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Structurally characterised intermediate of the oxidative addition of a heteroleptic germylene to gallanediyle

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I. Experimental Section

General Procedure. All experiments were performed either in a glovebox and using standard Schlenk-line techniques under Ar atmosphere. Toluene and *n*-hexane were dried using a mBraun Solvent Purification System (SPS), degassed and stored in Schlenk flasks under Ar atmosphere. Deuterated solvents were stored over molecular sieves (4 Å) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. LGa,[1], $\{Sn[N(Ar)(SiMe_3)]Cl\}_2$,[2] and $(DMPGeCl)_2$[3] were synthesized according to literature methods. Microanalyses were performed at the laboratory for microanalysis of the University of Duisburg-Essen. The melting points were measured using a Thermo Scientific 9300 apparatus.

Spectroscopic methods. ^1H (400 MHz) and $^{13}C\{^1H\}$ (100 MHz) NMR spectra were recorded using a Ascend™ 400 spectrometer The spectra were referenced to internal C_6D_5H (^1H: δ = 7.16, C_6D_6) and toluene-d_7 (^1H: δ = 2.08, toluene-d_8) or to natural-abundance carbon resonances C_6D_6 (^{13}C: δ = 128.06, C_6D_6) and toluene-d_8 (^{13}C: δ = 20.43, toluene-d_8). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module. The IR spectrometer was placed in a glovebox to guarantee measurements under inert gas conditions.

Synthesis of L'GeCl. Li[N(Ar)($SiMe_3$)] (100 mg, 0.39 mmol) and $GeCl_2$-dioxane (90 mg, 0.39 mmol) were dissolved in THF at -78 °C with rapid stirring. The resulting yellow solution was slowly warmed to r.t. over night. All residues were removed in vacuo and the colorless solid was extracted with 60 mL of *n*-pentane. The suspension was filtrated, and the solution was concentrated until initial crystallization. Colorless crystals were formed after storage at −20 °C for 16 hours. Yield: 68 mg (0.19 mmol, 48%), m.p. 116-118 °C. **Anal. Calcd for $C_{15}H_{26}ClGeNSi$:** C 50.53, N 3.93, H 7.35; **found:** C 49.8, N 3.93, H 6.75. **^1H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.03 (s 3H, Ar*H*), 3.18 (sept, $^3J_{HH}$ = 6.9 Hz, 2H, C*H*(CH_3)$_2$), 1.14 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 1.03 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 0.27 (s, 9H, Si(C*H*$_3$)$_3$). **^{13}C NMR (101 MHz, C_6D_6): δ [ppm] =** 145.8, 140.2, 128.4, 128.2, 126.7, 124.2 (Ar), 28.6 (*C*H(CH_3)$_2$), 26.2 (CH(*C*H$_3$)$_2$), 23.8 (CH(*C*H$_3$)$_2$), 3.2 (Si(*C*H$_3$)$_3$). **IR(ATR): *ν*[cm^{-1}]:** 2958, 2863, 1537, 1457, 1436, 1347, 1292, 1268, 1233, 1211, 1158, 1096, 1026, 968, 886, 868, 827, 788, 724, 671, 628, 558, 533, 439.

Synthesis of 1. LGa (100 mg, 0.21 mmol) and $\{Sn[N(Ar)(SiMe_3)]Cl\}_2$ (85 mg, 0.21 mmol) were dissolved in toluene (2 mL). Rapid stirring for 5 minutes gave a green solution. The solvent was evaporated until incipient crystallization and the resulting saturated stored at −20 °C for 16 h to yield colorless crystals. Yield 75 mg (0.09 mmol, 42 %), m.p. 175-176 °C. **Anal. Calcd for $C_{44}H_{67}ClGaN_3SiSn$:** C 59.38, N 4.72, H 7.59; **found:** C 59.0, N 4.86, H 7.29. **^1H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.08 (s, 7H, Ar-*H*), 7.06 (s, 1H, Ar-*H*), 7.00 (dd, $^3J_{HH}$ = 8.7, 6.3 Hz, 1H Ar-*H*), 5.10 (s, 1H, γ-C*H*), 3.55 (s, 6H, C*H*(CH_3)$_2$), 1.68 (s, 6H, C*H*$_3$), 1.38 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.23 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 1.14 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.03 (d, $^3J_{HH}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 0.18 (s, 9H, Si(C*H*$_3$)$_3$). **^{13}C NMR (101 MHz, C_6D_6, 298 K): δ [ppm] =** 167.7 (*CN*), 145.8, 144.0, 142.6, 127.9, 127.54, 124.9, 124.6, 123.7 (Ar), 98.9 (*γ-C*), 28.9

(*C*H(CH$_3$)$_2$), 27.8 (*C*H(CH$_3$)$_2$), 26.7 (CH(*C*H$_3$)$_2$), 25.6(CH(*C*H$_3$)$_2$), 24.6 (CH(*C*H$_3$)$_2$), 24.0 (CH(*C*H$_3$)$_2$), 23.9 (C*C*H$_3$), 3.9 (Si(*C*H$_3$)$_3$). **IR(ATR): *ν*[cm^{-1}]:** 3051, 2957, 2923, 2864, 1583, 1526, 1458, 1435, 1358, 1314, 1258, 1238, 1175, 1097,1054, 1021, 935, 907, 880, 841, 790, 757, 732, 695, 669, 630, 567, 527, 465, 430, 396.

Synthesis of 2. LGa (58 mg, 0.12 mmol) and (DMPGeCl)$_2$ (50 mg, 0.06 mmol) were dissolved in 5 mL of *n*-hexane with rapid stirring for five minutes to yield a dark red solution. The solvent was removed until incipient crystallization and the resulting saturated solution stored at -30 °C for 16 h to yield pale yellow crystals. Yield 47 mg (0.058 mmol, 43%), m.p. 113-115 °C. **Anal. Calcd for $C_{53}H_{66}ClGaGeN_2$:** C 70.04, N 3.08, H 7.32; **found:** C 67.50, N 2.70, H 7.57. **^{1}H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.12 (m, 8H, Ar-*H*), 6.84 (d, $^3J_{HH}$ = 7.5 Hz, 2H, *p*-C$_6$*H*$_3$), 6.79 (s, 4H, *m*-Mes), 5.04 (s, 1H, *γ*-C*H*), 3.17 (sept, $^3J_{HH}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 2.24 (s, 6H, *p*-C*H*$_3$), 2.08 (s, 12H, *o*-C*H*$_3$), 1.60 (s, 6H, C*H*$_3$), 1.19 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.12 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$). **^{13}C NMR (101 MHz, C_6D_6, 298 K): δ [ppm] =** 166.25, 146.68, 143.88, 143.37, 138.90, 136.88, 129.46, 128.75, 128.42, 128.18, 127.32, 124.48, 99.47, 28.86, 25.76, 24.46, 24.24, 21.76, 21.54. **IR(ATR): *ν*[cm^{-1}]:** 2961, 2913, 2855, 1620, 1515, 1443, 1371, 1314, 1281, 1266, 1175, 1103, 1017, 935, 855, 797, 739, 697, 634, 528, 429, 394.

Synthesis of 3. LGa (67 mg, 0.14 mmol) and [N(Ar)(SiMe$_3$)]GeCl (50 mg, 0.14 mmol) were dissolved in 2.5 mL of toluene with rapid stirring. The solution immediately turned purple. After five minutes stirring at r.t. the solution was concentrated until incipient crystallization and stored at −20 °C for 16 hours to yield purple crystals. The crystals were washed with cold *n*-hexane (3x 0.3 mL). Yield 57 mg (0.067 mmol, 48%), m.p. 128-129 °C. **Anal. Calcd for $C_{44}H_{67}ClGaGeN_3Si$:** C 62.62, N 4.98, H 8.00; **found:** C 62.30, N 4.73, H 7.93. **^{1}H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.07 (s, 6H, Ar-*H*), 6.99 (m, 3H, Ar-*H*), 5.12 (s, 1H, *γ*-C*H*), 3.77 (sept, $^3J_{HH}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 3.21 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 1.71 (s, 6H, C*H*$_3$), 1.37 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.18 (dd, $^3J_{HH}$ = 6.9 Hz, 18H, CH(C*H*$_3$)$_2$), 0.87 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 0.13 (s, 9H, Si(C*H*$_3$)$_3$). **^{13}C NMR (101 MHz, C_6D_6): δ [ppm] =** 167.8 (*C*N), 147.5, 144.9, 144.6, 143.3, 129.6, 128.8, 128.4, 128.2, 127.5, 125.9, 125.0, 124.0 (Ar), 98.5 (*γ*-*C*), 29.1 (*C*H(CH$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 26.7 (CH(*C*H$_3$)$_2$), 26.0 (*C*H(CH$_3$)$_2$), 24.9 (*C*H(CH$_3$)$_2$), 23.9 (C*C*H$_3$), 3.6 Si(*C*H$_3$)$_3$. **IR(ATR): *ν*[cm^{-1}]:** 3062, 2957, 2862, 1533, 1462, 1433, 1376, 1319, 1248, 1176, 1095, 1019, 943, 891, 862, 829, 796, 753, 729, 691, 634, 528, 438.

Synthesis of 4. CNCy (10 µL, 8.8 mg, 0.08 mmol) was added to a solution of **2** (73 mg, 0.08 mmol) in 0.5 mL of benzene. The color immediately turned from dark red to orange. The solution was stirred for 10 minutes, the solvent was removed in vacuo and 1 mL of *n*-hexane was added. Yellow crystals of **4** were obtained after storage for 16 hours at ambient temperature. After filtration the crystals were washed with n-hexane (3 x 0.3 mL) and dried in vacuo. Yield: 55 mg (0.056 mmol, 54%), m.p. 164 °C. **Anal. Calcd for $C_{60}H_{77}ClGaGeN_3$:** C 70.78, N 4.13, H 7.62; **found:** C 70.9, N 4.25, H 7.74. **^{1}H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.11 (t, 1H, *p*-C$_6$*H*$_3$), 7.04 (m, 4H, Ar-*H*), 6.90 (s, 4H, *m*-Mes), 6.84 (d, $^3J_{HH}$

= 7.5 Hz, 2H, *m*-C$_6$H$_3$), 5.01 (s, 1H, *γ*-C*H*), 4.03 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, C*H*(CH$_3$)$_2$), 3.30 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 2.87 (tt, $^3J_{HH}$ = 19.2, 3.7 Hz, 1H, Cy-C*H*), 2.37 (s, 6H, *p*-CH$_3$), 2.07 (br s, 12H, *o*-CH$_3$), 1.56 (m, 2H, Cy-CH$_2$), 1.43 (m, 1H, Cy-CH$_2$, overlapping with CH$_3$), 1.38 (s, 6H, CH$_3$), 1.30 (m, 1H, Cy-CH$_2$, overlapping with CH(CH$_3$)$_2$) 1.27 (d, $^3J_{HH}$ = 6.9 Hz, 6H), 1.16 (m, 2H, Cy-CH$_2$, overlapping with CH(CH$_3$)$_2$) 1.11 (dd , $^3J_{HH}$ = 6.5 Hz 12H, CH(CH$_3$)$_2$), 1.06 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 0.80 (m, 4H, Cy-CH$_2$). **^{13}C NMR (101 MHz, C$_6$D$_6$): δ [ppm] =** 167.6 (NC), 151.1 (CyNC), 149.4, 146.6, 144.5, 144.3, 144.1, 143.5, 136.0, 135.3, 128.8, 127.0, 124.4, 124.2 (Ar), 100.3 (*γ*-C), 55.7 (Cy), 31.7 (Cy-C), 28.7 (CH(CH$_3$)$_2$), 28.2 (CH(CH$_3$)$_2$), 27.4 (CH(CH$_3$)$_2$), 25.6 (Cy), 25.1 ((CH(CH$_3$)$_2$)), 24.8 (Cy), 24.7 (CH(CH$_3$)$_2$), 24.4 (CCH$_3$), 23.9 (CH(CH$_3$)$_2$), 23.7 (Cy), 22.8 (*p*-CH$_3$), 21.5 (*o*-CH$_3$).

Synthesis of 5. A solution of compound **1** (42 mg, 0.047 mmol) dissolved in 2 mL of fluorobenzene was added to a solution of Li[Al(OC(CF$_3$)$_3$)$_4$] (45 mg, 0.047 mmol) in 1 mL of fluorobenzene. The solution was stirred for five minutes at r.t., filtrated and concentrated in vacuo to roughly 0.5 mL and layered with 1 mL of *n*-hexane to yield orange crystals. Yield: 11 mg (0.006 mmol, 13%), m.p. 88-90 °C decomp. **^{1}H NMR (400 MHz, Tol-*d*$_8$, 298 K): δ [ppm] =** 7.14 − 6.79 (Ar*H*, overlapping with solvent resonances), 5.76 (s, 1H, *γ*-C*H*), 2.99 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, C*H*(CH$_3$)$_2$), 2.81 (sept, $^3J_{HH}$ = 6.6 Hz, 4H, C*H*(CH$_3$)$_2$), 1.93 (s, 6H, CH$_3$), 1.22 (d, $^3J_{HH}$ = 6.7 Hz, 12H), 1.19 (d, $^3J_{HH}$ = 6.8 Hz, 6H), 1.14 (d, $^3J_{HH}$ = 6.7 Hz, 12H), 0.95 (d, $^3J_{HH}$ = 6.8 Hz, 6H), −0.22 (s, 9H, Si(CH$_3$)$_3$). **^{13}C NMR (101 MHz, Tol-*d*$_8$): δ [ppm] =** 171.8 (CN), 145.9, 143.3, 139.9, 130.2, 127.3, 126.0, 125.6, 125.3, 124.6, 124.0, 121.1, (Ar), 104.2 (*γ*-CH), 29.4 (CH(CH$_3$)$_2$), 28.3 (CH(CH$_3$)$_2$), 26.9 (CH(CH$_3$)$_2$), 25.60(CH(CH$_3$)$_2$), 23.6 (CH(CH$_3$)$_2$), 23.1 (CH(CH$_3$)$_2$), 23.0 (CH$_3$), 2.8 (Si(CH$_3$)$_3$). **IR(ATR): *ν*[cm^{-1}]:** 2958, 1538, 1452, 1430, 1352, 1293, 1268, 1210, 1158, 1096, 1026, 966, 870, 828, 788, 750, 723, 673, 626, 556, 535, 439.

Synthesis of 6. A solution of compound **2** (43 mg, 0.047 mmol) in 2 mL of fluorobenzene was added to a solution of Li[Al(OC(CF$_3$)$_3$)$_4$] (45 mg, 0.047 mmol) in 1 mL of fluorobenzene and stirred for 10 minutes at r.t. The solution was filtrated, concentrated to 5 mL in vacuo and layered with 1 mL of *n*-hexane. After storage at r.t. for 16 hours orange crystals were obtained. Yield: 33 mg (0.018 mmol, 39%). m.p. 87-88 °C decomp. **^{1}H NMR (400 MHz, C$_6$D$_6$): δ [ppm] =** 6.65 – 7.45 (ArH, overlapping with solvent resonances), 5.57 (s, 1H, , *γ*-C*H*), 2.54 (sept, $^3J_{HH}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 2.32 (s, 6H, *p*-CH$_3$), 1.90 (s, 12H, *o*-CH$_3$), 1.73 (s, 6H, CH$_3$), 1.16 (d, $^3J_{HH}$ = 6.8 Hz, 12H, CH(CH$_3$)$_2$), 0.78 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH$_3$)$_2$). **^{13}C NMR (101 MHz, C$_6$D$_6$): δ [ppm] =** 169.0 (CN), 141.6, 140.6, 138.6, 138.3, 136.2, 135.6, 128.7, 128.3, 127.9, 127.8, 126.82, 126.58, 123.54, 122.37, 122.34, 121.81, 121.78, 113.78, 113.71, 113.57, 113.14, 113.07, 112.94, 112.87 (Ar), 101.30 (*γ*-C), 27.25 CH(CH$_3$)$_2$, 22.37 (CH(CH$_3$)$_2$), 21.41 (CH$_3$), 20.60 (CH(CH$_3$)$_2$), 18.67 (*p*-CH$_3$), 18.35 (*o*-CH$_3$). **IR(ATR): *ν*[cm^{-1}]:** 2963, 1543, 1431, 1351, 1292, 1270, 1209, 969, 854, 829, 799, 753, 742, 556, 533, 439.

Synthesis of 7. Compound **3** (30 mg, 0.0355 mmol) and Na[B(Ar^F)$_4$] (32 mg, 0.0355 mmol) were dissolved in 2 mL of fluorobenzene and stirred for five minutes. The solution was filtrated,

concentrated in vacuo, layered with 1 mL of *n*-hexane, and stored at r.t. for 16 hours to yield orange crystals. Yield: 15 mg (0.009 mmol, 25 %), m.p. 97 – 98 °C decomp. **^{1}H NMR (400 MHz, Tol-*d*$_8$, 298 K): δ [ppm] =** 8.19 (s, 8H, Ar*H*), 7.55 (s, 4H, Ar*H*), 7.11−6.45 (m, Ar*H*, overlapping with solvent resonances), 5.66 (s, 1H, *γ*-C*H)*, 2.72 (sept, $^{3}J_{HH}$ = 6.7 Hz, 4H, C*H*(CH$_3$)$_2$), 2.64 (sept, $^{3}J_{HH}$ = 6.7 Hz, 2H, C*H*(CH$_3$)$_2$), 1.78 (s, 6H, C*H*$_3$), 1.06 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, CH(C*H*$_3$)$_2$), 1.03 (d, $^{3}J_{HH}$ = 6.8 Hz, 18H, CH(C*H*$_3$)$_2$), 0.72 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, CH(C*H*$_3$)$_2$), −0.36 (s, 9H, Si(C*H*$_3$)$_3$). **^{13}C NMR (101 MHz, Tol-*d*$_8$): δ [ppm] =** 169.4 (*C*N), 143.0, 140.1, 137.2, 135.2, 132.9, 127.6, 127.4, 127.3, 126.8, 126.6, 126.3, 126.1, 125.9, 125.7, 125.5, 125.2, 124.0, 123.1, 122.8, 122.5, 122.0, 121.3, 115.0, 114.6 (Ar), 101.3 (*γ*-*C*), 26.8 (*C*H(CH$_3$)$_2$), 25.8 (*C*H(CH$_3$)$_2$), 23.7 (CH(*C*H$_3$)$_2$), 22.5 (CH(*C*H$_3$)$_2$, 20.8 (CH(*C*H$_3$)$_2$, 20.4 (*C*H$_3$), 20.1 (CH(*C*H$_3$)$_2$, −1.0 (Si(*C*H$_3$)$_3$. **IR(ATR): *ν*[cm^{-1}]:** 2960, 1604, 1537, 1514, 1456, 1430, 1348, 1270, 1155, 1116, 927, 884, 834, 797, 741, 709, 667, 574, 527, 445.

II. Spectroscopic characterization

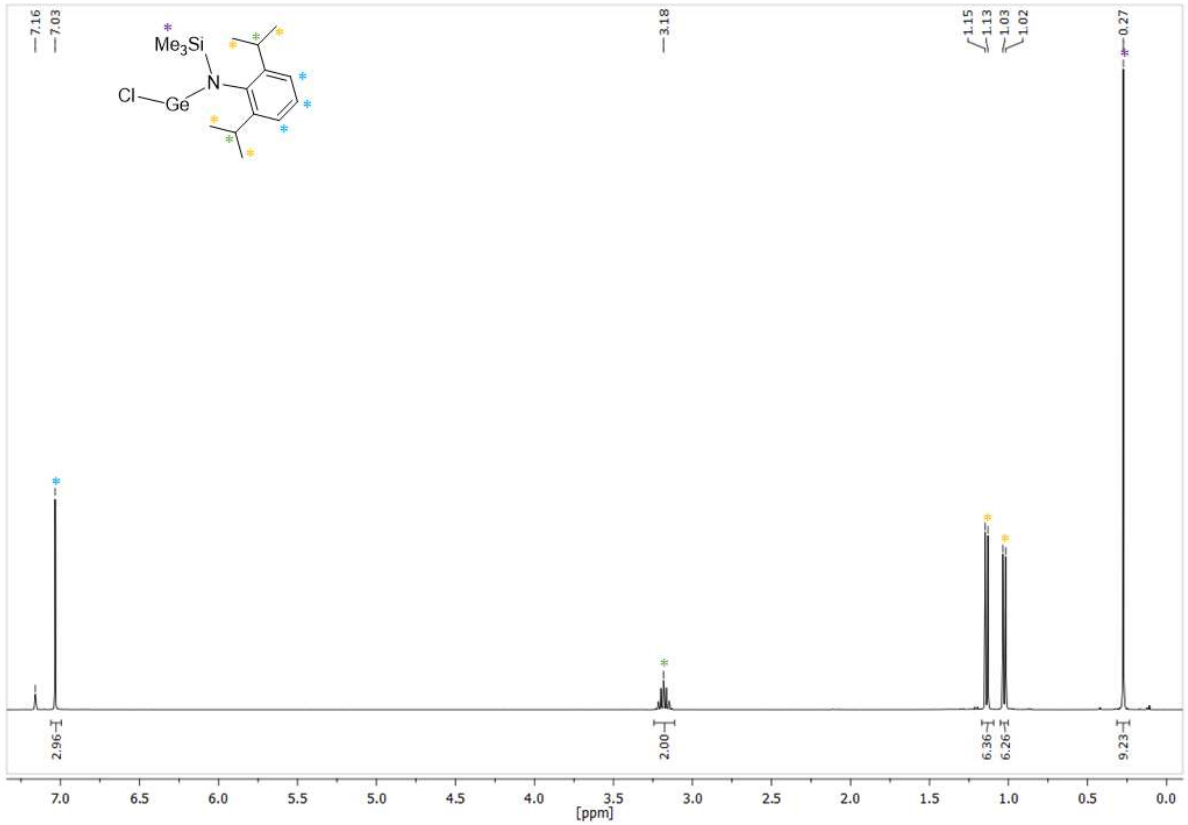


Figure S1: ^{1}H NMR spectrum of L'GeCl in C_6D_6.

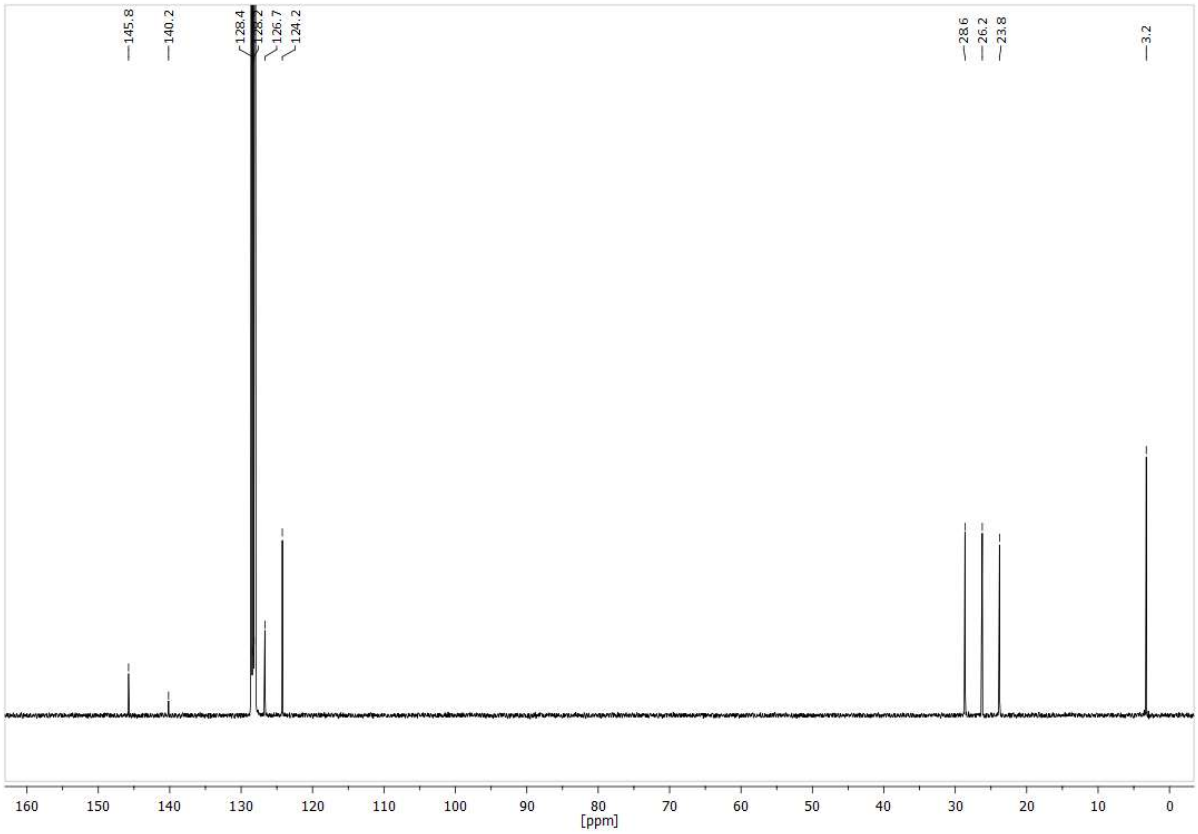


Figure S2: ^{13}C NMR spectrum of L'GeCl in C_6D_6.

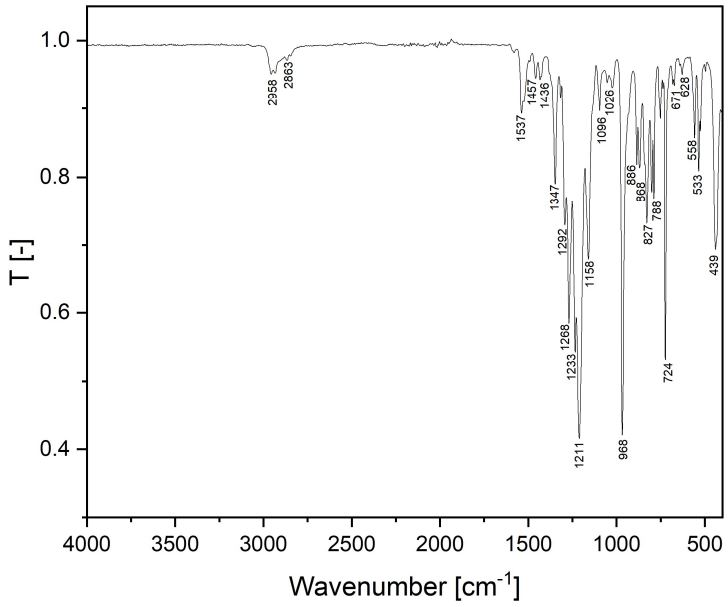


Figure S3: IR spectrum of L'GeCl.

