.83078	11.99721
H	-1.82876	4.36681	12.12281
C	-1.74442	6.62149	9.46224
H	-2.61902	7.21552	9.77092
H	-1.75413	6.54934	8.36398
H	-0.8443	7.18824	9.74885
C	-0.10481	0.84292	8.11833
H	-1.19541	0.72537	8.02638
C	0.39138	-0.23389	9.0853
H	0.15324	-1.24178	8.70949
H	-0.0692	-0.1274	10.08029
H	1.48286	-0.17362	9.2238
C	0.49722	0.6495	6.72637
H	0.2285	-0.33893	6.32139
H	1.5971	0.70981	6.74601
H	0.13599	1.41384	6.02164

[Ga(CGiso)]

Ga	4.13281	1.89877	5.16429
N	2.24957	1.02709	5.57384
C	1.6542	1.62662	4.52956
N	2.53819	2.38796	3.86375
C	1.67611	0.63157	6.791
N	0.33351	1.48225	4.19198
C	1.07991	1.57464	7.66263
C	0.60379	1.13336	8.90071
H	0.13827	1.84755	9.58323
C	0.71849	-0.19782	9.2879
H	0.34034	-0.52061	10.26085
C	1.32236	-1.11417	8.43286
H	1.41231	-2.15703	8.74421
C	1.80643	-0.72302	7.1825
C	1.02524	3.04791	7.29743
H	0.96277	3.12	6.20158
C	2.31477	3.75452	7.72198
H	2.31735	4.80619	7.39327
H	3.2069	3.26727	7.29524
H	2.42949	3.73303	8.81736
C	-0.1939	3.77592	7.85844
H	-1.12894	3.24452	7.62401
H	-0.26132	4.7891	7.43287
H	-0.13904	3.88975	8.95243
C	2.48414	-1.71402	6.25552
H	2.30212	-1.35932	5.22622
C	4.00007	-1.70315	6.46665
H	4.41948	-0.69412	6.33451
H	4.5033	-2.3749	5.75262
H	4.25194	-2.03585	7.48633
C	1.93462	-3.13343	6.36587
H	2.2034	-3.60557	7.32414
H	2.35209	-3.76696	5.56809
H	0.83744	-3.15448	6.27929
C	2.54541	2.72092	2.5015
C	2.56723	4.09208	2.14855
C	2.66707	4.44069	0.79978
H	2.67941	5.4947	0.51431
C	2.74334	3.46609	-0.19007
H	2.81602	3.75506	-1.24128
C	2.73293	2.12118	0.16533
