Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

On the σ-complex character of bis(gallyl)/digallane transition metal species

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1. Experimental Methods and Data

a. General Considerations

All analysis and manipulations were carried out under an dry oxygen free argon atmosphere using standard Schlenk techniques or in an MBraun inert atmosphere glovebox containing an atmosphere of high purity argon, using flame dried glassware. All syringes, magnetic stirring bars and needles were rigorously dried. THF and diethyl ether were dried by distillation over a sodium/benzophenone mixture, degassed by standard procedures and stored over activated 4Å mol sieves. C_6D_6 and THF-d_8 were dried, degassed by standard procedures, and stored over a potassium mirror, molecular sieve prior to use, respectively. All other solvents were dried over activated 4Å mol sieves and degassed by standard procedures, prior to use. ^{PhiP}DippNK ([[$Ph_2PCH_2Si(^iPr)_2$](Dipp)NK]), [1] $Ni(COD)_2$, [2] $Pd(COD)(CH_2TMS)_2$ [3] were synthesized according to known literature procedures. All other reagents were used as received, unless mentioned otherwise. If compounds were sensitive to oxygen and/ or moisture, they were stored in a glovebox (MBraun Labmaster dp) under dry argon atmosphere.

NMR. NMR spectra were recorded on a Bruker AV 400 Spectrometer. The spectra were processed using the MestReNova 14.3.0 software suite. All chemical shifts δ are given in ppm. The ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to the residual solvent signals as internal standards. ^{29}Si{^{1}H} NMR spectra were externally calibrated with $SiMe_4$. ^{31}P{^{1}H} NMR spectra were externally calibrated with H_3PO_4. The coupling constants J are given in Hz. For signal multiplicities, the following abbreviations were used: s = singlet, d = doublet, t = triplet, q = quartet, p = pentad, h = heptad, m = multiplet, br = broard and combinations thereof.

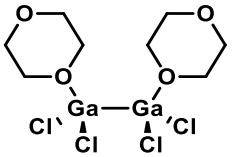
LIFDI-MS. Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) was measured directly from an inert atmosphere glovebox with a Thermo Fisher Scientific Exactive Plus Orbitrap equipped with an ion source from Linden CMS.[4]

Raman. Raman spectra were measured using an *inVia* Raman microscope (Renishaw, RE04). The powdery samples were filled into a 0.5 mm glass capillary and irradiated with a 532 nm laser beam for 1 s at 0.5 % laser power using a microscope equipped with a 50-fold magnifying objective and a grating with 1800 lines mm^{-1}. 150 such measurements were averaged to yield the final Raman spectra.

UV-Vis. Absorption spectra (UV/vis) were recorded on an Agilent Cary 60 UV/vis spectrophotometer. In an inert cuvette with all samples being prepared in an MBraun Labmaster dp inert atmosphere glovebox containing an dry atmosphere of high purity argon.

Elemental Analysis. Elemental analyses (C, H, N) were performed with a combustion analyzer (elementar vario EL, Bruker).

b. Experimental Procedures

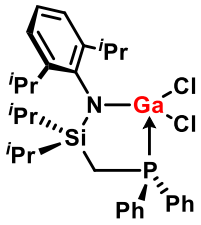


Ga_2Cl_4·(dioxane)$_2$. *This was accessed via modified literature procedures.*[5,6]

A high pressure Schlenk flask was loaded with gallium trichloride (4.00 g, 22.72 mmol) and excess of elemental gallium (1.58 g, 22.72 mmol). Subsequently 30 mL of benzene were added, and the reaction mixture was heated to 60 °C for 24 h, without stirring. After 24 h two layers had formed, characteristic for group 13 benzene adducts. The reaction mixture was filtered to separate it from the excess of elemental gallium, and dioxane (15.65 g, 15.20 mL, 181.74 mmol) was added to the filtrate dropwise at 0 °C. This resulted in the formation of a grey precipitate. Subsequently the solution was filtered off, and the crude product was purified by washing with benzene (2 x 10 mL), and the solid dried *in vacuo*, yielding **Ga_2Cl_4·(dioxane)$_2$** as an off-white powder. The filtrate and wash solutions were concentrated and stored at room temperature for two days, leading to a further crop of crystalline **Ga_2Cl_4·(dioxane)$_2$**. The combined yield was 8.32 g (81%).

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ = 3.32 (s).

^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 298 K): δ = 67.2 (O-*C*H_2).



^{PhiP}DippGaCl$_2$, 1.

Method A: A Schlenk flask was loaded with ^{PhiP}DippNK (1.00 g, 1.90 mmol) and gallium trichloride (0.335 g, 1.90 mmol). Subsequently 20 mL of toluene were added at -80 °C. The suspension was subsequently allowed to slowly warm up to room temperature overnight under continuous stirring. Afterwards the reaction mixture was filtered, and all volatiles were removed *in vacuo*, yielding an off-white solid. The crude product was purified by washing with pentane (2x10 mL) and dried *in vacuo* afterwards. Yielding **1** (0.38 g, 0.60 mmol, 30 %) as an off-white powder.

Method B: A Schlenk flask was loaded with gallium trichloride (0.335 g, 1.90 mmol) and 15 mL of THF were added at -80 °C. Subsequently a solution of ^{PhiP}DippK (1.00 g, 1.90 mmol) in 20 mL of THF was added dropwise over the course of 30 min, while maintaining a temperature of -80 °C. The solution was subsequently allowed to slowly warm up to room temperature overnight under continuous stirring. Afterwards the reaction mixture was filtered, and all volatiles were removed *in vacuo*, yielding an off-white solid. The crude product was purified by washing with pentane (10 mL) and dried *in vacuo* afterwards. Yielding **1** (1.00 g, 1.58 mmol, 80 %) as an off-white powder.

N.B. Colorless crystals of **1** *suitable for single crystal X-Ray diffraction analysis were obtained from a concentrated pentane solution at room temperature.*

^{1}H NMR (THF-d_8, 400 MHz, 298 K): δ = 7.93 (dt, $^{3}J_{HH}$ = 12.0, 5.5 Hz, 4H, Ar-C*H*), 7.55 (m, 6H, Ar-C*H*), 6.93 (m, 3H, Ar-C*H*), 3.33 (p, $^{3}J_{HH}$ = 6.8 Hz, 2H, Dipp-iPr-C*H*), 2.11 (d, $^{3}J_{HP}$ = 14.8 Hz, 2H, Si-CH_2-P), 1.17 (m, 8H, Si-iPr-C*H* /Si-iPr-CH_3), 1.08 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, Dipp-iPr-CH_3), 0.94 (d, $^{3}J_{HH}$ = 6.6 Hz, 6H, Dipp-iPr-CH_3), 0.83 (d, $^{3}J_{HH}$ = 7.0 Hz, 6H, Si-iPr-CH_3).

^{13}C{^{1}H} NMR (THF-d_8, 101 MHz, 298 K): δ = 147.7, 143.2, 143.1, 134.0, 133.9, 133.1, 133.1, 130.5, 130.4, 128.8, 128.4, 124.7 and 124.3 (Ar-*C*), 28.5 (Dipp-iPr-*C*H), 27.2 and 24.1 (Dipp-iPr-*C*H_3), 19.6 and 18.9 (Si-iPr-*C*H_3), 16.3 (Si-iPr-*C*H), 4.0 (d, $^{1}J_{CP}$ = 20.2 Hz, Si-*C*H_2-P).

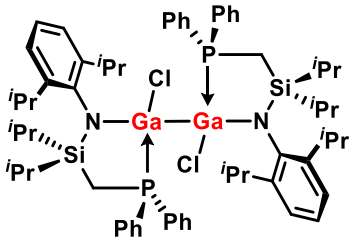
^{31}P{^{1}H} NMR (THF-d_8, 162 MHz, 298 K): δ = -20.6 (s, CH_2-*P*-(Ph)$_2$).

^{29}Si{^{1}H} NMR (THF-d_8, 400 MHz, C_6D_6, 298 K): δ = 0.1 (s, CH_2-*Si*-(^{i}Pr)$_2$)

MS/LIFDI-HRMS found (calcd.) m/z: 629.1495 (629.1521) for [^{PhiP}DippNGaCl$_2$]$^{+}$.

Anal. calcd. $C_{31}H_{43}Cl_2GaNPSi$: C, 59.16%; H, 6.89%; N, 2.23%; found: C, 57.10%; H, 6.83%; N, 2.47%.

N.B. Repeated element analysis gave variable but consistently low values for C, possibly due to Si-carbide formation.[7]



(^{PhiP}DippGaCl)$_2$, 2. A Schlenk flask was loaded with ^{PhiP}DippNK (1.50 g, 2.84 mmol) and tetrachlorodigallane·(dioxane)$_2$ (0.643 g, 1.42 mmol). Subsequently 30 mL of toluene were added at -80 °C. The suspension was subsequently allowed to slowly warm up to room temperature overnight under continuous stirring. After this time, the reaction mixture was filtered, and all volatiles were removed *in vacuo*, yielding an off-white solid. The crude product was purified by washing with pentane (2 x 10 mL) and dried in *vacuo* afterwards. Yielding **2** (1.28 g, 1.08 mmol, 76 %) as a white powder.

N.B. Colorless crystals of **2** *suitable for single crystal X-Ray diffraction analysis were obtained from a concentrated diethyl ether solution at room temperature.*

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ = 7.94 (t, $^{3}J_{HH}$ = 8.6 Hz, 4H, Ar-C*H*), 7.69 (t, $^{3}J_{HH}$ = 8.9 Hz, 3H, Ar-C*H*), 7.21 (m, 4H, Ar-C*H*), 7.11 (m, 6H, Ar-C*H*), 7.03 (m, 6H, Ar-C*H*), 6.88 (dd, $^{3}J_{HH}$ = 8.5, 6.6 Hz, 2H, Ar-C*H*), 4.16 (p, $^{3}J_{HH}$ = 6.8 Hz, 2H, Dipp-^{i}Pr-C*H*), 3.06 (p, $^{3}J_{HH}$ = 6.9 Hz, 2H, Dipp-^{i}Pr-C*H*), 1.92 (m, 2H, Si-CH_2-P), 1.57 (m, 10H, Si-^{i}Pr-CH_3 /Si-^{i}Pr-C*H* /Si-CH_2-P), 1.42 (d, *J* = 7.0 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.35 (d, $^{3}J_{HH}$ = 6.6 Hz, 6H, Dipp-^{i}Pr-CH_3), 0.97 (d, $^{3}J_{HH}$ = 7.1 Hz, 6H, Si-^{i}Pr-CH_3), 0.87 (m, 12H, Dipp-^{i}Pr-CH_3 /Si-^{i}Pr-CH_3), 0.72 (q, $^{3}J_{HH}$ = 7.3

Hz, 2H, Si-^{i}Pr-C*H*), 0.47 (d, $^{3}J_{HH}$ = 7.3 Hz, 6H, Si-^{i}Pr-CH_3), 0.36 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3).

^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 298 K): δ = 147.0, 146.5, 145.0, 135.1, 135.0, 135.0, 133.8, 133.7, 133.7, 131.4, 131.0, 129.3, 128.9, 128.8, 128.7, 128.7, 124.2, 124.1 and 124.0 (Ar-*C*), 28.3 (Dipp-^{i}Pr-*C*H$_3$), 27.5 (Dipp-^{i}Pr-*C*H), 27.2 (Dipp-^{i}Pr-*C*H$_3$), 27.0 (Dipp-^{i}Pr-*C*H), 24.0 and 23.7 (Dipp-^{i}Pr-*C*H$_3$), 20.5, 19.9, 18.2 and 15.0 (Si-^{i}Pr-*C*H$_3$), 14.8 (Si-^{i}Pr-*C*H), 4.2 (Si-*C*H$_2$-P).

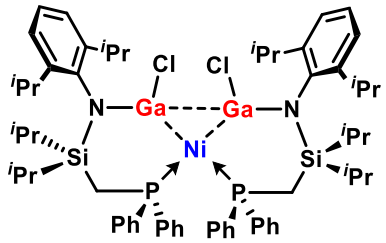
^{31}P{^{1}H} NMR (C_6D_6, 162 MHz, 298 K): δ = -13.1 (s, CH$_2$-*P*-(Ph)$_2$).

^{29}Si{^{1}H} NMR (C_6D_6, 99 MHz, 298 K): δ = 3.6 (s, CH$_2$-*Si*-(^{i}Pr)$_2$).

MS/LIFDI-HRMS found (calcd.) m/z: 1186.3651 (1186.3679) for [(^{PhiP}DippNGaCl)$_2$]$^{+}$.

Raman *ν*/cm^{-1} (ATR): 151.6, 179.3, 218.6, 256.4, 268.0, 340.0, 363.0, 389.6, 443.7, 486.2, 506.0, 535.6, 545.5, 556.5, 594.4, 617.5, 628.4, 646.5, 688.5, 715.9, 747.9, 790.3, 796.2, 842.9, 881.0, 906.3, 953.2, 971.3, 987.1, 999.6, 1014.2, 1025.4, 1040.0, 1072.27, 1092.2, 1100.0, 1149.4, 1158.2, 1176.7, 1184.3, 1237.3.

Anal. calcd. $C_{62}H_{86}Cl_2Ga_2N_2P_2Si_2$: C, 62.69%; H, 7.30%; N, 2.36%; found: C, 63.09%; H, 7.36%; N, 2.36%.



[(^{PhiP}DippGaCl)$_2$Ni], 3.

Method A: A Schlenk flask was loaded with **2** (450 mg, 0.38 mmol) and Ni(COD)$_2$ (105 mg, 0.38 mmol). Toluene (15 mL) was added, and the solution was stirred for 72 h at room temperature. Afterwards the reaction mixture was filtered, and all volatiles were removed *in vacuo*, resulting in the formation of a reddish solid. Then the crude product was purified by extraction with pentane and subsequent crystallization from the concentrated pentane solution at room temperature, yielding **3** (76 mg, 0.06 mmol, 16 %) as orange to yellow crystals suitable for single crystal X-Ray diffraction analysis.

Method B: A Schlenk flask was loaded with **2** (300 mg, 0.26 mmol) and Ni(COD)$_2$ (70 mg, 0.26 mmol). Then THF 15 mL was added and the solution was stirred for 16 h at room temperature. Afterwards the reaction mixture was filtered, and all volatiles were removed *in vacuo*, resulting in the formation of a reddish solid. The crude product was purified by extraction with pentane and subsequent crystallization from the concentrated pentane solution at room temperature, yielding **3** (56 mg, 0.04 mmol, 17 %) as orange to yellow crystals suitable for single crystal X-Ray diffraction analysis.

^{1}H NMR (THF-d$_8$, 400 MHz, 193 K): δ = 7.97 (m, 1H, Ar-C*H*), 7.82 (m, 3H, Ar-C*H*), 7.65 (m, 2H, Ar-C*H*), 7.46 (m, 6H, Ar-C*H*), 6.98 (d, $^{3}J_{HH}$ = 7.7 Hz, 3H, Ar-C*H*), 6.90 (m, 6H, Ar-C*H*), 6.98 (d, $^{3}J_{HH}$ = 7.6 Hz, 5H, Ar-C*H*), 4.05 (p, *J* = 6.7 Hz, 2H, Dipp-^{i}Pr-C*H*), 2.35 (m, 4H, Dipp/Si-

^{i}Pr-C*H*), 2.17 (m, 4, Si-CH_2-P), 1.72 (d, *J* = 8.6 Hz, 6H, Si-^{i}Pr-CH_3), 1.42 (d, *J* = 7.3 Hz, 6H, Si-^{i}Pr-CH_3), 1.25 (m, 8H, Si-^{i}Pr-C*H* /Dipp-^{i}Pr-CH_3), 1.14 (m, 12H, Si-^{i}Pr-CH_3), 0.96 (d, *J* = 6.8 Hz, 6H, Dipp-^{i}Pr-CH_3), 0.59 (d, *J* = 7.2 Hz, 6H, Si-^{i}Pr-CH_3), 0.04 (d, *J* = 6.4 Hz, 6H, Dipp-^{i}Pr-CH_3).

^{13}C{^{1}H} NMR (THF-d_8, 101 MHz, 298 K) δ = 146.8, 143.3, 139.5, 134.0, 133.9, 133.1, 130.5, 129.7 (br), 124.3 and 124.0 (br, Ar-*C*), 28.5 (br), 27.0 (br), 19.6, 18.9 and 16.3 (Ali-*C*), 14.9 (Si-*C*H_2-P).

^{31}P{^{1}H} NMR (THF-d_8, 162 MHz, 298 K): δ = 8.5 (s, CH_2-*P*-$(Ph)_2$).

λ_{max}, nm (*ε*, Lmol^{-1} cm^{-1}): 350 (172,800)

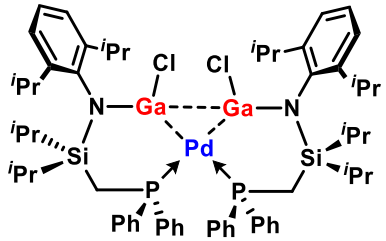
MS/LIFDI-HRMS found (calcd.) m/z: 1244.2999 (1244.3033) for [(^{PhiP}DippNGaCl)$_2$Ni]$^{+}$.