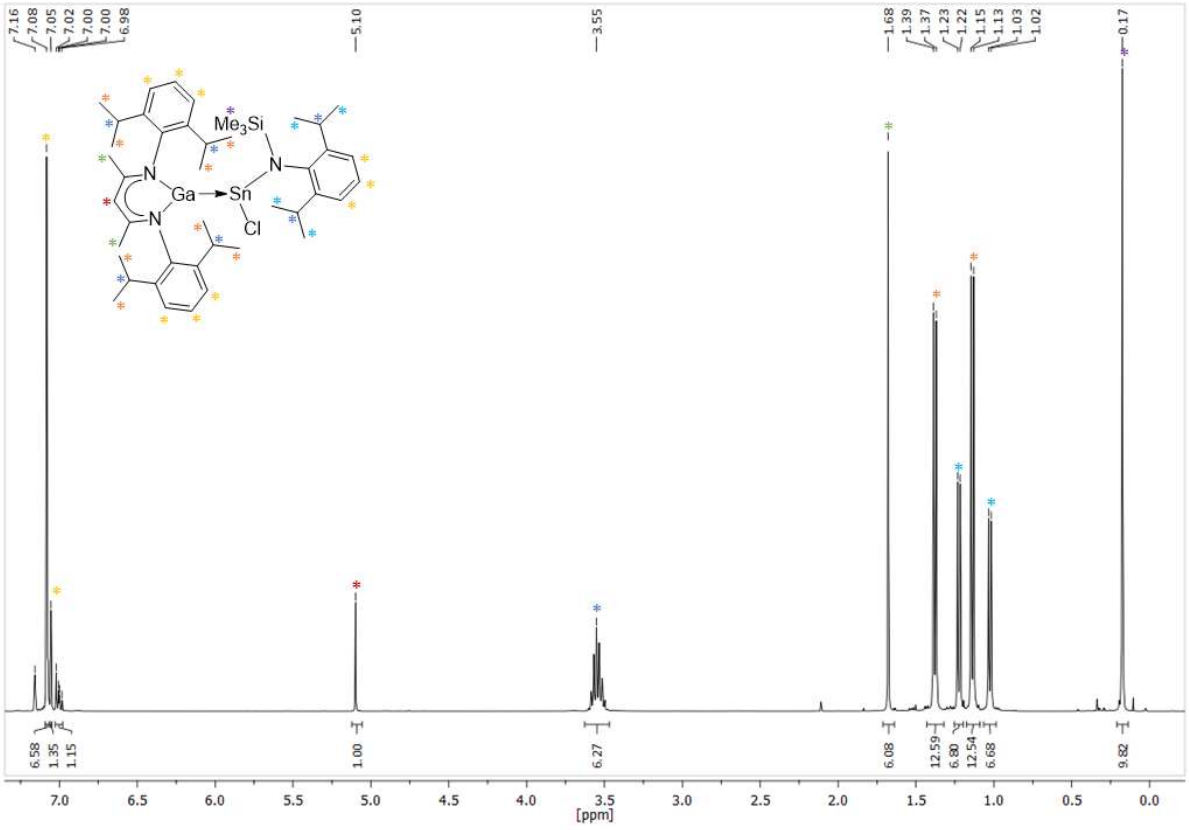


Figure S4: ^{1}H NMR spectrum of **1** in C_6D_6.

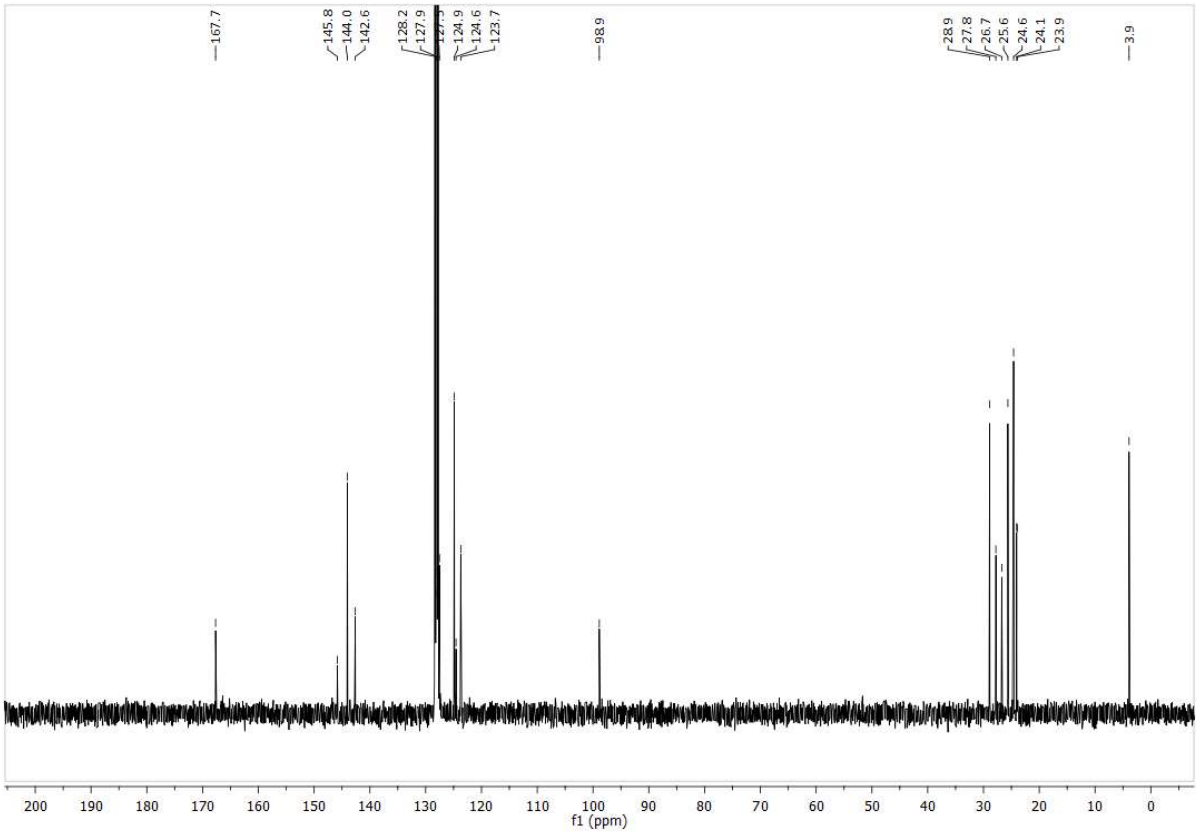


Figure S5: ^{13}C NMR spectrum of **1** in C_6D_6.

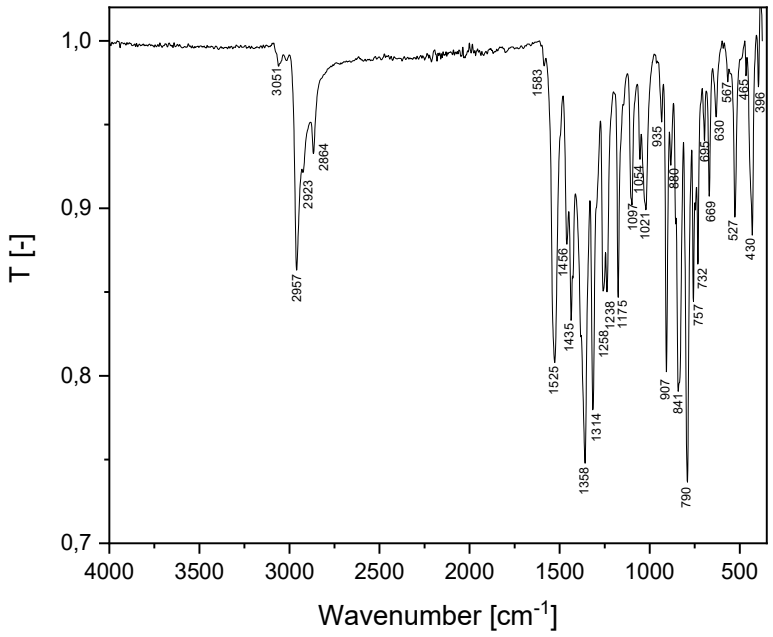


Figure S6: IR spectrum of **1**.

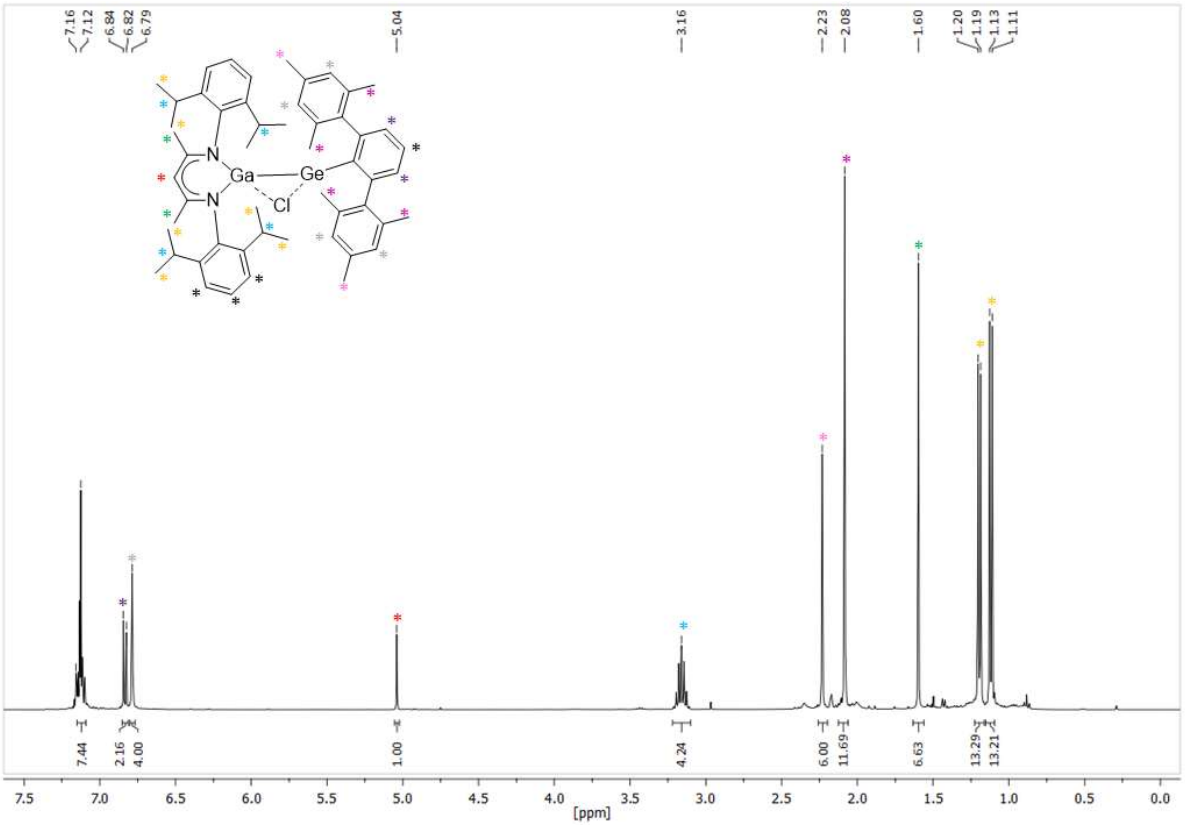


Figure S7: ^{1}H-NMR spectrum of **2** in C_6D_6.

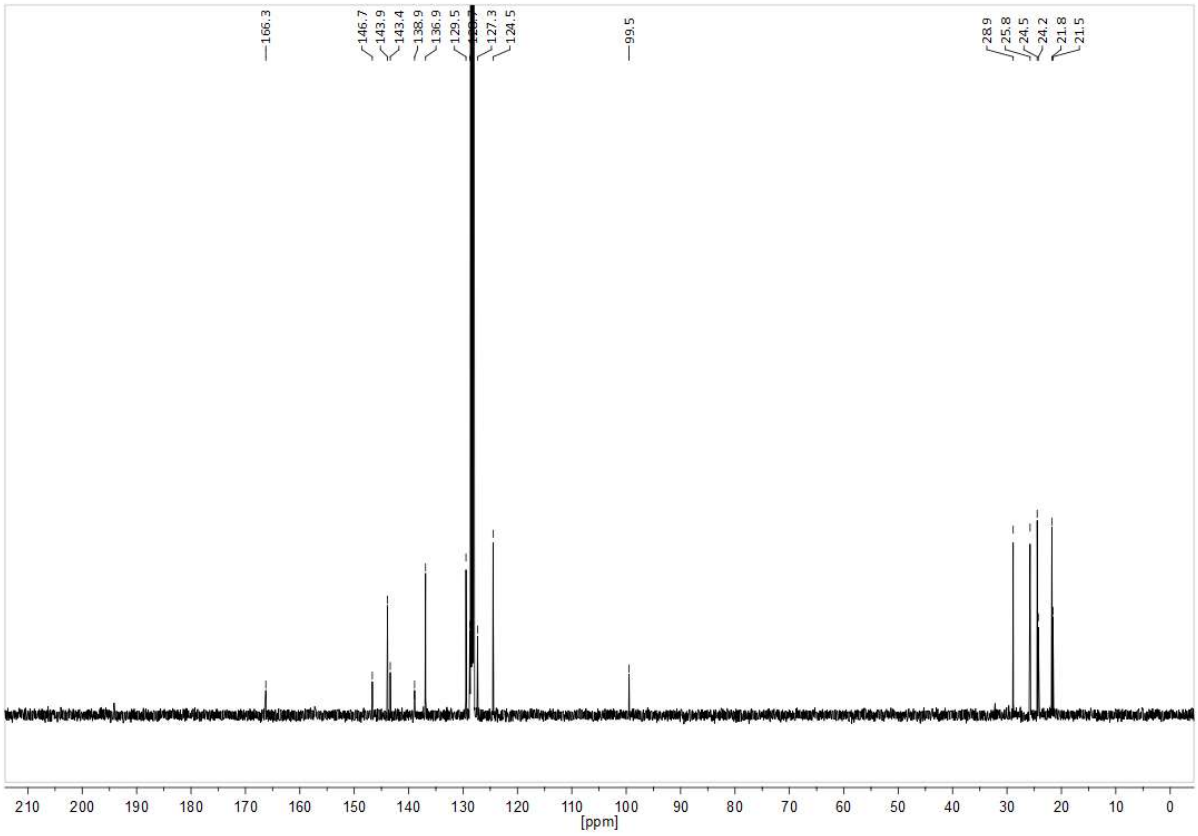


Figure S8: ^{13}C-NMR spectrum of **2** in C_6D_6.

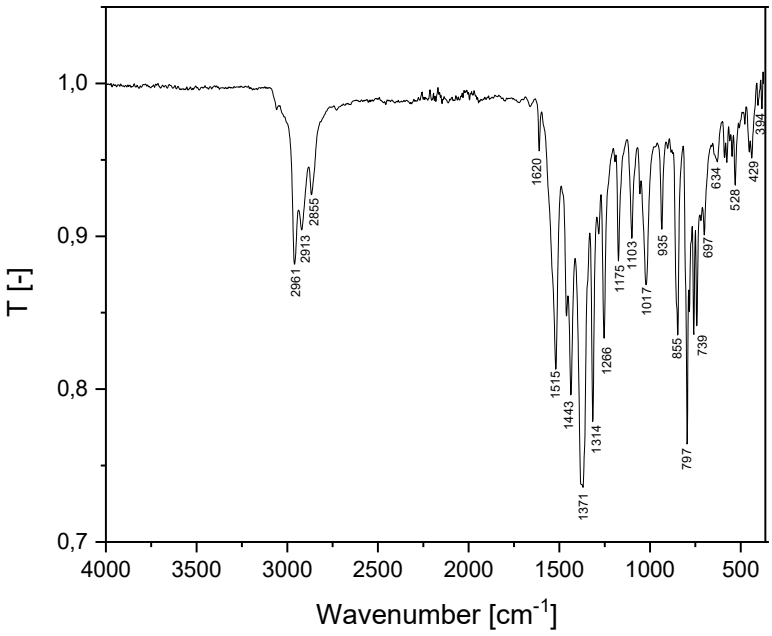


Figure S9: IR spectrum of **2**.

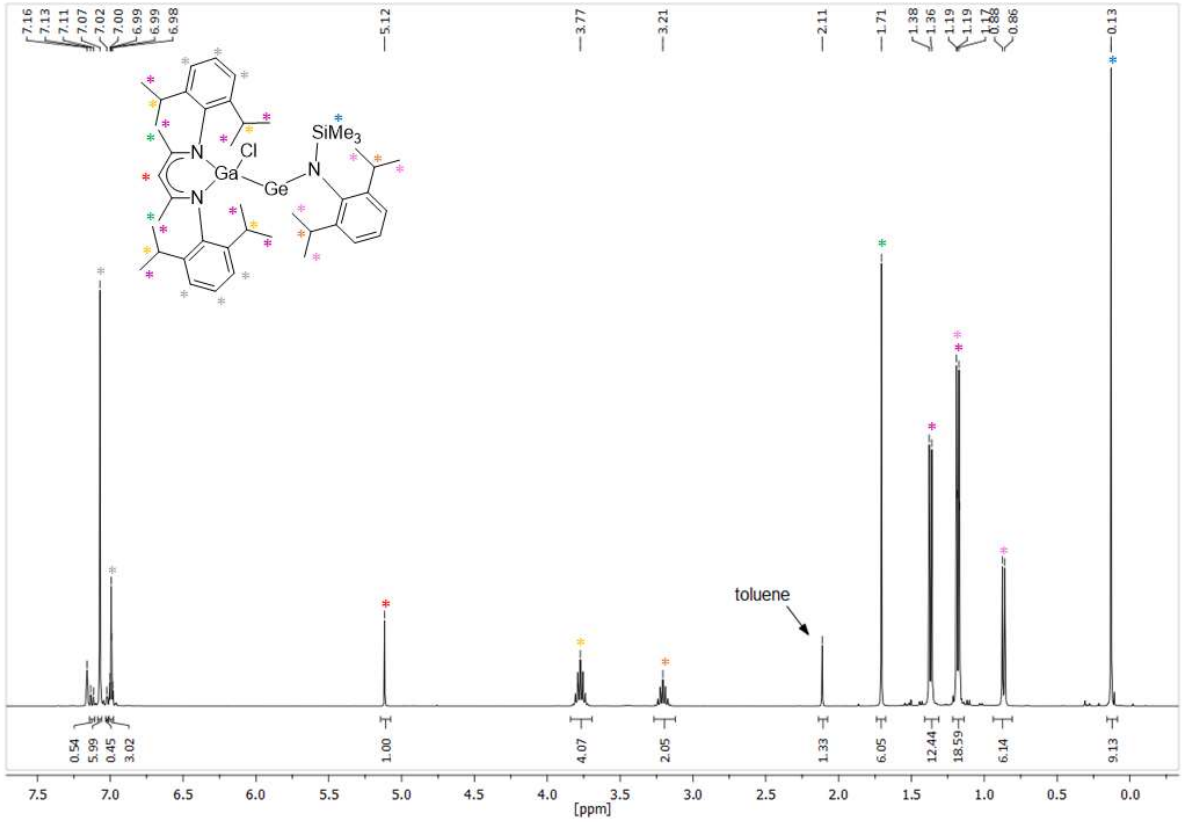


Figure S10: ^{1}H NMR spectrum of **3** in C_6D_6.

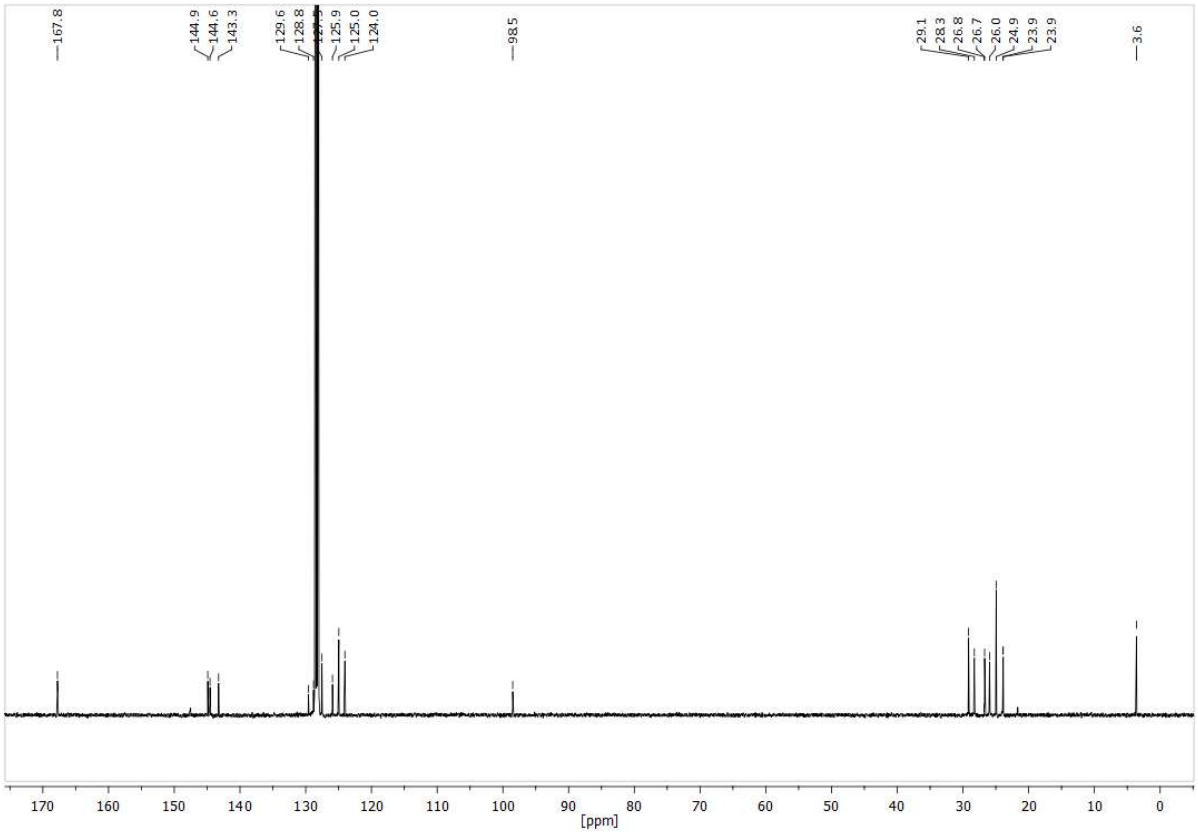


Figure S11: ^{13}C NMR spectrum of **3** in C_6D_6.

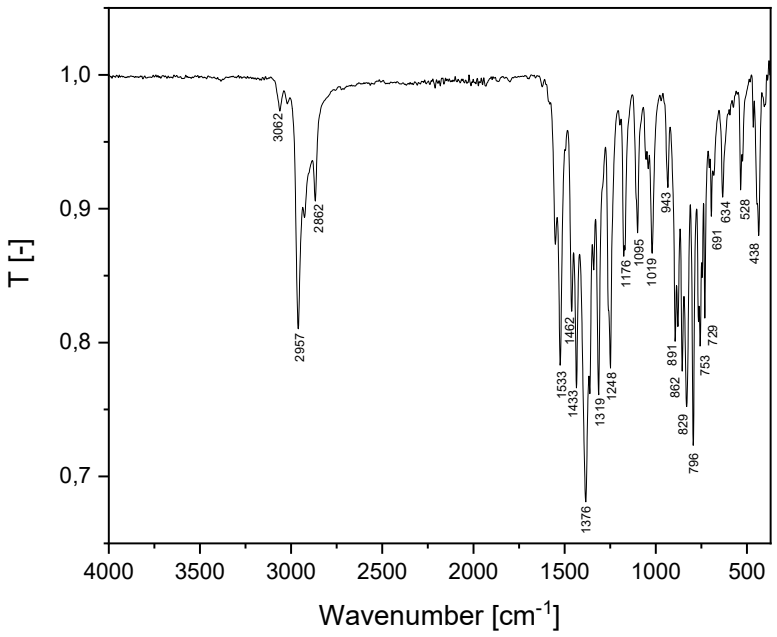


Figure S12: IR spectrum of **3**.

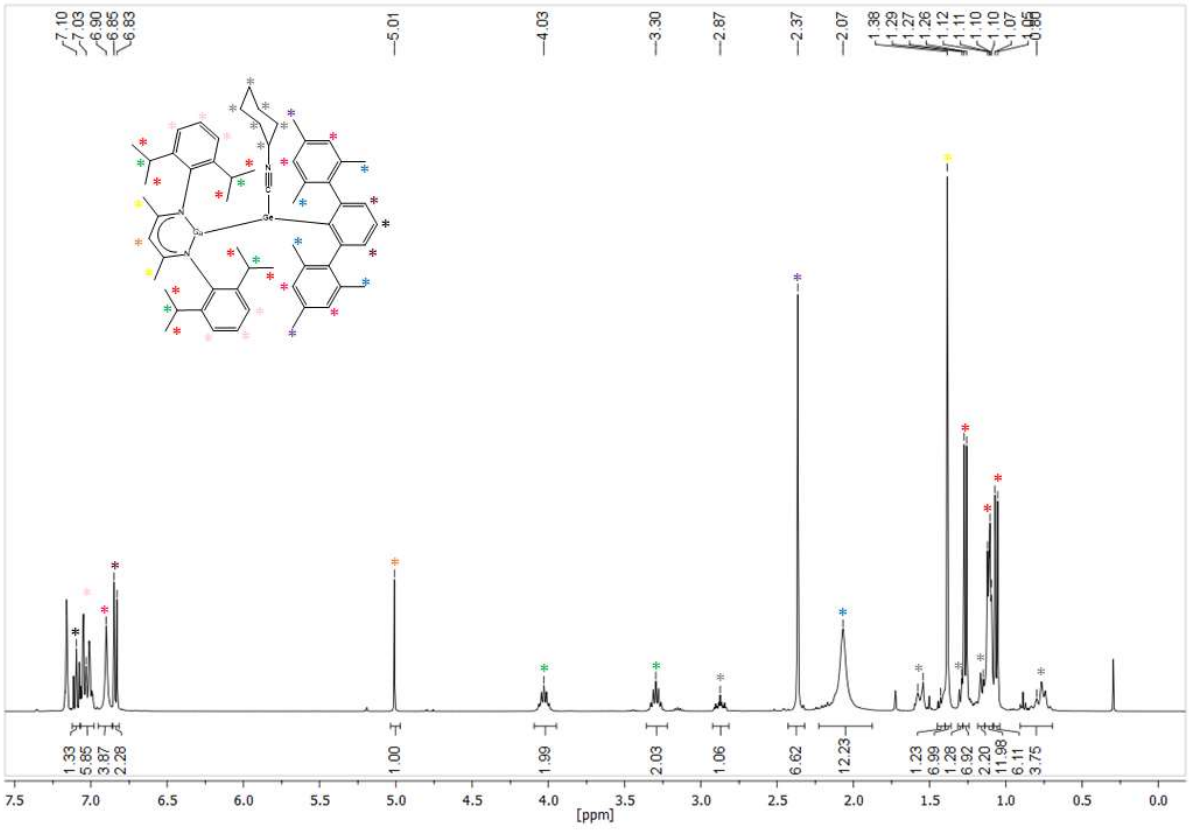


Figure S13: ^{1}H NMR spectrum of **4** in C_6D_6.

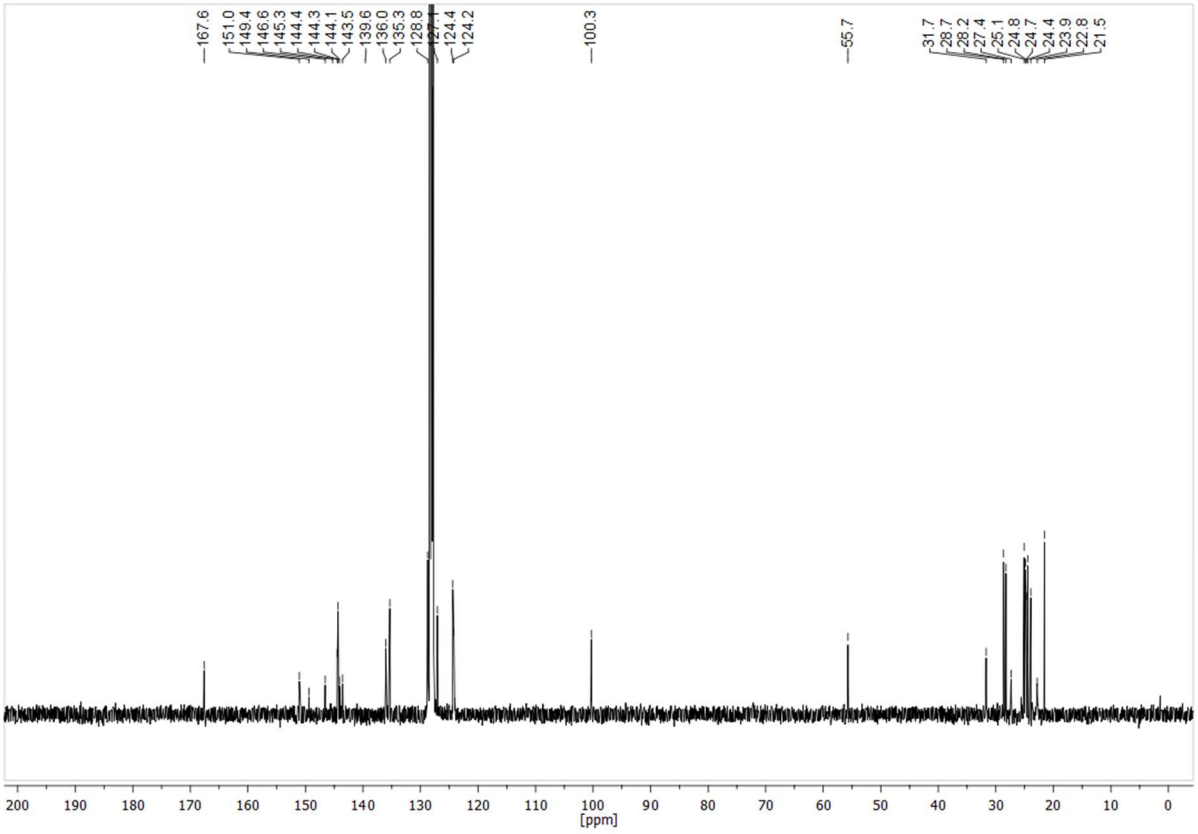


Figure S14: ^{13}C NMR spectrum of **4** in C_6D_6.