H	2.8047	1.36364	-0.61799
C	2.64196	1.72258	1.50219
C	2.50646	5.15066	3.23307
H	1.93535	4.71308	4.0702
C	3.90757	5.45997	3.76596
H	4.41025	4.55201	4.13262
H	3.86364	6.18169	4.59752
H	4.53833	5.89009	2.97159
C	1.7986	6.4321	2.80209
H	2.38651	6.99814	2.06223
H	1.64956	7.09513	3.66827
H	0.8131	6.2247	2.35763
C	2.72174	0.25221	1.87433
H	2.162	0.11198	2.81086
C	4.1712	-0.15355	2.15148
H	4.78571	-0.05179	1.24292
H	4.23149	-1.19837	2.49614
H	4.63246	0.48222	2.92506
C	2.09356	-0.67902	0.84023
H	1.07348	-0.36272	0.57369
H	2.04026	-1.70539	1.2351
H	2.68388	-0.72212	-0.08846
C	-0.35348	0.24339	4.5842
H	0.4293	-0.34619	5.07602
C	-1.48164	0.37949	5.60866
H	-1.1626	1.02631	6.43756
H	-2.36372	0.84708	5.1432
C	-1.872	-1.00192	6.12964
H	-1.01218	-1.43078	6.67353
H	-2.68579	-0.90952	6.86656
C	-2.2856	-1.93117	4.99215
H	-2.51105	-2.93833	5.37938
H	-3.22273	-1.55545	4.54188
C	-1.21355	-2.00696	3.9085
H	-1.56069	-2.62663	3.06583
H	-0.31678	-2.50945	4.31305
C	-0.82361	-0.61802	3.40778
H	-1.69714	-0.15774	2.92005
H	-0.03136	-0.68594	2.64854
C	-0.32004	2.57358	3.45532
H	0.46293	3.3361	3.36688
C	-1.4595	3.25696	4.21785
H	-1.15854	3.44524	5.2584
H	-2.34464	2.60272	4.253
C	-1.83869	4.56125	3.51976
H	-2.66452	5.05096	4.06081
H	-0.98236	5.25763	3.5665
C	-2.2222	4.32479	2.06152
H	-3.16093	3.74182	2.02911
H	-2.4366	5.28346	1.56136
C	-1.13573	3.56146	1.30971
H	-0.22932	4.18543	1.21991
H	-1.46092	3.34342	0.27987
C	-0.76737	2.26382	2.02535
H	0.03365	1.74162	1.48427
H	-1.64703	1.60092	2.03715