Raman *v*/cm^{-1} (ATR): 151.6, 176.7, 225.2, 277.1, 343.9, 357.9, 392,13, 445.0, 577.7, 595.60, 617.5, 686.1, 713.6, 745.6, 793.9, 837.1, 879.9, 999.6, 1026.5, 1039.9, 1096.7, 1103.3, 1159.3, 1183.3.

Anal. calcd. $C_{62}H_{86}Cl_2Ga_2N_2P_2Si_2Ni$: C, 59.74%; H, 6.95%; N, 2.25%; found: C, 56.12%; H, 6.53%; N, 2.08%.

*N.B. Due to the conformationally locked nature of **3**, highly broadened NMR signals for the ligands in this compound are observed at room temperature. This precluded the observation of any signal in the ^{29}Si-NMR-spectrum.*

N.B. Repeated element analysis gave variable but consistently low values for C, possibly due to Si-carbide/Ni-carbide formation.[7]



[(^{PhiP}DippGaCl)$_2$Pd], 4.

A Schlenk flask was loaded with **2** (250 mg, 0.21 mmol, 1.0 eq.) and Pd(COD)$(CH_2TMS)_2$ (82 mg, 0.21 mmol, 1.0 eq). THF (15 mL) was subsequently added, and the solution was stirred for 24 h at room temperature. All volatiles were then removed *in vacuo*, yielding an off-white to light pink solid. The crude product was purified by washing with pentane (10 mL* 2 times), yielding **4** (217 mg, 0.17 mmol, 79%) as an analytically pure off-white to light pink solid.

*N. B. Colorless crystals of **4** suitable for single crystal X-Ray diffraction analysis were obtained from a concentrated pentane solution stored at room temperature.*

^{1}H NMR (THF-d_8, 400 MHz, 193 K): δ = 7.89 (m, 4H, Ar-C*H*), 7.55 (d, $^{3}J_{HH}$ = 7.3 Hz, 6H, Ar-C*H*), 6.98 (d, $^{3}J_{HH}$ = 7.3 Hz, 3H, Ar-C*H*), 6.88 (m, 10H, Ar-C*H*), 6.76 (m, 3H, Ar-C*H*), 4.00 (p, *J* = 6.8 Hz, 2H, Dipp-^{i}Pr-C*H*), 2.42 (m, 4H, Dipp/Si-^{i}Pr-C*H*), 2.25 (m, 2H, Si-CH_2-P), 1.98 (m,

2H, Si-CH_2-P), 1.66 (d, *J* = 7.3 Hz, 6H, Si-^{i}Pr-CH_3), 1.33 (d, *J* = 7.4 Hz, 6H, Si-^{i}Pr-CH_3), 1.24 (d, *J* = 6.4 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.14 (d, *J* = 6.5 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.07 (d, *J* = 7.5 Hz, 6H, Si-^{i}Pr-CH_3), 0.99 (d, *J* = 6.6 Hz, 6H, Dipp-^{i}Pr-CH_3), 0.86 (d, *J* = 7.2 Hz, 2H, Si-^{i}Pr-C*H*), 0.12 (d, *J* = 6.4 Hz, 6H, Dipp-^{i}Pr-CH_3).**^{13}C{^{1}H} NMR** (THF-d_8, 101 MHz, 298 K): K δ = 146.6, 143.5, 138.6, 138.5, 138.3, 129.8 (br), 124.4 and 123.9 (br, Ar-*C*), 29.1 (br), 24.1 (br), 19.6 (br), 23.7 and 16.6 (br, Ali-*C*).

^{31}P{^{1}H} NMR (THF-d_8, 162 MHz, 298 K): δ = 4.3 (s, CH_2-*P*-$(Ph)_2$).

MS/LIFDI-HRMS found (calcd.) m/z: 1294.2700 (1294.2718) for $[(^{PhiP}DippNGaCl)_2Pd]^+$.

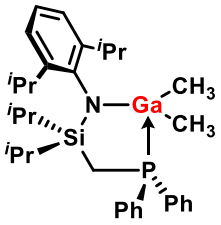
λ$_{max}$, nm (*ε*, Lmol^{-1} cm^{-1}): 275 (689760)

Raman *v*/cm^{-1} (ATR): 151.6, 166.37, 219.9, 260.3, 271.9, 309.3, 360.4, 434.9, 453.7, 517.1, 566.3, 591.9, 617.5, 686.1, 701.6, 718.3, 785.7, 793.9, 830.1, 837.1, 881.3, 898.3, 952.0, 999.6, 1027.6, 1038.8, 1058.9, 1097.8, 1104.4, 1127.5, 1159.3, 1175.6, 1210.4, 1237.3.

Anal. calcd. $C_{62}H_{86}Cl_2Ga_2N_2P_2Si_2Pd$: C, 57.54%; H, 6.70%; N, 2.16%; found: C, 54.85%; H, 6.22%; N, 2.25%.

*N.B. Due to the conformationally locked nature of **3**, highly broadened NMR signals for the ligands in this compound are observed at room temperature. This precluded the observation of any signal in the ^{29}Si-NMR-spectrum.*

N.B. Repeated element analysis gave variable but consistently low values for C, possibly due to Si-carbide/Pd-carbide formation.[7]



^{PhiP}DippGaMe$_2$, 6.

Method A: A Schlenk flask was loaded with **2** (0.313 g, 0.263 mmol). Diethyl ether (15 mL) was added and the solution was cooled to -80 °C. A stock solution of MeLi (1.6 M in Et_2O, 0.35 mL, 0.553 mmol) was then added dropwise at -80 °C, with rapid stirring. The reaction mixture was then stirred for 3 h at room temperature, resulting in the deposition of elemental gallium in the form of a gallium mirror. The reaction mixture was then filtered, and all volatiles were removed *in vacuo*, resulting in the formation of an off-white solid. The crude product was purified by crystallization from a concentrated diethyl ether solution (~7 mL) at room temperature, yielding **6** (0.102 g, 0.173 mmol, 66 %) as colorless crystals, which were suitable for single crystal X-Ray diffraction analysis.

Method B: A Schlenk flask was loaded with **1** (0.300 g, 0.477 mmol), and diethyl ether (10 mL) was added. The solution was cooled to -80 °C, and a stock solution of MeLi (1.6 M in Et_2O, 0.66 mL, 1.05 mmol) was added dropwise at -80 °C. The reactions mixture was subsequently allowed to slowly warm up to room temperature over the cause of 16 h. The reaction mixture was then filtered, and all volatiles removed *in vacuo*, resulting in the

formation of an off-white solid. The crude product was purified by extracting with pentane (20 mL), filtration, and solvent removal *in vacuo*, yielding analytically pure **6** (0.197 g, 0.335 mmol, 70 %) as an off-white powder.

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ = 7.57 (t, $^{3}J_{HH}$ = 8.2 Hz, 1H, Ar-C*H*), 7.47 (t, $^{3}J_{HH}$ = 8.9 Hz, 3H, Ar-C*H*), 7.10 (m, 3H, Ar-C*H*), 7.02 (m, 6H, Ar-C*H*), 3.65 (p, $^{3}J_{HH}$ = 7.1 Hz, 2H, Dipp-iPr-C*H*), 1.66 (d, $^{3}J_{HH}$ = 12.6 Hz, 2H, Si-CH_2-P), 1.28 (d, $^{3}J_{HH}$ = 6.9 Hz, 6H, Dipp-iPr-CH_3), 1.22 (m, 2H, Si-iPr-C*H*), 1.13 (d, $^{3}J_{HH}$ = 7.6 Hz, 12H, Si-iPr-CH_3), 1.06 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, Dipp-iPr-CH_3), 0.11 (d, $^{3}J_{HP}$ = 5.4 Hz, 6H, Ga-CH_3)

^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 298 K): δ = 147.1, 147.0, 146.5, 141.9, 140.3, 133.6, 133.4, 132.9, 133.6, 132.8, 132.5, 130.5, 130.5, 129.2, 129.1, 123.7, 122.9, 122.8 and 116.0 (Ar-*C*), 27.9 (Dipp-iPr-*C*H), 26.3, 25.2 and 24.2 (Dipp-iPr-*C*H_3), 19.7 (Si-iPr-*C*H_3), 19.6 (Si-iPr-*C*H), 19.0, 16.9 and 16.8 (Si-iPr-*C*H_3), 7.3 (Si-*C*H_2-P), -3.7 (d, $^{2}J_{CP}$ = 20.2 Hz, Ga-*C*H_3).

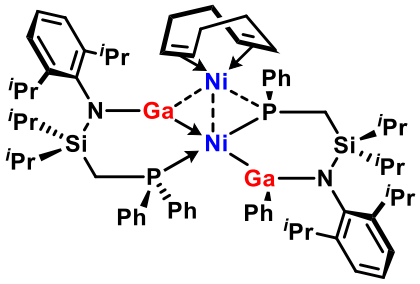
^{31}P{^{1}H} NMR (C_6D_6, 162 MHz, 298 K): δ = -17.4 (s, CH_2-*P*-(Ph)$_2$).

^{29}Si{^{1}H} NMR (C_6D_6, 99 MHz, 298 K): δ = -0.3 (d, $^{2}J_{SiP}$ = 9.9 Hz, 1Si, CH_2-*Si*-(^{i}Pr)$_2$)

MS/LIFDI-HRMS found (calcd.) m/z: 572.2378 (572.2387) for $[M\text{-}CH_3]^+$.

Anal. calcd. $C_{33}H_{46}GaNPSi$: C, 67.35%; H, 8.29%; N, 2.38%; found: C, 65.88%; H, 8.29%; N, 2.65%.

N.B. Repeated element analysis gave variable but consistently low values for C, possibly due to Si-carbide formation.[7]



[(^{PhiP}DippNGa)(Ni$_2$(COD)(^{PhiP}DippNGaPh)], 7.

A Schlenk flask was loaded with **2** (200 mg, 0.17 mmol, 1.0 eq) and Ni(COD)$_2$ (56 mg, 0.17 mmol, 1.0 eq), and diethyl ether (15 mL) was added. The reaction mixture was stirred for 24 h at room temperature, leading to the formation of a deep red solution over a colourless precipitate. After this time, the suspension was filtered, and all volatiles were removed *in vacuo*, yielding a red-purple solid. The so formed crude product was further purified by extraction with pentane (15 mL), filtration, and concentration to ~6 mL, leading to crystallization of **7** (84 mg, 0.06 mmol, 74 % based on Ni) as red crystals, which were suitable for single crystal X-Ray diffraction analysis.

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ = 7.58 (m, 2H, Ar-C*H*), 7.42 (m, 2H, Ar-C*H*), 7.08 (m, 12H, Ar-C*H*), 7.00 (m, 3H, Ar-C*H*) , 6.93 (m, 1H, Ar-C*H*), 6.77 (m, 4H, Ar-C*H*), 6.70 (m, 2H, Ar-C*H*), 4.24 (m, 1H, HC=C*H*), 4.08 (m, 1H, HC=C*H*), 3.79 (m, 1H, HC=C*H*), 3.64 (p, $^{3}J_{HH}$ = 6.7 Hz, 1H, Dipp-^{i}Pr-C*H*), 3.54 (p, $^{3}J_{HH}$ = 6.7 Hz, 1H, Dipp-^{i}Pr-C*H*), 2.90 (m, 4H, HC=C*H*/

Dipp-^{i}Pr-C*H*/ CH_2-CH_2), 2.42 (m, 6H, Si-CH_2-P/ CH_2-CH_2), 2.14 (m, 1H, CH_2-CH_2), 2.05 (m, 1H, CH_2-CH_2), 1.94 (m, 1H, CH_2-CH_2), 1.86 (m, 1H, CH_2-CH_2), 1.75 (m, 1H, CH_2-CH_2), 1.66 (d, $^{3}J_{HH}$ = 7.0 Hz, 3H, Si-^{i}Pr-CH_3), 1.53 (p, $^{3}J_{HH}$ = 6.6 Hz, 2H, Si-^{i}Pr-C*H*), 1.36 (m, 5H, Si-^{i}Pr-C*H*/ Si-^{i}Pr-CH_3), 1.23 (m, 12H, Si-^{i}Pr-CH_3), 1.15 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, Dipp-^{i}Pr-CH_3), 1.02 (m, 15H, Si-^{i}Pr-CH_3), 0.68 (d, $^{3}J_{HH}$ = 7.2 Hz, 3H, Si-^{i}Pr-CH_3), 0.63 (d, $^{3}J_{HH}$ = 6.7 Hz, 3H, Dipp-^{i}Pr-CH_3), -0.14 (d, $^{3}J_{HH}$ = 6.6 Hz, 3H, Dipp-^{i}Pr-CH_3).

^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 298 K): δ = 151.8, 148.0, 147.0, 145.9, 145.8, 145.5, 144.5, 141.3, 140.2, 139.8, 137.4, 134.6, 134.4, 131.7, 130.9, 130.8, 130.5, 128.8, 128.7, 127.79, 127.7, 127.6, 127.1, 126.2, 124.8, 124.7, 124.5, 123.3 and 123.0 (Ar-*C*), 86.9, 83.0, 80.6 and 75.5 (H*C*=CH), 35.8, 32.0, 30.7 and 29.1 (CH_2-*C*H_2), 28.5, 28.2 and 27.8 (Dipp-^{i}Pr-*C*H), 27.7 (Si-^{i}Pr-*C*H_3), 27.2 (Dipp-^{i}Pr-*C*H), 26.5 (Dipp-^{i}Pr-*C*H_3), 26.2, 26.1, 25.2, 25.0 and 23.2 (Si-^{i}Pr-*C*H_3), 23.2 (Dipp-^{i}Pr-*C*H_3), 20.5 and 20.4 (Si-^{i}Pr-*C*H_3), 20.1 (Si-^{i}Pr-*C*H), 19.9, 19.3, 19.1, 18.9 and 18.7 (Si-^{i}Pr-*C*H_3), 14.5 (Si-^{i}Pr-*C*H), 14.0 and 14.0 (Si-^{i}Pr-*C*H_3), 12.5, 12.3 and 9.4 (Si-*C*H_2-P).

^{31}P{^{1}H} NMR (C_6D_6, 162 MHz, 298 K): δ = 67.8 (d, $^{2}J_{PP}$= 111.3 Hz, 1P, CH_2-*P*-Ph), 17.5 (d, $^{2}J_{PP}$ = 110.8 Hz, 1P, CH_2-*P*-(Ph)$_2$).

^{29}Si{^{1}H} NMR (C_6D_6, 99 MHz, 298 K): δ = 3.27 (dd, $^{2}J_{SiP}$/ $^{4}J_{SiP}$ = 9.9 Hz/ 1.2 Hz, 1Si, CH_2-*Si*-(^{i}Pr)$_2$), -0.5 (d, $^{2}J_{SiP}$= 3.7 Hz, 1Si, CH_2-*Si*-(^{i}Pr)$_2$).

λ_{max}, nm (***ε***, Lmol^{-1} cm^{-1}): 599 (26880), 450 (195630), 331 (462409)

MS/LIFDI-HRMS found (calcd.) m/z: 1342.3902 (1342.3903) for [(^{PhiP}DippNGa)(^{PhiP}DippNGaPh)(Ni)(Ni)(COD)]$^{+}$

Anal. calcd. $C_{70}H_{98}Ga_2N_2P_2Si_2Ni_2$: C, 62.63%; H, 7.36%; N, 2.09%; found: C, 58.52%; H, 7.24%; N, 1.87%.