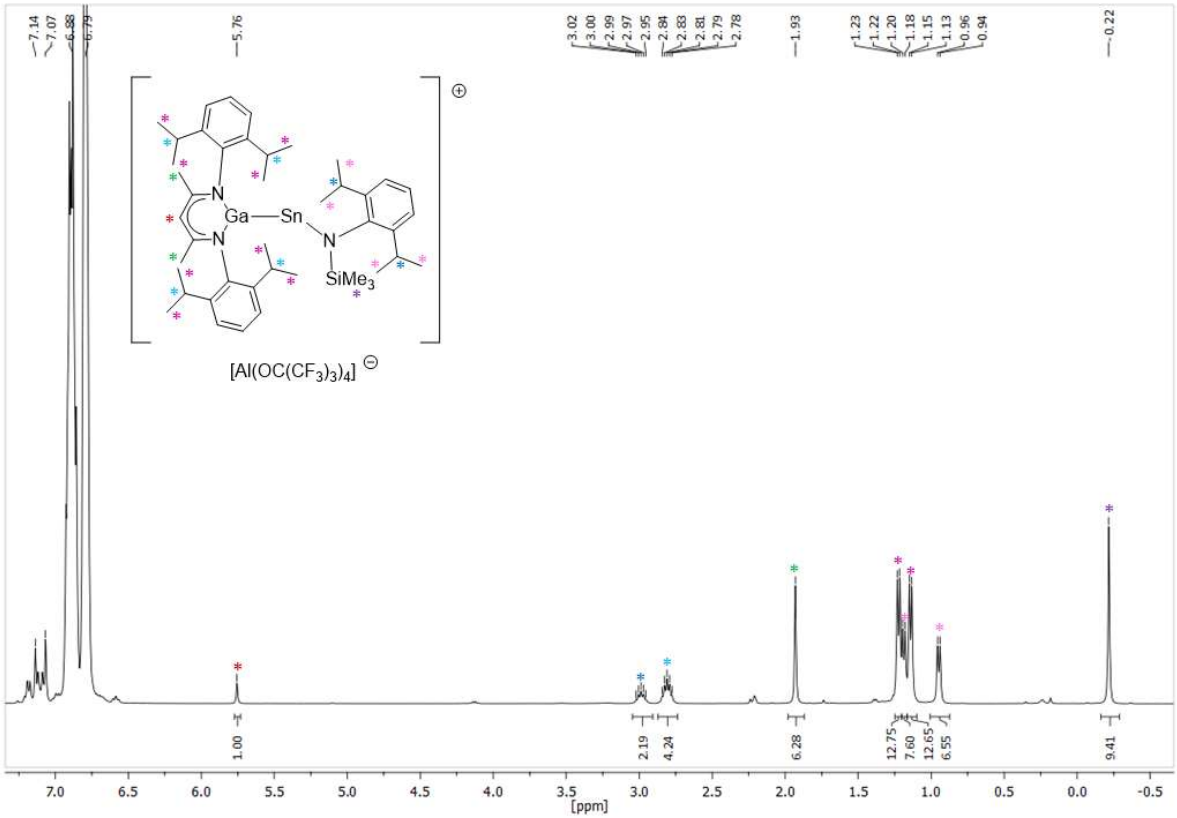


Figure S15: ^{1}H NMR spectrum of **5** in toluene-d_8 and 1,2-difluorobenzene.

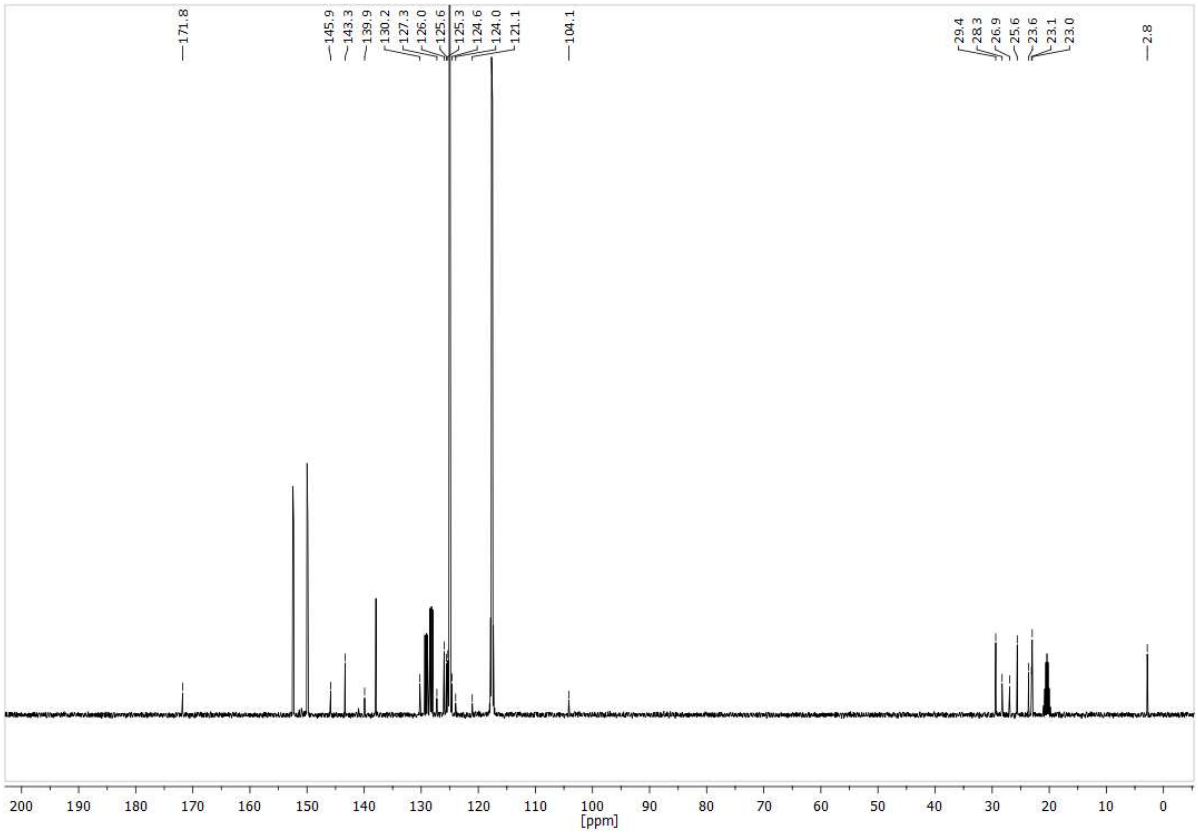


Figure S16: ^{13}C NMR spectrum of **5** in toluene-d_8 and 1,2-difluorobenzene.

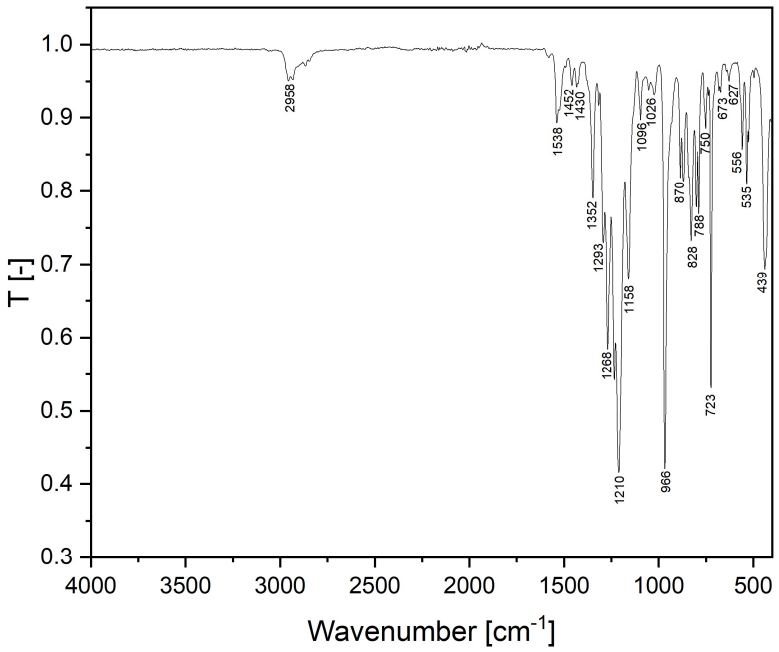


Figure S17: IR spectrum of **5**.

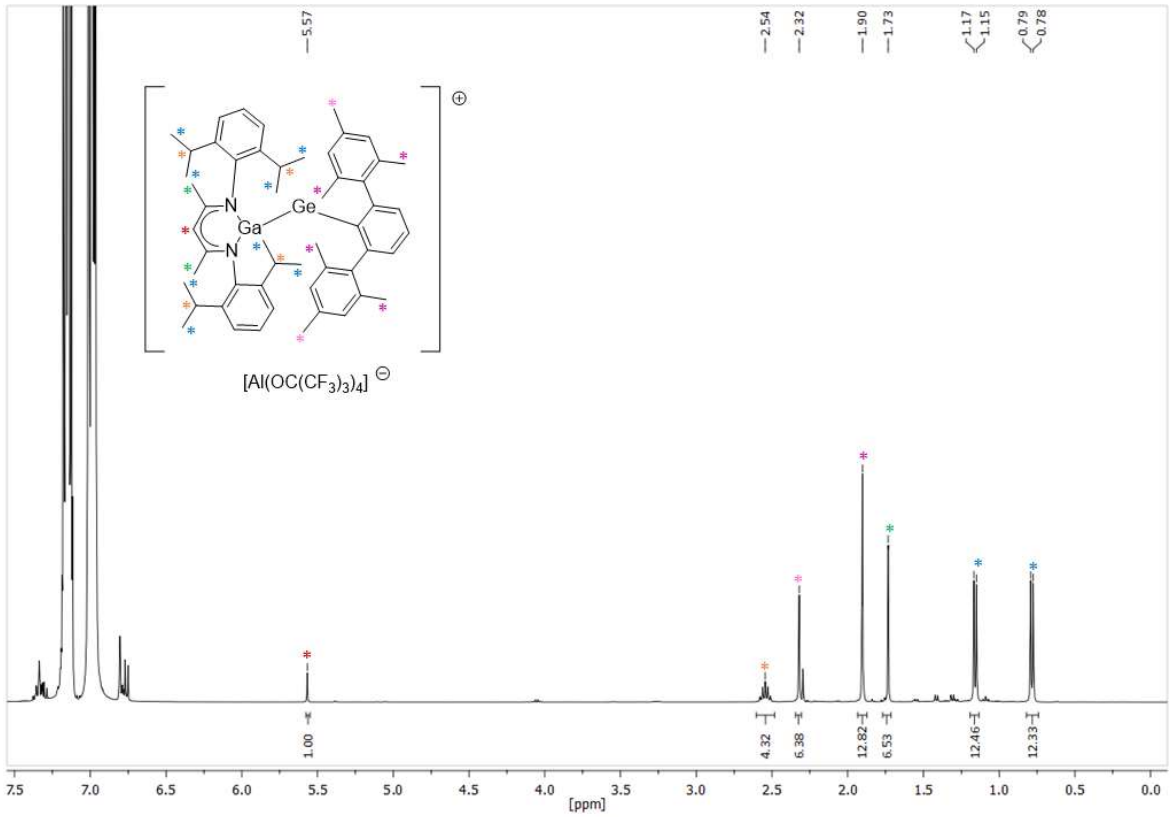


Figure S18: ^{1}H NMR spectrum of **6** in C_6D_6 and fluorobenzene.

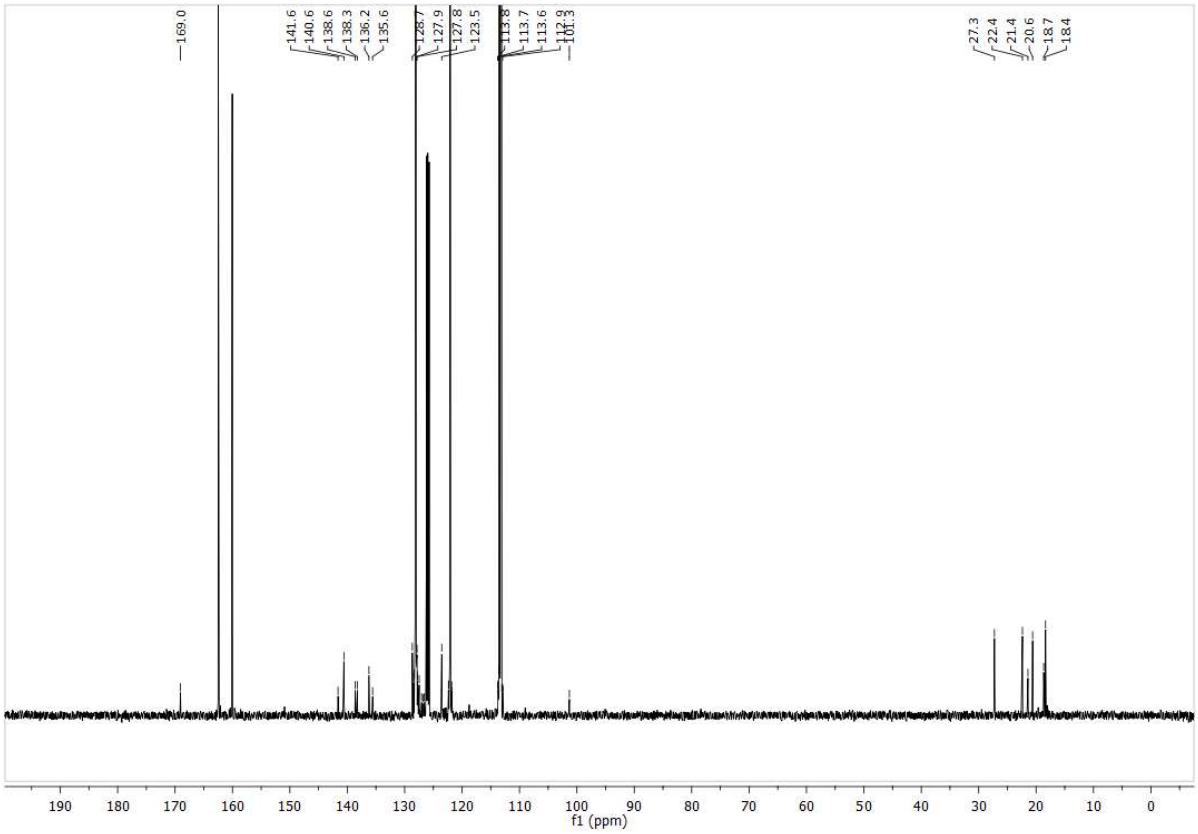


Figure S19: ^{13}C NMR spectrum of **6** in C_6D_6 and fluorobenzene.

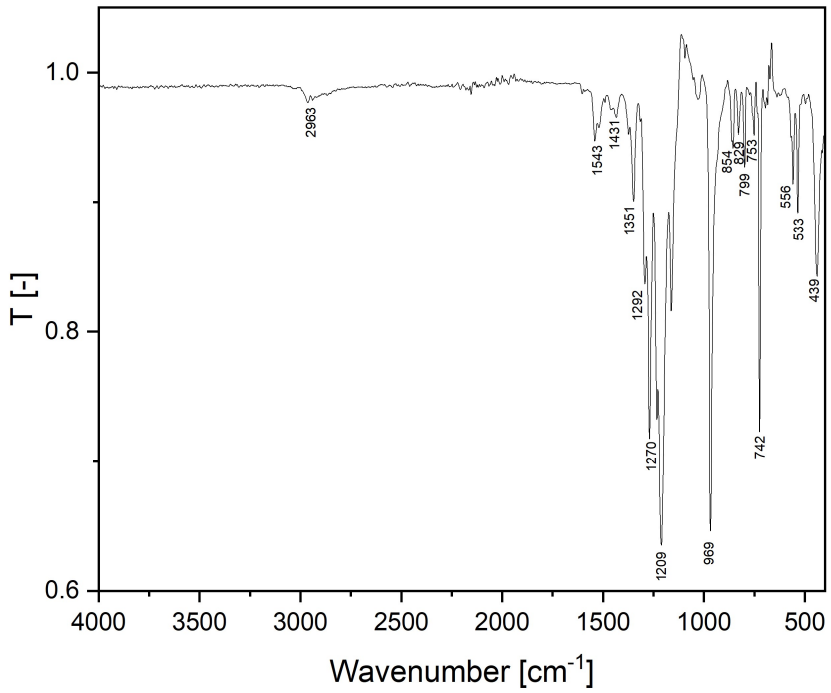


Figure S20: IR spectrum of **6**.

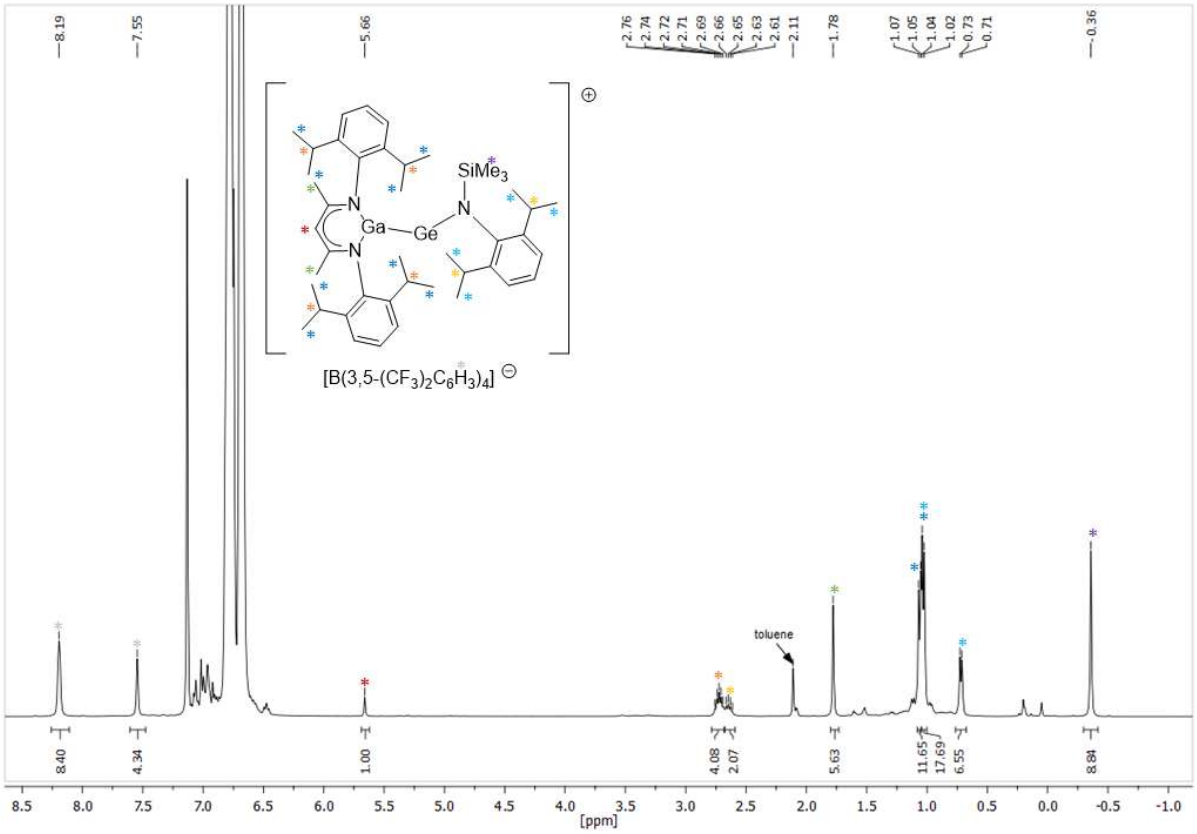


Figure S21: ^{1}H NMR spectrum of **7** in toluene-d_8 and 1,2-difluorobenzene.

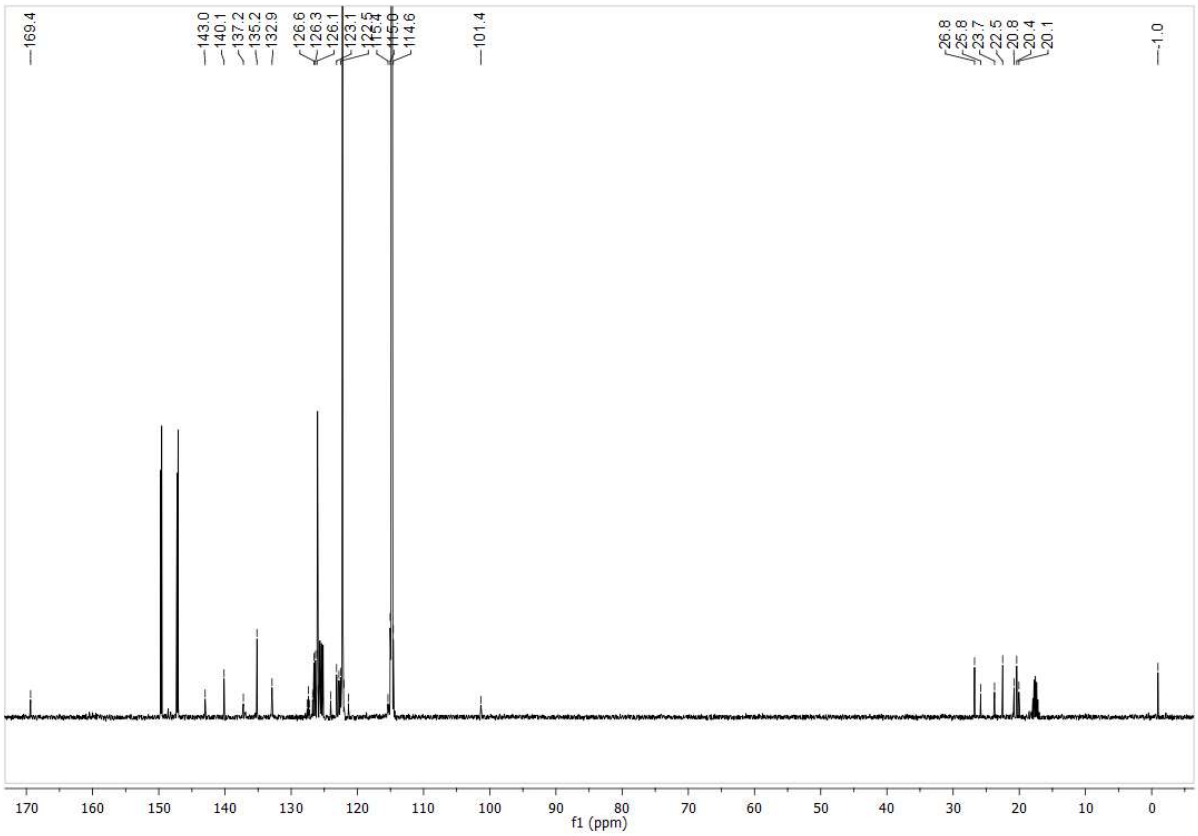


Figure S22: ^{13}C NMR spectrum of **7** in toluene-d_8 and 1,2-difluorobenzene.

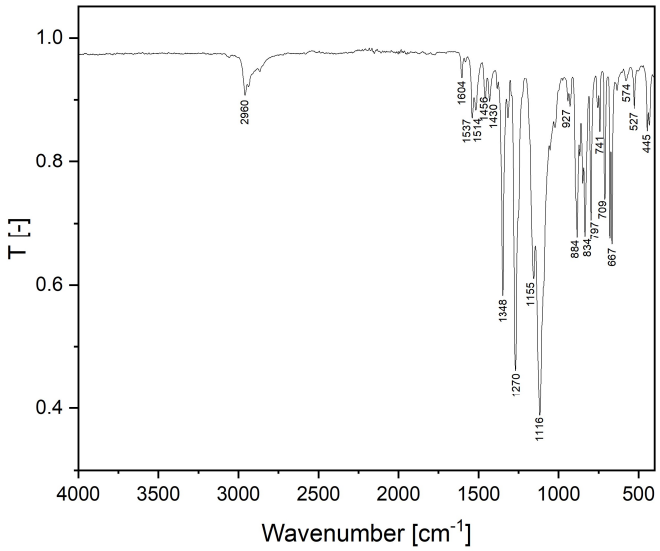


Figure S23: IR spectrum of **7**.

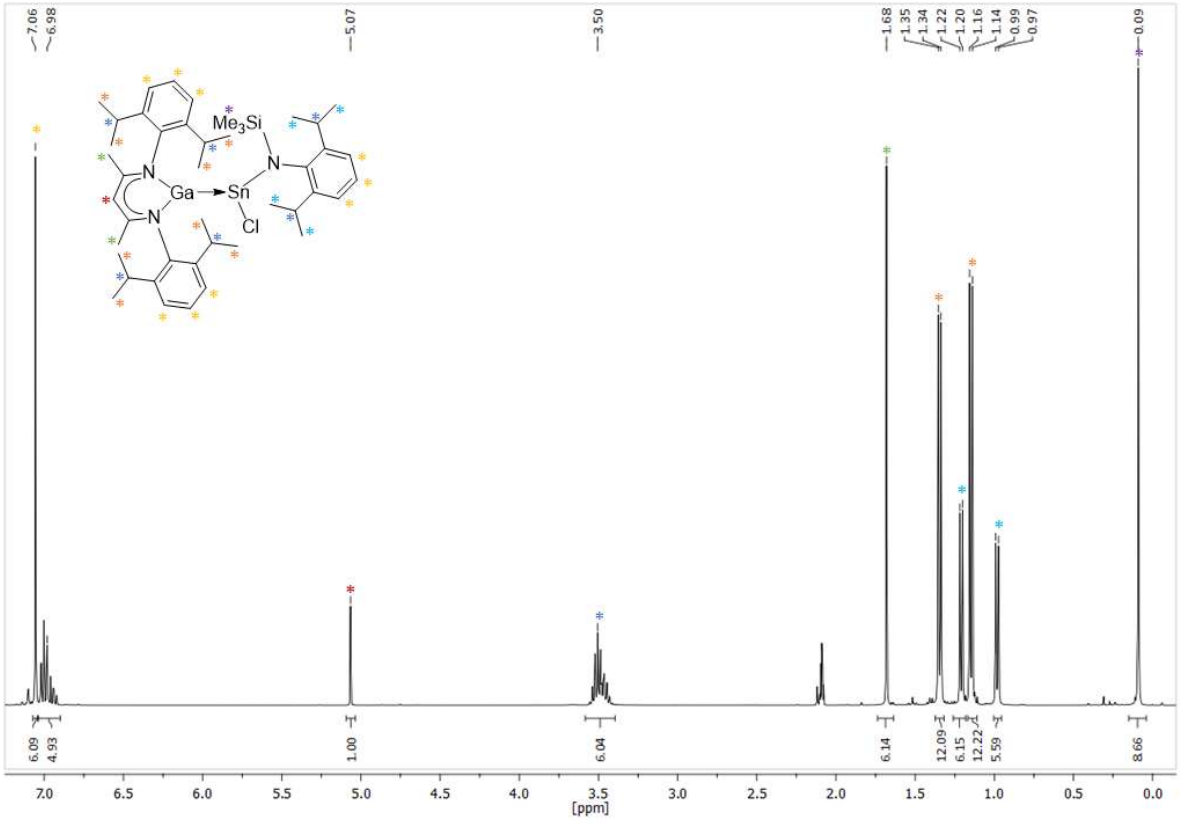


Figure S24: Initial *in situ* ^{1}H NMR spectrum of the reaction of LGa with L'SnCl in toluene-d_8 at r.t.