[In(CGiso)]

In	4.44204	1.90427	5.20138
N	2.32771	0.99799	5.57514
C	1.74603	1.60518	4.52955
N	2.60691	2.37177	3.84291
C	1.74043	0.60754	6.78422
N	0.4146	1.45795	4.19865
C	1.14526	1.55115	7.65879
C	0.66501	1.11204	8.89599
H	0.2015	1.82919	9.577
C	0.7721	-0.21902	9.28553
H	0.38966	-0.53987	10.2574
C	1.37616	-1.13639	8.43195
H	1.46303	-2.17964	8.74359
C	1.86468	-0.74753	7.18281
C	1.09879	3.02657	7.3014
H	1.06221	3.10593	6.20507
C	-0.13071	3.75216	7.84357
H	-1.0604	3.21873	7.59402
H	-0.19412	4.76601	7.41882
H	-0.09371	3.86367	8.93856
C	2.37697	3.73031	7.76361
H	2.45835	3.71081	8.86205
H	2.39548	4.78131	7.43306
H	3.28003	3.23713	7.36862
C	2.54691	-1.7448	6.26559
H	2.4033	-1.3756	5.23566
C	4.05531	-1.77165	6.52355
H	4.50044	-0.76973	6.4247
H	4.56828	-2.44148	5.81454
H	4.26838	-2.12573	7.54493
C	1.96582	-3.15387	6.34664
H	2.19609	-3.63967	7.3081
H	2.39294	-3.7895	5.55553
H	0.87174	-3.15108	6.22814
C	2.58086	2.69528	2.48137
C	2.59417	4.06575	2.118
C	2.67221	4.41021	0.76694
H	2.677	5.4638	0.47884
C	2.73633	3.43381	-0.2218
H	2.79132	3.71922	-1.27501
C	2.73739	2.09072	0.14033
H	2.80136	1.3301	-0.64086
C	2.66769	1.69609	1.4796
C	2.55306	5.13265	3.19549
H	2.03089	4.68791	4.05994
C	1.79705	6.39364	2.78534
H	1.6697	7.06161	3.65132
H	0.79873	6.1588	2.38625
H	2.33809	6.96598	2.0152
C	3.96811	5.48397	3.66113
H	4.51497	4.59167	4.00246
H	3.94532	6.20621	4.4932
H	4.54872	5.92872	2.83706
C	2.76424	0.22616	1.84925
H	2.23785	0.08453	2.80452
C	4.22407	-0.1754	2.07328
H	4.80246	-0.08253	1.14034
H	4.30168	-1.21595	2.42743
H	4.71536	0.47133	2.81833
C	2.10814	-0.70764	0.83455
H	2.67302	-0.75205	-0.10978
H	1.08187	-0.39081	0.59462
H	2.06466	-1.73351	1.23207
C	-0.26567	0.21058	4.57376
H	0.52225	-0.3859	5.04886
C	-0.74511	-0.63328	3.38769
H	0.03944	-0.68607	2.62018
H	-1.62445	-0.16763	2.91595
C	-1.12788	-2.03191	3.86597
H	-1.47881	-2.63762	3.01462
H	-0.2273	-2.53928	4.25563
C	-2.19339	-1.97824	4.95726
H	-2.41382	-2.99251	5.32882
H	-3.1342	-1.59764	4.51889
C	-1.7754	-1.06674	6.10726
H	-2.58569	-0.98755	6.84967
H	-0.91287	-1.50304	6.64039
C	-1.38923	0.32354	5.60752
H	-1.06901	0.9569	6.44606
H	-2.27503	0.79602	5.15437
C	-0.255	2.55486	3.48601
H	0.52042	3.32556	3.40148
C	-0.718	2.26481	2.05589
H	0.07852	1.75532	1.49677
H	-1.59352	1.59655	2.06908
C	-1.10512	3.56895	1.36245
H	-0.20477	4.20088	1.26978
H	-1.44084	3.36224	0.33357
C	-2.18843	4.31389	2.13678
H	-2.41484	5.27841	1.65321
H	-3.12348	3.72493	2.10588
C	-1.7909	4.53053	3.59427
H	-2.61483	5.00514	4.15167
H	-0.93985	5.23313	3.64317
C	-1.39416	3.21854	4.26734
H	-2.27411	2.55725	4.2991
H	-1.08704	3.39264	5.30791