N.B. Repeated element analysis gave variable but consistently low values for C, possibly due to Si-carbide/Ni-carbide formation.[7]

c. Spectroscopic data

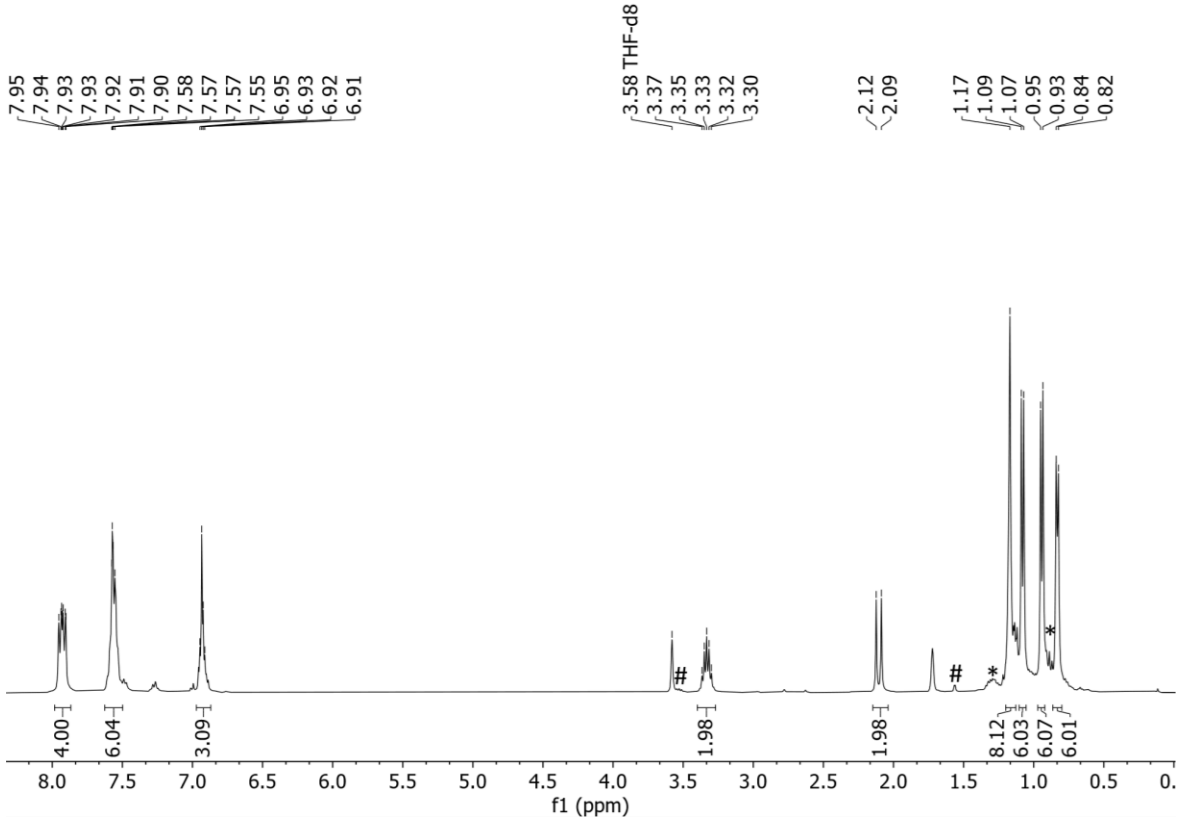


Figure S1. ^{1}H-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **1**. * Denotes minor amounts of pentane. # denotes minor amounts of coordinated THF.

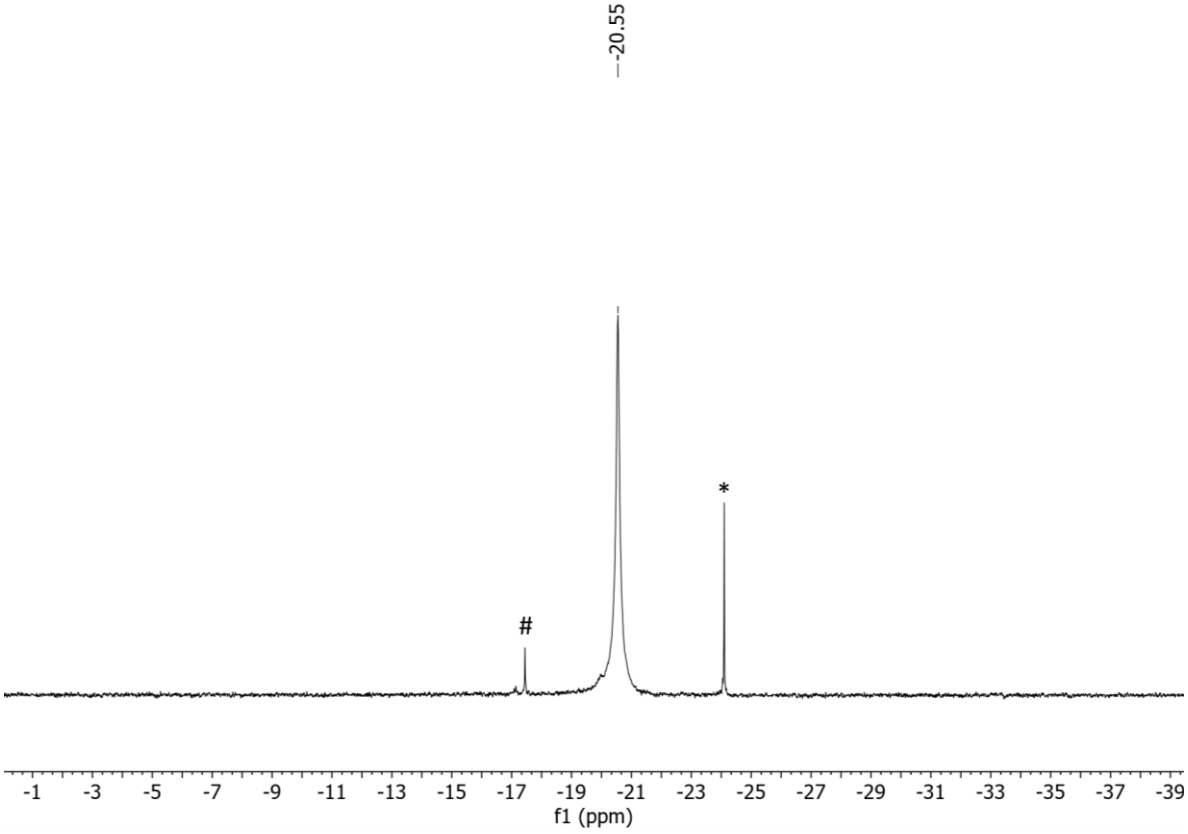


Figure S2. ^{31}P{^{1}H}-NMR-spectrum (162 MHz, THF-d_8, 298 K) of **1**. * Denotes minor amounts of decomposition product ^{PhiP}DippNH and # denotes minor amounts of starting material ^{PhiP}DippNK.

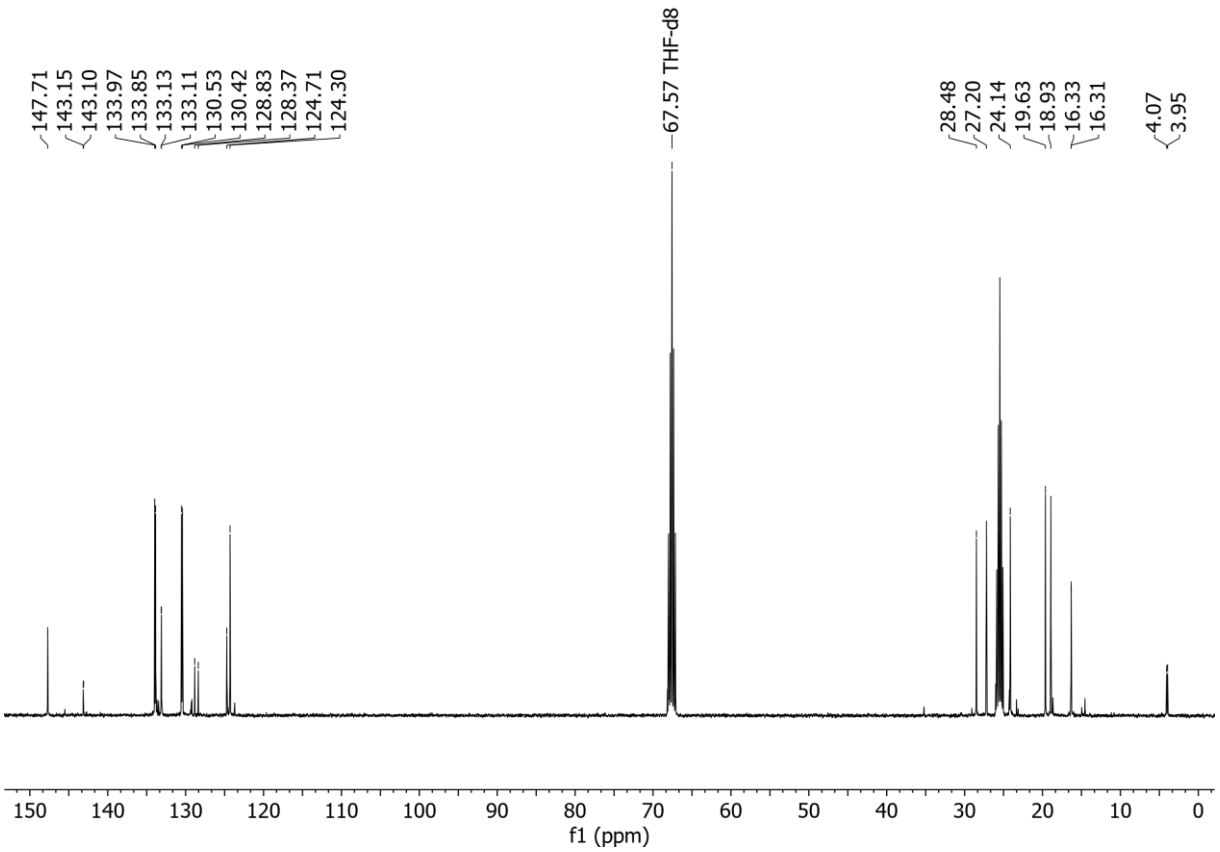


Figure S3. ^{13}C-NMR-spectrum (101 MHz, THF-d_8, 298 K) of **1**.

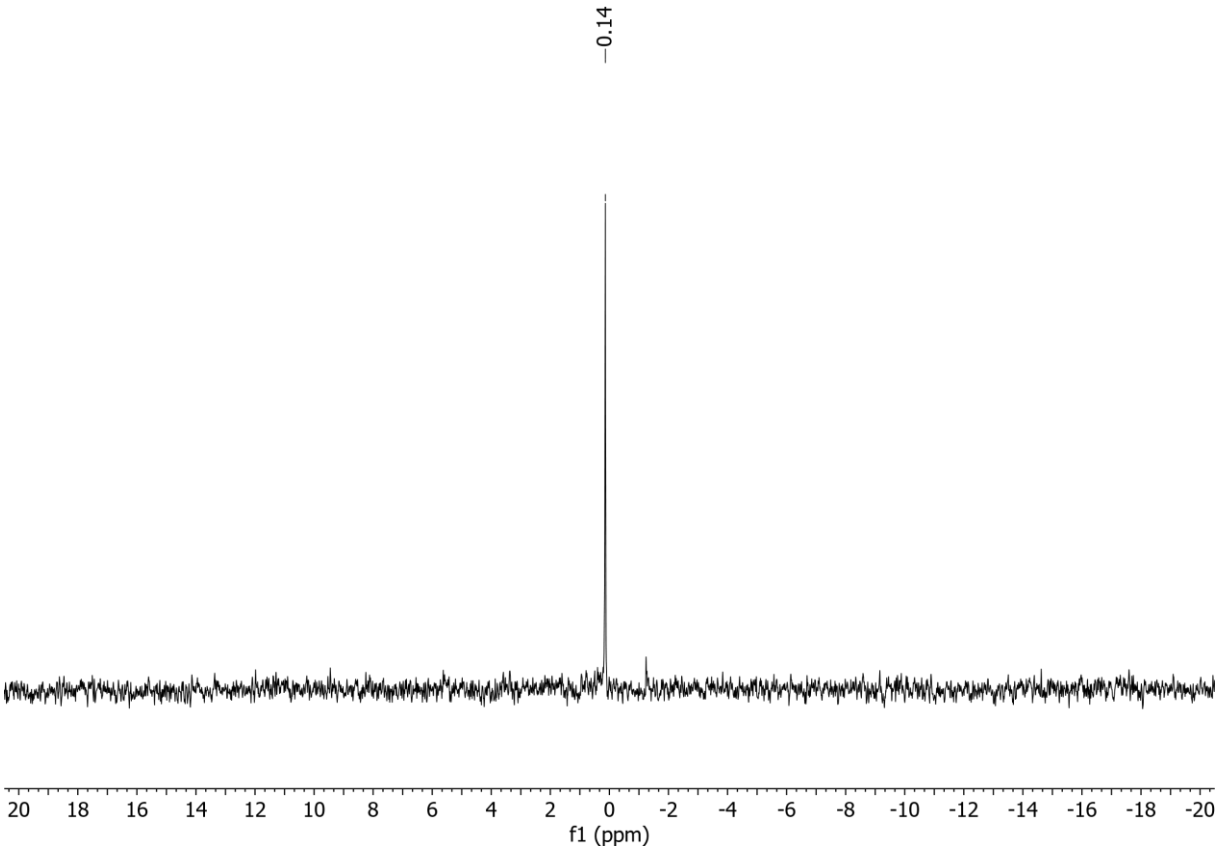


Figure S4. ^{29}Si{^{1}H}-NMR-spectrum (99 MHz, THF-d_8, 298 K) of **1**.

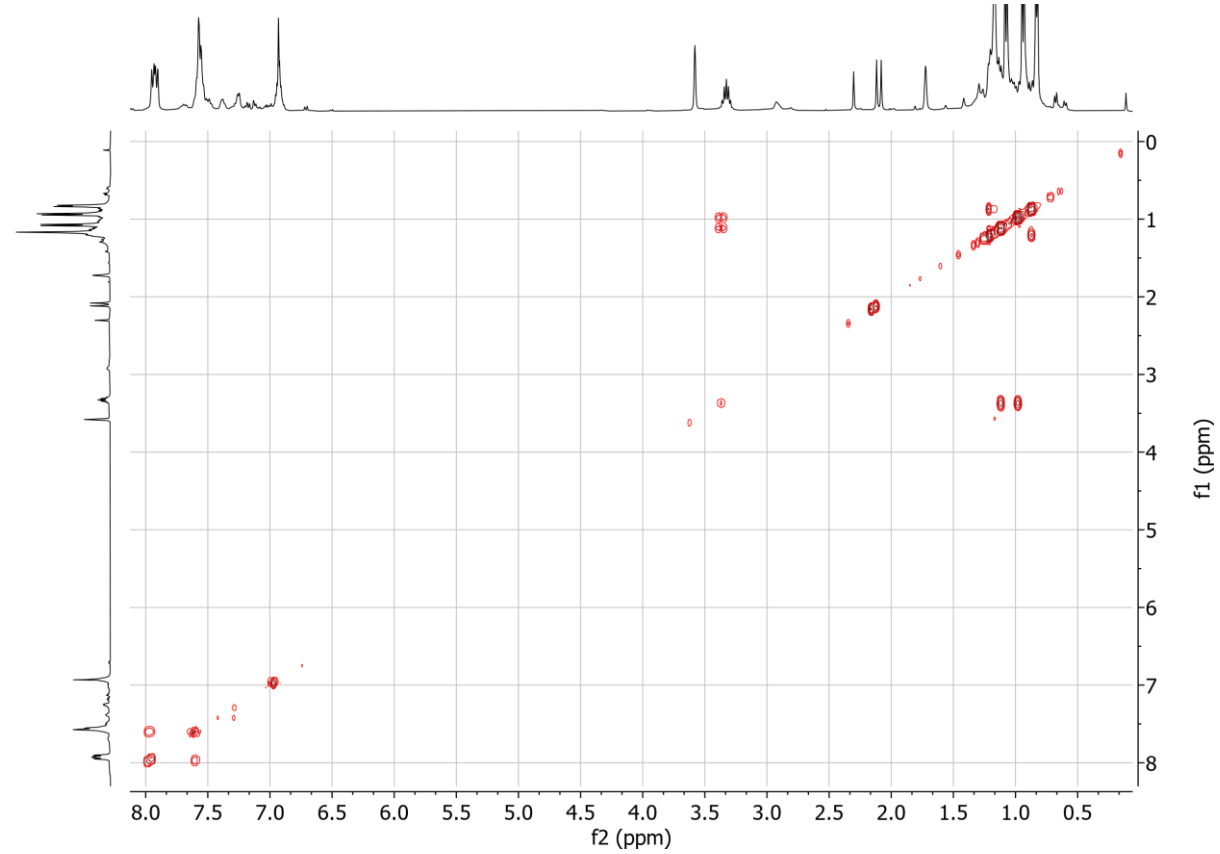


Figure S5. COSY-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **1**.