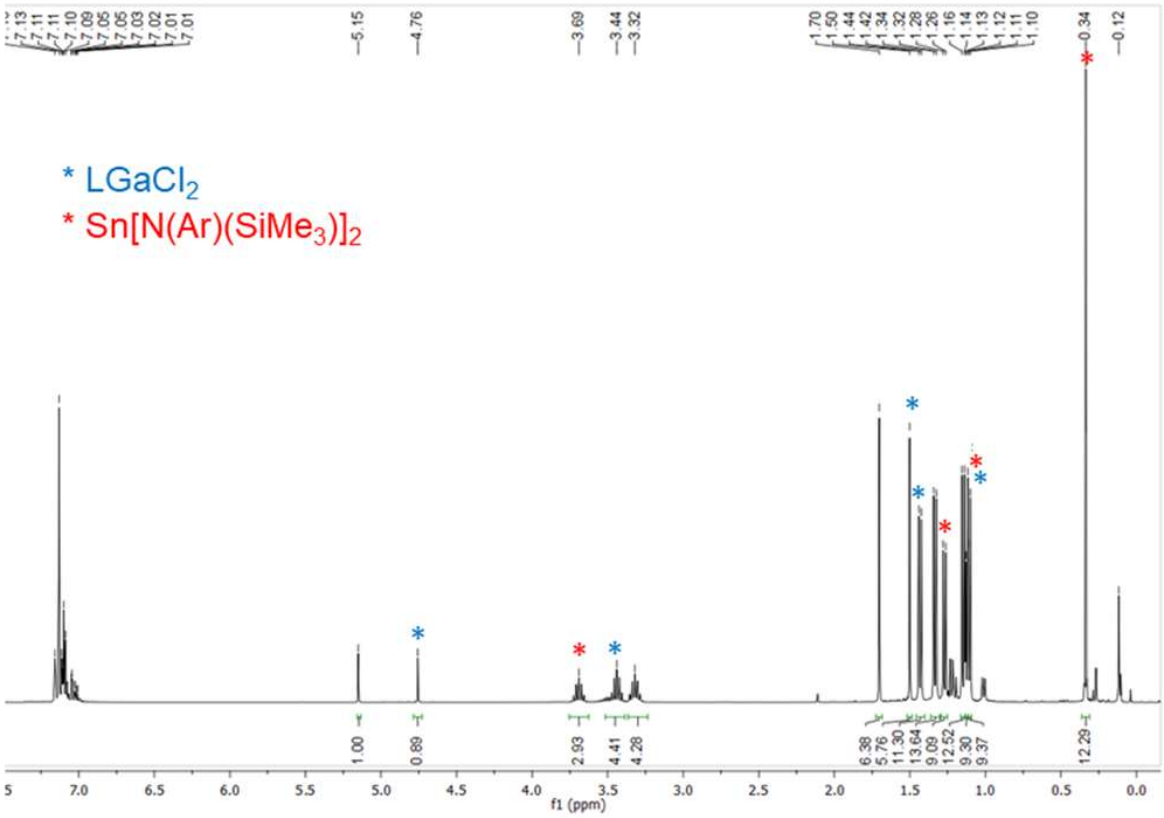


Figure S25: Decomposition of **1** in a C_6D_6 solution after 4 days at r.t.

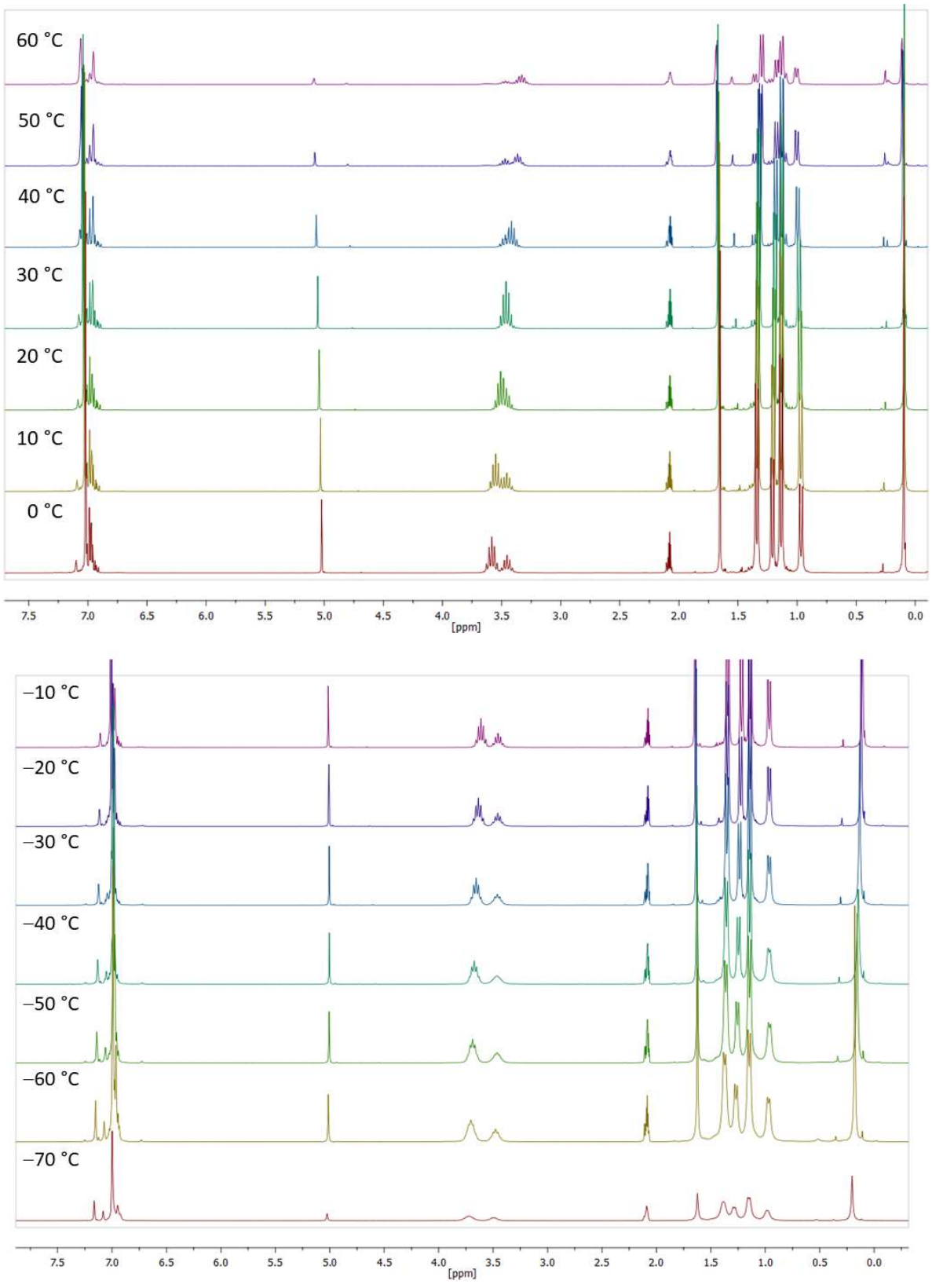


Figure S26: Temperature-dependent *in situ* ^{1}H NMR spectra of **1** in toluene-d_8.

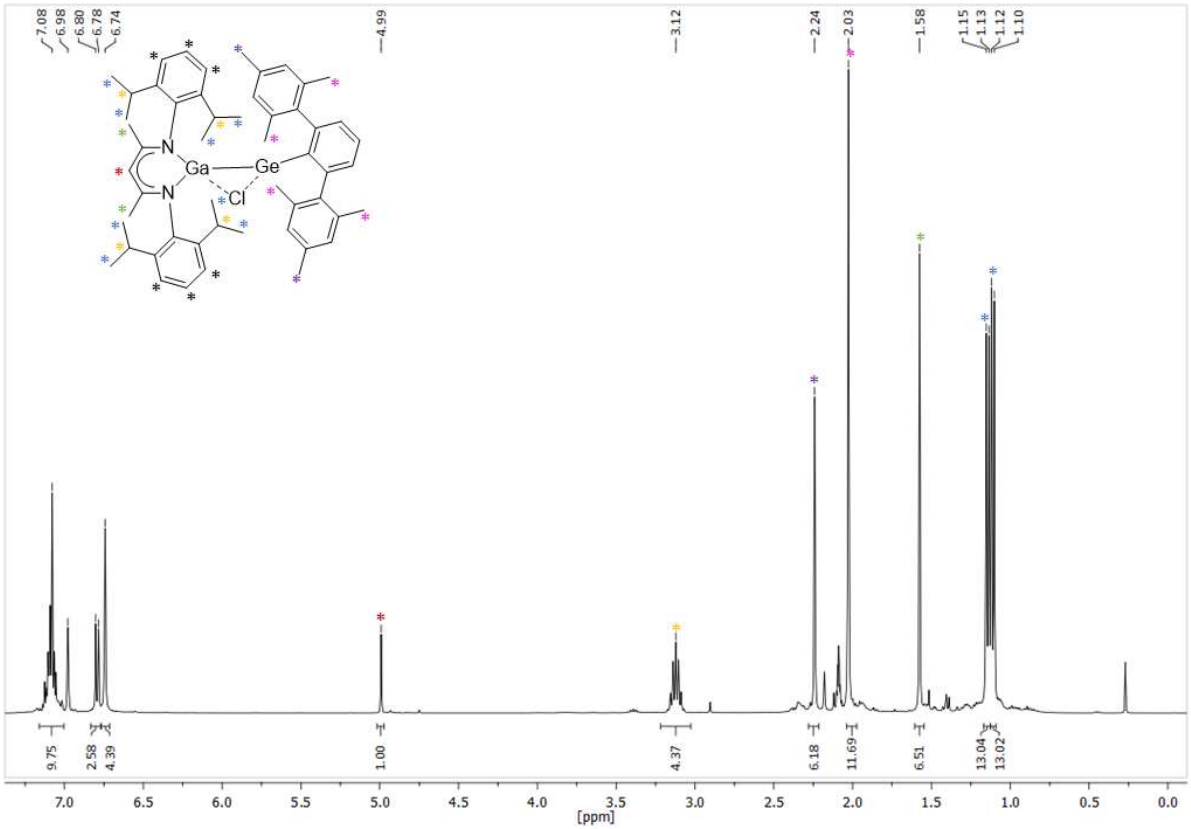


Figure S27: Initial *in situ* ^{1}H NMR spectrum of the reaction of LGa with DMPGeCl in toluene-d_8 at r.t.

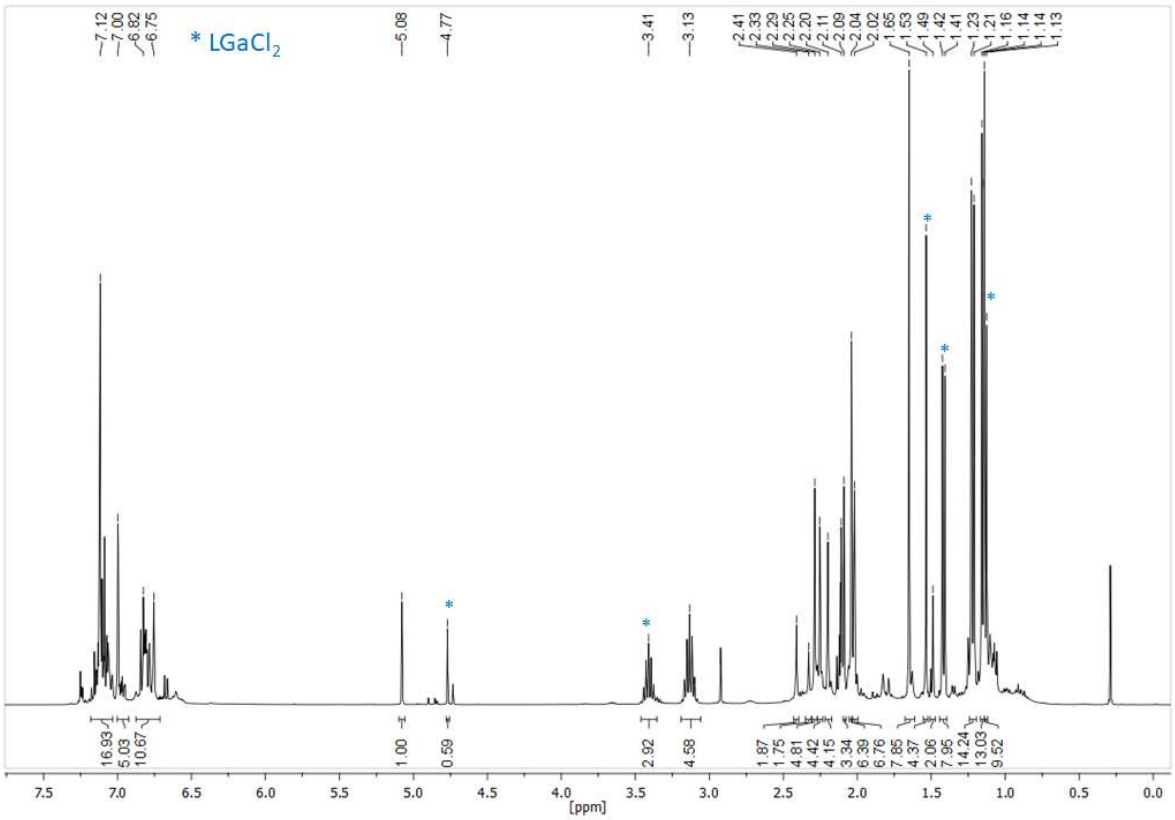


Figure S28: Decomposition of **2** in toluene-d_8 after 90 minutes at ambient temperature.

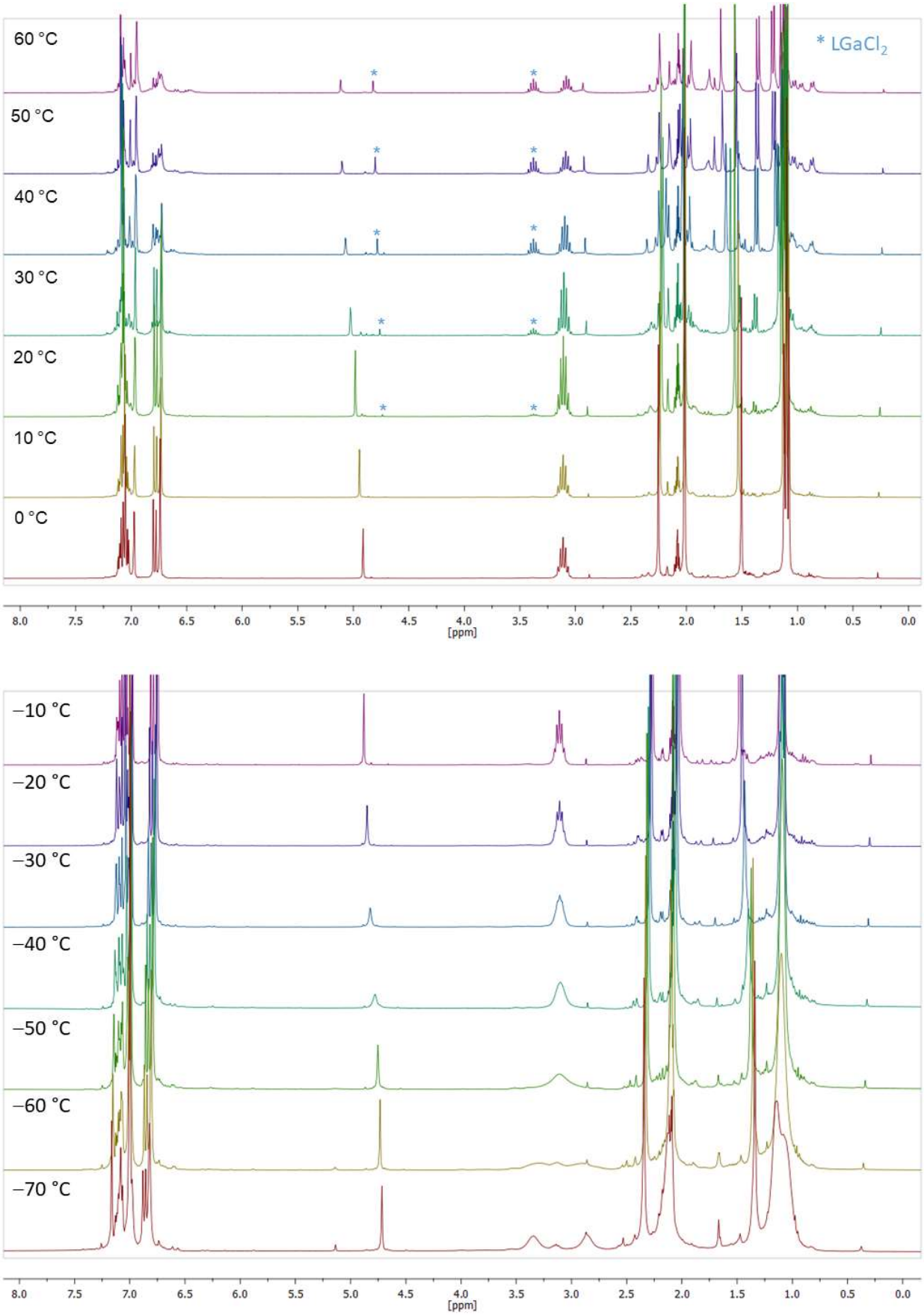


Figure S29: Temperature-dependent *in situ* ^{1}H NMR spectra of **2** in toluene-d_8.

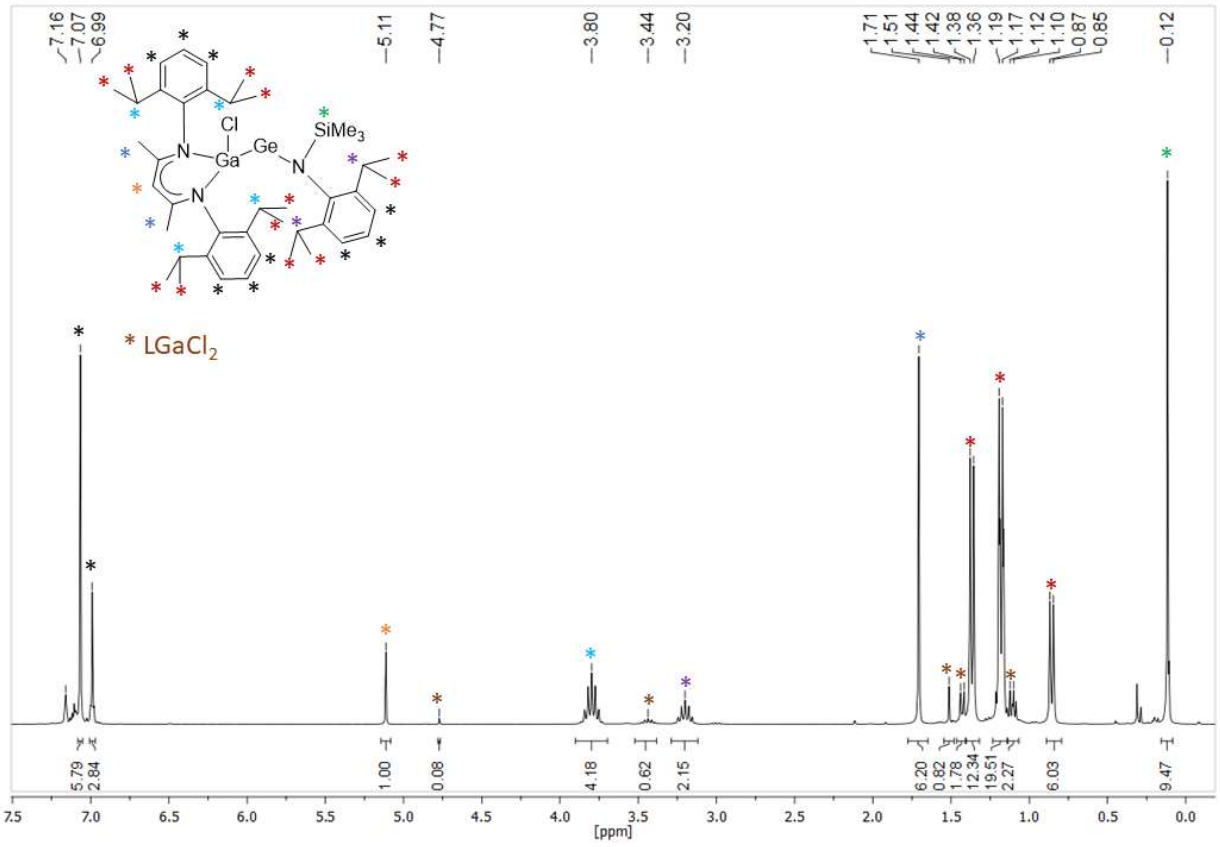


Figure S30: Initial *in situ* ^{1}H NMR spectrum of the reaction of LGa with L'GeCl in C_6D_6 at r.t.

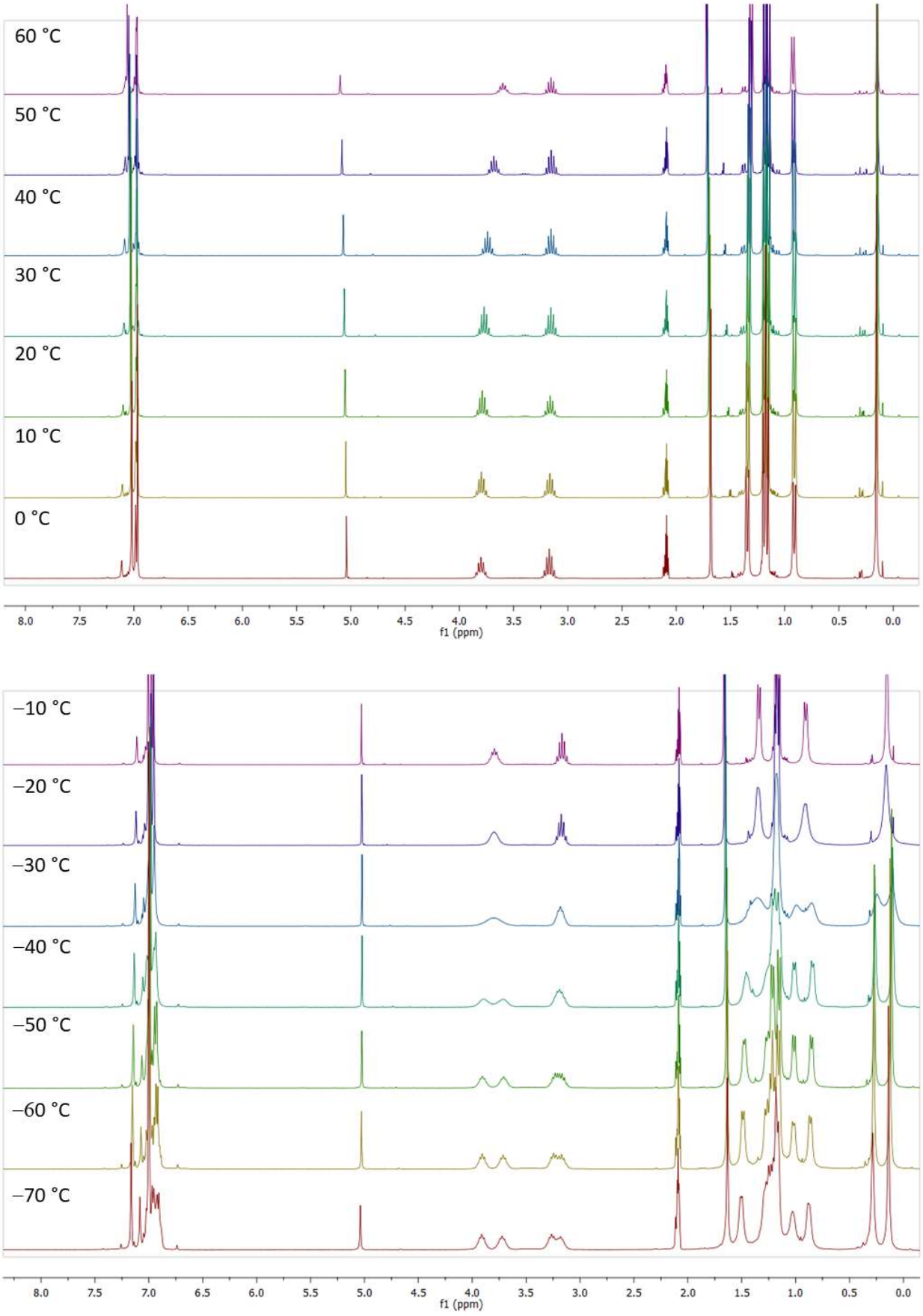


Figure S31: Temperature-dependent *in situ* ^{1}H NMR spectra of **3** in toluene-d_8.

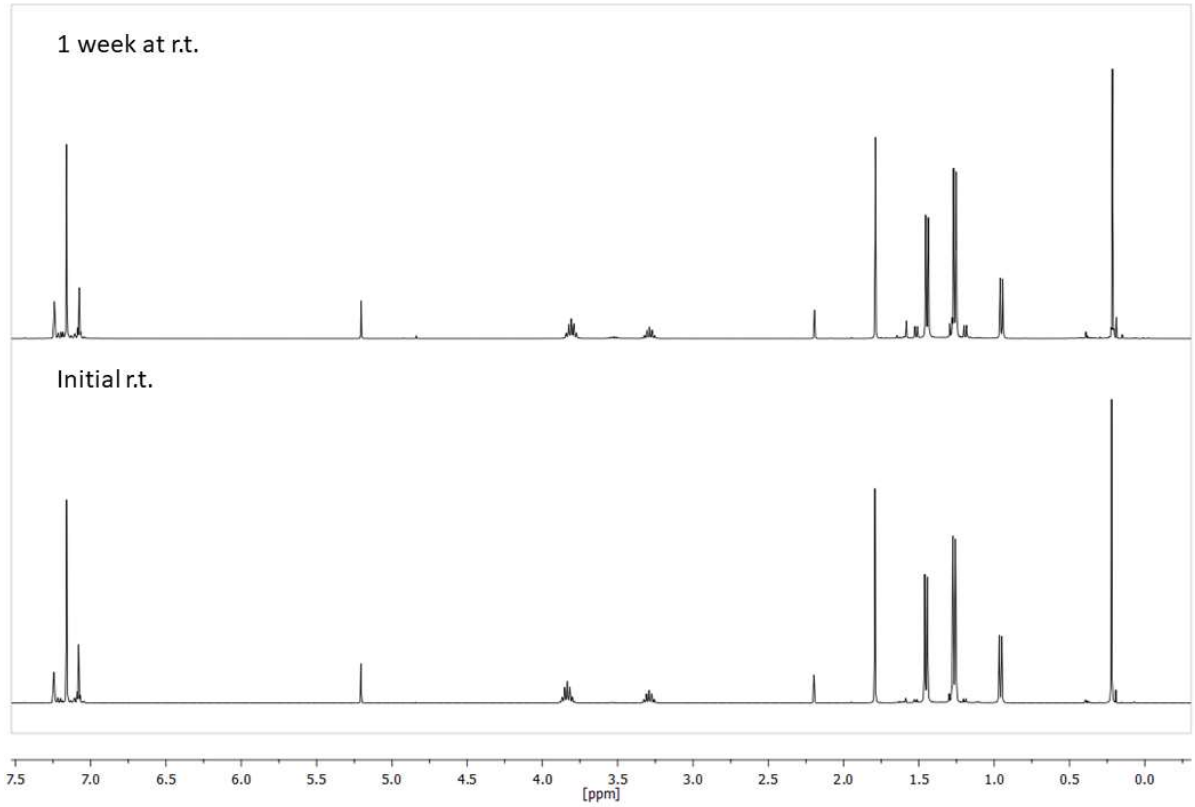


Figure S32: Time-dependent *in situ* ^{1}H NMR spectra of **3** in C_6D_6.