[Ga(N_3Dmp$_2$)]

Ga	4.76019	2.68253	7.04237
N	5.60865	3.80591	4.70561
N	6.28749	3.00552	5.45165
N	4.4595	3.98404	5.25821
C	7.99854	1.36853	5.47939
C	9.30519	0.95081	5.2327
H	9.59075	-0.07182	5.49311
C	9.84992	3.12781	4.3718
H	10.58377	3.83508	3.97625
C	10.23257	1.8234	4.66714
H	11.25725	1.49504	4.4789
C	7.89714	7.25922	5.22739
H	7.77126	7.93026	6.08251
C	7.60365	2.68127	5.13258
C	7.8747	7.78999	3.93738
C	7.01252	0.46105	6.12896
C	8.54665	3.5869	4.60099
C	8.2563	5.02832	4.36766
C	3.23612	4.77198	3.24635
C	8.08417	5.89392	5.46472
C	6.03196	-0.18995	5.35556
C	8.08913	5.37417	6.8737
H	8.20472	6.19105	7.5997
H	8.89674	4.64449	7.03567
H	7.14263	4.85602	7.10766
C	2.18815	5.56874	2.76805
H	1.98611	5.56463	1.69363
C	8.24803	5.54215	3.05661
C	8.41264	4.62881	1.87579
H	9.42367	4.19611	1.8274
H	8.23133	5.1644	0.93354
H	7.70579	3.78707	1.93176
C	8.05996	6.91207	2.86662
H	8.04833	7.30577	1.84556
C	2.64627	5.4857	5.51265
C	4.36524	1.73067	1.30325
H	4.18374	0.65158	1.30078
C	3.48403	4.75868	4.63568
C	5.08818	-0.9961	5.9986
H	4.32507	-1.49745	5.39504
C	1.61535	6.26812	4.99523
H	0.98567	6.83573	5.68546
C	2.86739	5.38032	6.98154
C	2.05533	4.52265	7.74816
C	5.20442	2.28135	0.33428
C	5.10095	-1.18909	7.3834
C	7.04312	0.28541	7.52582
C	5.39982	3.66454	0.34917
H	6.05239	4.11939	-0.40247
C	6.09269	-0.54682	8.12653
H	6.11741	-0.67794	9.21251
C	7.62403	9.2519	3.70167
H	8.20144	9.62885	2.84418
H	7.88572	9.85582	4.58277
H	6.55861	9.43612	3.48201
C	3.96268	3.90671	2.27685
C	4.7974	4.48701	1.3025
C	4.05128	-2.02584	8.05631
H	3.18442	-1.40656	8.34261
H	4.43449	-2.4946	8.97451
H	3.68042	-2.82153	7.39368
C	4.12373	5.94836	8.96711
H	4.9346	6.51108	9.44021
C	3.73938	2.51654	2.27589
C	1.38933	6.32287	3.62146
H	0.57792	6.93328	3.21867
C	2.8528	1.8708	3.30174
H	2.58392	0.8464	3.00846
H	1.92715	2.44475	3.4589
H	3.35871	1.81183	4.28133
C	3.90665	6.10623	7.59533
C	6.01094	-0.0207	3.86541
H	5.21436	-0.62157	3.40536
H	6.97203	-0.3198	3.41923
H	5.84972	1.02975	3.57871
C	3.32853	5.10542	9.74967
C	2.29403	4.40978	9.12194
H	1.66344	3.73941	9.71362
C	4.759	7.03633	6.78411
H	5.30928	6.49932	5.99641
H	5.49416	7.55692	7.41319
H	4.14385	7.79243	6.27214
C	5.0589	5.96597	1.3014
H	5.84437	6.22787	0.57888
H	5.38299	6.30605	2.2967
H	4.15804	6.54332	1.04272
C	0.97012	3.71367	7.09473
H	0.48475	3.0416	7.81589
H	1.37402	3.10174	6.27178
H	0.19713	4.3571	6.64744
C	5.90523	1.41423	-0.672
H	5.38064	0.45902	-0.82
H	6.93017	1.17782	-0.33898
H	5.98916	1.91391	-1.64875
C	8.05998	1.00907	8.36326
H	8.01197	2.09663	8.19078
H	9.08665	0.70355	8.10998
H	7.89901	0.82395	9.43431
C	3.60859	4.91952	11.21315
H	4.32577	4.09623	11.37055
H	4.04596	5.82417	11.66056
H	2.69513	4.66765	11.77147