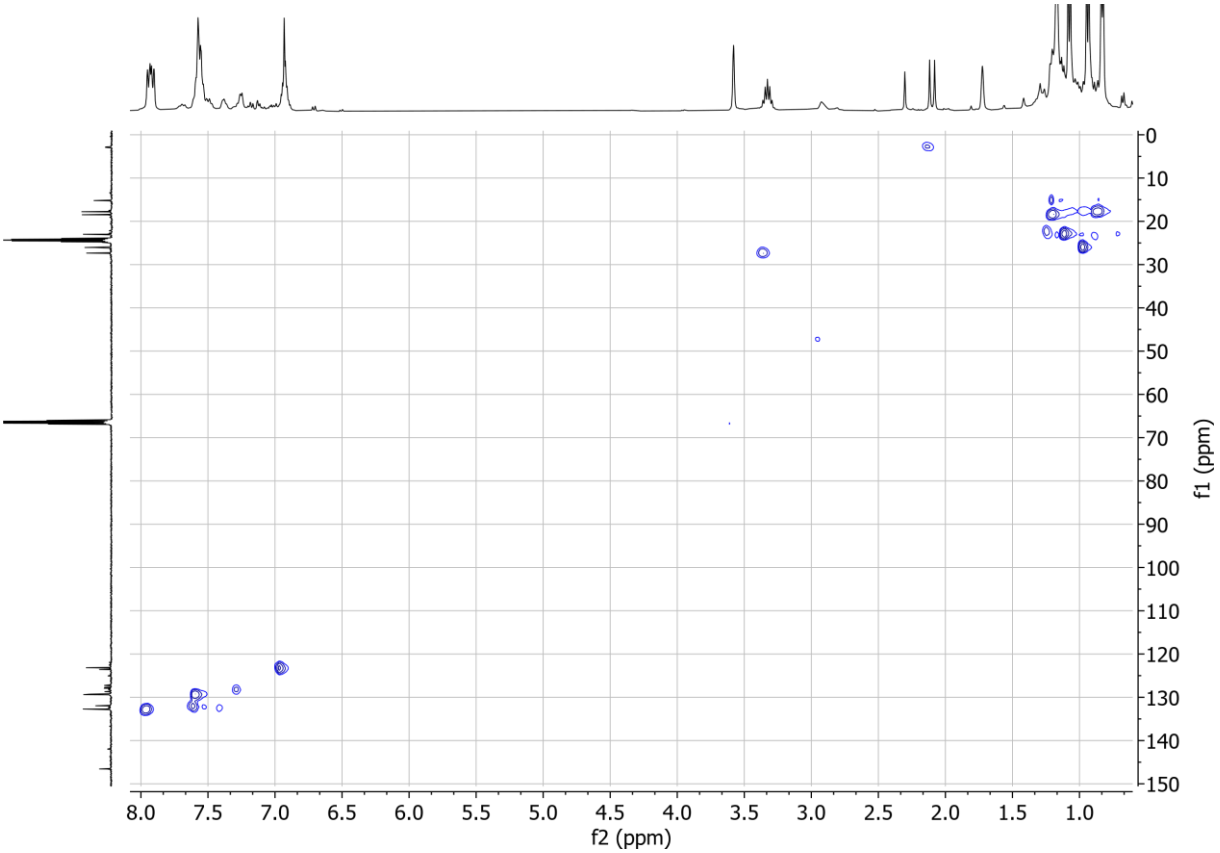


Figure S6. HSQC-NMR-spectrum (400/ 101 MHz, THF-d_8, 298 K) of **1**.

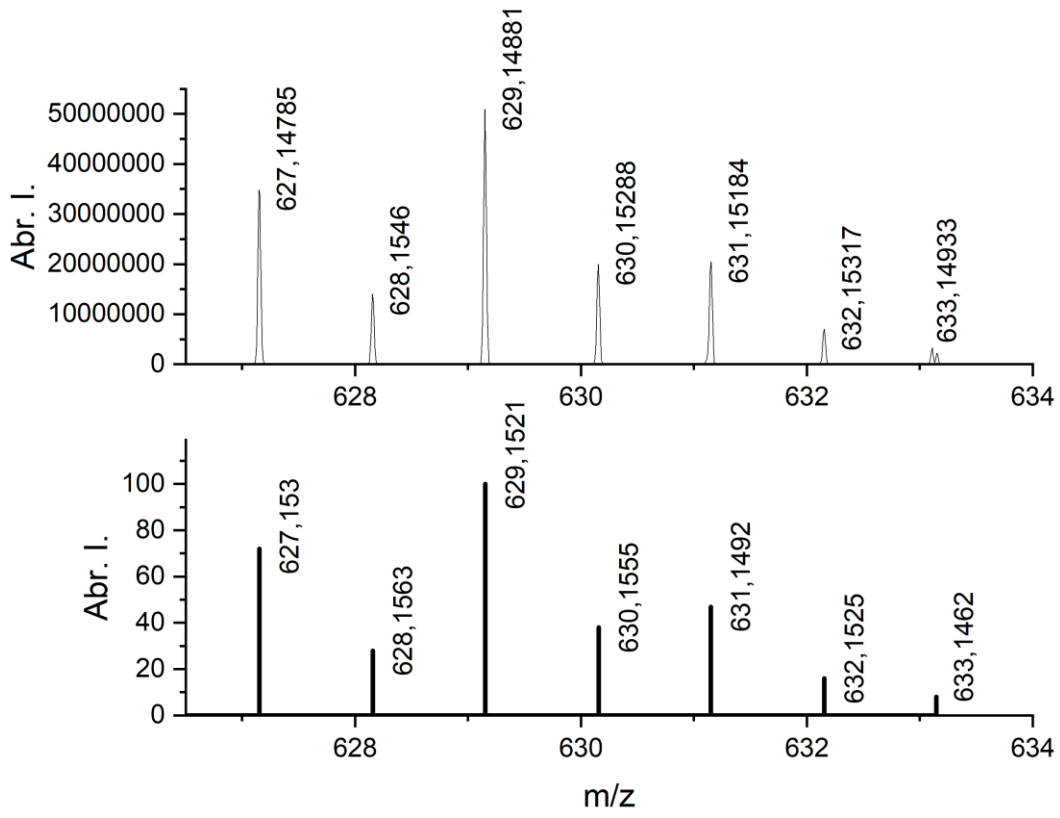


Figure S7. Cutout from LIFDI/MS of **1**; Top: found MS for [^{PhiP}DippNGaCl$_2$]+; Bottom: Calculated MS spectrum of [^{PhiP}DippNGaCl$_2$]+.

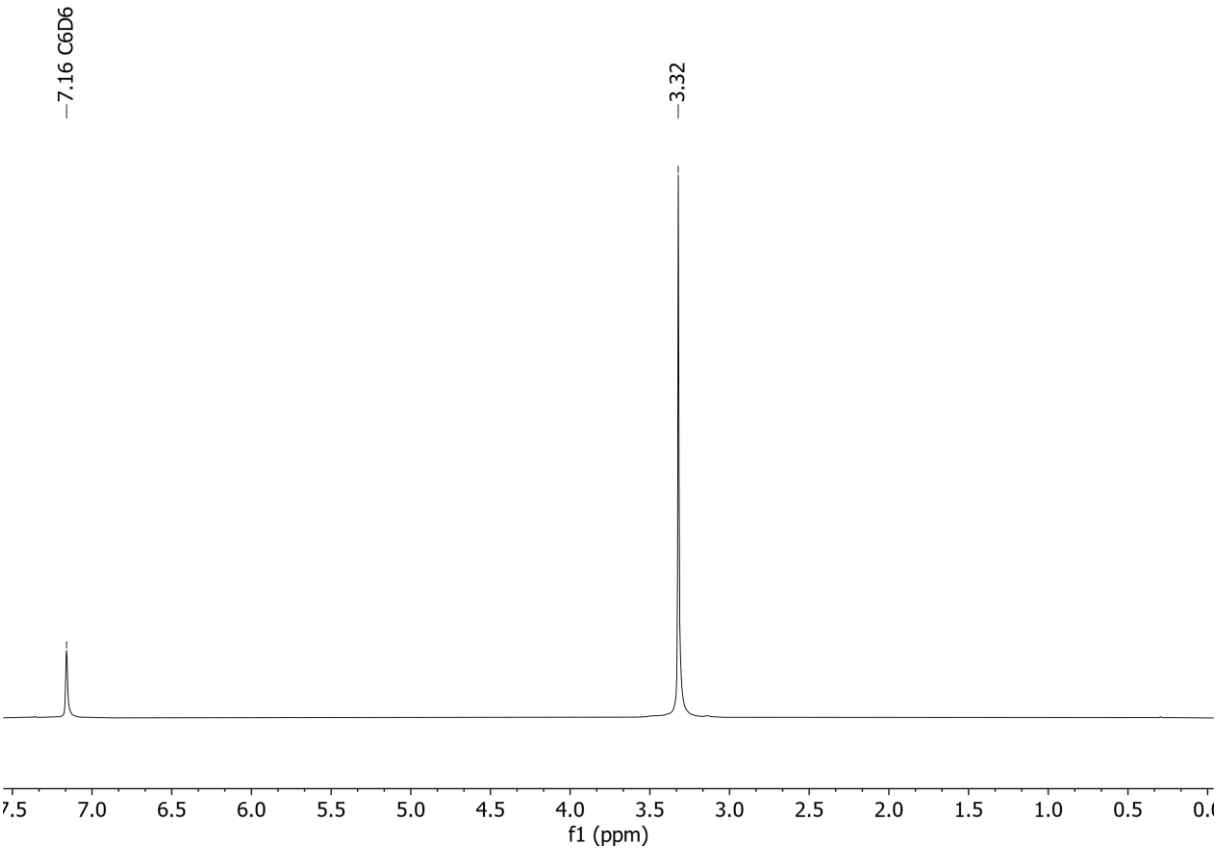


Figure S8. ^{1}H NMR-spectrum (400 MHz, C_6D_6, 298 K) of Ga_2Cl_4*(dioxane)$_2$.

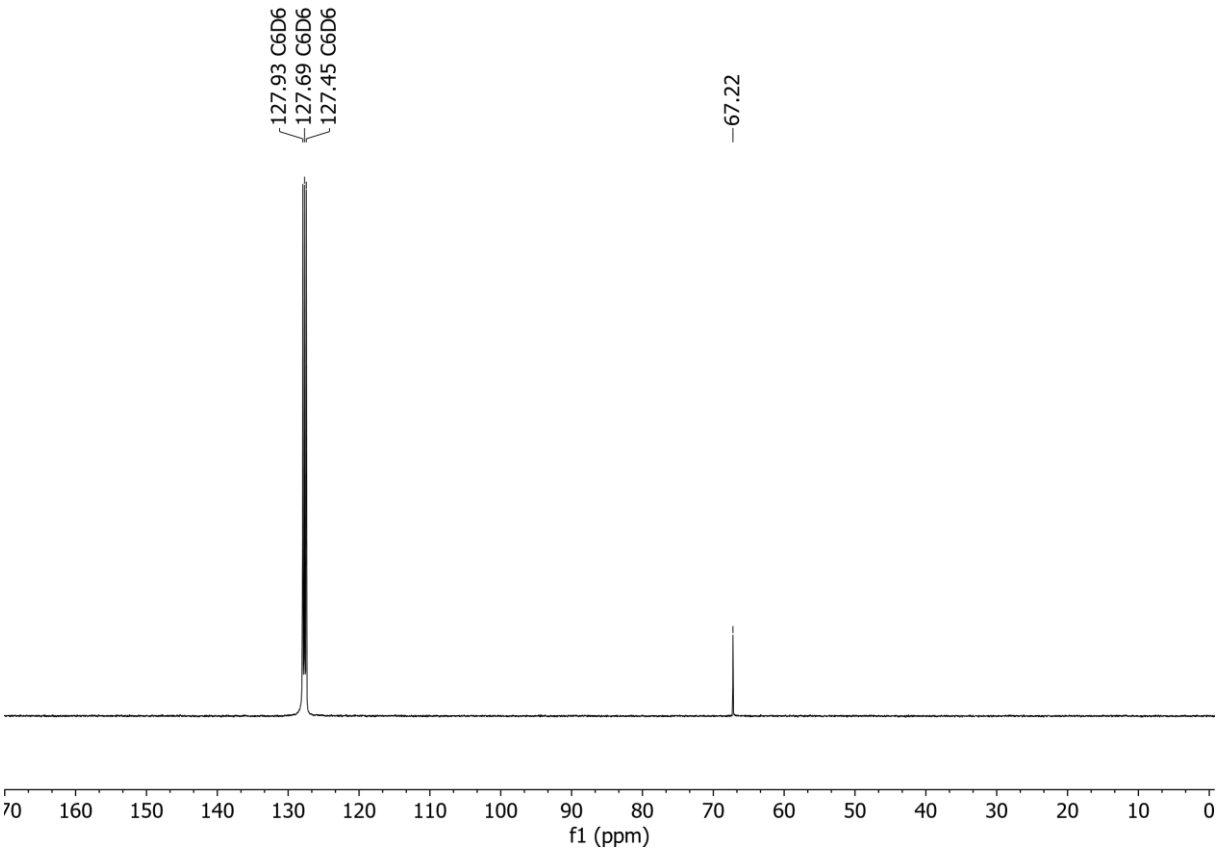


Figure S9. ^{13}C NMR-spectrum (101 MHz, C_6D_6, 298 K) of Ga_2Cl_4*(dioxane)$_2$.

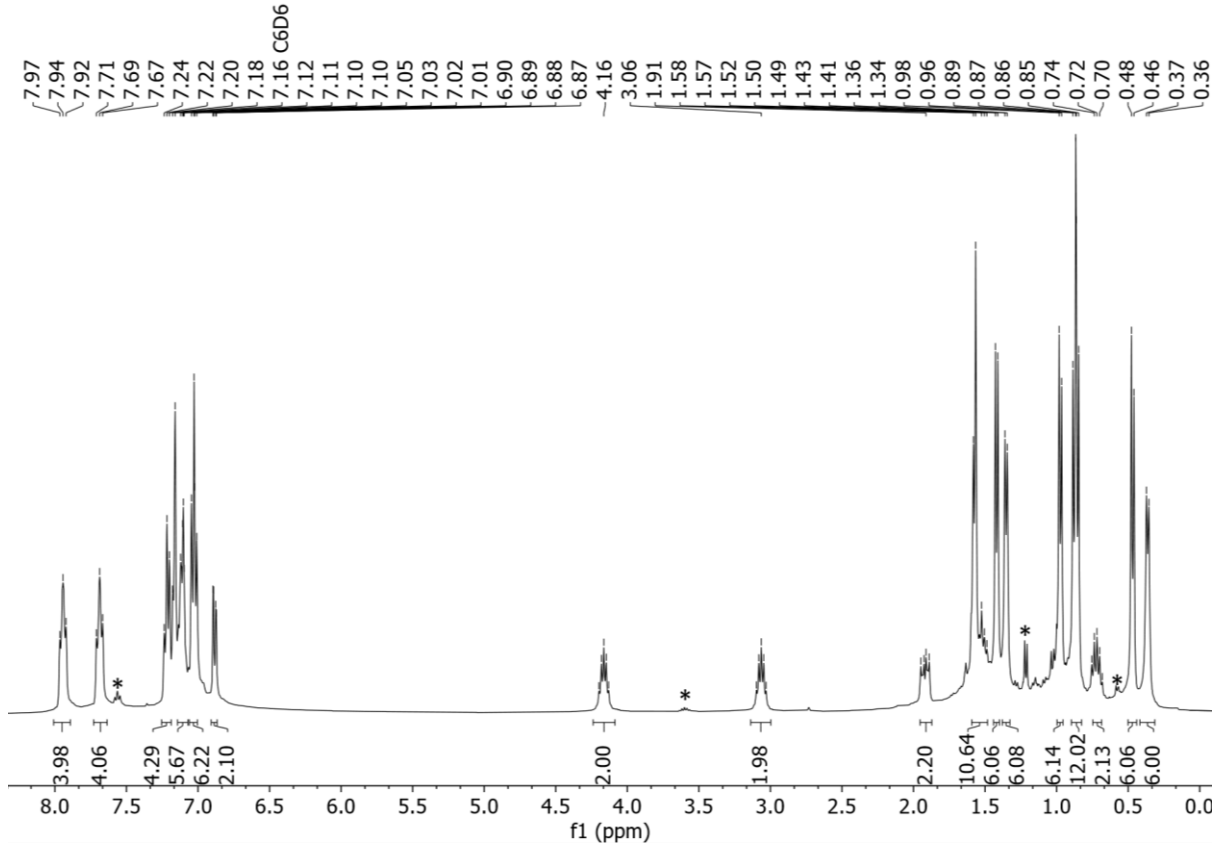


Figure S10. ^{1}H NMR-spectrum (400 MHz, C_6D_6, 298 K) of **2**.. * Denotes minor amounts of decomposition product ^{PhiP}DippNH.