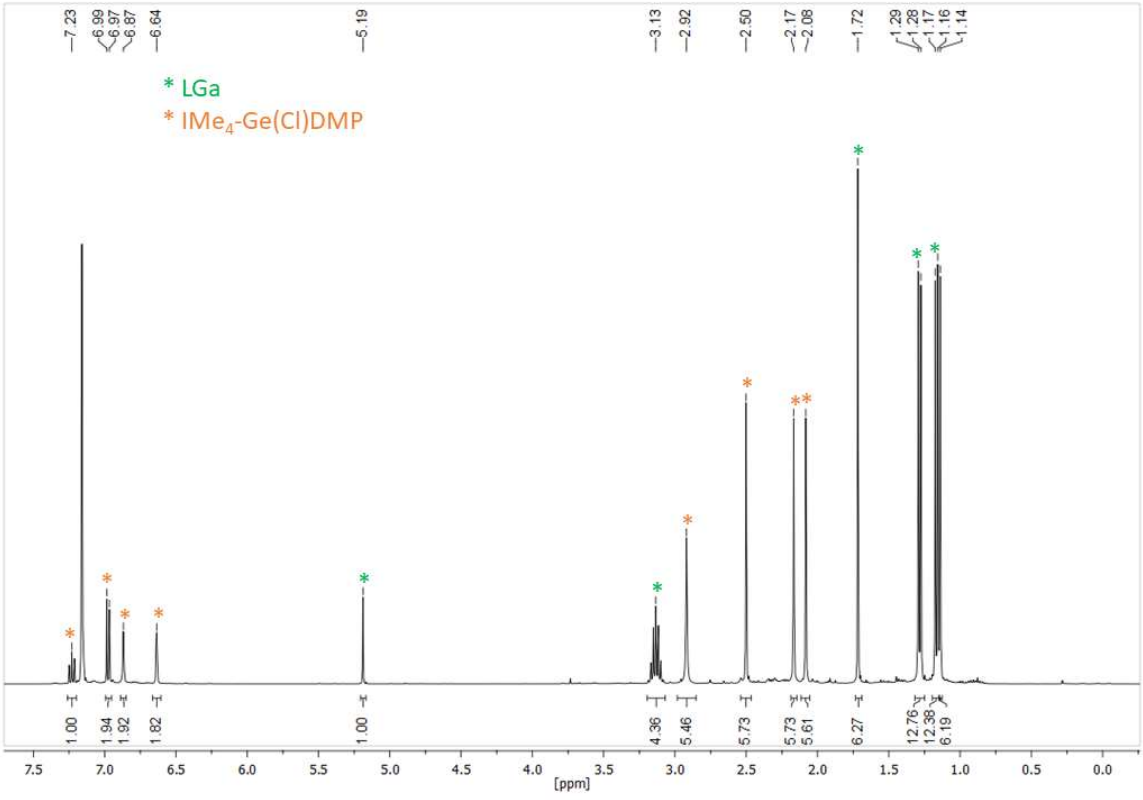


Figure S33: Reaction of **2** with IMe_4 in C_6D_6 at r.t., yielding LGa and IMe_4-Ge(Cl)DMP.

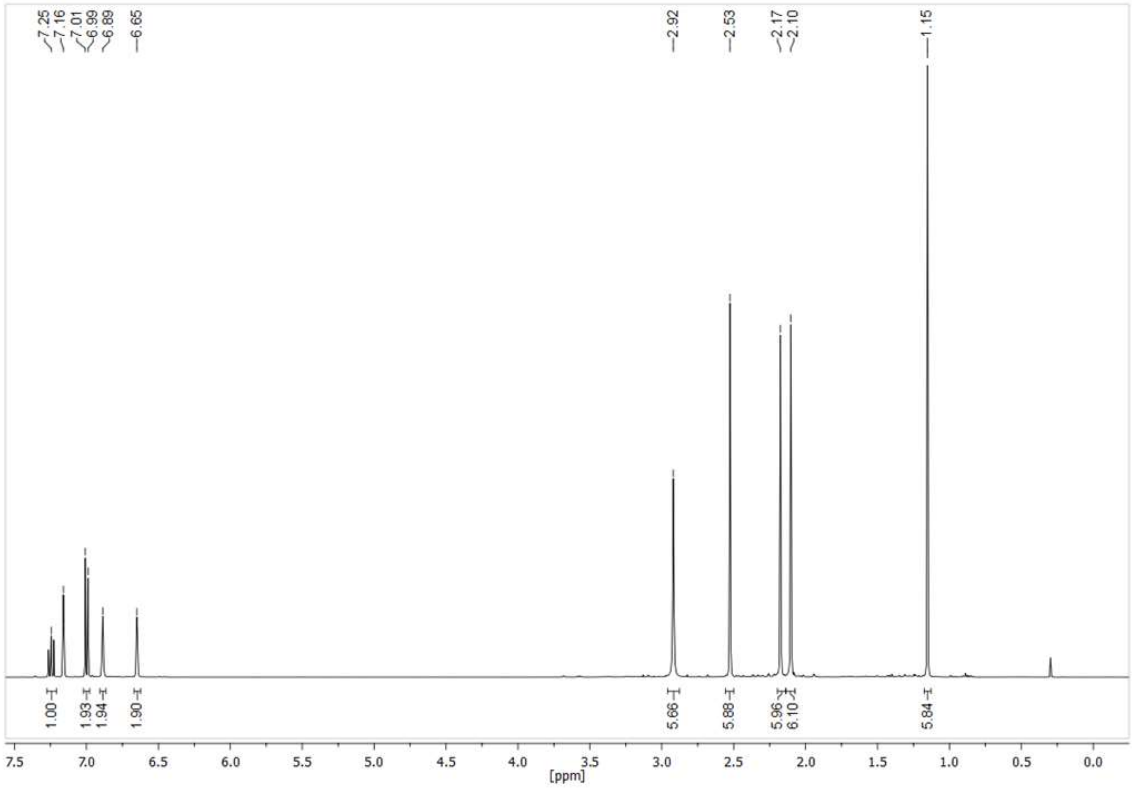


Figure S34: ^{1}H NMR spectra of IMe_4-Ge(Cl)DMP in C_6D_6 for comparison.

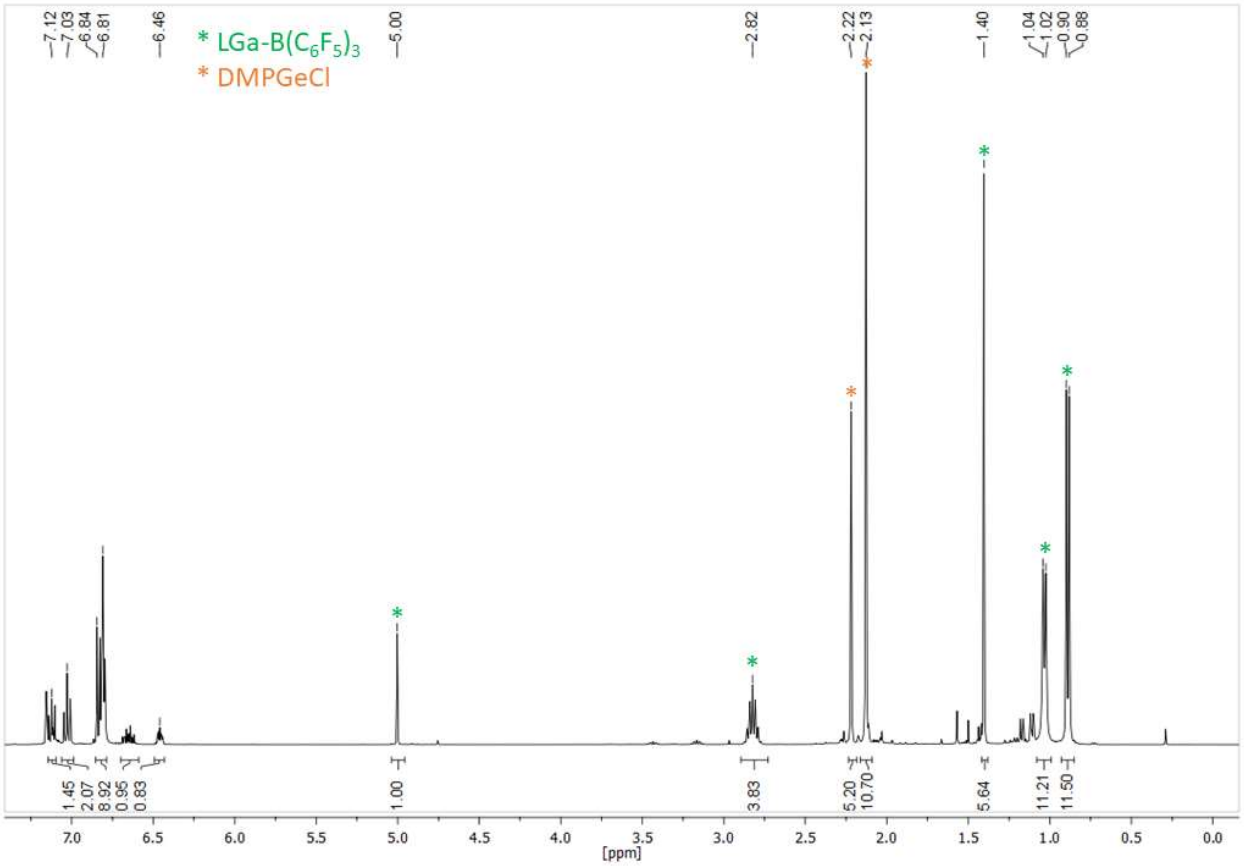


Figure S35: Reaction of **2** with $B(C_6F_5)_3$ in C_6D_6 at r.t., yielding LGa-$B(C_6F_5)_3$ and DMPGeCl.

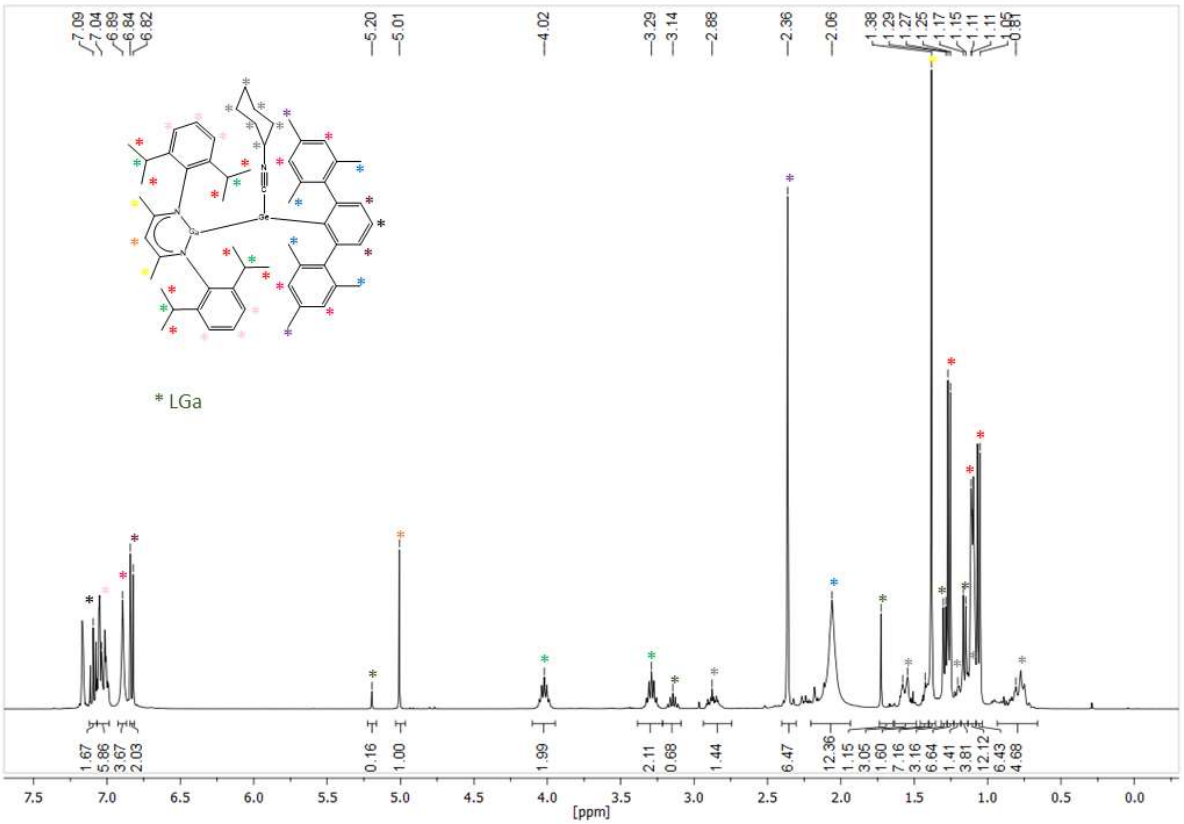


Figure S36: Reaction of **2** with CNCy in C_6D_6 at r.t.

III Crystallographic Part

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data of **2** (ab_167) were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) while those of **1** (ab_006), **3** (ab_191), **4** (ab_265), **5** (ab_047b), **6** (ab_248), and **7** (ab_230) were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $Cu_{K\alpha}$ radiation, λ = 1.54178 Å, microfocus source) at low temperature (details see Tables X1 and X2). The structures were solved by Direct Methods (SHELXS-2013)[1] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017).[2,3] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups.

In **1** (ab_006) the toluene molecule is disordered over a two-fold rotational axis. The central Sn–Cl moiety is disordered over two positions. The Sn–Cl bond lengths of both components were restrained to be equal (SADI). The toluene molecule of **3** (ab_191) is disordered over a centre of inversion. For the refinement the local symmetry was ignored (negative PART). The phenyl ring was constrained to a regular hexagon with edges of 1.39 Å of length. The angles to the methyl group were restrained to be equal (SADI) and RIGU, SIMU and ISOR restraints were applied to the anisotropic displacement parameters of the toluene's atoms. The displacement parameters suggest further disorder but the electron density is too featureless to identify further alternate positions. In **4** (ab_265) an isopropyl group is disordered over two positions. Its bond length and angles were restrained to be equal (SADI) and RIGU restraints were applied to its displacement parameters. The anion in **5** (ab_047b) shows a severe full-body disorder. The individual $–OC(CF_3)_3$ groups were crudely modelled with two alternate sites. All bond corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints were applied to the displacement parameters. Atoms in close proximity were refined with common displacement parameters (EADP) to avoid correlations. The displacement parameters of residue 9 were refined with an additional ISOR restraint due to the low occupancy of this residue. In addition, the structure contains highly disordered solvent – possibly *n*-hexane. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE[4] run. Since the nature and amount of the solvent is not clear it was not included in the sum formula. In **6** (ab_248) both anions show severe full body disorder and were crudely modelled with two alternate sites. All corresponding bond lengths and angles of the $–OC(CF_3)_3$ groups were restrained to be equal (SADI). RIGU and SIMU restraints were applied to all displacement parameters. The oxygen atoms of neighbouring components were refined with common displacement parameters (EADP) to avoid correlations. Furthermore, the fluorobenzene molecule is disordered over two positions. All its corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU and SIMU restraints were used for the displacement parameters. In addition, all its atoms were restrained to lie on a common plane (FLAT). The structure also contains a fluorobenzene molecule highly disordered over a centre of inversion molecules. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.[4] The molecule was included in the sum formula for completeness. All CF_3 groups of **7** (ab_230) show signs of rotational disorder. In two cases this was pronounced enough to be refined with two alternate sites. For one of the groups bond lengths and angles had to be restrained to be equal (SADI) and RIGU restraints were necessary for the refinement of the displacement parameters. For C48 and C48' additional SIMU restraints were applied.

CCDC-2160059 **1** (ab_006), -2160060 **2** (ab_167), -2160061 **3** (ab_191), -2179253 **4** (ab_265), -2160062 **5** (ab_047b), -2160063 **6** (ab_248), and -2160064 **7** (ab_230), contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1: Crystallographic data of **1–4**.

Identification code	**1 ab_006m**	**2 ab_167m**	**3 ab_191m**	**4 ab_265m**
Empirical formula	$C_{47.50}H_{71}ClGaN_3SiSn$	$C_{53}H_{66}ClGaGeN_2$	$C_{47.50}H_{71}ClGaGeN_3Si$	$C_{60}H_{77}ClGaGeN_3$
M	936.02	908.83	889.92	1018.00
Crystal size [mm]	0.110 × 0.069 × 0.046	0.112 × 0.056 × 0.038	0.192 × 0.103 × 0.092	0.117 × 0.107 × 0.055
T [K]	100(2)	100(2)	102(2)	100(2)
Crystal system	monoclinic	triclinic	triclinic	triclinic
Space group	*P*2/*c*	*P-1*	*P-1*	*P-1*
a [Å]	21.6428(13)	10.8257(9)	10.2306(5)	10.8534(10)
b [Å]	11.8899(8)	11.4854(9)	12.1923(6)	12.7554(11)
c [Å]	19.3967(11)	21.0914(18)	20.7888(10)	20.8891(18)
α [°]	90	87.639(4)	81.3746(13)	81.618(3)
β [°]	107.608(3)	87.473(4)	85.1409(14)	83.685(3)
γ [°]	90	65.602(4)	67.7274(13)	70.885(3)
V [Å^3]	4757.5(5)	2385.2(3)	2371.4(2)	2697.2(4)
Z	4	2	2	2
D_{calc} [g·cm^{-3}]	1.307	1.265	1.246	1.253
μ(MK_α [mm^{-1}])	5.872 (M=Cu)	1.287 (M=Mo)	2.482(M=Cu)	2.045(M=Cu)
Transmissions	0.75/0.57	0.75/0.70	0.75/0.63	0.75/0.64
F(000)	1956	956	942	1076
Index ranges	-27 ≤ *h* ≤ 27	-15 ≤ *h* ≤ 15	-13 ≤ *h* ≤ 13	-13 ≤ *h* ≤ 13
	-13 ≤ *k* ≤ 15	-16 ≤ *k* ≤ 16	-14 ≤ *k* ≤ 15	-15 ≤ *k* ≤ 16
	-24 ≤ *l* ≤ 24	-30 ≤ *l* ≤ 30	-26 ≤ *l* ≤ 26	-26 ≤ *l* ≤ 26
ϑ_{max} [°]	81.424	30.870	80.765	80.678
Reflections collected	216210	118858	136125	131791
Independent reflections	10454	14952	10317	11693
R_{int}	0.1331	0.1006	0.0285	0.0561
Refined parameters	548	539	529	641
R_1 [$I > 2\sigma(I)$]	0.0506	0.0433	0.0239	0.0294
wR_2 [all data]	0.1564	0.0990	0.0632	0.0822
GooF	1.043	1.029	1.027	1.036
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.687/-0.783	0.834/-0.573	0.606/-0.525	0.741/-0.544

Table S2: Crystallographic data of **5–7**.

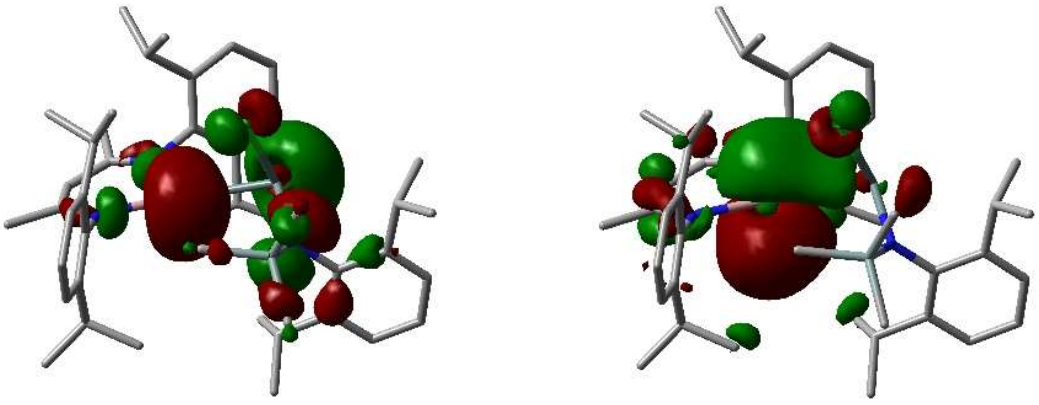
Identification code	**5 ab_047bm_sq**	**6 ab_248m_sq**	**7 ab_230m**
Empirical formula	$C_{60}H_{67}AlF_{36}GaN_3O_4SiSn$	$C_{73.50}H_{69.75}AlF_{36.75}GaGeN_2O_4$	$C_{76}H_{79}BF_{24}GaGeN_3Si$
M	1821.64	1912.60	1671.63
Crystal size [mm]	0.439 × 0.404 × 0.385	0.303 × 0.219 × 0.201	0.454 × 0.307 × 0.164
T [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	*P-1*
a [Å]	21.3750(16)	25.1362(16)	12.5504(12)
b [Å]	19.8369(15)	17.4140(11)	16.4542(16)
c [Å]	20.6724(17)	36.805(2)	20.1733(19)
α [°]	90	90	100.150(4)
β [°]	113.542(3)	96.472(2)	106.824(4)
γ [°]	90	90	93.386(4)
V [Å^3]	8035.8(11)	16007.7(18)	3898.3(7)
Z	4	8	2
D_{calc} [g·cm^{-3}]	1.506	1.587	1.424
μ(MK_α [mm^{-1}])	4.285	2.205	1.937
Transmissions	0.75/0.44	0.75/0.60	0.75/0.55
F(000)	3648	7708	1708
Index ranges	-26 ≤ *h* ≤ 27	-31 ≤ *h* ≤ 31	-16 ≤ *h* ≤ 16
	-25 ≤ *k* ≤ 24	-20 ≤ *k* ≤ 21	-20 ≤ *k* ≤ 20
	-26 ≤ *l* ≤ 25	-46 ≤ *l* ≤ 46	-25 ≤ *l* ≤ 25
ϑ_{max} [°]	79.850	79.639	80.798
Reflections collected	228480	454318	208405
Independent reflections	17440	34579	16862
R_{int}	0.0871	0.0532	0.0516
Refined parameters	1436	3179	1046
R_1 [$I > 2\sigma(I)$]	0.0502	0.0477	0.0358
wR_2 [all data]	0.1436	0.1262	0.0976
GooF	1.024	1.021	1.023
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.823/-0.760	1.457/-0.864	1.139/-0.762

IV. Computational Details

All calculations were performed by using the program package Gaussian 16[8]. The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP[9] together with the dispersion correction with Becke-Johnson damping[10] (D3BJ) using Gaussian 16. The basis set def2-TZVP was applied. For all structures C1 symmetry was applied. Frequency calculations were carried out at each of the stationary points to verify the nature of the stationary point. It turned out that all products have no imaginary frequency. Natural bond orbital analysis was performed using the NBO[11] version 3.1 implemented in Gaussian 16. Quantum theory of atoms in molecules (QTAIM)[12] analyses (B3LYP-D3BJ/TZP) were performed using Amsterdam Density Functional (ADF)

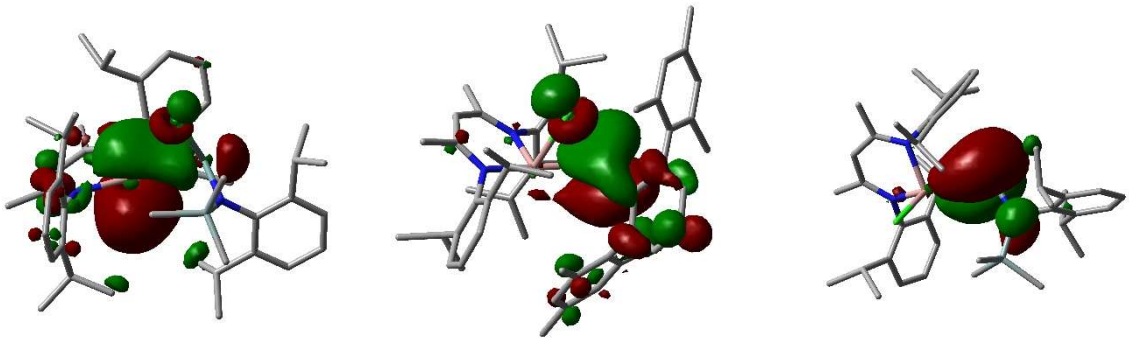
Table S3: Calculated bond length [Å] and bond angles [°] of **1**–**3** and **5**–**8**.

	Ga–Cl	**E–Cl**	**E–Ga**	**E–C/N**	**Ga–E–C/N**
1	–	2.4978	2.9478	2.1253	105.35
2	2.5018	2.6039	2.4943	2.0194	111.26
3	2.2662	–	2.5864	1.8592	108.52
7	–	2.3335	2.7434	1.9086	108.41
	–	–	–	–	–
5	–	–	2.8296	2.0576	101.38
6	–	–	2.6355	2.0056	99.62
7	–	–	2.6095	1.8299	106.12

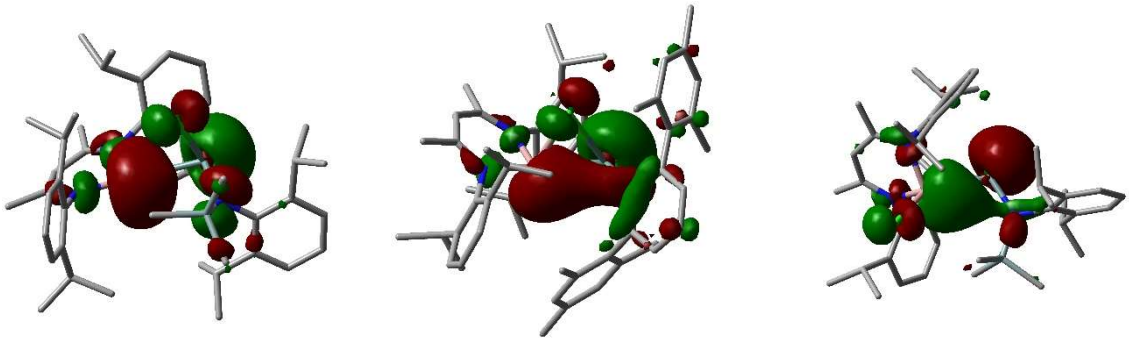


HOMO (-0.1977 au) LUMO+1 (-0.0544 au)

Figure S37: Selected orbitals of **1** calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03). Hydrogen atoms are omitted for clarity.



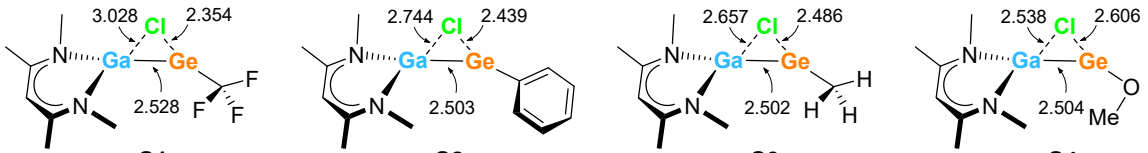
LUMO+1 (-0.0500 au) LUMO+1 (-0.0413 au) LUMO (-0.0814 au)



HOMO (-0.1914 au) HOMO (-0.1817 au) HOMO (-0.1951 au)

8 **2** **3**

Figure S38: Selected orbitals of **8** (left), **2** (middle), and **3** (right) calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03). Hydrogen atoms are omitted for clarity.