[In(N_3Dmp$_2$)]

In	0.09068	2.49741	11.81104
N	-0.85274	1.27436	14.3273
N	-1.52629	2.09761	13.60356
N	0.29515	1.06706	13.7844
C	1.23548	0.26835	14.42921
C	-3.51508	-0.49121	15.97226
C	-2.27359	4.65403	12.95971
C	-3.50487	0.05758	14.6755
C	0.74115	1.12359	16.78748
C	-2.8368	2.41641	13.9487
C	-3.23812	3.73509	13.62574
C	-5.07926	1.96736	14.7307
H	-5.81122	1.25512	15.12083
C	0.99458	2.50881	16.79064
C	1.45739	0.24262	15.82447
C	-3.34429	-1.86806	16.12785
H	-3.34516	-2.28809	17.13847
C	0.73137	-0.87614	10.0537
H	-0.07943	-1.40718	9.54514
C	-3.7809	1.50699	14.4765
C	1.59725	-0.07188	9.30547
C	-3.17096	-2.1561	13.76039
H	-3.04985	-2.80657	12.88878
C	-0.10532	0.56144	17.76238
C	-0.42294	6.34781	11.66637
C	-1.2661	5.29516	13.70706
C	-5.46188	3.27798	14.4658
H	-6.48225	3.60709	14.67481
C	0.8792	-1.03838	11.43466
C	-3.34072	-0.78329	13.55765
C	-4.5389	4.15438	13.89973
H	-4.82423	5.18175	13.65793
C	2.08169	-0.47412	13.57085
C	-3.16116	-2.72022	15.0365
C	1.90464	3.13344	15.77262
H	2.82749	2.54849	15.64049
H	2.17799	4.15909	16.05736
H	1.41633	3.18023	14.78362
C	3.08058	-1.28473	14.10761
H	3.7128	-1.86294	13.42837
C	-3.68641	0.39009	17.17643
H	-2.99108	1.24212	17.14079
H	-3.4974	-0.16769	18.10415
H	-4.70294	0.80801	17.23908
C	-0.35326	6.12202	13.04498
H	0.42974	6.61554	13.62926
C	-2.362	4.86367	11.56943
C	-0.47333	2.77632	18.7257
C	0.38099	3.30852	17.75956
H	0.58521	4.38359	17.76209
C	3.27453	-1.35266	15.48533
H	4.06135	-1.98448	15.90352
C	1.91878	-0.35451	12.09526
C	-0.69467	1.39722	18.7126
H	-1.35752	0.95613	19.4635
C	-3.34247	-0.22856	12.16234
H	-4.16017	0.493	12.0139
H	-3.44114	-1.02815	11.41493
H	-2.403	0.31161	11.95187
C	0.59413	7.20742	10.9725
H	0.18012	7.67309	10.0663
H	1.46614	6.6067	10.66269
H	0.96551	8.00689	11.63033
C	2.8011	0.46435	11.36345
C	3.8952	1.22361	12.06129
H	3.49401	1.82397	12.89375
H	4.41728	1.8977	11.36796
H	4.63871	0.54467	12.50616
C	-1.44047	5.71589	10.94938
H	-1.51203	5.87408	9.86902
C	2.47598	-0.58027	16.32202
H	2.65625	-0.58188	17.40034
C	-0.39044	-0.91321	17.77088
H	-0.7015	-1.25755	16.77311
H	-1.19171	-1.15668	18.48235
H	0.49629	-1.50219	18.05137
C	2.63033	0.58235	9.97896
H	3.3174	1.22045	9.41496
C	-0.04447	-1.93197	12.20688
H	-0.77988	-2.41419	11.54823
H	-0.59475	-1.37395	12.97937
H	0.51687	-2.71863	12.73443
C	-1.16114	3.6591	19.72736
H	-0.61255	4.59945	19.88385
H	-1.26874	3.15919	20.70167
H	-2.17577	3.92427	19.38446
C	-3.41339	4.16118	10.75608
H	-3.38965	3.07332	10.93013
H	-3.27357	4.34337	9.68141
H	-4.42645	4.4917	11.03207
C	-1.18598	5.09489	15.19078
H	-2.12712	5.38952	15.68035
H	-0.36825	5.68183	15.6313
H	-1.02174	4.03752	15.44744
C	-2.92702	-4.19041	15.23494
H	-1.8601	-4.39454	15.42834
H	-3.21494	-4.77082	14.34612
H	-3.49251	-4.57841	16.09536
C	1.39382	0.11692	7.8297
H	0.95177	-0.77619	7.36413
H	2.34038	0.339	7.31574
H	0.70985	0.96034	7.6347

[Tl(N_3Dmp$_2$)]