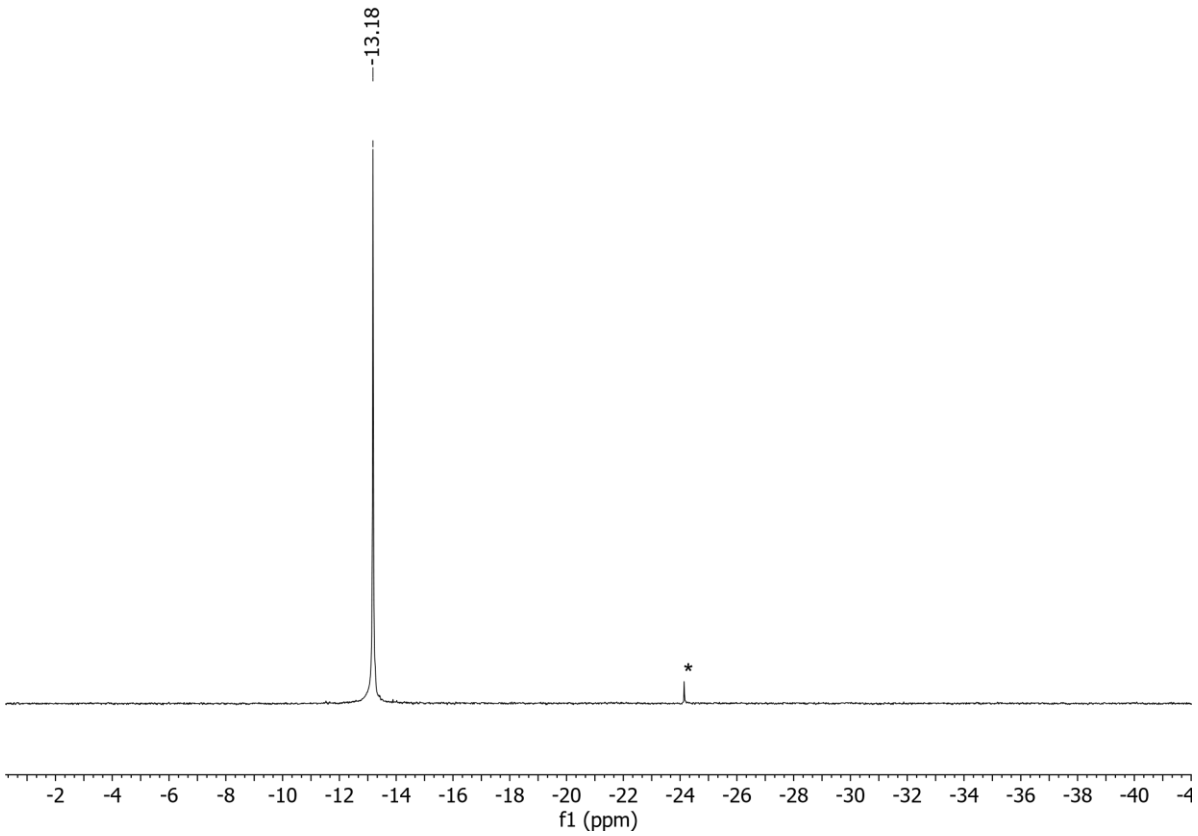


Figure S11. $^{31}P\{^{1}H\}$ NMR-spectrum (162 MHz, C_6D_6, 298 K) of **2**. * Denotes minor amounts of decomposition product ^{PhiP}DippNH.

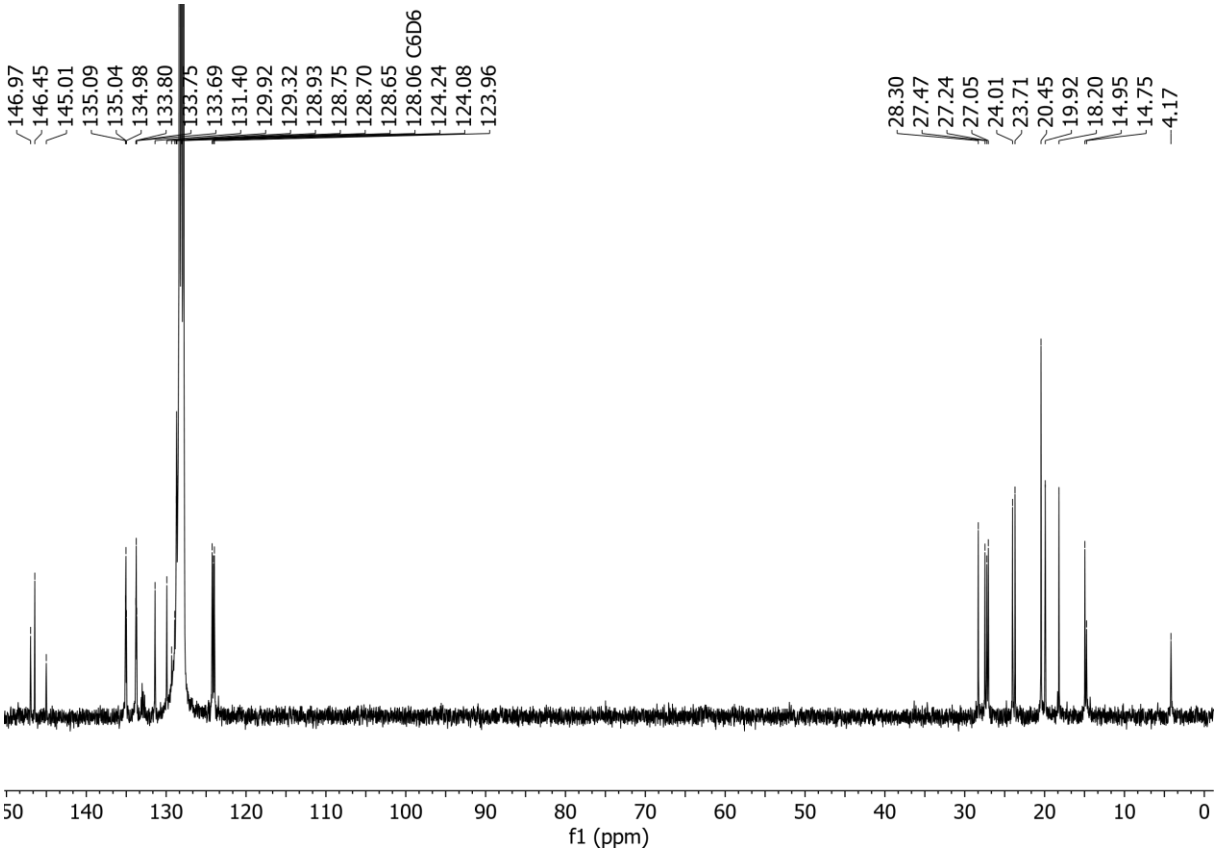


Figure S12: $^{13}C\{^{1}H\}$ NMR-spectrum (101 MHz, C_6D_6, 298 K) of **2**.

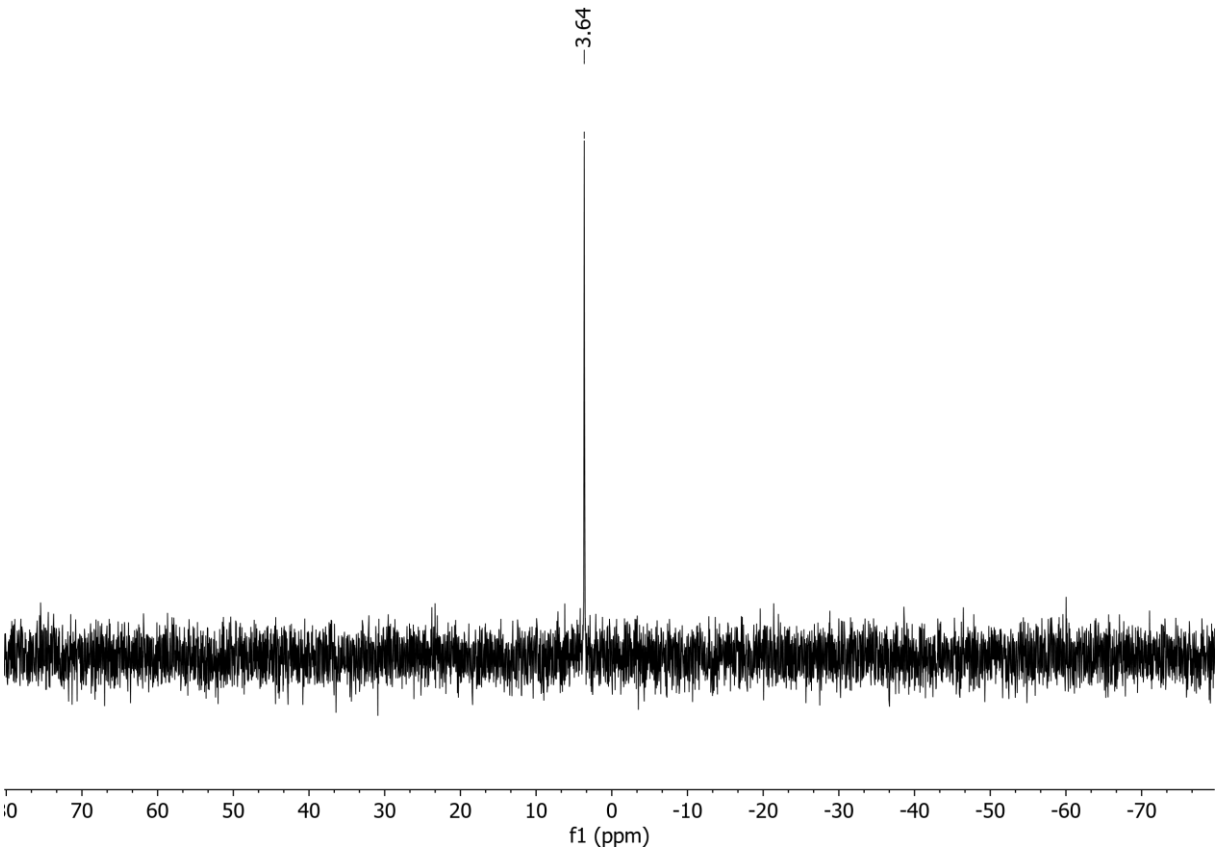


Figure S13. $^{29}Si\{^{1}H\}$ NMR-spectrum (99 MHz, C_6D_6, 298 K) of **2**.

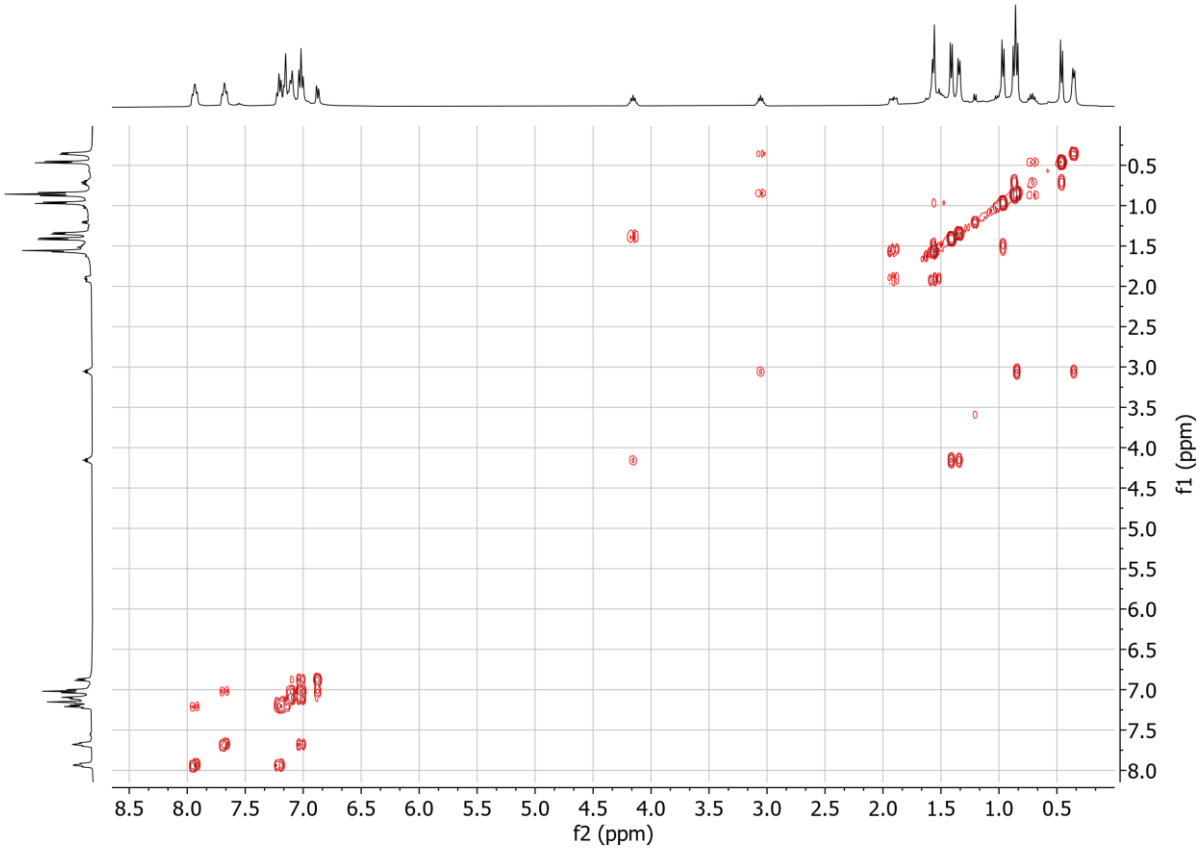


Figure S14. COSY-NMR-spectrum (400 MHz, C_6D_6, 298 K) of $(^{PhiP}DippNGaCl)_2$.

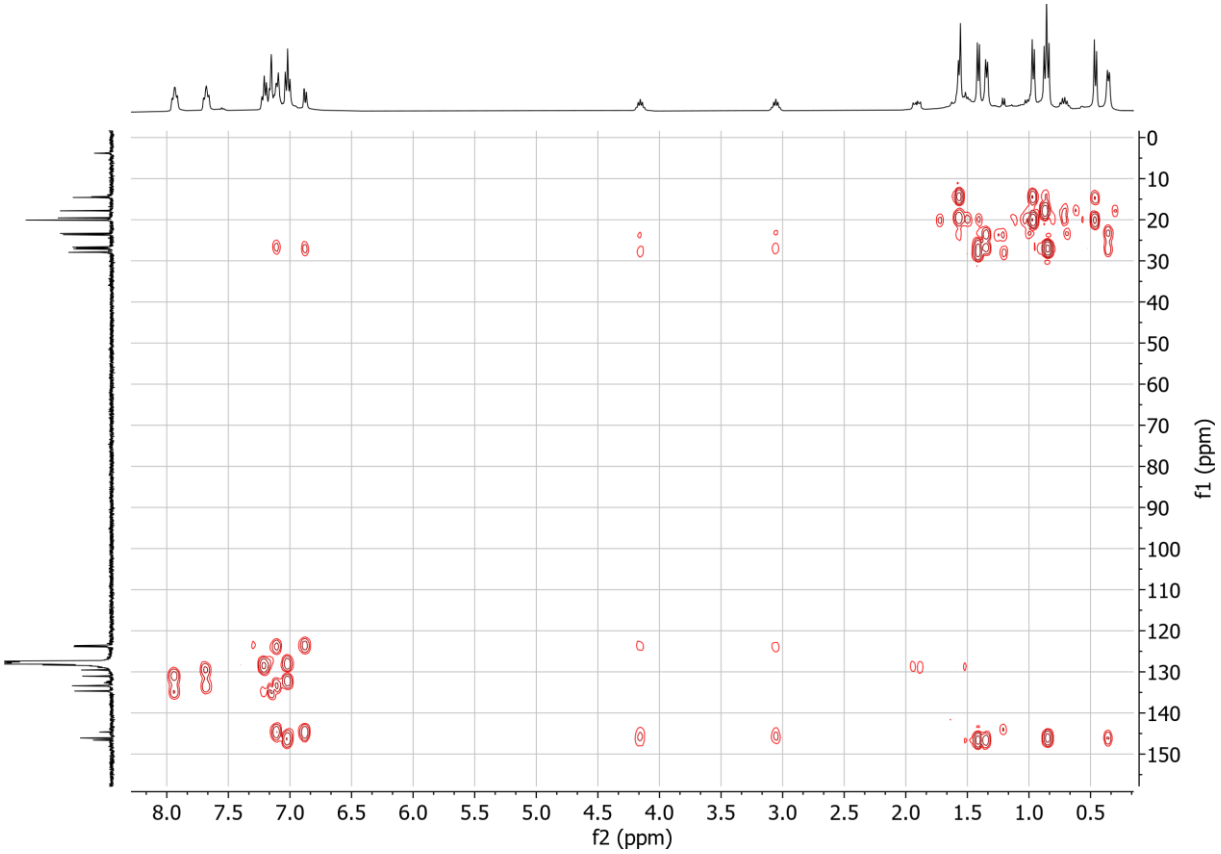


Figure S15. HSQC-NMR-spectrum (400/101 MHz, C_6D_6, 298 K) of **2**.