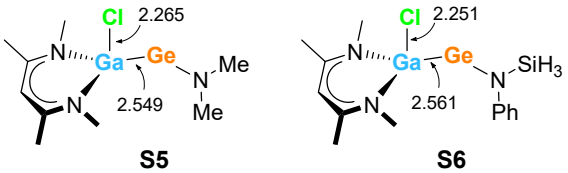
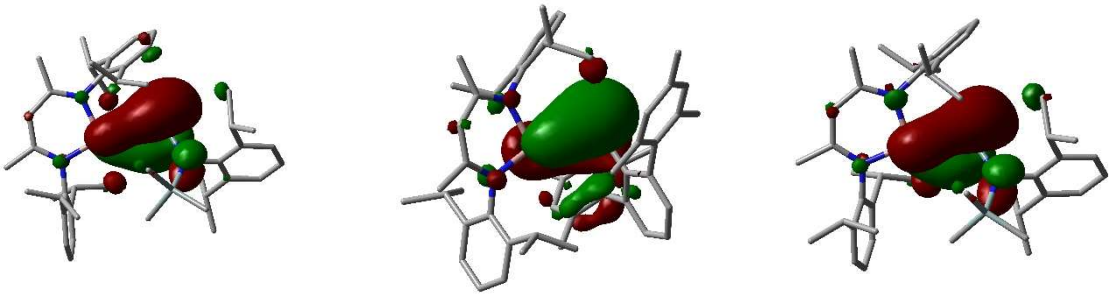
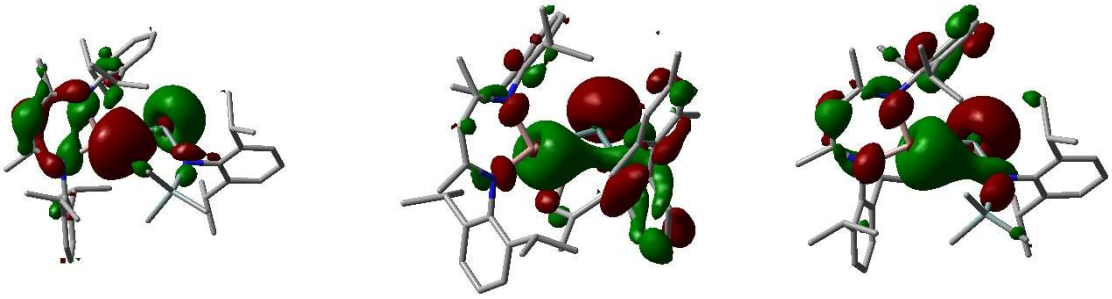


Figure S39: Calculated (B3LYP-D3BJ/def2-TZVP) bond lengths [Å] of the reference compounds **S1–S6**.



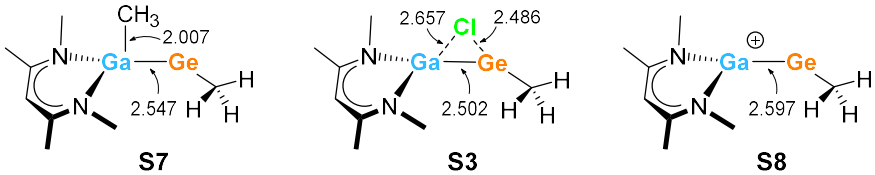
LUMO (-0.1933 au) LUMO (-0.1954 au) LUMO (-0.1903 au)



HOMO-2 (-0.3280 au) HOMO (-0.3054 au) HOMO-2 (-0.3251 au)

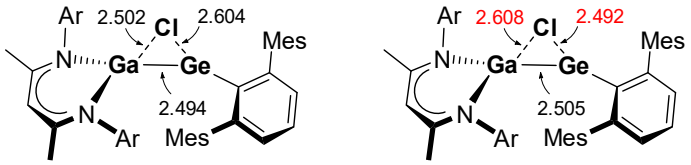
5^{+} **6**$^{+}$ **7**$^{+}$

Figure S40: Selected orbitals of **5** (left), **6** (middle), and **7** (right) calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.03). Hydrogen atoms are omitted for clarity.



S7 **S3** **S8**

Figure S41: Calculated (B3LYP-D3BJ/def2-TZVP) bond lengths [Å] of the reference compounds **S3**, **S7** and **S8**.



2 **2**-fix

ΔE = 0.0 kcal/mol ΔE = 0.3 kcal/mol

Figure S42: Germylene compounds **2** and **2**-fix. In **2**, all structural parameters were optimized using B3LYP-D3BJ/def2-TZVP. For system **2**-fix, all structural parameters were optimized using B3LYP-D3BJ/def2-TZVP with two exceptions: for the bond lengths for Ga-Cl and Ge-Cl, the experimental data were used. The bond lengths are given in Å. The energy of **2**-fix is only 0.3 kcal/mol higher than that of **2**; i.e., the energy hypersurface is very flat in this region. Ga and Ge compete strongly for bonding to the chlorine atom, so that the weakening of one bond (e.g. Ga-Cl) is compensated energetically by the strengthening of the other bond (Ge-Cl).

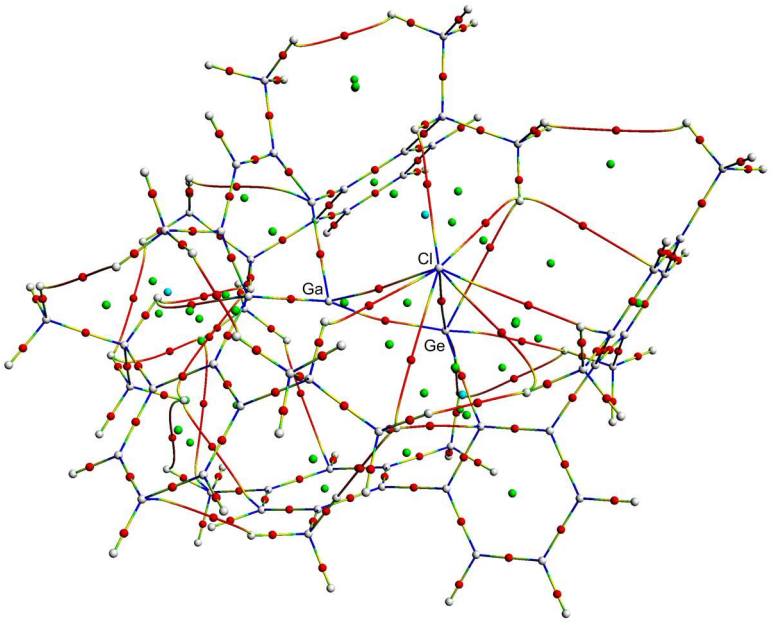


Figure S43: Molecular graphs of **2** showing the bond paths (lines) as well as the nuclear (white dots), bond (red dots), ring (green dots) and cage (blue dots) critical points (B3LYP-D3BJ/TZP).

Table S4: Selected bond distances and distances [Å] between the bond critical points (BCP) and the atoms of the bonds in **2** (B3LYP-D3BJ/TZP).

Bond A-B	$d_{(A\text{-}B)}$ [Å]	$d_{(A\text{-}BCP)}$ [Å]	$d_{(BCP\text{-}B)}$ [Å]	$\alpha_{(A\text{-}BCP\text{-}B)}$ [°]
Ga-Ge	2.4943	1.2610	1.2460	168.5
Ga-Cl	2.5018	1.1193	1.3853	174.5
Ge-Cl	2.6038	1.1769	1.4291	175.4

Table S5: Topological and energetic properties of the electron density $\rho(\mathbf{r})$ calculated at the bond critical points of selected bonds of **2**. The electron density (ρ_{CP}), the Laplacian of the electron density ($\nabla^2\rho_{CP}$), the electron kinetic (G_{CP}), potential (V_{CP}) and total (H_{CP}) energy densities at the critical points are given in a.u. (B3LYP-D3BJ/TZP).

Bond A-B	ρ_{CP}	$\nabla^2\rho_{CP}$	G_{CP}	V_{CP}	H_{CP}
Ga-Ge	0.06118675	-0.00919826	0.02574611	-0.05379179	-0.002804568
Ga-Cl	0.04705063	0.09992949	0.03426161	-0.04354084	-0.009279232
Ge-Cl	0.04220239	0.06911158	0.02620663	-0.03513537	-0.008928738

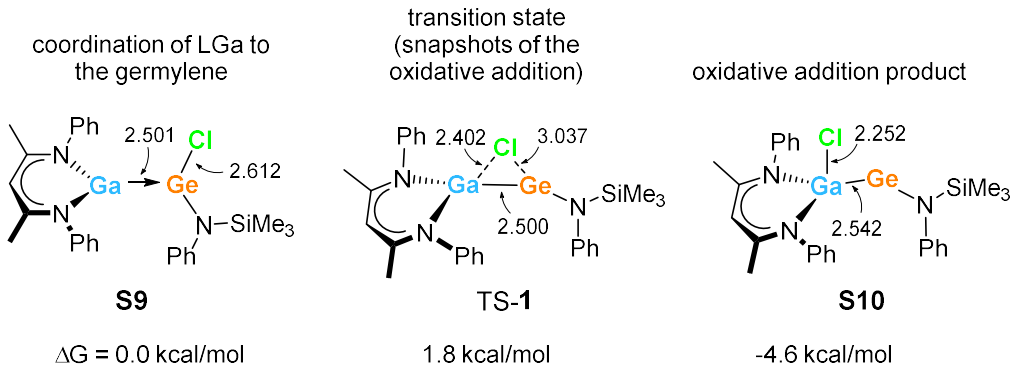


Figure S44: Oxidative addition calculated with B3LYP-D3BJ/def2-TZVP. Coordination of LGa to the germylene leads to **S9**. Migration of the chlorine substituents via the transition state TS-**1** leads to the oxidative addition product **S10**. In the transition state TS-**1**, the chlorine atom is bonded to both the Ge and Ga atoms, resembling compound **2**. The free enthalpies are given relative to **S9**.

V. Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S6: Absolute energies [au] calculated by means B3LYP-D3BJ/def2-TZVP.

	E
1	-4771.560922
2	-6632.354697
3	-6634.228168
5	-4311.083567
6	-6171.874446
7	-6173.740173
8	-6634.213361
S1	-5184.356499
S2	-5078.320529
S3	-4886.492624
S4	-4961.769863
S5	-4981.216984
S6	-5424.470362
S7	-4466.117686
S8	-4425.983730
2-fix	-6632.354289
S9	-5926.190301
TS-**1**	-5926.189544
S10	-5926.193785

Cartesian coordinates of the optimized geometry for 1 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Sn	1.33625900	-1.05721300	-0.59564100
Cl	0.50429300	-0.54668800	-2.89475900
Ga	-1.24300400	-0.00273100	0.36623300
Si	2.69560700	2.07609700	-1.30572000
N	-2.75015500	1.29760500	0.52080500
N	-2.44708600	-1.53773300	0.90255500
N	2.70103400	0.56432600	-0.43735900
C	-3.93063300	1.05442900	1.09492800
C	-4.31343000	-0.19310700	1.58542500
H	-5.28746800	-0.23976700	2.04738400
C	-3.66334200	-1.42192600	1.41698700
C	-4.93834400	2.17033600	1.20642800
H	-4.59572800	2.93057000	1.90863800
H	-5.89642600	1.78837000	1.54928600

H	-5.07409300	2.66765600	0.24675700
C	-4.45317000	-2.64889300	1.79738000
H	-5.13910100	-2.90665200	0.98876400
H	-5.05336600	-2.44507900	2.68316600
H	-3.81697200	-3.50983900	1.97948800
C	-2.51264500	2.57576900	-0.08902900
C	-2.14221500	3.67395100	0.70090500
C	-1.92793000	4.89680600	0.06917600
H	-1.63867700	5.75746500	0.65678000
C	-2.06795600	5.02528800	-1.30203500
H	-1.89910900	5.98326400	-1.77662200
C	-2.39456700	3.91981800	-2.07175600
H	-2.46196500	4.02539400	-3.14450700
C	-2.60841000	2.67355300	-1.48954400
C	-1.90162200	3.53776400	2.19377500
H	-2.38401100	2.62144700	2.53295100
C	-2.48733700	4.69384800	3.00945500
H	-2.38761000	4.48792600	4.07665600
H	-3.54530500	4.84643700	2.78934300
H	-1.96865700	5.63264600	2.80970000
C	-0.40110700	3.38222500	2.46869300
H	0.00890200	2.52188900	1.94044500
H	-0.21593000	3.24637100	3.53588600
H	0.14911000	4.26463500	2.13676500
C	-2.92169900	1.45715500	-2.34814400
H	-2.40576000	0.60119000	-1.90231800
C	-4.42112300	1.13018200	-2.35578200
H	-4.99241000	1.97476600	-2.74740600
H	-4.79630100	0.89819000	-1.36069300
H	-4.61494300	0.26641100	-2.99394800
C	-2.39614200	1.56827100	-3.77900500
H	-2.95447500	2.30732600	-4.35764600
H	-2.50306600	0.60691300	-4.28118500
H	-1.33988800	1.83219200	-3.79762200
C	-1.92464000	-2.82605200	0.54814200
C	-0.93714600	-3.41608800	1.36037900
C	-0.40056200	-4.63510500	0.95706600
H	0.36143000	-5.10820200	1.55857400
C	-0.81023000	-5.24735900	-0.21798700
H	-0.37128800	-6.19011400	-0.51773200
C	-1.76857200	-4.64397100	-1.01253700
H	-2.07109800	-5.11881800	-1.93640300
C	-2.34450200	-3.42735600	-0.65054500
C	-0.47099900	-2.75006900	2.64438600
H	-0.46939600	-1.67114300	2.46695800
C	0.94981200	-3.14216300	3.05186300
H	1.00250200	-4.18377400	3.37392500
H	1.27556000	-2.52711200	3.89040100
H	1.65797900	-3.00036500	2.23504600
C	-1.44069600	-3.00957600	3.80576300
H	-1.53496500	-4.08159900	3.99216400
H	-2.43354600	-2.61257100	3.60436800
H	-1.07136100	-2.53789100	4.71848100
C	-3.37622900	-2.79518600	-1.57056000
H	-3.75294700	-1.89071300	-1.09466600
C	-2.74807200	-2.37968600	-2.90584300
H	-2.37351000	-3.24957700	-3.44861200
H	-1.90911100	-1.69990600	-2.76785400
H	-3.49262000	-1.88939500	-3.53644700
C	-4.57325800	-3.72500700	-1.80922600
H	-4.27805700	-4.60966900	-2.37596200
H	-5.34394600	-3.20750400	-2.38367100
H	-5.01609000	-4.06720900	-0.87327200
C	0.95919900	2.77087200	-1.34451700
H	0.28363100	2.09920100	-1.87152100
H	0.94364600	3.72979500	-1.86722100
H	0.56170300	2.93664000	-0.34358300
C	3.29247500	1.92095200	-3.08192400
H	4.34923600	1.65734100	-3.13986900
H	3.16214400	2.87551500	-3.60013400

H	2.71852800	1.16460300	-3.61844300
C	3.83180600	3.30133800	-0.43993700
H	4.83130700	2.88831500	-0.29162300
H	3.44676700	3.59927100	0.53597700
H	3.92975100	4.20357600	-1.04930500
C	3.82142300	0.19539100	0.36216700
C	4.88121300	-0.56699900	-0.18117900
C	5.93934800	-0.94995700	0.64194200
H	6.74880700	-1.53586500	0.22453500
C	5.97750900	-0.59713600	1.97986900
H	6.80786700	-0.90312200	2.60356900
C	4.94017500	0.15299600	2.51317500
H	4.96956600	0.42666900	3.56011100
C	3.86310600	0.55595600	1.72993400
C	4.90004200	-0.98483900	-1.64000200
H	4.03093700	-0.53895600	-2.11834400
C	4.78393300	-2.50615000	-1.79668500
H	4.74979200	-2.78137500	-2.85300900
H	3.87783700	-2.88444600	-1.31935600
H	5.63474200	-3.01735100	-1.34079900
C	6.14392600	-0.45802300	-2.36463500
H	7.05592600	-0.91830300	-1.97867700
H	6.24142000	0.62156000	-2.24357400
H	6.08517300	-0.67771400	-3.43271600
C	2.72483500	1.33179900	2.36492600
H	2.15069400	1.77352600	1.55285300
C	1.79058200	0.37759800	3.11685600
H	1.39970700	-0.38685600	2.44589000
H	0.94493000	0.91216100	3.55459200
H	2.32452500	-0.13394200	3.92035500
C	3.19812200	2.46179300	3.28213600
H	3.69049000	2.07868700	4.17808300
H	2.34841000	3.06350500	3.60992900
H	3.90275500	3.11699100	2.76942300

Cartesian coordinates of the optimized geometry for 2 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.41922200	-0.07853500	0.79614400
Ga	0.64416400	0.48641600	-0.48638900
Cl	-1.44335000	0.07668300	-1.80304700
N	0.55611700	2.50827000	-0.63122800
N	2.05246200	0.32227700	-1.85309900
C	1.05071900	3.17266800	-1.65393100
C	1.75003700	2.55886900	-2.71126700
H	2.02298300	3.21467300	-3.52381300
C	2.26850900	1.27368600	-2.77250000
C	0.92707800	4.67244200	-1.74753000
H	0.23119300	4.93013100	-2.54717300
H	1.89316800	5.10596700	-2.00482300
H	0.56992300	5.11588200	-0.82369700
C	3.16259900	0.95105400	-3.94223300
H	2.73988000	0.13044200	-4.52209400
H	4.14762700	0.62550300	-3.61079600
H	3.27608600	1.81660600	-4.58953000
C	-0.11767200	3.16308300	0.45161400
C	0.55510400	3.24477200	1.68700500
C	-0.11424800	3.80575400	2.76977500
H	0.38126400	3.87677900	3.72693400
C	-1.41362200	4.27412400	2.64353800
H	-1.91970700	4.70555800	3.49769600
C	-2.06214800	4.17800700	1.42647100
H	-3.08085600	4.53120000	1.33746000
C	-1.44119300	3.61655400	0.31117800
C	1.98998300	2.76425600	1.82888600
H	2.09485200	1.85809800	1.22600800
C	2.97733300	3.79846400	1.27073000
H	2.79603500	4.00465400	0.21754300
H	4.00382000	3.44073600	1.37015700
H	2.89107200	4.73902700	1.81901300
C	2.37057800	2.38204600	3.25799400

H	2.41508400	3.25464400	3.91256000
H	3.35730000	1.92014100	3.26572600
H	1.66430600	1.66737900	3.67808700
C	-2.23223800	3.51277800	-0.98223400
H	-1.62126000	2.98838300	-1.71477100
C	-2.58669400	4.89933900	-1.54049600
H	-3.07582100	4.79988100	-2.51173600
H	-1.71068100	5.53432800	-1.66342700
H	-3.27784400	5.41953400	-0.87423100
C	-3.51747500	2.69513400	-0.79791700
H	-4.23080300	3.22061900	-0.15930200
H	-3.31824000	1.72494400	-0.35184700
H	-3.99326600	2.52461300	-1.76462900
C	2.91049500	-0.82767800	-1.83504200
C	4.12088600	-0.74147300	-1.12249100
C	4.95522000	-1.85604100	-1.09648600
H	5.89112200	-1.80768400	-0.55469100
C	4.61209700	-3.02220900	-1.76285200
H	5.27292600	-3.87911900	-1.73363300
C	3.41973700	-3.08758600	-2.46401800
H	3.15688200	-4.00107700	-2.98094700
C	2.54912400	-2.00020000	-2.51587200
C	4.55812200	0.53726300	-0.42610900
H	3.77276300	1.27891300	-0.55963400
C	5.83571100	1.11080600	-1.05232600
H	5.71179000	1.29350000	-2.12015800
H	6.67887400	0.42883000	-0.92641700
H	6.09732800	2.05831000	-0.57693200
C	4.73773800	0.32959600	1.07903600
H	3.81086100	-0.00606300	1.53999700
H	5.04524500	1.26138500	1.55673800
H	5.50445800	-0.41891500	1.28857300
C	1.26174000	-2.10993900	-3.31121300
H	0.78619800	-1.13030300	-3.32285900
C	1.52291000	-2.52431800	-4.76529200
H	0.59570500	-2.47770500	-5.33911000
H	1.89938800	-3.54705000	-4.82857700
H	2.25440800	-1.87432100	-5.24782000
C	0.27802500	-3.08133300	-2.65151500
H	-0.04309000	-2.72134800	-1.67511900
H	0.72427200	-4.06969400	-2.52360000
H	-0.61132100	-3.18911300	-3.27214200
C	-1.65319300	-2.07737400	0.96308900
C	-0.77266800	-2.88747600	1.69831200
C	-1.04453800	-4.24811600	1.85043700
H	-0.35852900	-4.86380500	2.41903200
C	-2.19208600	-4.80624000	1.30730100
H	-2.39274000	-5.86319400	1.42944000
C	-3.10512800	-3.99445100	0.64843900
H	-4.03223200	-4.41050800	0.27353100
C	-2.86082200	-2.63125000	0.49415600
C	0.41177200	-2.32209600	2.40755800
C	0.23434700	-1.53738800	3.55771800
C	1.35621000	-1.06864600	4.24178200
H	1.21000600	-0.47173800	5.13513700
C	2.64742500	-1.36174700	3.82682300
C	2.80265900	-2.14654700	2.68691100
H	3.79990900	-2.38948600	2.33923700
C	1.71238600	-2.63118200	1.97516800
C	-1.13219500	-1.20560200	4.10160700
H	-1.84690700	-2.00531900	3.91719600
H	-1.53902000	-0.29831900	3.64544000
H	-1.07967800	-1.02595300	5.17567000
C	3.84457800	-0.87039300	4.59294100
H	3.56095100	-0.12313500	5.33399300
H	4.58570100	-0.42371200	3.92743000
H	4.33817700	-1.69173900	5.11918400
C	1.94369500	-3.48011300	0.75818700
H	1.75191400	-4.53587900	0.96464100
H	2.96940500	-3.38503200	0.41040000

H	1.28065800	-3.19509600	-0.05429500
C	-3.93516100	-1.76628900	-0.08513400
C	-4.71517700	-0.96773500	0.77124400
C	-5.70032800	-0.14831800	0.22744100
H	-6.29272000	0.46848400	0.89423600
C	-5.94461200	-0.10101800	-1.14000000
C	-5.19750100	-0.93360400	-1.96457800
H	-5.38175100	-0.92684700	-3.03308800
C	-4.20738500	-1.77153200	-1.46113200
C	-4.52273200	-0.98184300	2.26457100
H	-5.42763900	-0.64099600	2.76771700
H	-3.71004100	-0.31473400	2.56379300
H	-4.27460200	-1.97714300	2.63128900
C	-6.96821600	0.84214600	-1.70925000
H	-7.34461400	0.48894400	-2.66998000
H	-6.53408600	1.83324500	-1.86995600
H	-7.81624400	0.96479500	-1.03364200
C	-3.45565200	-2.67639600	-2.39558500
H	-3.88227000	-3.68363800	-2.39502000
H	-2.41460200	-2.76439900	-2.10193500
H	-3.49486600	-2.29653000	-3.41633900

Cartesian coordinates of the optimized geometry for 3 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.09824000	0.10588600	0.66470200
Ga	1.17261100	0.33363200	-0.55215300
Cl	1.72323100	0.51095100	-2.74324200
Si	-1.90534400	-1.88140800	-1.84962100
N	2.82795500	-0.59786200	0.08956500
N	1.76193700	2.10943300	0.15070200
N	-2.24385700	-0.89376300	-0.40524900
C	3.96169500	0.06817400	0.24774800
C	4.07161100	1.46625900	0.17305800
H	5.07782300	1.85294000	0.22762000
C	3.05314400	2.42084300	0.19382300
C	5.24254400	-0.67662100	0.53033200
H	5.78545300	-0.83151500	-0.40358600
H	5.05892600	-1.65219100	0.97226700
H	5.88050200	-0.09428000	1.19220000
C	3.46063400	3.86990700	0.26246300
H	3.37220400	4.30571200	-0.73573800
H	4.49168200	3.97466900	0.59151500
H	2.81160600	4.44455200	0.91949700
C	2.74891200	-2.01845400	0.24728500
C	2.14973000	-2.51571200	1.42144500
C	1.99990300	-3.89132900	1.56257000
H	1.54323700	-4.29107900	2.45678300
C	2.42588900	-4.76139200	0.57009000
H	2.29967700	-5.82932600	0.69363700
C	3.00351400	-4.25801400	-0.58091100
H	3.32236800	-4.94088100	-1.35720200
C	3.17304900	-2.88668700	-0.77326200
C	1.70727200	-1.57161200	2.52376300
H	1.38591200	-0.64619100	2.04467800
C	2.87472500	-1.20428000	3.44845200
H	3.68434100	-0.72450900	2.90053800
H	3.27448800	-2.09827100	3.93187400
H	2.54292200	-0.51532200	4.22763500
C	0.51999700	-2.09543900	3.32814400
H	0.12906900	-1.31049900	3.97505900
H	0.79720500	-2.93756100	3.96504500
H	-0.28609000	-2.42262800	2.67269200
C	3.78527900	-2.40306600	-2.07599600
H	3.85173400	-1.31741100	-2.04130700
C	5.19649400	-2.97090400	-2.28286100
H	5.65692700	-2.52151600	-3.16480200
H	5.16771400	-4.05090200	-2.44007800
H	5.84307200	-2.78217000	-1.42586500
C	2.89666600	-2.75794800	-3.27517000
H	1.90743500	-2.31840600	-3.17589900

H	2.79022600	-3.84001900	-3.37835200
H	3.33923300	-2.37141100	-4.19491500
C	0.75698200	3.06388200	0.51135300
C	0.36591400	3.13690500	1.86560200
C	-0.63176200	4.04017400	2.21911100
H	-0.94610000	4.11056700	3.25106000
C	-1.24184500	4.84359400	1.26738700
H	-2.02154000	5.53480200	1.56053000
C	-0.86105100	4.74701200	-0.05908900
H	-1.34917700	5.36677100	-0.79966800
C	0.13720400	3.86154200	-0.46376500
C	1.02359800	2.26655900	2.92340100
H	1.41698600	1.38771100	2.41370100
C	2.21712200	2.97546300	3.57892200
H	1.89585200	3.90167800	4.06057400
H	2.99095100	3.22161400	2.85453800
H	2.66597500	2.33471100	4.34078400
C	0.04536900	1.78236500	3.99643700
H	-0.29080900	2.59939800	4.63719400
H	0.53673900	1.05153700	4.64105900
H	-0.83108000	1.31297100	3.54979300
C	0.50977200	3.77627600	-1.93041600
H	1.35664600	3.10090500	-2.02562700
C	0.93134000	5.13542500	-2.49994900
H	0.10203500	5.84554800	-2.50469500
H	1.27494300	5.02017200	-3.52961100
H	1.74158100	5.57749700	-1.91795600
C	-0.63759600	3.17467500	-2.75021300
H	-1.50960700	3.83215000	-2.74739900
H	-0.94249800	2.20828600	-2.35028400
H	-0.32678100	3.01820100	-3.78377500
C	-3.62210200	-0.83524000	0.01569300
C	-4.13578200	-1.78481300	0.92006000
C	-5.48566400	-1.72395600	1.25897300
H	-5.89052600	-2.44907500	1.95297900
C	-6.31853500	-0.75006100	0.73342400
H	-7.36579000	-0.72296800	1.00599200
C	-5.79692100	0.19788900	-0.13097700
H	-6.44298200	0.97261400	-0.52287100
C	-4.45394500	0.17763800	-0.50075900
C	-3.25663700	-2.82312100	1.59302800
H	-2.28459000	-2.80490500	1.10160600
C	-3.80498200	-4.24904600	1.47867900
H	-4.74991900	-4.36059400	2.01323900
H	-3.09731400	-4.95910700	1.91160600
H	-3.97602000	-4.53260700	0.44038300
C	-3.04741800	-2.44714900	3.06705700
H	-2.60498800	-1.45458700	3.15942900
H	-2.39176000	-3.16502800	3.56360000
H	-4.00110900	-2.43689100	3.59839000
C	-3.91594200	1.27656800	-1.39847300
H	-2.91616500	0.98893900	-1.71281800
C	-3.78655700	2.58696600	-0.61227400
H	-3.38629500	3.37975700	-1.24505300
H	-3.11740100	2.47221400	0.24258000
H	-4.75753300	2.90963900	-0.23045300
C	-4.74756900	1.47038700	-2.66902900
H	-5.74959800	1.84223000	-2.44742700
H	-4.85393900	0.53312800	-3.21764600
H	-4.26445000	2.19614800	-3.32619800
C	-3.41832900	-2.92037000	-2.23317700
H	-4.29965400	-2.30175200	-2.40799800
H	-3.65959400	-3.62209100	-1.43608800
H	-3.22714900	-3.49812100	-3.14150700
C	-0.47156300	-3.01769100	-1.46681900
H	0.43703500	-2.47573800	-1.21284800
H	-0.24316700	-3.65087900	-2.32687700
H	-0.70834000	-3.67048600	-0.62438700
C	-1.57065400	-0.81844900	-3.34884900
H	-2.46609600	-0.26850000	-3.64293000