Tl	4.519	2.54042	7.54604
N	5.54451	3.85506	4.81519
N	4.41452	4.10987	5.3717
N	6.20729	2.99948	5.50807
C	7.50432	2.67102	5.13695
C	8.19782	5.02255	4.40774
C	3.49785	4.92666	4.72345
C	8.45424	3.56788	4.5927
C	7.90323	1.34886	5.45785
C	3.27509	4.96229	3.32639
C	6.95267	0.44227	6.16024
C	8.21793	5.58647	3.11758
C	3.96532	4.06262	2.3619
C	2.65677	5.68168	5.57939
C	7.08106	0.24967	7.5501
C	9.74185	3.09163	4.31462
H	10.47574	3.79567	3.91328
C	8.04582	5.85436	5.53467
C	2.2755	5.8083	2.82923
H	2.09602	5.81481	1.75075
C	10.115	1.77661	4.57116
H	11.12704	1.43525	4.34235
C	2.79253	5.54254	7.05617
C	5.91673	-0.19975	5.45364
C	5.1284	2.37151	0.4235
C	9.19291	0.91344	5.15882
H	9.47195	-0.11596	5.40019
C	8.38238	4.71866	1.90248
H	9.40154	4.30968	1.8237
H	8.17979	5.28508	0.98287
H	7.69401	3.86119	1.93648
C	6.17222	-0.58784	8.21069
H	6.27505	-0.73212	9.29072
C	8.06485	6.96723	2.97723
H	8.07229	7.39835	1.97128
C	4.80281	4.60188	1.36654
C	5.36637	3.74755	0.41679
H	6.0232	4.17151	-0.34915
C	5.01957	-1.013	6.15331
H	4.21232	-1.50358	5.60019
C	3.69201	2.68065	2.37591
C	7.88956	7.80938	4.07727
C	1.87989	4.73272	7.76054
C	5.13219	-1.22702	7.53169
C	7.89186	7.23096	5.34715
H	7.77835	7.87325	6.22591
C	4.28122	1.86187	1.4082
H	4.06245	0.78967	1.42078
C	3.83624	6.1907	7.74605
C	8.04607	5.2846	6.92378
H	7.11369	4.72637	7.118
H	8.12982	6.07731	7.68037
H	8.87388	4.57336	7.06779
C	1.67783	6.51605	5.04288
H	1.05274	7.1017	5.72262
C	1.49134	6.5966	3.6647
H	0.72	7.24697	3.2462
C	3.05553	5.21414	9.84981
C	2.02321	4.5885	9.14724
H	1.31253	3.95691	9.68932
C	5.10621	6.07273	1.33287
H	4.22927	6.66733	1.03367
H	5.91512	6.29264	0.62232
H	5.41422	6.43228	2.32599
C	3.95538	6.00575	9.12694
H	4.7723	6.50618	9.65656
C	8.15679	0.96153	8.32294
H	9.15985	0.6153	8.03042
H	8.04249	0.80405	9.40478
H	8.14021	2.04474	8.12152
C	2.78437	2.08093	3.41069
H	3.2743	2.06711	4.39989
H	2.51307	1.04753	3.15314
H	1.86025	2.66794	3.52582
C	5.78392	-0.00343	3.97386
H	5.62185	1.05598	3.72475
H	4.94554	-0.58373	3.56427
H	6.70462	-0.30677	3.45199
C	4.17828	-2.13761	8.25061
H	4.49934	-3.18938	8.16632
H	3.16405	-2.07423	7.82873
H	4.11931	-1.89822	9.32236
C	4.80207	7.06069	7.00027
H	5.34508	6.48827	6.23338
H	5.54046	7.51387	7.67613
H	4.2755	7.86823	6.46862
C	0.7864	4.00235	7.03103
H	0.05673	4.70093	6.59383
H	0.24623	3.31888	7.70135
H	1.19112	3.4206	6.18726
C	5.79113	1.46753	-0.57625
H	5.90807	1.96008	-1.55322
H	5.21895	0.54025	-0.72683
H	6.79991	1.17852	-0.23515
C	3.18487	5.06653	11.33894
H	2.67327	4.16376	11.70295
H	2.73881	5.93013	11.86005
H	4.23926	5.01173	11.64912
C	7.67158	9.28419	3.89485
H	8.23999	9.6751	3.03762
H	7.96756	9.85193	4.78927
H	6.6067	9.50255	3.70553

[GeH(N_3Dmp$_2$)]