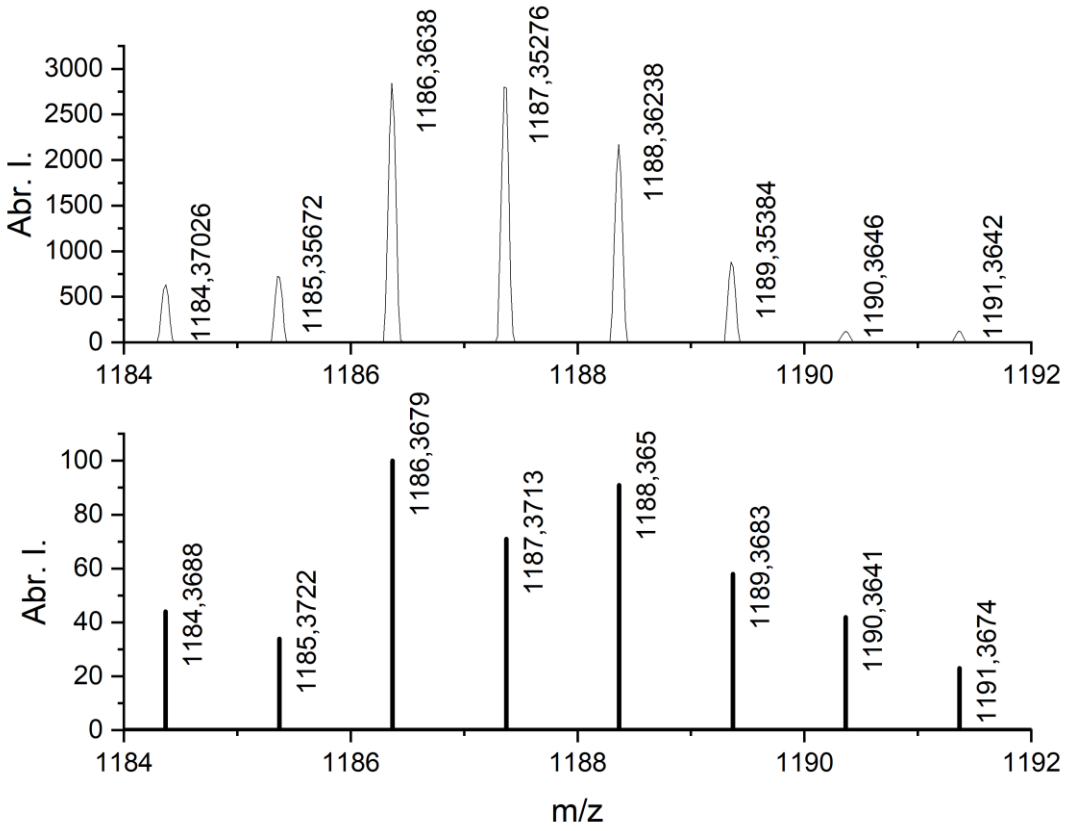


Figure S16. Cutout from LIFDI/MS of **2**; Top: found MS for [(^{PhiP}DippNGaCl)$_2$]+; Bottom: Calculated MS spectrum of [(^{PhiP}DippNGaCl)$_2$]+.

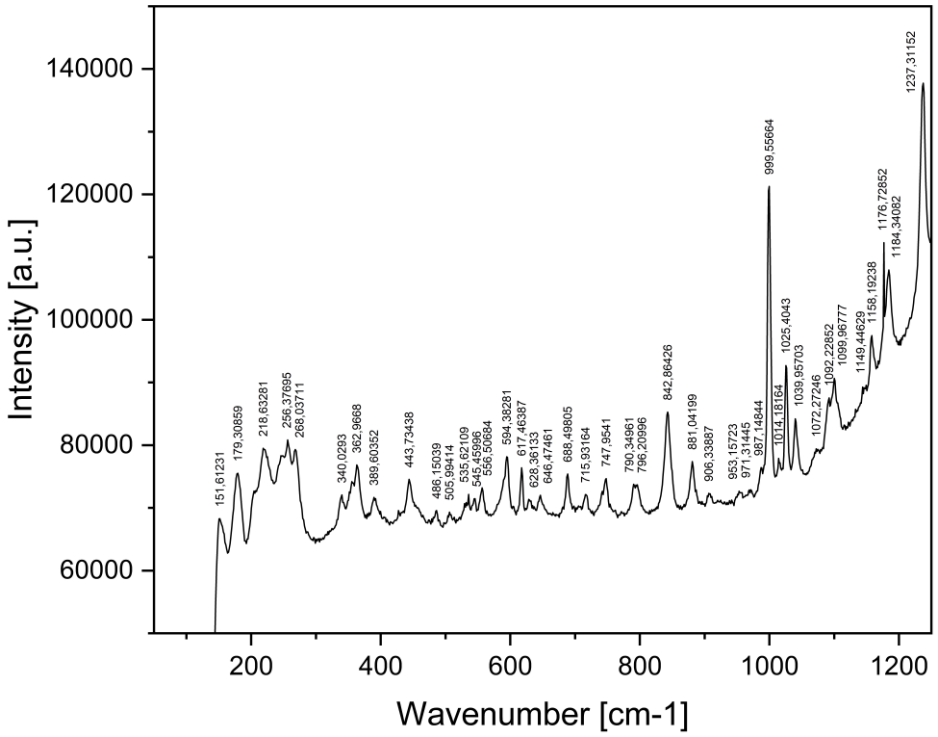


Figure S17. Raman-Spectra of **2**.

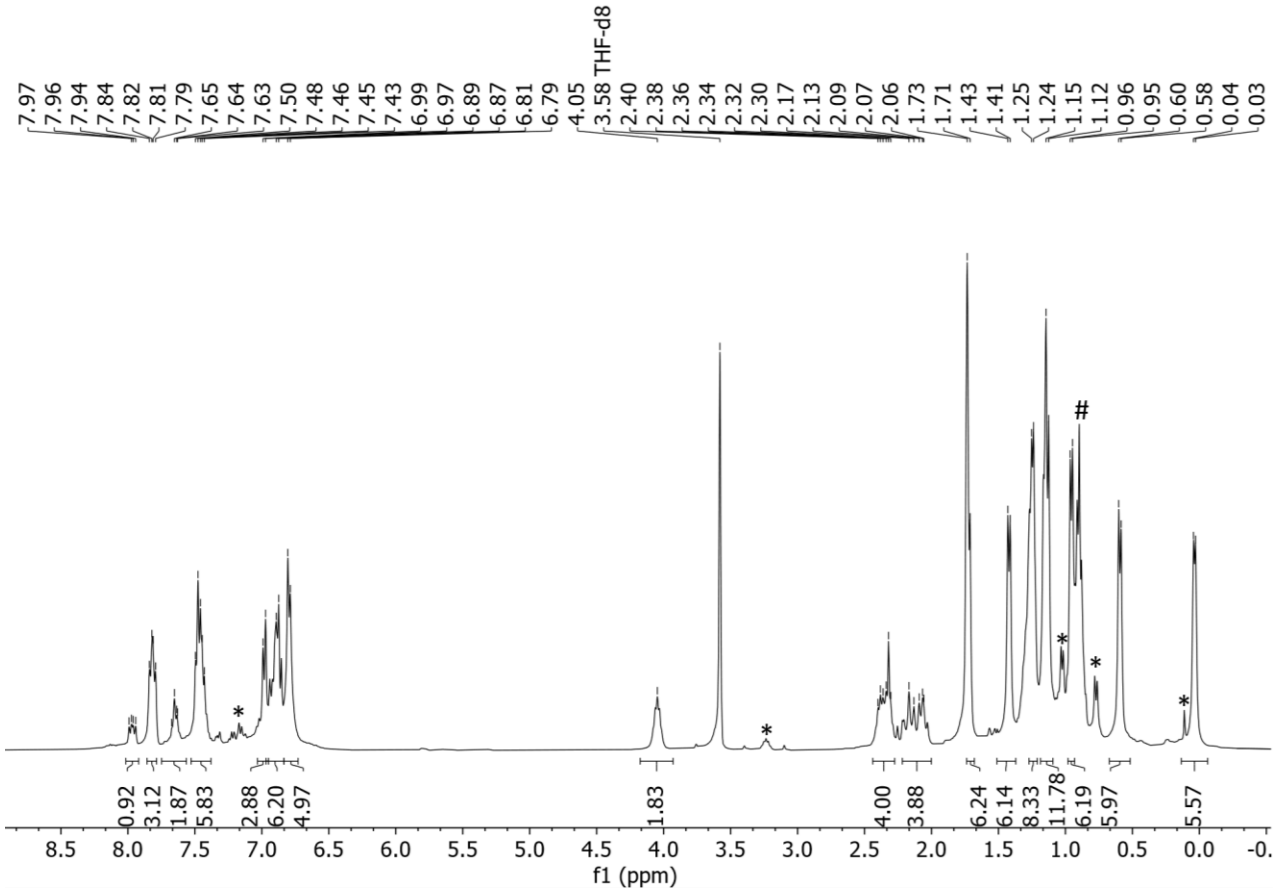


Figure S18. ^{1}H-NMR-spectrum (400 MHz, THF-d_8, 193 K) of **3**. * Denotes minor amounts of decomposition product ^{PhiP}DippNH. # denotes minor amounts of pentane.

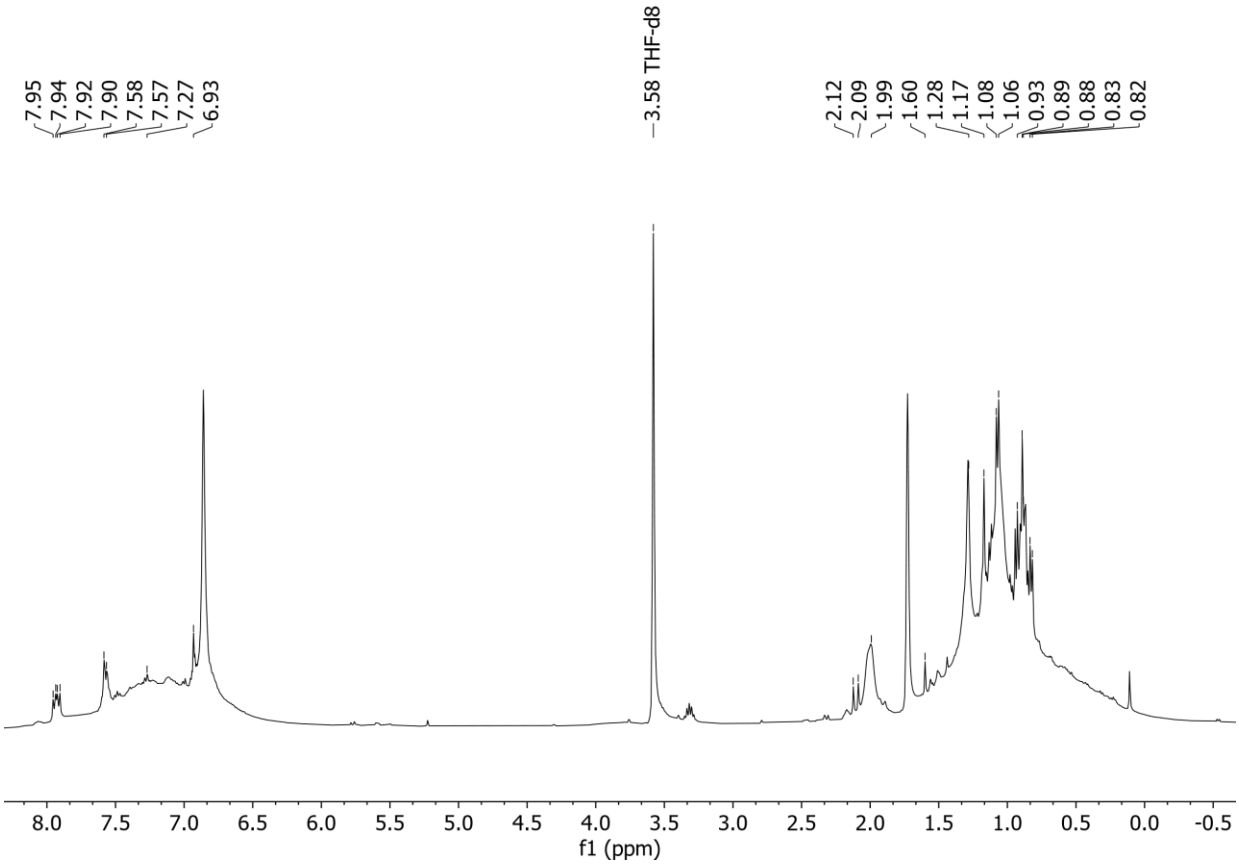


Figure S19. ^{1}H-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **3**.

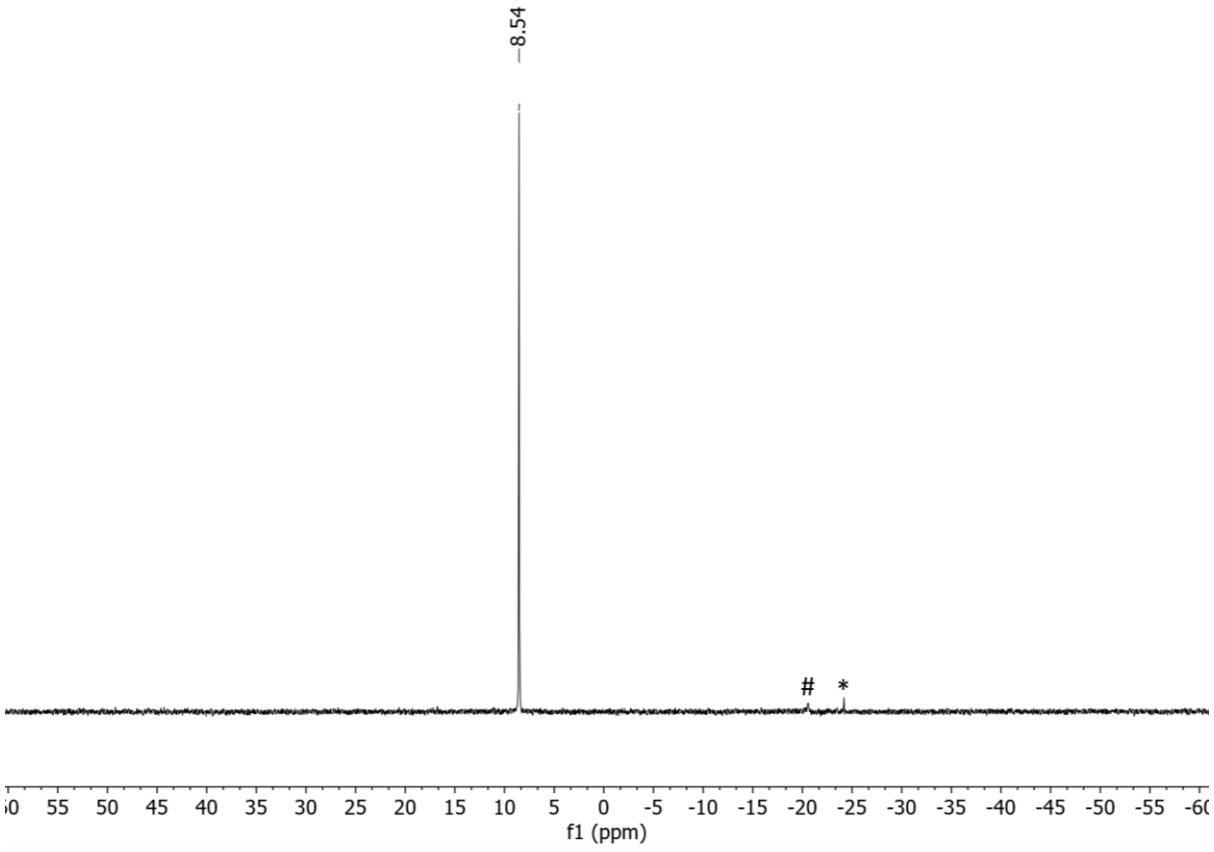


Figure S20. ^{31}P{^{1}H}-NMR-spectrum (162 MHz, THF-d_8, 298 K) of **3**. * Denotes minor amounts of decomposition product ^{PhiP}DippNH. # denotes minor amounts of ^{PhiP}DippNGaCl$_2$.