H	-1.28766400	-1.46074000	-4.18745300
H	-0.75741900	-0.11183300	-3.19766000

Cartesian coordinates of the optimized geometry for 5 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Sn	1.29190900	-0.79553700	0.74127100
Ga	-1.33311300	-0.23011900	-0.15114700
Si	1.89934700	1.87015300	-1.43901400
N	-2.97914100	0.77602300	-0.22361100
N	-2.19525200	-1.98705000	-0.23530400
N	2.37548500	0.65041500	-0.24297000
C	-4.19931200	0.21956200	-0.22495400
C	-4.43092300	-1.15043900	-0.35767500
H	-5.46713300	-1.44607700	-0.41546900
C	-3.50334400	-2.19707300	-0.35458000
C	-5.39840900	1.10246200	-0.01095600
H	-5.47638000	1.33740900	1.05371400
H	-6.31059700	0.59434900	-0.31256400
H	-5.31717300	2.04865300	-0.53829200
C	-4.03724200	-3.60114300	-0.43022900
H	-3.28936900	-4.29947800	-0.79628300
H	-4.91445600	-3.63705200	-1.07364000
H	-4.34456400	-3.93762800	0.56243600
C	-2.84145000	2.20790000	-0.12388200
C	-2.72854000	2.79739100	1.14344600
C	-2.59939500	4.18352200	1.21005900
H	-2.51138400	4.66561700	2.17410900
C	-2.58440800	4.95349500	0.05984600
H	-2.49643400	6.02952000	0.13005400
C	-2.65620500	4.34559000	-1.18445500
H	-2.60689400	4.95845600	-2.07264600
C	-2.76496000	2.96293900	-1.30772300
C	-2.68302800	1.97190400	2.41809600
H	-2.99543500	0.95491700	2.17704900
C	-3.63936600	2.48915400	3.49716900
H	-3.63990300	1.81557900	4.35546700
H	-4.66041500	2.56197900	3.12064500
H	-3.34669000	3.47645600	3.85593700
C	-1.24449400	1.90009900	2.95278700
H	-0.55863800	1.50543900	2.19879400
H	-1.18732000	1.26176900	3.83575800
H	-0.88064800	2.89195200	3.22500200
C	-2.76458400	2.30343900	-2.67913800
H	-2.27889800	1.32969900	-2.56714600
C	-4.18022700	2.04265700	-3.21410500
H	-4.75200700	2.97182900	-3.25240400
H	-4.73013500	1.33078900	-2.60250800
H	-4.12976100	1.63716100	-4.22587400
C	-1.96160000	3.09290900	-3.71650600
H	-2.48179400	4.00232600	-4.02046700
H	-1.82148900	2.48749300	-4.61259800
H	-0.98005800	3.37556600	-3.33852200
C	-1.24705500	-3.03822600	-0.01696500
C	-1.14298300	-3.60463900	1.26561200
C	-0.10022500	-4.49839400	1.50340700
H	0.00283400	-4.94767400	2.48110900
C	0.82168100	-4.80459900	0.51599600
H	1.63020400	-5.49229800	0.72467100
C	0.71342700	-4.22565000	-0.73951100
H	1.44166600	-4.47126300	-1.49789800
C	-0.31825700	-3.33424900	-1.03661800
C	-2.07243400	-3.20294100	2.40010000
H	-2.97037700	-2.76348800	1.97102600
C	-1.42454900	-2.11735600	3.27096500
H	-0.48808000	-2.46976100	3.70594800
H	-2.09219000	-1.82845700	4.08424400
H	-1.20386600	-1.21766300	2.69134900
C	-2.51948600	-4.39354000	3.25313800
H	-1.69432500	-4.81839400	3.82570200
H	-2.94264700	-5.18733600	2.63620900

H	-3.27936200	-4.07539300	3.96794700
C	-0.45596700	-2.74029500	-2.42895800
H	-0.84199500	-1.72164400	-2.32170600
C	0.86803200	-2.63528700	-3.18461500
H	1.25498100	-3.61674900	-3.46140600
H	1.63091400	-2.12489700	-2.59687600
H	0.72138400	-2.07349100	-4.10687900
C	-1.48855000	-3.51937200	-3.25550200
H	-1.18204100	-4.56145900	-3.36290600
H	-1.58098900	-3.08759800	-4.25309800
H	-2.47316200	-3.50396200	-2.79087900
C	0.80391500	3.16872900	-0.65059300
H	-0.06118900	2.74402100	-0.14100800
H	0.42446600	3.85742500	-1.40780300
H	1.36175600	3.75994800	0.07640200
C	0.98552600	1.03086800	-2.84684200
H	1.60565200	0.26511700	-3.31326900
H	0.72444500	1.76057100	-3.61496300
H	0.05787400	0.55553800	-2.52167200
C	3.43273100	2.69484100	-2.11472700
H	4.07399500	1.99446400	-2.64991500
H	4.02855000	3.15147000	-1.32349000
H	3.14330200	3.48319100	-2.81391300
C	3.73499200	0.69060100	0.24775400
C	4.74108500	-0.03397200	-0.42358300
C	6.03760400	0.00122800	0.08038500
H	6.81985300	-0.55140200	-0.42201900
C	6.34738500	0.73120200	1.21808800
H	7.36194000	0.74696800	1.59365800
C	5.35247200	1.43830000	1.87076000
H	5.59977100	2.00486800	2.75892700
C	4.03811000	1.43460700	1.40589000
C	4.42471800	-0.88188500	-1.64218800
H	3.47168500	-0.53585300	-2.04066400
C	4.24938100	-2.35277800	-1.24038500
H	4.00253000	-2.96790700	-2.10793300
H	3.45525500	-2.48007800	-0.49955300
H	5.16703900	-2.74218300	-0.79629500
C	5.46324700	-0.75142800	-2.75952500
H	6.42324500	-1.18434500	-2.47554300
H	5.63461000	0.29237300	-3.02411600
H	5.12164800	-1.27790200	-3.65245300
C	2.98221300	2.22109600	2.16304700
H	2.06348100	2.18415200	1.58223300
C	2.68458000	1.58814700	3.52797400
H	2.35828300	0.54935200	3.42406700
H	1.89871900	2.14040100	4.04707100
H	3.57086400	1.58267300	4.16438000
C	3.35845900	3.69900300	2.31129700
H	4.24512400	3.82913700	2.93315400
H	2.54279300	4.25397600	2.77884400
H	3.56610800	4.15126700	1.34053200

Cartesian coordinates of the optimized geometry for 6 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.19695800	-0.07907600	1.35773100
Ga	0.55180300	0.49716800	-0.52787900
N	0.26738000	2.40721900	-0.92284900
N	1.85171800	0.21670100	-1.94229800
C	0.71411000	3.02124700	-2.01194400
C	1.45028300	2.35776400	-3.00254600
H	1.69275100	2.94589600	-3.87377900
C	2.02611900	1.09432500	-2.95021100
C	0.44201000	4.48387300	-2.22960500
H	-0.47713200	4.60508600	-2.80621600
H	1.25035000	4.93948900	-2.79712700
H	0.31201500	5.01500700	-1.29054700
C	2.95165900	0.72167900	-4.07630400
H	2.76231100	-0.29240200	-4.42122100
H	3.99031300	0.75112200	-3.74632800

H	2.83561800	1.41290200	-4.90669000
C	-0.43846500	3.11606700	0.11110900
C	0.23431400	3.36186700	1.32340500
C	-0.48215900	3.95307400	2.35941700
H	0.00623000	4.15595600	3.30071900
C	-1.82104300	4.28272300	2.20873900
H	-2.36101700	4.73703000	3.02887800
C	-2.46381500	4.02933600	1.01069600
H	-3.50894400	4.28556900	0.90293600
C	-1.79003800	3.44386900	-0.06046400
C	1.70504700	3.02047500	1.49424000
H	1.88970300	2.06597200	0.98643300
C	2.60067300	4.06642700	0.81702000
H	2.40994700	4.13767700	-0.25223500
H	3.65349000	3.81594600	0.95341500
H	2.42748400	5.05057900	1.25596300
C	2.12245400	2.81975600	2.94889700
H	2.10390600	3.75720600	3.50634600
H	3.14270700	2.44107900	2.98952900
H	1.47506800	2.10398000	3.45414000
C	-2.54827700	3.14401800	-1.33844100
H	-1.83640000	2.81676900	-2.09498500
C	-3.27289900	4.37897300	-1.88771000
H	-3.71293300	4.15498900	-2.86066800
H	-2.59628900	5.22609400	-2.00490900
H	-4.08204100	4.69296500	-1.22718600
C	-3.53265100	1.99381600	-1.12369900
H	-4.27230500	2.24042600	-0.36167500
H	-3.02714700	1.08005500	-0.80380300
H	-4.06156600	1.76531200	-2.04747000
C	2.79832700	-0.87101800	-1.83700800
C	4.05092900	-0.59204000	-1.25740300
C	4.98949100	-1.61797200	-1.19376400
H	5.95952600	-1.42477600	-0.75568300
C	4.70638200	-2.88020300	-1.69093400
H	5.45264300	-3.66223500	-1.64413000
C	3.46425000	-3.13780700	-2.24279200
H	3.24860600	-4.12697200	-2.62315400
C	2.48474800	-2.14813300	-2.32355500
C	4.41258600	0.77494000	-0.69651500
H	3.61553000	1.47443600	-0.94394900
C	5.70540600	1.33388000	-1.30241100
H	5.65746700	1.37222800	-2.39099400
H	6.57108600	0.72893800	-1.03010000
H	5.88323100	2.34680000	-0.93783500
C	4.51365400	0.71938500	0.83173800
H	3.57555400	0.39529600	1.28176800
H	4.76735600	1.70054800	1.23504500
H	5.28950500	0.01910300	1.14590100
C	1.14191100	-2.49706100	-2.93918600
H	0.50768700	-1.61067900	-2.89267700
C	1.27784700	-2.88392100	-4.41799100
H	0.29322000	-3.06737200	-4.85079000
H	1.86753700	-3.79448200	-4.53400700
H	1.76105600	-2.10018800	-5.00191700
C	0.45094700	-3.62022800	-2.15477500
H	0.18165100	-3.30671900	-1.14740500
H	1.09527800	-4.49575200	-2.07166900
H	-0.46192500	-3.93136100	-2.65943600
C	-1.44276800	-2.03716500	1.00005400
C	-0.51494600	-2.82970500	1.68751100
C	-0.58033500	-4.21521200	1.59903900
H	0.13061400	-4.83113000	2.13458300
C	-1.58363600	-4.80375000	0.83694000
H	-1.64241300	-5.88173500	0.76417800
C	-2.53523500	-4.01684600	0.19921400
H	-3.34011400	-4.48599600	-0.35276900
C	-2.49065500	-2.62371700	0.28681500
C	0.46454800	-2.09676500	2.54301600
C	0.00238500	-1.36113100	3.66372300

C	0.92155800	-0.61346000	4.41337700
H	0.55679500	-0.05229200	5.26578700
C	2.27743000	-0.63456600	4.14239300
C	2.72006300	-1.41266300	3.06823600
H	3.78076900	-1.45767500	2.85522100
C	1.85054100	-2.12841100	2.26291600
C	-1.38993200	-1.51501000	4.22994000
H	-2.07338700	-2.01032200	3.54883400
H	-1.81229500	-0.55124700	4.51596100
H	-1.33399900	-2.12430600	5.13540000
C	3.26247000	0.10404600	5.00229700
H	2.77765700	0.88399200	5.58789900
H	4.04821700	0.56238700	4.40074700
H	3.74924600	-0.58180200	5.70024800
C	2.39441500	-2.95064300	1.13205400
H	2.40946100	-4.01215000	1.38781400
H	3.41108700	-2.65328900	0.88868200
H	1.78804900	-2.85326700	0.23662300
C	-3.60171300	-1.80998800	-0.29116500
C	-4.61400000	-1.32949700	0.55926400
C	-5.70218100	-0.65799000	0.00728200
H	-6.48386600	-0.30061200	0.66751700
C	-5.82771900	-0.45880900	-1.36215700
C	-4.81693900	-0.94269000	-2.18715900
H	-4.89199700	-0.79574700	-3.25864700
C	-3.70678600	-1.60437000	-1.67680200
C	-4.56986800	-1.55121200	2.04818000
H	-5.55453900	-1.39764400	2.48715600
H	-3.88560600	-0.85338900	2.53800000
H	-4.23634300	-2.55856000	2.29666200
C	-6.99679700	0.29254500	-1.93258200
H	-7.25516900	-0.06846800	-2.92833300
H	-6.76470800	1.35827200	-2.02143700
H	-7.87700100	0.20316100	-1.29607200
C	-2.63853300	-2.09386900	-2.61328800
H	-2.64306800	-3.18225200	-2.69321500
H	-1.64707400	-1.81183200	-2.26022200
H	-2.77937800	-1.68424100	-3.61280200

Cartesian coordinates of the optimized geometry for 7 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.24439800	0.21406900	0.78773900
Ga	1.18989900	0.32988800	-0.14516000
Si	-1.70905300	-1.79836900	-1.81010800
N	2.93606900	-0.50077800	-0.12090500
N	1.83289200	2.15185800	0.04219300
N	-2.19052700	-0.82052500	-0.38831400
C	4.08441700	0.18510900	-0.04823800
C	4.15737200	1.57870600	-0.08275600
H	5.15312400	1.99281000	-0.08536900
C	3.11624200	2.50960000	-0.02389900
C	5.37325400	-0.57350100	0.09948200
H	5.62155200	-1.10190100	-0.82074700
H	5.28644300	-1.32746000	0.88162500
H	6.18979400	0.10101100	0.34099500
C	3.47849400	3.96737800	-0.03034500
H	3.33748700	4.36557200	-1.03783000
H	4.51936900	4.11181300	0.24688400
H	2.84141100	4.54638900	0.63416500
C	2.93135800	-1.93997500	-0.03758600
C	2.52373100	-2.53780600	1.16706300
C	2.45274600	-3.92850900	1.21930800
H	2.14725500	-4.41141100	2.13785500
C	2.77018400	-4.70219000	0.11612000
H	2.70775300	-5.78067200	0.17411300
C	3.16797000	-4.09289400	-1.06333200
H	3.40793300	-4.70621600	-1.92095700
C	3.25692900	-2.70732300	-1.16845400
C	2.17344400	-1.73140400	2.40600300
H	2.23807800	-0.67128800	2.15550200

C	3.18036100	-1.96953800	3.53799400
H	4.19460100	-1.72256600	3.22211400
H	3.17482500	-3.01312900	3.85561700
H	2.93451800	-1.35322200	4.40442300
C	0.74149400	-2.00935500	2.87425600
H	0.45598300	-1.33147500	3.67934200
H	0.63068100	-3.02982000	3.24225200
H	0.02653700	-1.89284800	2.05574200
C	3.64485900	-2.07997900	-2.49627500
H	3.84902400	-1.02277600	-2.32945800
C	4.90842600	-2.70519800	-3.09751800
H	5.21451500	-2.15120600	-3.98595000
H	4.73963700	-3.73923500	-3.40010800
H	5.73956600	-2.70101600	-2.39093900
C	2.47649000	-2.15949600	-3.48595600
H	1.58807100	-1.67612400	-3.08452700
H	2.22012200	-3.19812600	-3.70209200
H	2.73506200	-1.67160200	-4.42727800
C	0.80212300	3.11067300	0.35198700
C	0.38879400	3.21502300	1.69726100
C	-0.63285300	4.11223800	1.99528000
H	-0.96995400	4.21770300	3.01617200
C	-1.23315300	4.87189500	1.00179100
H	-2.02475600	5.56403200	1.25622000
C	-0.83098000	4.73296600	-0.31473700
H	-1.31877500	5.31573700	-1.08427800
C	0.18639800	3.84769900	-0.66860800
C	1.04081500	2.39301600	2.79869800
H	1.36802200	1.44718000	2.35636100
C	2.29852800	3.08091000	3.34875600
H	2.04534500	4.05759600	3.76486000
H	3.05540400	3.22824100	2.58078300
H	2.74252600	2.47917300	4.14346800
C	0.08862200	2.04180000	3.94400400
H	-0.16000200	2.91675600	4.54569500
H	0.56564100	1.32124800	4.60983500
H	-0.84092000	1.60575800	3.57776600
C	0.55666100	3.67707900	-2.12936000
H	1.41859400	3.01118100	-2.18452300
C	0.95058800	5.00155600	-2.79261800
H	0.10606700	5.69055400	-2.83588300
H	1.28599900	4.82723500	-3.81605000
H	1.75457100	5.50023800	-2.25044600
C	-0.59418300	3.00737600	-2.89152300
H	-1.46554200	3.66247600	-2.93331800
H	-0.90236900	2.08103200	-2.40785600
H	-0.29843300	2.77521700	-3.91578700
C	-3.58774600	-0.88859500	0.01048600
C	-4.00684700	-1.86779500	0.92724800
C	-5.35487600	-1.90397300	1.28143600
H	-5.69795600	-2.64938600	1.98660000
C	-6.26150800	-1.00300000	0.75016500
H	-7.30377200	-1.04883700	1.03692700
C	-5.83002500	-0.03870400	-0.14818500
H	-6.54414200	0.66479700	-0.55338800
C	-4.49535100	0.03815100	-0.53480100
C	-3.04798800	-2.86276500	1.55603300
H	-2.07244700	-2.72518300	1.09414100
C	-3.46596000	-4.31426700	1.29769800
H	-4.42201700	-4.54700800	1.76825300
H	-2.72162400	-5.00120200	1.70477300
H	-3.56470700	-4.51485800	0.23013100
C	-2.88499500	-2.59273900	3.05722100
H	-2.53796000	-1.57371400	3.24032100
H	-2.16401000	-3.28437800	3.49671900
H	-3.83232500	-2.71561300	3.58416100
C	-4.03554100	1.13086400	-1.48298100
H	-3.08460400	0.81656100	-1.90974500
C	-3.77966700	2.43271600	-0.71302100
H	-3.43824000	3.22175900	-1.38406200

H	-3.01986500	2.30564000	0.06323900
H	-4.69035100	2.77290500	-0.21687000
C	-4.99654800	1.36747400	-2.65036500
H	-5.94529200	1.79193200	-2.31992200
H	-5.21241200	0.43974100	-3.18189900
H	-4.55632900	2.07104900	-3.35907500
C	-3.24370400	-2.58449000	-2.52056600
H	-3.96119700	-1.83660600	-2.85999100
H	-3.75107700	-3.22348200	-1.79808400
H	-2.96927800	-3.20027100	-3.38060500
C	-0.50022800	-3.11442400	-1.26252800
H	0.36515000	-2.70810200	-0.73943000
H	-0.12682900	-3.66689900	-2.12704100
H	-0.98266700	-3.83173000	-0.59729600
C	-0.94941100	-0.69181000	-3.11636800
H	-1.68213400	0.01827000	-3.50114000
H	-0.60683500	-1.29973400	-3.95642200
H	-0.09269100	-0.12095800	-2.75529700

Cartesian coordinates of the optimized geometry for 8 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	1.37246000	-0.84373900	-0.57990100
Cl	0.46856500	-0.56372200	-2.71292500
Ga	-1.06737700	-0.04444200	0.38672600
Si	2.52754400	2.13323600	-1.47390900
N	-2.70088600	1.10140000	0.56837800
N	-2.10679300	-1.69347600	0.94825300
N	2.55719200	0.65199600	-0.53673400
C	-3.81669800	0.75478800	1.21314700
C	-4.04073300	-0.51299500	1.74670600
H	-4.97347500	-0.64522400	2.27326100
C	-3.29034400	-1.67916800	1.54453600
C	-4.92391000	1.76669800	1.36640200
H	-4.62840800	2.55714100	2.05651900
H	-5.82528400	1.29399200	1.74791900
H	-5.14700600	2.24690000	0.41455300
C	-3.93895300	-2.96359200	1.99790200
H	-4.71797300	-3.25100900	1.29043700
H	-4.41798000	-2.81178400	2.96488100
H	-3.23090500	-3.78329800	2.06873100
C	-2.62262400	2.37491200	-0.08783000
C	-2.31922300	3.53182400	0.64508800
C	-2.24546400	4.74452700	-0.03698800
H	-2.00866100	5.64846500	0.50799100
C	-2.45777300	4.80958600	-1.40296400
H	-2.39716200	5.76027500	-1.91677700
C	-2.72200400	3.65161200	-2.11780500
H	-2.85195800	3.71096700	-3.18842500
C	-2.79644500	2.41440800	-1.48456000
C	-2.00459800	3.48369300	2.12944900
H	-2.33010200	2.51753200	2.51411100
C	-2.72794700	4.56960100	2.93232000
H	-2.55716600	4.42388300	4.00051500
H	-3.80434900	4.55401300	2.75417700
H	-2.36571700	5.56663900	2.67715100
C	-0.48926900	3.56741700	2.34677200
H	0.02540700	2.75951300	1.82861400
H	-0.24694400	3.50029200	3.40905200
H	-0.09268000	4.51060900	1.96624700
C	-3.05332000	1.14655700	-2.28485900
H	-2.45985200	0.34753300	-1.83229600
C	-4.52475800	0.71639800	-2.21177900
H	-5.17120900	1.50272000	-2.60785500
H	-4.83796500	0.50092400	-1.19177100
H	-4.68489500	-0.18453100	-2.80631100
C	-2.59903900	1.24143600	-3.74117100
H	-3.23158700	1.91852100	-4.31908700
H	-2.66002200	0.25764200	-4.20618100
H	-1.56586500	1.57785100	-3.81584000
C	-1.50735100	-2.93710300	0.55238000

C	-0.42584600	-3.44959100	1.29326100
C	0.17081500	-4.62736700	0.85482400
H	1.00509200	-5.03853400	1.40405200
C	-0.27226900	-5.27522600	-0.28821500
H	0.21303200	-6.18495300	-0.61731900
C	-1.32542200	-4.74820900	-1.01390300
H	-1.65675100	-5.25019400	-1.91329400
C	-1.96333300	-3.57526000	-0.61386600
C	0.07289100	-2.75364200	2.54730600
H	-0.08527600	-1.68229500	2.40601700
C	1.56635700	-2.96083800	2.80437300
H	1.78776300	-3.99271800	3.08276900
H	1.89095800	-2.32714500	3.62961600
H	2.16209000	-2.70472300	1.92817800
C	-0.74137800	-3.16408000	3.78208800
H	-0.66717600	-4.24105600	3.94804600
H	-1.79497600	-2.91129900	3.67635400
H	-0.36236500	-2.65669900	4.67154800
C	-3.10777500	-3.03638400	-1.45689900
H	-3.49240300	-2.13615700	-0.97906400
C	-2.63153100	-2.64214300	-2.85982300
H	-2.26288000	-3.51241900	-3.40599500
H	-1.82330500	-1.91467300	-2.82025300
H	-3.45858600	-2.21761200	-3.43268300
C	-4.26364000	-4.04166800	-1.55266900
H	-3.96459700	-4.92991300	-2.11197600
H	-5.11250400	-3.59344500	-2.07284800
H	-4.59998100	-4.37119400	-0.56954600
C	0.79743000	2.84092600	-1.49120600
H	0.09811100	2.16420200	-1.97791500
H	0.78389000	3.78397500	-2.04270800
H	0.42823400	3.04442000	-0.48632100
C	3.09718400	1.89217100	-3.24762900
H	4.15291000	1.62334500	-3.30250900
H	2.96602100	2.82513700	-3.80348600
H	2.51761800	1.11562000	-3.74618400
C	3.69309900	3.38322400	-0.68978900
H	4.69086600	2.96780700	-0.53832700
H	3.32934800	3.73983500	0.27395100
H	3.78845700	4.24929400	-1.35000700
C	3.70803700	0.32716100	0.25203500
C	4.74241000	-0.46955600	-0.28589600
C	5.82941900	-0.80522400	0.52034500
H	6.62166500	-1.41940300	0.11132600
C	5.91563800	-0.37067300	1.83154500
H	6.76747200	-0.64146200	2.44247400
C	4.90028300	0.41412200	2.35637000
H	4.96759200	0.74995300	3.38306800
C	3.79489200	0.77133100	1.59013600
C	4.70624500	-0.97974800	-1.71495800
H	3.83052200	-0.55086100	-2.19632400
C	4.55658000	-2.50552700	-1.76535700
H	4.48697600	-2.84833900	-2.79989600
H	3.65630300	-2.82829700	-1.24000700
H	5.41158600	-3.00190400	-1.30074600
C	5.93520500	-0.52591700	-2.51095100
H	6.85116700	-0.97975700	-2.12706700
H	6.05750000	0.55701600	-2.46398400
H	5.83557500	-0.81269200	-3.55981700
C	2.68189200	1.58567700	2.22132100
H	2.06815700	1.97028700	1.40907700
C	1.78875700	0.68415200	3.08067300
H	1.37170900	-0.12348800	2.48147200
H	0.96358500	1.24822600	3.51952200
H	2.36221000	0.23177700	3.89244800
C	3.19130400	2.77640800	3.03745200
H	3.71588200	2.45421200	3.93901500
H	2.35456600	3.40189500	3.35382400
H	3.87712000	3.39221900	2.45550700

Cartesian coordinates of the optimized geometry for S1 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.98719200	-1.02697900	-0.55630100
Ga	0.35292000	-0.07161400	-0.55993600
Cl	-1.12593000	-1.68577000	1.53253000
N	1.90454800	-1.22798300	-0.33674300
N	1.29083000	1.59561200	-0.20826700
C	3.09460100	-0.80186100	0.07140300
C	3.39350700	0.54327700	0.31787700
H	4.39903400	0.74564900	0.65072300
C	2.56219400	1.65841600	0.18666600
C	4.19478000	-1.80467600	0.29261000
H	5.10040800	-1.31667100	0.64187900
H	4.42412700	-2.34133300	-0.63025100
H	3.89426900	-2.55102100	1.03050000
C	3.15752000	3.00217100	0.51196400
H	2.57666500	3.50675800	1.28615300
H	3.15352600	3.65234000	-0.36533500
H	4.18205300	2.89808000	0.85813400
C	0.50892200	2.82727500	-0.33575900
H	0.34447400	3.30112700	0.63407600
H	0.99812800	3.54402200	-0.99794200
H	-0.46603900	2.58952700	-0.75148900
C	1.67214100	-2.65766200	-0.53646200
H	1.74184700	-3.20762300	0.40378200
H	0.66583100	-2.80246200	-0.92243200
H	2.37712200	-3.08561200	-1.25200400
C	-2.71382100	0.81507000	0.16785100
F	-1.99812600	1.48191600	1.11767000
F	-2.83871000	1.69910700	-0.87905100
F	-3.96179900	0.67933400	0.68127200

Cartesian coordinates of the optimized geometry for S2 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.22127800	-1.90796800	-0.23817200
Ga	0.65744900	-0.28485000	-0.55369000
Cl	-0.02301000	-1.44915800	1.83585200
N	2.56303200	-0.69607300	-0.40054700
N	0.84471400	1.63735700	-0.25793200
C	3.48678500	0.19242800	-0.05914600
C	3.21815000	1.54990100	0.15389600
H	4.06652700	2.15733200	0.42637200
C	1.99473800	2.22237300	0.06304600
C	4.90973800	-0.26526900	0.12276500
H	5.55313300	0.56584600	0.39823900
H	5.29571000	-0.71394300	-0.79482300
H	4.97294200	-1.02687600	0.90268400
C	2.00396000	3.70125100	0.34818900
H	1.31134100	3.94449800	1.15604300
H	1.68405300	4.26871000	-0.52823000
H	2.99858000	4.03535200	0.63040000
C	-2.54790100	-0.38099600	-0.03618100
C	-3.27569200	-0.02941100	-1.17841800
C	-4.22948300	0.98073300	-1.14661500
H	-4.77165700	1.24244100	-2.04736400
C	-4.48998500	1.65241300	0.04403000
H	-5.23407400	2.43822100	0.07517900
C	-3.79336900	1.29875300	1.19373000
H	-3.99676900	1.80998800	2.12732100
C	-2.83189100	0.29349400	1.15257800
H	-3.08995500	-0.54214000	-2.11840400
H	-2.28296800	0.04384500	2.05172700
C	-0.38148100	2.43294900	-0.33277300
H	-0.67216400	2.81581900	0.64804600
H	-0.27349800	3.27650000	-1.01770100
H	-1.19289000	1.80492900	-0.68836600
C	2.91703600	-2.10527400	-0.54145600
H	3.25356000	-2.53008900	0.40707500
H	2.03388700	-2.65947600	-0.85411100
H	3.69751800	-2.25899500	-1.29019600