N	0.618792	1.000371	13.744048
N	-1.093572	2.121198	13.717067
N	-0.461052	1.234117	14.412684
C	-3.088945	0.191903	14.917472
C	-2.422979	2.467769	13.967923
C	-2.791065	3.761958	13.538861
C	-4.699133	2.061645	14.644016
H	-5.449217	1.380018	15.053477
C	1.679594	0.263616	14.265810
C	1.221391	0.918197	16.697318
C	-2.870474	-0.793411	13.937516
C	-3.384777	1.594846	14.516850
C	-3.094265	-0.152839	16.282743
C	-4.110255	4.186649	13.685213
H	-4.379887	5.193639	13.356893
C	1.995754	0.209671	15.641262
C	-5.067461	3.341009	14.241172
H	-6.102288	3.673836	14.349076
C	-2.872214	-1.481834	16.643473
H	-2.878113	-1.747191	17.705138
C	1.237308	-1.107547	11.291670
C	2.515409	-0.370208	13.318975
C	-2.626765	-2.475956	15.692574
C	-0.859880	5.344378	13.760229
C	2.207048	-0.262770	11.867207
C	-2.634347	-2.110167	14.345789
H	-2.464314	-2.876112	13.582772
C	0.476399	0.168881	17.628412
C	1.292238	2.318896	16.808006
C	-1.759761	4.646226	12.930184
C	3.633372	-1.081281	13.751622
H	4.262732	-1.574017	13.006096
C	2.877400	0.693318	11.080289
C	-1.674953	4.763736	11.529821
C	0.951292	-0.976410	9.932459
H	0.195305	-1.630043	9.486530
C	-0.667565	5.567191	10.981011
H	-0.594019	5.649911	9.892441
C	-3.312270	0.895174	17.336590
H	-2.593109	1.720213	17.217524
H	-3.181056	0.475987	18.343276
H	-4.319753	1.334491	17.278511
C	-0.194032	0.838998	18.651837
H	-0.772792	0.254278	19.373563
C	3.133185	-0.508771	16.029294
H	3.386435	-0.532194	17.092369
C	2.554463	0.793368	9.722065
H	3.068204	1.542061	9.111530
C	0.119035	6.143080	13.170707
H	0.819028	6.682922	13.815938
C	3.946135	-1.157535	15.106320
H	4.828658	-1.707534	15.440612
C	2.092961	3.132506	15.832539
H	3.082372	2.685205	15.651623
H	2.237850	4.159472	16.196190
H	1.591094	3.196877	14.851806
C	0.592048	2.949743	17.841451
H	0.648077	4.039310	17.927175
C	-2.881579	-0.448769	12.475913
H	-3.722981	0.214240	12.223352
H	-2.952756	-1.352560	11.854716
H	-1.961613	0.081954	12.175268
C	3.918116	1.593556	11.687320
H	3.534798	2.103393	12.584577
H	4.245620	2.360227	10.971503
H	4.803698	1.021861	12.006446
C	-0.160519	2.230815	18.771175
C	0.385348	-1.326306	17.513590
H	0.050254	-1.619475	16.506854
H	-0.329982	-1.734586	18.240235
H	1.357924	-1.812689	17.683997
C	0.516262	-2.115922	12.138141
H	1.222616	-2.792004	12.644190
H	-0.174479	-2.722583	11.535959
H	-0.068695	-1.624827	12.932329
C	1.591818	-0.026579	9.131184
C	0.241938	6.257772	11.782094
C	1.346705	7.074895	11.176662
H	1.125730	7.349455	10.135161
H	2.293200	6.508641	11.175874
H	1.522989	8.000187	11.745582
C	-2.657638	4.057684	10.635818
H	-2.770650	2.998086	10.911531
H	-2.341200	4.104788	9.584605
H	-3.658949	4.511155	10.711691
C	-0.950010	5.212215	15.252384
H	-1.958484	5.460754	15.617276
H	-0.226935	5.869022	15.755935
H	-0.746583	4.177973	15.572619
C	-2.332055	-3.885673	16.117498
H	-2.991162	-4.206777	16.938409
H	-1.294511	-3.974758	16.482582
H	-2.450832	-4.594857	15.285714
C	1.220378	0.133155	7.685232
H	0.977287	-0.834059	7.220687
H	2.031297	0.598239	7.106219
H	0.330683	0.776984	7.583389
C	-0.940808	2.925848	19.849589
H	-2.012423	2.970204	19.589891
H	-0.595394	3.958737	20.000522
H	-0.863895	2.394975	20.810705
H	1.084535	3.279148	12.613967
Ge	0.139274	2.117517	12.068993

[SnH(N_3Dmp$_2$)]