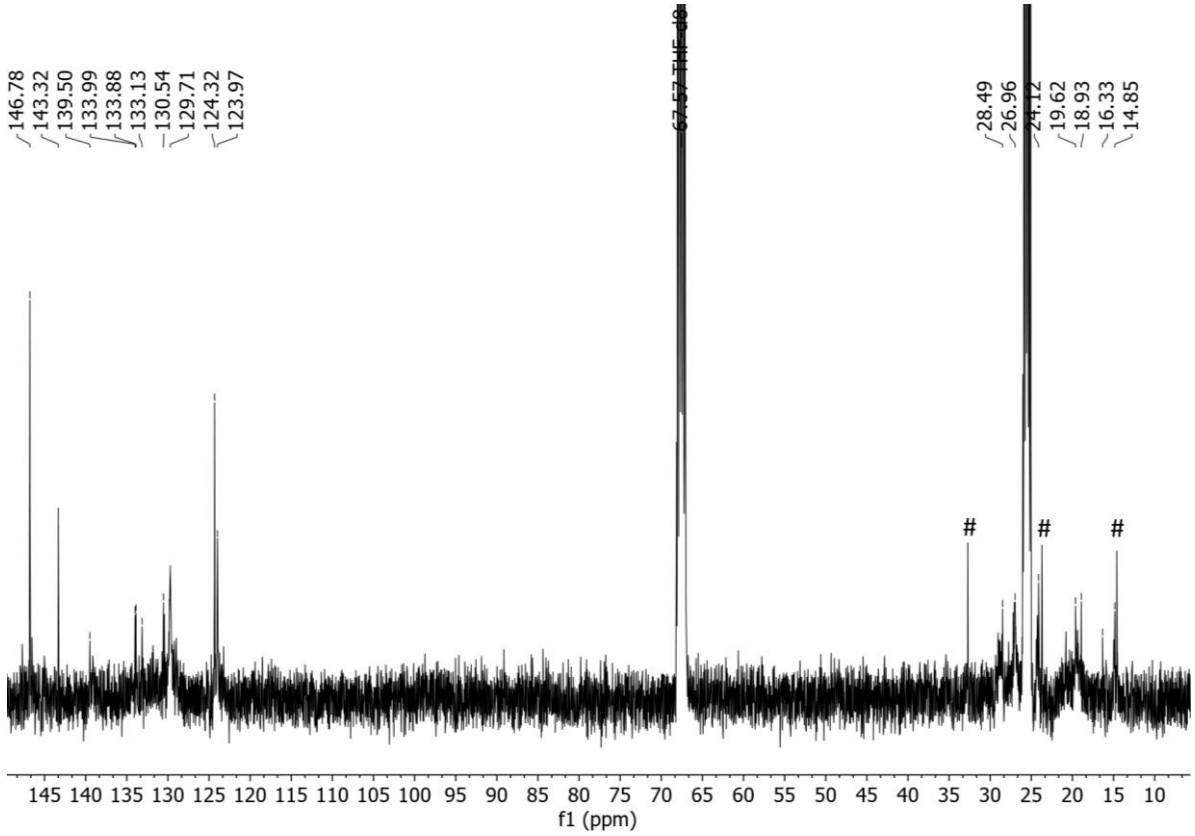


Figure S21. $^{13}C\{^{1}H\}$-NMR-spectrum (101 MHz, THF-d_8, 298 K) of **3**. # denotes minor amounts of pentane.

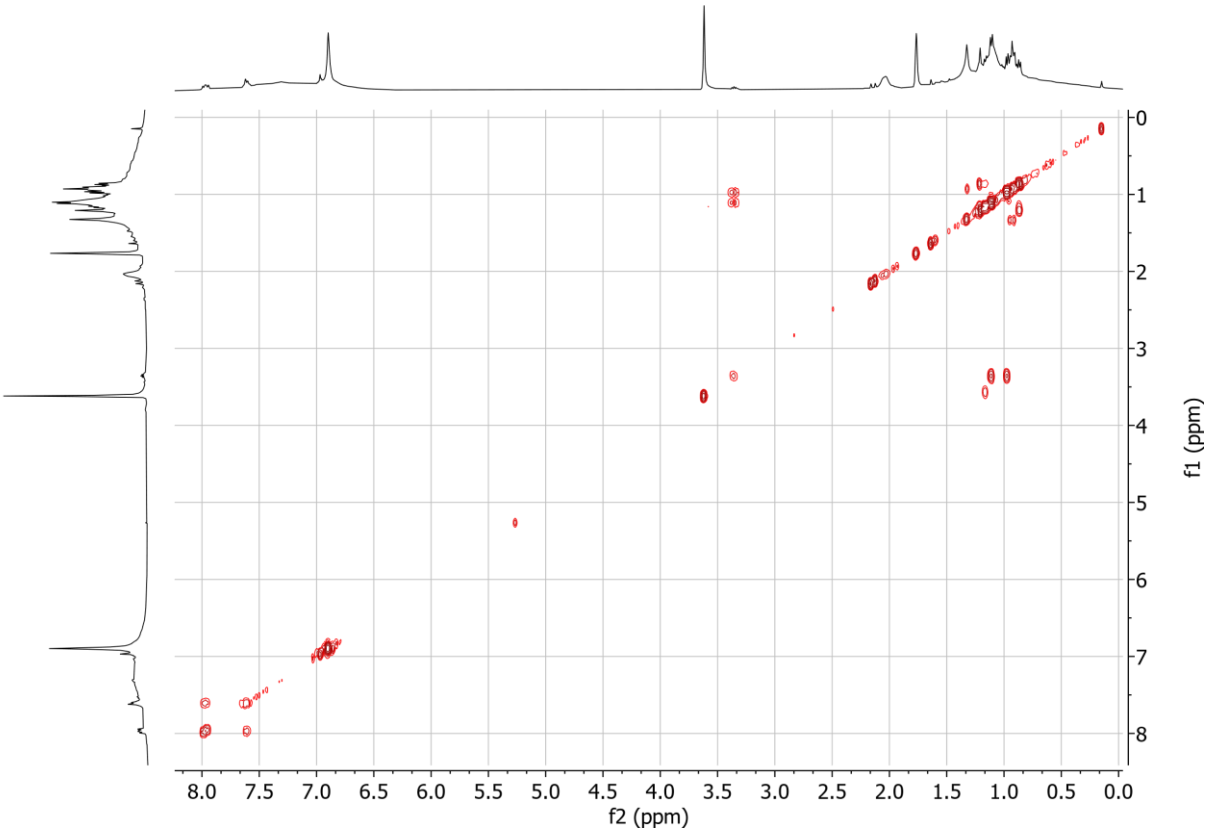


Figure S22. COSY-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **3**.

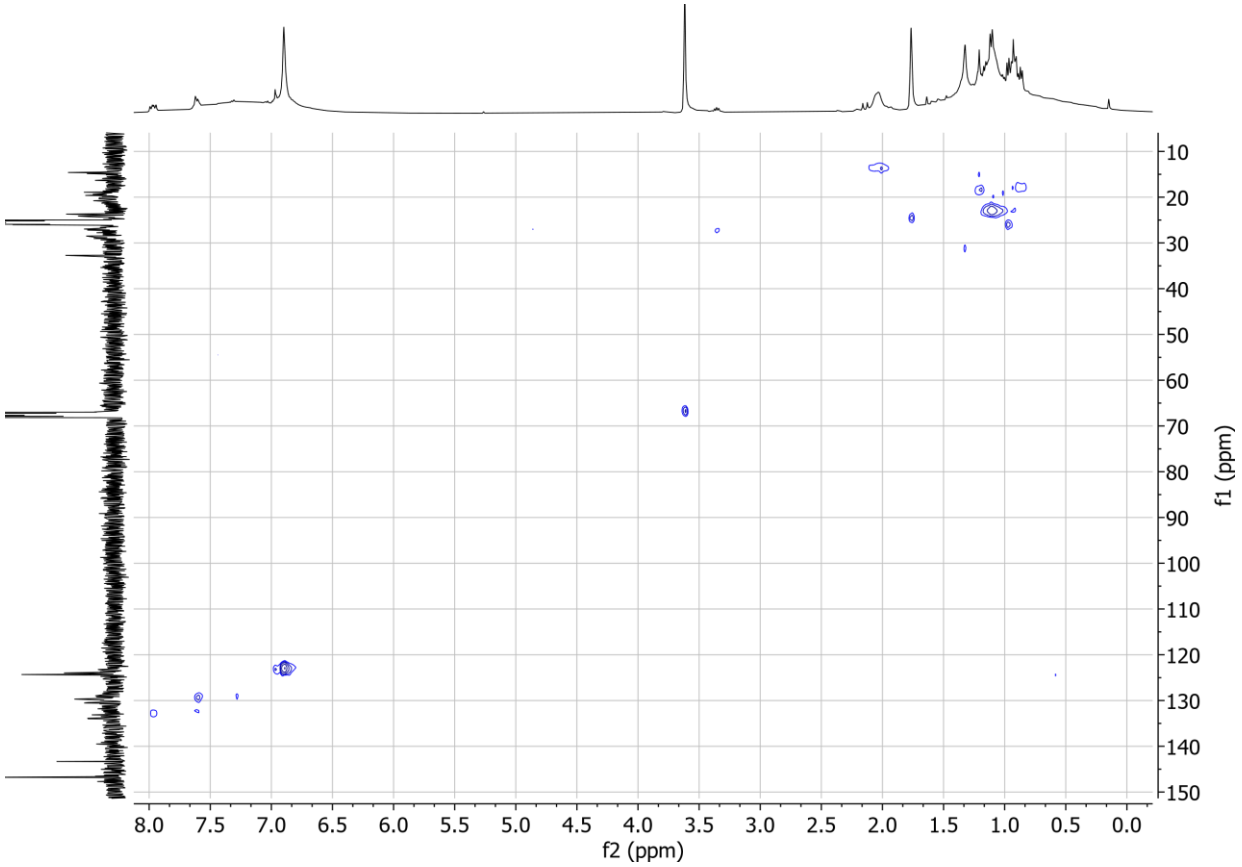


Figure S23. HSQC-NMR-spectrum (400/101 MHz, THF-d_8, 298 K) of **3**.

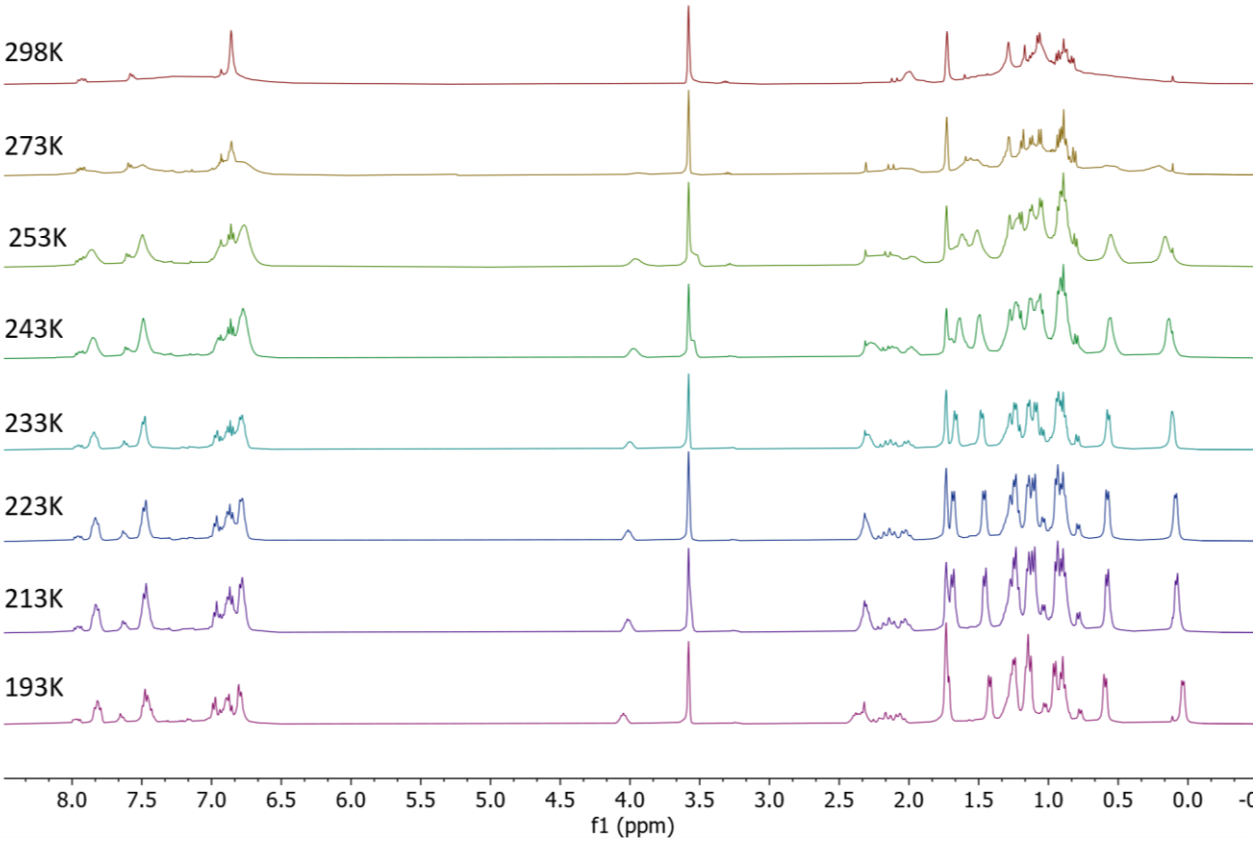


Figure S24. ^{1}H-NMR-spectrum (400 MHz, THF-d_8) of **3** from 193 – 298K, bottom to top.

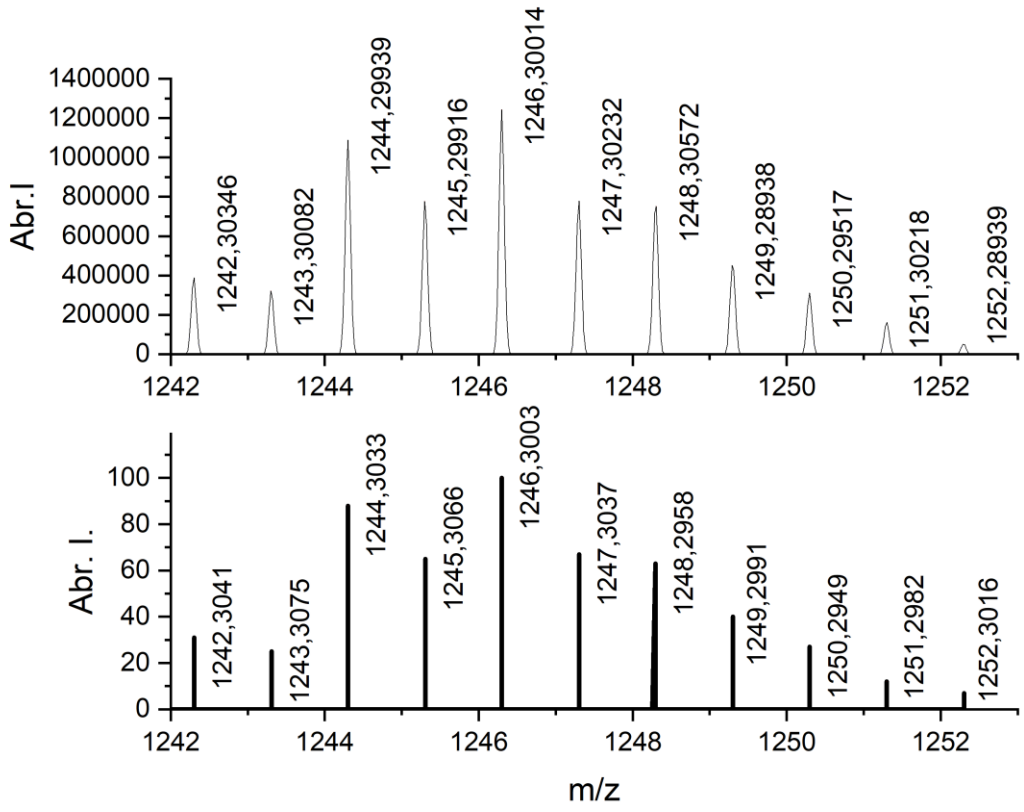


Figure S25. Cutout from LIFDI/MS of **3**, Top: found MS for [(^{PhiP}DippNGaCl)$_2$Ni]+; Bottom: Calculated MS spectrum of [(^{PhiP}DippNGaCl)$_2$Ni]+.

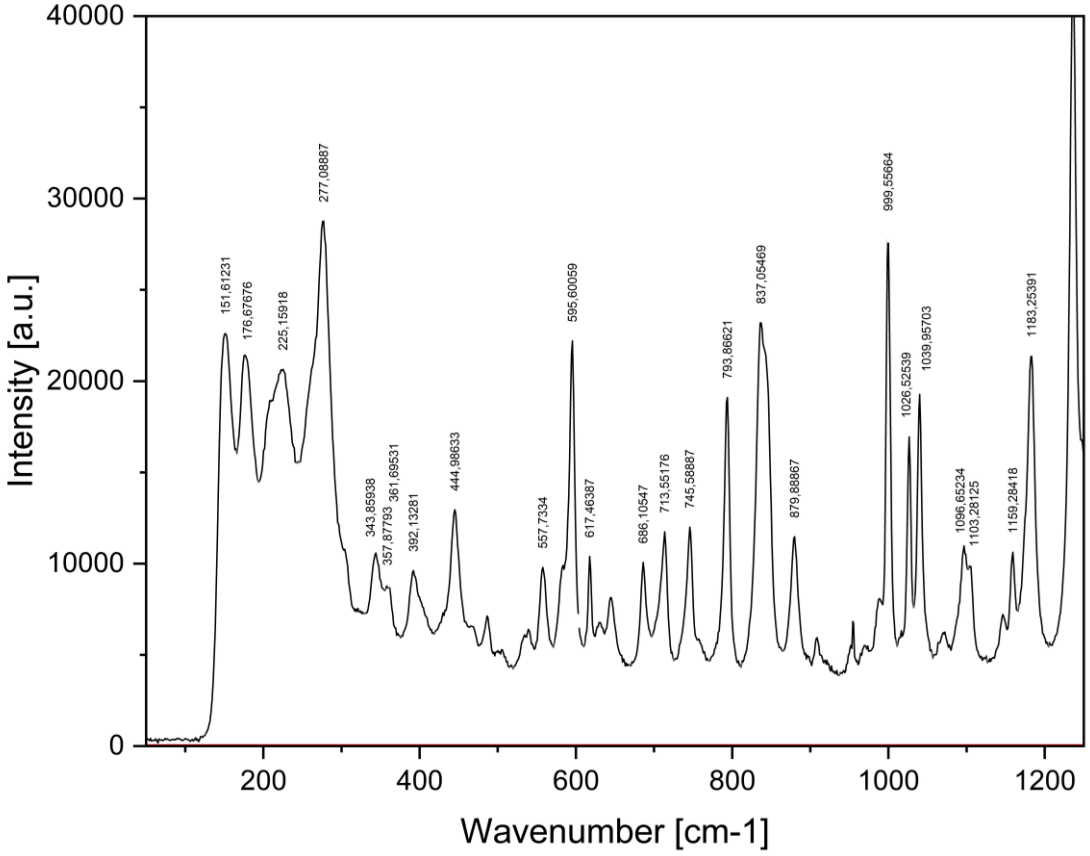


Figure S26. Raman-Spectra of **3**.