Cartesian coordinates of the optimized geometry for S3 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	2.81335000	-0.54460900	0.00012300
Ga	0.26220400	-0.05720400	0.00005300
N	-0.88671300	1.47063500	0.00001100
N	-1.08142700	-1.42000300	0.00005700
C	-2.22368000	1.37237400	0.00002000
C	-2.90498100	0.15352800	-0.00010400
H	-3.98067100	0.22593000	-0.00018000
C	-2.39252300	-1.14665100	-0.00011800
C	-3.04416700	2.62954200	0.00013700
H	-4.10532400	2.39998700	0.00006400
H	-2.82254700	3.23946300	-0.87791000
H	-2.82262300	3.23920900	0.87838200
C	-3.37390400	-2.28234300	-0.00028400
H	-3.23527800	-2.91640900	0.87769700
H	-3.23501400	-2.91636500	-0.87825400
H	-4.39504800	-1.91356100	-0.00042900
C	-0.63605800	-2.81865600	0.00011800
H	-0.98772200	-3.34932900	0.88571300
H	-0.98746200	-3.34933800	-0.88557400
H	0.45170200	-2.84699600	0.00027800
C	-0.26035500	2.79789400	0.00011400
H	-0.53840300	3.37095100	0.88558500
H	0.82040900	2.68019400	0.00009100
H	-0.53842500	3.37109100	-0.88526000
C	3.40724200	1.36455200	-0.00058700
H	3.03643900	1.89486200	0.88098000
H	4.49585200	1.40077400	-0.00077000
H	3.03613900	1.89450100	-0.88223500

Cartesian coordinates of the optimized geometry for S4 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-2.33289600	-0.86041900	-0.34342200
Ga	0.08645900	-0.21905500	-0.40821400
Cl	-0.96242200	-0.64577000	1.86293100
N	1.73633400	-1.25518200	-0.29105900
N	0.91606700	1.53310200	-0.19741400
C	2.92763500	-0.71156700	-0.06886700
C	3.14864000	0.66441100	0.05097200
H	4.17164300	0.96069200	0.22017800
C	2.21385500	1.70885800	0.00274100
C	4.12486500	-1.61500400	0.07006200
H	5.02721300	-1.03780100	0.25208500
H	4.27129900	-2.21127400	-0.83299700
H	3.98772400	-2.31451700	0.89723000
C	2.73692000	3.10718700	0.19992200
H	2.27602000	3.57117900	1.07429100
H	2.49718500	3.73726200	-0.65884000
H	3.81470400	3.10342300	0.33769700
C	0.00125000	2.67537600	-0.18774000
H	0.01453100	3.18535300	0.77877600
H	0.25596300	3.40152900	-0.96395300
H	-1.01102100	2.31718000	-0.36434400
C	1.58780300	-2.70533800	-0.34265500
H	1.80528400	-3.16788600	0.62347600
H	0.55615100	-2.94420500	-0.59578900
H	2.23300000	-3.15950800	-1.09825600
C	-4.09408100	1.28792000	0.06811500
H	-3.98784500	1.66541000	1.09064200
H	-4.51480900	2.08233600	-0.55441100
H	-4.80942000	0.45456400	0.08802900
O	-2.83776700	0.90524700	-0.45693700

Cartesian coordinates of the optimized geometry for S5 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	-1.95306500	-0.80379100	-1.00765700
Ga	0.12385600	-0.15212900	0.31921400
Cl	0.12616300	-0.01223100	2.58009900

N	1.65851500	-1.32939800	-0.06916800
N	1.00753900	1.50995500	-0.27921200
C	2.86623400	-0.87354800	-0.35991900
C	3.16559400	0.48047100	-0.56937000
H	4.19735800	0.70009100	-0.79334100
C	2.30401500	1.58533200	-0.53933500
C	4.00689900	-1.85129600	-0.48085000
H	4.93897700	-1.33642000	-0.69709400
H	3.81860200	-2.57288500	-1.27880000
H	4.12945800	-2.41972200	0.44336800
C	2.91414000	2.93308100	-0.82959800
H	2.73236800	3.62681100	-0.00632600
H	2.47420100	3.37561100	-1.72606400
H	3.98674500	2.84857100	-0.98140600
C	0.18931200	2.71447400	-0.25295600
H	0.41007300	3.33730700	0.61902800
H	0.31543600	3.32234500	-1.15151700
H	-0.85923100	2.42562200	-0.19363000
C	1.44403200	-2.75084700	0.16315100
H	1.93297100	-3.09210400	1.08002100
H	0.37585800	-2.93258900	0.27851500
H	1.79849900	-3.36507800	-0.66784300
N	-3.24916900	0.16916900	-0.13288300
C	-4.60589300	0.14114500	-0.66331200
H	-4.65316100	-0.48458100	-1.55358200
H	-5.30767700	-0.25413000	0.08062400
H	-4.94237400	1.15038100	-0.92982600
C	-3.16459000	0.99328700	1.06250600
H	-3.39258500	2.04130300	0.82898900
H	-3.89767000	0.66070500	1.80687600
H	-2.18073300	0.93331200	1.51664400

Cartesian coordinates of the optimized geometry for S6 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	0.97547400	0.77537000	-0.65783700
Ga	-1.23390100	0.01204700	0.38964100
Cl	-1.55508600	-0.37983900	2.58289100
Si	1.97599200	-1.33158800	1.60626700
N	-2.20184400	-1.40174900	-0.58559400
N	-2.54641000	1.43925300	0.00687000
N	2.25704900	-0.25555100	0.23788500
C	-3.44671800	-1.25363500	-1.01865600
C	-4.16205900	-0.05061700	-0.97123400
H	-5.16828300	-0.09163500	-1.35676400
C	-3.74353300	1.20367500	-0.50275000
C	-4.15763300	-2.44356500	-1.61150200
H	-4.17798700	-3.27590200	-0.90533500
H	-3.64561100	-2.79653600	-2.50936900
H	-5.17982800	-2.19015200	-1.87864500
C	-4.73489100	2.33466000	-0.59785600
H	-4.92476100	2.76659600	0.38687900
H	-5.67832500	1.99099600	-1.01306600
H	-4.35105400	3.13694000	-1.23174200
C	3.61137300	-0.04382000	-0.15375500
C	3.99959200	-0.22374300	-1.48269200
C	5.31409600	-0.00053900	-1.87091800
H	5.59572400	-0.14447800	-2.90621800
C	6.26555300	0.39270200	-0.93783500
H	7.29068400	0.56061600	-1.24013900
C	5.88813100	0.56509200	0.38929400
H	6.61853700	0.87524100	1.12559300
C	4.57330900	0.35199700	0.77925900
H	1.81680600	-0.58721800	2.87252300
H	0.77354300	-2.14105300	1.34703000
H	3.15299300	-2.22562900	1.72156600
H	4.28131400	0.51127000	1.80975300
H	3.26286000	-0.55156200	-2.20450400
C	-1.54455500	-2.69916600	-0.67827400
H	-1.97328100	-3.42390700	0.02004600
H	-1.59729500	-3.11844400	-1.68536100

H	-0.49395900	-2.58160500	-0.42034800
C	-2.20611300	2.76420100	0.50519700
H	-1.15258900	2.77843400	0.78431200
H	-2.36265400	3.54271500	-0.24489900
H	-2.77938000	3.02238100	1.39993800

Cartesian coordinates of the optimized geometry for S7 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	2.28742000	-0.43489500	-0.83449300
Ga	0.39494400	-0.18920500	0.85291100
N	-0.69409300	1.44899400	0.46576700
N	-0.98500500	-1.44147500	0.10766600
C	-1.76880400	1.45309700	-0.30040900
C	-2.36709100	0.29565600	-0.82730400
H	-3.23743300	0.45998300	-1.44271200
C	-2.02919100	-1.04791000	-0.60029500
C	-2.42561800	2.76909700	-0.63549000
H	-3.28438000	2.62227100	-1.28491800
H	-1.72281800	3.43931000	-1.13515100
H	-2.76156500	3.27748600	0.27097700
C	-2.93888400	-2.08871400	-1.20449900
H	-3.36893600	-2.72603400	-0.42877000
H	-2.38766300	-2.74203600	-1.88441000
H	-3.75102900	-1.62314700	-1.75625900
C	-0.73792200	-2.85816300	0.32922500
H	-1.52174700	-3.32241800	0.93583600
H	-0.65432600	-3.42034000	-0.60508700
H	0.20303800	-2.97386200	0.86567000
C	-0.17286200	2.69613200	1.00220600
H	-0.89146900	3.19680500	1.65794100
H	0.71544800	2.48260500	1.59544100
H	0.11714100	3.39874100	0.21548200
C	2.16179200	1.46485600	-1.53018800
H	2.45965600	2.16028200	-0.73881100
H	2.79604900	1.62948600	-2.40037300
H	1.12493900	1.70287500	-1.78302800
C	0.45750700	-0.42205500	2.84517200
H	0.88080100	-1.39155500	3.11581000
H	1.07365000	0.34484300	3.31919200
H	-0.54992000	-0.35790800	3.26216500

Cartesian coordinates of the optimized geometry for S8 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	2.81335000	-0.54460900	0.00012300
Ga	0.26220400	-0.05720400	0.00005300
N	-0.88671300	1.47063500	0.00001100
N	-1.08142700	-1.42000300	0.00005700
C	-2.22368000	1.37237400	0.00002000
C	-2.90498100	0.15352800	-0.00010400
H	-3.98067100	0.22593000	-0.00018000
C	-2.39252300	-1.14665100	-0.00011800
C	-3.04416700	2.62954200	0.00013700
H	-4.10532400	2.39998700	0.00006400
H	-2.82254700	3.23946300	-0.87791000
H	-2.82262300	3.23920900	0.87838200
C	-3.37390400	-2.28234300	-0.00028400
H	-3.23527800	-2.91640900	0.87769700
H	-3.23501400	-2.91636500	-0.87825400
H	-4.39504800	-1.91356100	-0.00042900
C	-0.63605800	-2.81865600	0.00011800
H	-0.98772200	-3.34932900	0.88571300
H	-0.98746200	-3.34933800	-0.88557400
H	0.45170200	-2.84699600	0.00027800
C	-0.26035500	2.79789400	0.00011400
H	-0.53840300	3.37095100	0.88558500
H	0.82040900	2.68019400	0.00009100
H	-0.53842500	3.37109100	-0.88526000
C	3.40724200	1.36455200	-0.00058700
H	3.03643900	1.89486200	0.88098000
H	4.49585200	1.40077400	-0.00077000

H	3.03613900	1.89450100	-0.88223500

Cartesian coordinates of the optimized geometry for **2**-fix at B3LYP-D3BJ/def2-TZVP level of theory:

Ge	-1.44992800	-0.03701900	0.73049600
Ga	0.70296700	0.46978300	-0.44620300
Cl	-1.50280200	0.01584500	-1.76078200
N	0.61359500	2.48406800	-0.68308300
N	2.06253600	0.24167400	-1.85497200
C	1.11089100	3.11100400	-1.72890700
C	1.79155600	2.45708200	-2.77339800
H	2.06911800	3.08548800	-3.60580500
C	2.28481600	1.16110600	-2.80440600
C	1.01327000	4.60963300	-1.86506600
H	0.32776400	4.85687800	-2.67670700
H	1.98877800	5.01805800	-2.12818800
H	0.65946300	5.08586100	-0.95656400
C	3.15916100	0.78871100	-3.97410300
H	2.72033900	-0.04597200	-4.52067500
H	4.14474200	0.46336000	-3.64369200
H	3.27405400	1.63079200	-4.65143000
C	-0.03943400	3.18546400	0.38398400
C	0.64886000	3.30086800	1.60813700
C	0.00242300	3.91544400	2.67581800
H	0.51014900	4.01376200	3.62411700
C	-1.28938500	4.40296200	2.54567500
H	-1.77743600	4.87644600	3.38796000
C	-1.95402000	4.27183000	1.34048500
H	-2.96714800	4.64010600	1.24923600
C	-1.35656100	3.65695400	0.24074400
C	2.07668500	2.79985700	1.75434300
H	2.15968900	1.86823200	1.18717400
C	3.07806800	3.79147400	1.14633900
H	2.89100900	3.95909500	0.08741700
H	4.09837200	3.41789800	1.25132500
H	3.01490300	4.75456700	1.65736700
C	2.46602900	2.46557100	3.19304800
H	2.53700200	3.36204900	3.81201500
H	3.44275400	1.98282000	3.20759300
H	1.74950700	1.78360000	3.64843900
C	-2.16371200	3.52163600	-1.04012000
H	-1.57545500	2.94861600	-1.75484300
C	-2.48438600	4.89335700	-1.65340900
H	-2.98789100	4.76706500	-2.61411700
H	-1.59299200	5.49763800	-1.81271700
H	-3.15263700	5.46028200	-1.00203200
C	-3.47229000	2.75331500	-0.81135500
H	-4.16655900	3.33164900	-0.19783700
H	-3.30094000	1.80101600	-0.31762700
H	-3.95732200	2.54944700	-1.76688000
C	2.89150800	-0.92943500	-1.81971400
C	4.11284800	-0.85647400	-1.12470000
C	4.91572500	-1.99313700	-1.07535300
H	5.85884400	-1.95603900	-0.54532100
C	4.53202500	-3.16752400	-1.70420400
H	5.16863000	-4.04179300	-1.65727000
C	3.33060700	-3.21876300	-2.39104600
H	3.03644000	-4.13862400	-2.87898000
C	2.48975000	-2.10941800	-2.46389600
C	4.59341700	0.42917000	-0.47082600
H	3.83447800	1.19280100	-0.63099000
C	5.89051600	0.93777100	-1.11278300
H	5.77491600	1.08557300	-2.18701900
H	6.71110100	0.23425200	-0.95965300
H	6.18166300	1.89278000	-0.67077400
C	4.76342000	0.26590600	1.04089200
H	3.82591100	-0.02568200	1.51045200
H	5.09948200	1.20267900	1.48888500

H	5.50542500	-0.49966500	1.27628500
C	1.19140300	-2.20390500	-3.24319000
H	0.74180900	-1.21245800	-3.27395800
C	1.42678800	-2.66019200	-4.68922600
H	0.49539700	-2.60260500	-5.25519100
H	1.77505100	-3.69398100	-4.73055100
H	2.17057600	-2.04246600	-5.19480600
C	0.18853900	-3.13216700	-2.55146400
H	-0.11261700	-2.74084700	-1.58094200
H	0.60843500	-4.12965400	-2.40615600
H	-0.70982700	-3.22815200	-3.16076300
C	-1.70356500	-2.02585900	1.00841700
C	-0.82943800	-2.81572200	1.77320800
C	-1.12551500	-4.16220600	1.99484300
H	-0.44349300	-4.76239600	2.58434900
C	-2.29032500	-4.72465800	1.49528500
H	-2.50871800	-5.77025100	1.67240700
C	-3.19695200	-3.92853800	0.80918600
H	-4.13731300	-4.34367500	0.46764200
C	-2.92753900	-2.58023700	0.58384000
C	0.37547900	-2.24684000	2.44462200
C	0.22766200	-1.40250400	3.55619000
C	1.36598600	-0.93868300	4.21524700
H	1.24158800	-0.29827600	5.08134400
C	2.64621300	-1.29047300	3.81135100
C	2.77238000	-2.12926500	2.70720600
H	3.76024200	-2.41767700	2.36723300
C	1.66420300	-2.61480500	2.02336300
C	-1.12483400	-0.99903100	4.08516000
H	-1.86575100	-1.78367600	3.94476500
H	-1.50260500	-0.10440300	3.58143500
H	-1.06246200	-0.76472800	5.14813200
C	3.86009100	-0.80660100	4.55578800
H	3.60359600	-0.01395200	5.25859200
H	4.61874700	-0.42135500	3.87206200
H	4.32146100	-1.61898800	5.12359800
C	1.86741400	-3.53351600	0.85236100
H	1.69781200	-4.57671100	1.13116000
H	2.88097400	-3.44928300	0.46767800
H	1.17548700	-3.30849800	0.04556900
C	-3.99188000	-1.72254400	-0.02368800
C	-4.74274400	-0.86585800	0.80206300
C	-5.71273900	-0.04759200	0.22986600
H	-6.28236000	0.61450600	0.87262600
C	-5.97014400	-0.05764300	-1.13596200
C	-5.25354300	-0.94699400	-1.92773400
H	-5.44881700	-0.98487400	-2.99366200
C	-4.27890500	-1.78495100	-1.39509000
C	-4.53679300	-0.81715200	2.29326500
H	-5.43029300	-0.43560400	2.78756600
H	-3.70822100	-0.15476500	2.55669700
H	-4.30634600	-1.80026900	2.70186800
C	-6.97511500	0.88465800	-1.73892500
H	-7.37105200	0.49717200	-2.67834900
H	-6.51722300	1.85542100	-1.95008000
H	-7.81221300	1.06111800	-1.06160000
C	-3.55727300	-2.74852100	-2.29402600
H	-4.02141600	-3.73854200	-2.26137100
H	-2.52149900	-2.86577400	-1.99164400
H	-3.57851300	-2.40302700	-3.32752900

Cartesian coordinates of the optimized geometry for **S9** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	0.17578600	-1.99450200	-0.05077100
Cl	0.54047200	-0.76404400	2.22433400
Ga	0.91731800	0.39335900	-0.09793700
Si	-2.78650300	-2.47826900	0.88877900
N	0.37723100	2.23316900	0.32884300

N	2.85671000	0.78024800	-0.02483100
N	-1.71587600	-1.68250100	-0.25327500
C	1.22922800	3.19640800	0.68252800
C	2.61960300	3.05335400	0.69808200
H	3.17390000	3.92151400	1.01661000
C	3.38657000	1.93272800	0.36442300
C	0.67867600	4.53204200	1.11368200
H	0.18564500	5.03685600	0.28237700
H	1.47489400	5.17011500	1.48755200
H	-0.07344000	4.40300300	1.89256700
C	4.88392000	2.05275200	0.47150300
H	5.28630300	1.25360100	1.09538700
H	5.16532100	3.01312100	0.89539800
H	5.35082400	1.95149400	-0.50916300
C	-1.03086600	2.49495500	0.36922900
C	-1.64803300	3.19138400	-0.66512000
C	-3.00173300	3.48561800	-0.59076100
H	-3.47628700	4.02630800	-1.39882600
C	-3.74797800	3.07132900	0.50592100
H	-4.80421800	3.30025800	0.56152000
C	-3.13863200	2.33872000	1.51656200
H	-3.71700900	1.99140000	2.36236700
C	-1.78271100	2.04396300	1.45000400
C	3.68620500	-0.33617000	-0.35109100
C	4.25394600	-0.44649800	-1.61788900
C	5.00820300	-1.56546900	-1.94638900
H	5.44591000	-1.64612600	-2.93300700
C	5.19008100	-2.58330800	-1.01671800
H	5.77163400	-3.45799000	-1.27647200
C	4.61022800	-2.47865500	0.24182100
H	4.73471500	-3.27352900	0.96548300
C	3.85740400	-1.36027700	0.57713400
C	-3.37087400	-1.33618200	2.26092400
H	-2.50889500	-0.88091100	2.75131400
H	-3.92659300	-1.90670900	3.01017700
H	-4.01993200	-0.53654700	1.90370200
C	-1.82610200	-3.87049400	1.70161900
H	-1.43635800	-4.58577900	0.97529200
H	-2.50211700	-4.41049900	2.37078000
H	-0.99354500	-3.50575500	2.30580700
C	-4.25943800	-3.20581300	-0.01789700
H	-3.92688400	-3.91889800	-0.77536300
H	-4.85836900	-2.44514800	-0.51904400
H	-4.90840400	-3.73689800	0.68321900
C	-2.18058800	-0.84873600	-1.27454100
C	-1.47773200	-0.74256300	-2.48887000
C	-1.91781000	0.08324600	-3.51258900
H	-1.34954800	0.13462800	-4.43325400
C	-3.09157600	0.81461300	-3.37535600
H	-3.44426600	1.44748800	-4.17887200
C	-3.80646600	0.71089000	-2.18846000
H	-4.71696700	1.28046200	-2.05379400
C	-3.35682900	-0.09314200	-1.15281900
H	4.09165000	0.34217000	-2.34140500
H	3.38079100	-1.27953500	1.54472200
H	-1.29760000	1.46883500	2.22649200
H	-1.06330400	3.49637800	-1.52291200
H	-3.90931300	-0.11380600	-0.22613700
H	-0.59418800	-1.34966000	-2.64314400

Cartesian coordinates of the optimized geometry for TS-**1** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 1):

Ge	-0.09549100	-2.03503200	-0.12633000
Cl	-0.75958800	-0.32309600	-2.54525500
Ga	-0.91278500	0.32526700	-0.23774200
Si	2.97132400	-2.55294300	-0.64603000
N	-0.41164000	2.23041900	-0.33509400
N	-2.84160800	0.66984700	0.03172700

N	1.73912600	-1.71021000	0.29877800
C	-1.31147600	3.19904400	-0.50630600
C	-2.69668400	3.01618500	-0.43003100
H	-3.29079600	3.89858400	-0.60641900
C	-3.41639600	1.85115200	-0.14427800
C	-0.84023300	4.59625000	-0.82924500
H	-0.43621200	5.09125100	0.05424400
H	-1.66772300	5.19215800	-1.20583500
H	-0.04501100	4.57417900	-1.57384000
C	-4.91622600	1.96080700	-0.05575500
H	-5.39338000	1.18594500	-0.65669700
H	-5.25101000	2.93703300	-0.39698900
H	-5.25459800	1.81831900	0.97159800
C	0.98291400	2.53666700	-0.39226000
C	1.58524000	3.29585000	0.60772900
C	2.92930100	3.62560700	0.51727400
H	3.38695800	4.21950800	1.29765700
C	3.69044900	3.17637300	-0.55541600
H	4.73992300	3.43195500	-0.62262900
C	3.10041600	2.37999800	-1.52870900
H	3.68736100	2.00992900	-2.35921100
C	1.75118000	2.05803600	-1.45184800
C	-3.60388700	-0.48981700	0.35706100
C	-4.06751400	-0.69289700	1.65522800
C	-4.74760500	-1.86002900	1.97708900
H	-5.10403700	-2.01129700	2.98791200
C	-4.95793800	-2.83652400	1.00953000
H	-5.48146700	-3.74874400	1.26357400
C	-4.48093600	-2.64070600	-0.28088100
H	-4.62859700	-3.40152100	-1.03614600
C	-3.80375500	-1.47306600	-0.60998200
C	3.59497000	-1.47869300	-2.05480600
H	2.74768800	-1.10665600	-2.63546900
H	4.23370300	-2.06146800	-2.72381500
H	4.16927400	-0.61659500	-1.71438100
C	2.18884200	-4.07815100	-1.40512500
H	1.73858200	-4.72689600	-0.65199300
H	2.97065300	-4.64765900	-1.91602000
H	1.42251300	-3.83763600	-2.14343900
C	4.38147700	-3.08415200	0.46865000
H	4.01376400	-3.73877100	1.26186500
H	4.88404400	-2.24025500	0.94093800
H	5.12537200	-3.63985100	-0.10787800
C	2.08375400	-0.77748700	1.29085400
C	1.28690100	-0.65346800	2.44157000
C	1.60013600	0.25168400	3.44464600
H	0.96340900	0.31856700	4.31800800
C	2.74023300	1.04001300	3.34870600
H	2.99781200	1.73330300	4.13840400
C	3.54703000	0.91865700	2.22420000
H	4.43148200	1.53339700	2.12395100
C	3.22033600	0.03756800	1.20515000
H	-3.87856300	0.06131900	2.40829100
H	-3.41100100	-1.31864400	-1.60607100
H	1.28106000	1.45014100	-2.21232700
H	0.99751300	3.61669000	1.45718200
H	3.83884500	0.00210900	0.32198100
H	0.43462700	-1.31059400	2.56373300

Cartesian coordinates of the optimized geometry for **S9** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ge	0.65345100	0.77014100	-0.95316800
Ga	-1.21409400	-0.28320600	0.41265100
Cl	-1.72329900	-0.72774300	2.56103900
Si	2.31300200	0.53335500	1.87267900
N	-1.48959200	-2.05345400	-0.46730800
N	-2.91282900	0.45421200	-0.31810000
N	2.16863600	0.80780200	0.11830900

C	-2.66068100	-2.48513100	-0.91223700
C	-3.79772200	-1.67240000	-1.00645100
H	-4.69314000	-2.15924200	-1.35941500
C	-3.90309700	-0.29234800	-0.78682400
C	-2.78495800	-3.91527100	-1.37034300
H	-2.67609500	-4.59917000	-0.52714100
H	-1.99392400	-4.16026900	-2.08043300
H	-3.75001500	-4.09029000	-1.83865000
C	-5.22382100	0.35783600	-1.11442300
H	-5.49759300	1.08479000	-0.34989700
H	-6.00671700	-0.39258700	-1.19443700
H	-5.16903400	0.89417000	-2.06307200
C	-0.33518000	-2.88287400	-0.42687500
C	0.68319100	-2.68203000	-1.35822100
C	1.86879600	-3.40077600	-1.26645400
H	2.65258900	-3.23328500	-1.99384100
C	2.04510400	-4.32718700	-0.24615300
H	2.96934400	-4.88472800	-0.17101200
C	1.03213700	-4.52540900	0.68595500
H	1.17088000	-5.23117100	1.49454700
C	-0.15068500	-3.80336500	0.60312100
C	-2.99509900	1.87081900	-0.25238900
C	-2.96944000	2.64168300	-1.41496800
C	-2.96413700	4.02754200	-1.33367300
H	-2.94247100	4.61663800	-2.24150000
C	-2.96956000	4.65677100	-0.09347700
H	-2.95947300	5.73699600	-0.03202400
C	-2.97534500	3.89021000	1.06588000
H	-2.97037600	4.37141000	2.03530900
C	-2.98512600	2.50284300	0.99145100
C	3.37251000	1.09339900	-0.59707700
C	4.22104100	0.05379500	-0.98157100
C	5.39741500	0.32171900	-1.66897900
H	6.04527900	-0.49529300	-1.96081100
C	5.74087400	1.63085800	-1.98815100
H	6.65651700	1.83904000	-2.52576700
C	4.89563800	2.66929600	-1.61540700
H	5.15086200	3.69182800	-1.86317400
C	3.72062000	2.40375600	-0.92315800
C	4.06289600	0.97710400	2.38332100
H	4.31488000	2.00436000	2.11417000
H	4.80500000	0.32322600	1.92350900
H	4.15543500	0.88136900	3.46830300
C	2.00476600	-1.26498800	2.27335300
H	0.96715600	-1.55320100	2.11857400
H	2.24125500	-1.45871100	3.32295200
H	2.63463000	-1.91075200	1.65883700
C	1.13374100	1.67815200	2.76468600
H	1.36275900	2.71772800	2.51887500
H	1.23563200	1.55510500	3.84591200
H	0.09286700	1.48117700	2.51402100
H	0.53539400	-1.96636400	-2.15820000
H	-0.92326200	-3.91667100	1.35152300
H	-2.98523900	1.89763600	1.88834400
H	-2.93257600	2.14661800	-2.37649400
H	3.06041900	3.20814300	-0.62563500
H	3.94274100	-0.96286900	-0.73524200

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