N	5.320391	3.749244	4.839264
N	4.205912	3.992921	5.439653
N	5.931938	2.835061	5.507704
C	7.954719	4.795009	4.368795
C	3.730012	4.100181	2.445553
C	7.252158	2.491409	5.231350
C	2.961315	4.848572	3.472135
C	4.843974	-1.313625	6.028071
H	4.150371	-1.866611	5.401444
C	3.215867	4.779814	4.852305
C	9.517495	2.905432	4.545696
H	10.259114	3.594966	4.157324
C	6.641758	0.270281	6.232394
C	1.869548	4.450400	7.991908
C	2.623978	5.341420	7.218708
C	6.622549	0.105888	7.624511
C	2.375523	5.451332	5.758236
C	7.629719	1.190371	5.613609
C	8.215034	3.372453	4.706839
C	1.068182	6.301866	3.925110
H	0.234979	6.889099	3.557235
C	8.019447	5.208889	3.032769
C	1.315006	6.208083	5.285310
H	0.682748	6.726492	5.997874
C	9.886360	1.617905	4.890823
H	10.909448	1.286954	4.756578
C	3.602606	6.144152	7.822683
C	5.080298	2.720297	0.411901
C	3.600462	2.710549	2.338369
C	1.885425	5.621281	3.040328
H	1.680637	5.659633	1.976016
C	5.167334	4.102123	0.519421
H	5.777427	4.651975	-0.191356
C	5.746951	-0.446482	5.426349
C	4.285953	2.044971	1.327881
H	4.184282	0.966368	1.248449
C	3.097097	5.137625	9.973597
C	3.813975	6.034629	9.188322
H	4.575372	6.654655	9.652678
C	7.577942	7.071280	5.041987
H	7.417562	7.798265	5.832976
C	7.713960	5.322807	6.825263
H	6.794103	4.781513	7.069687
H	7.768677	6.193410	7.480402
H	8.545263	4.655925	7.067307
C	8.936764	0.766681	5.431386
H	9.203838	-0.242963	5.724158
C	7.748398	5.734482	5.385448
C	7.621270	7.502351	3.723420
C	4.513077	4.804127	1.522338
C	4.796334	-1.483474	7.406894
C	7.857388	6.555132	2.735668
H	7.904814	6.871752	1.697695
C	5.694622	-0.767927	8.186988
H	5.674632	-0.886529	9.266489
C	2.128142	4.358463	9.359631
H	1.550634	3.657906	9.955670
C	0.772752	3.628793	7.377345
H	-0.108079	4.245480	7.175651
H	0.472762	2.819031	8.043709
H	1.075445	3.193416	6.422356
C	4.411864	7.096622	6.999102
H	5.009824	6.562929	6.255740
H	5.090682	7.676350	7.625756
H	3.771037	7.789745	6.448036
C	2.735769	1.934563	3.283955
H	3.215805	1.812564	4.260670
H	2.530706	0.936339	2.894748
H	1.783620	2.439761	3.461625
C	4.663034	6.293300	1.612768
H	3.737509	6.811583	1.348810
H	5.447091	6.642978	0.940829
H	4.926051	6.598412	2.627924
C	5.764149	-0.273187	3.938938
H	6.744614	-0.520854	3.523810
H	5.558915	0.763238	3.658225
H	5.016478	-0.908245	3.462077
C	8.246847	4.220652	1.928230
H	9.260376	3.812258	1.949863
H	8.093469	4.688054	0.955098
H	7.557765	3.377218	2.011569
C	7.586231	0.851317	8.501567
H	8.604971	0.475225	8.374001
H	7.314699	0.747870	9.552809
H	7.609994	1.915603	8.256532
C	3.783018	-2.388724	8.037858
H	2.831957	-1.864863	8.174019
H	4.111122	-2.735330	9.019914
H	3.590577	-3.264339	7.414702
C	3.391762	5.000057	11.436087
H	4.318843	4.439669	11.590809
H	2.592439	4.470689	11.957345
H	3.520040	5.976445	11.909035
C	5.845111	1.983025	-0.644963
H	5.821424	2.514894	-1.598896
H	5.443578	0.980476	-0.803382
H	6.896662	1.876313	-0.359031
C	7.390758	8.940035	3.368741
H	6.349649	9.104115	3.071496
H	8.019666	9.250455	2.531357
H	7.598241	9.598771	4.214129
Sn	4.291271	2.398747	7.072765
H	5.258122	3.415366	8.159024

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