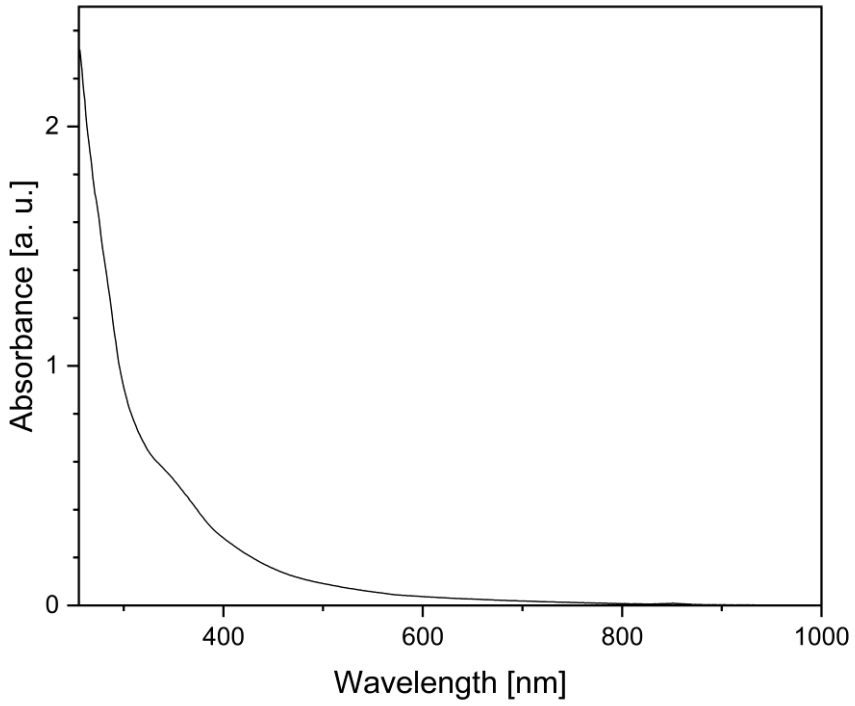


Figure S27. UV/Vis spectrum of a 3.125x10^{-6} M solution of **3** in THF at ambient temperature.

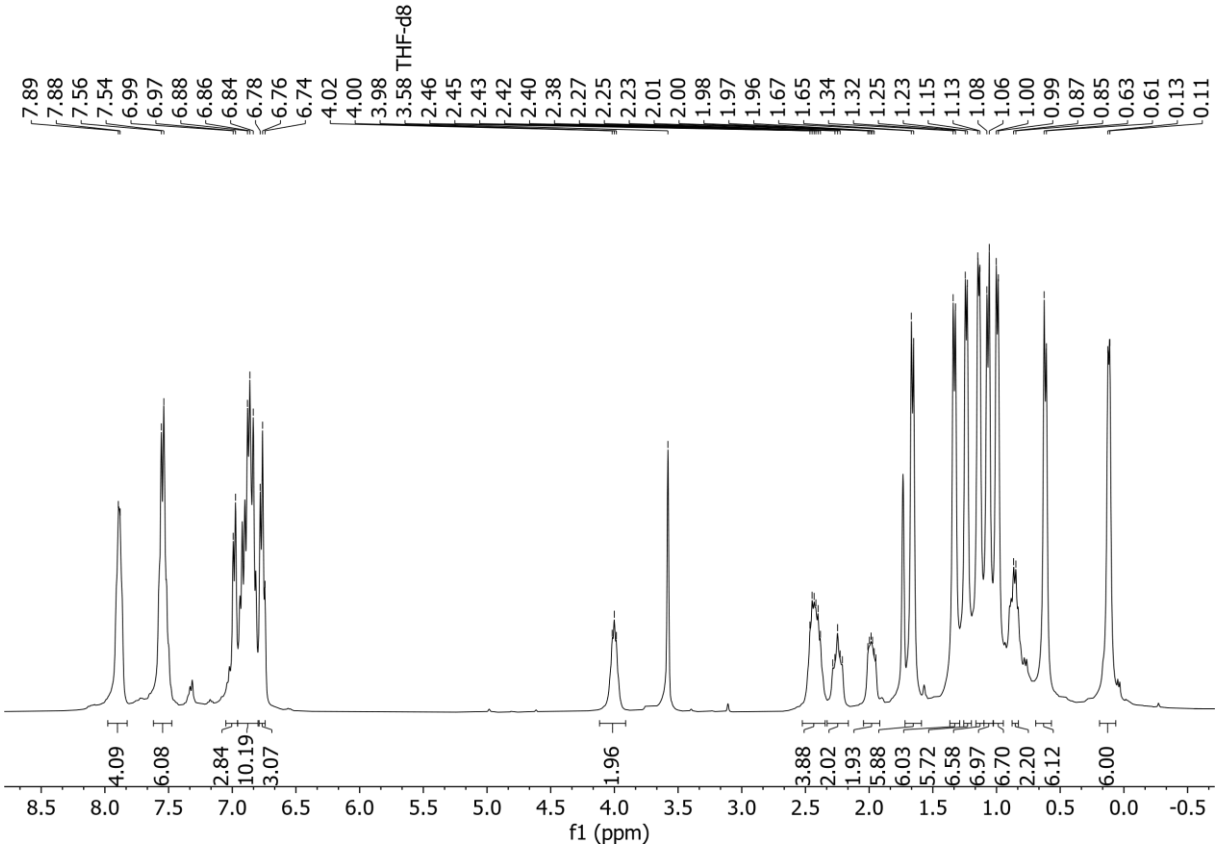


Figure S28. ^{1}H-NMR-spectrum (400 MHz, THF-d_8, 193 K) of **4**.

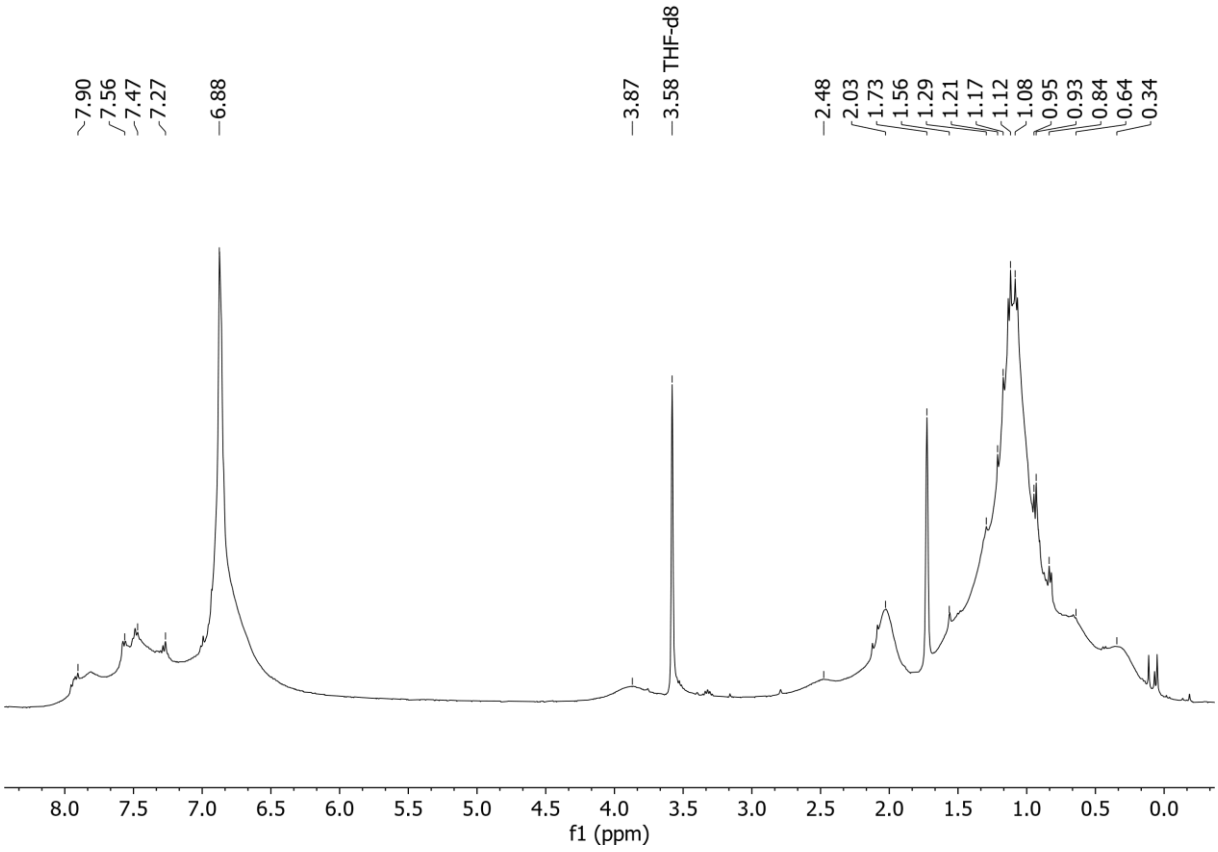


Figure S29. ^{1}H-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **4**.

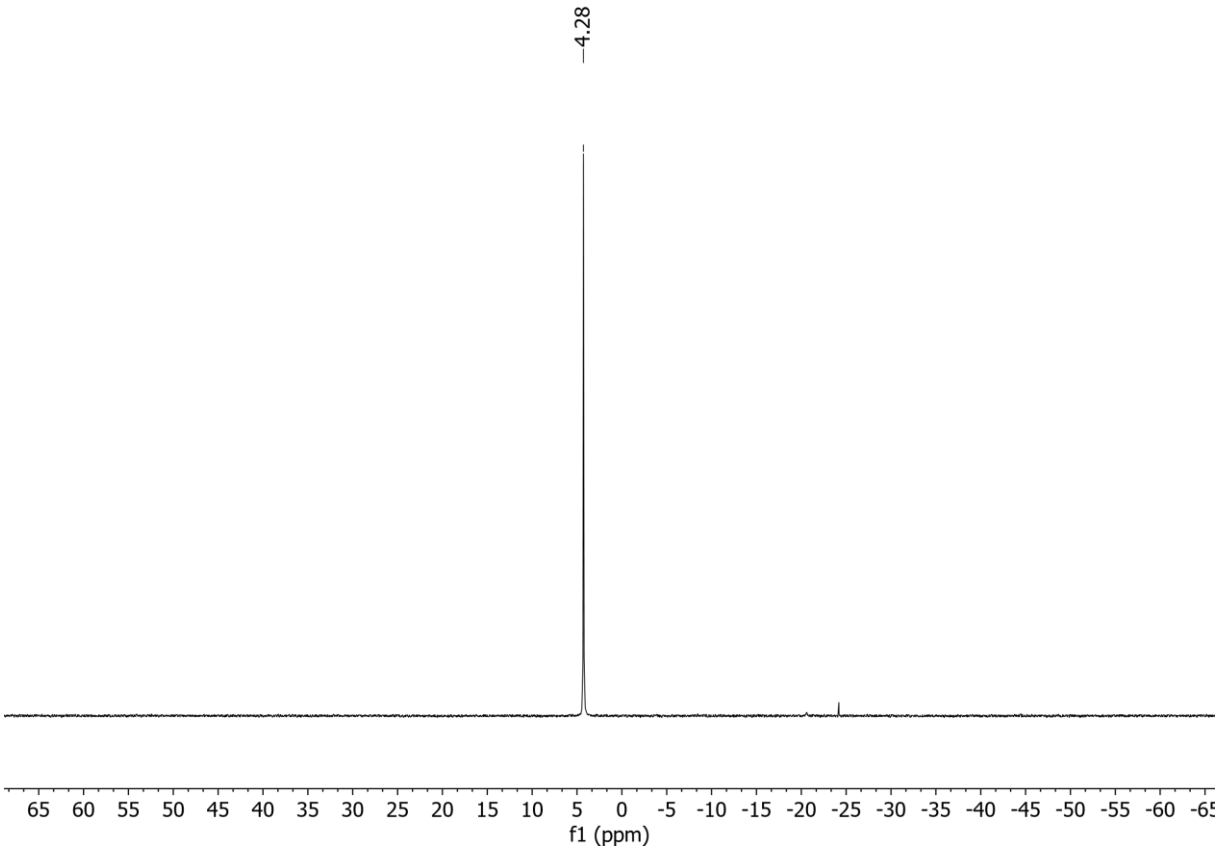


Figure S30. ^{31}P{^{1}H}-NMR-spectrum (162 MHz, THF-d_8, 298 K) of **4**.

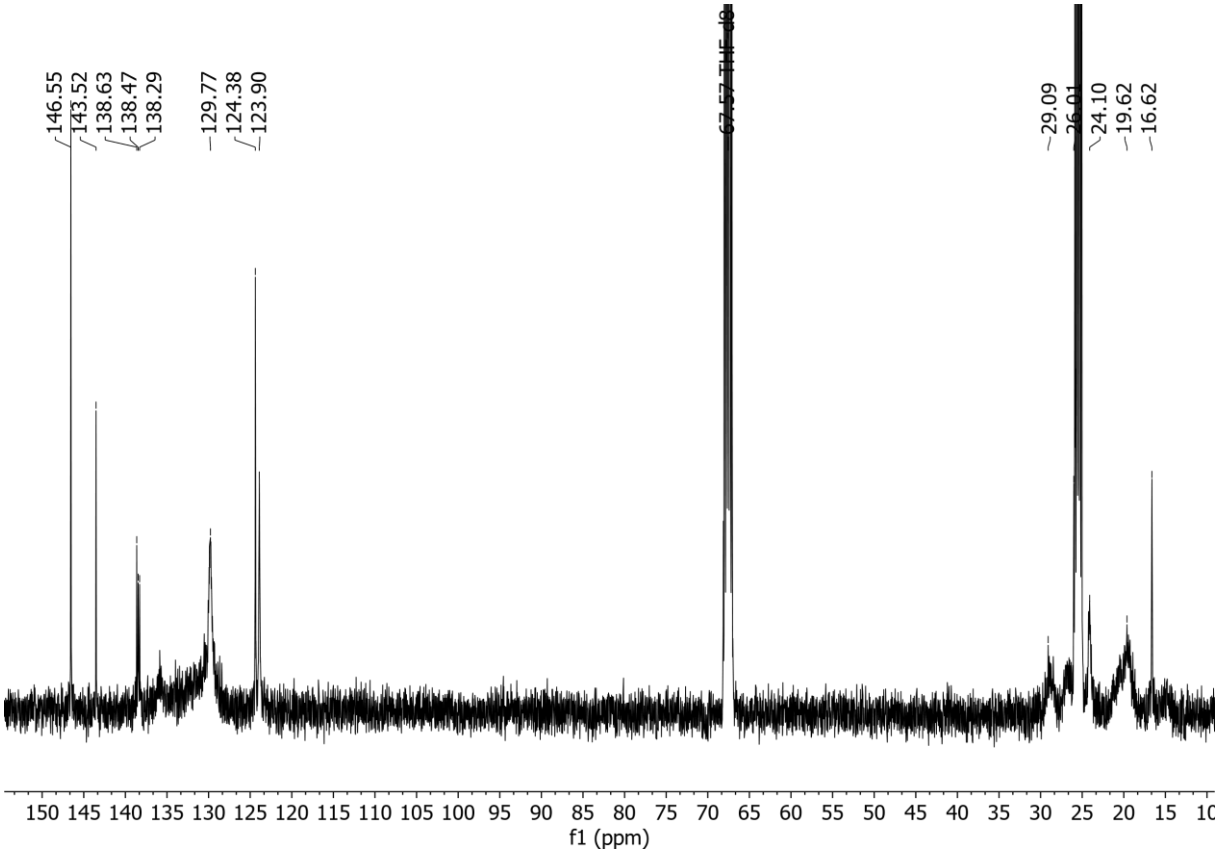


Figure S31. $^{13}C\{^{1}H\}$-NMR-spectrum (101 MHz, THF-d_8, 298 K) of **4**.

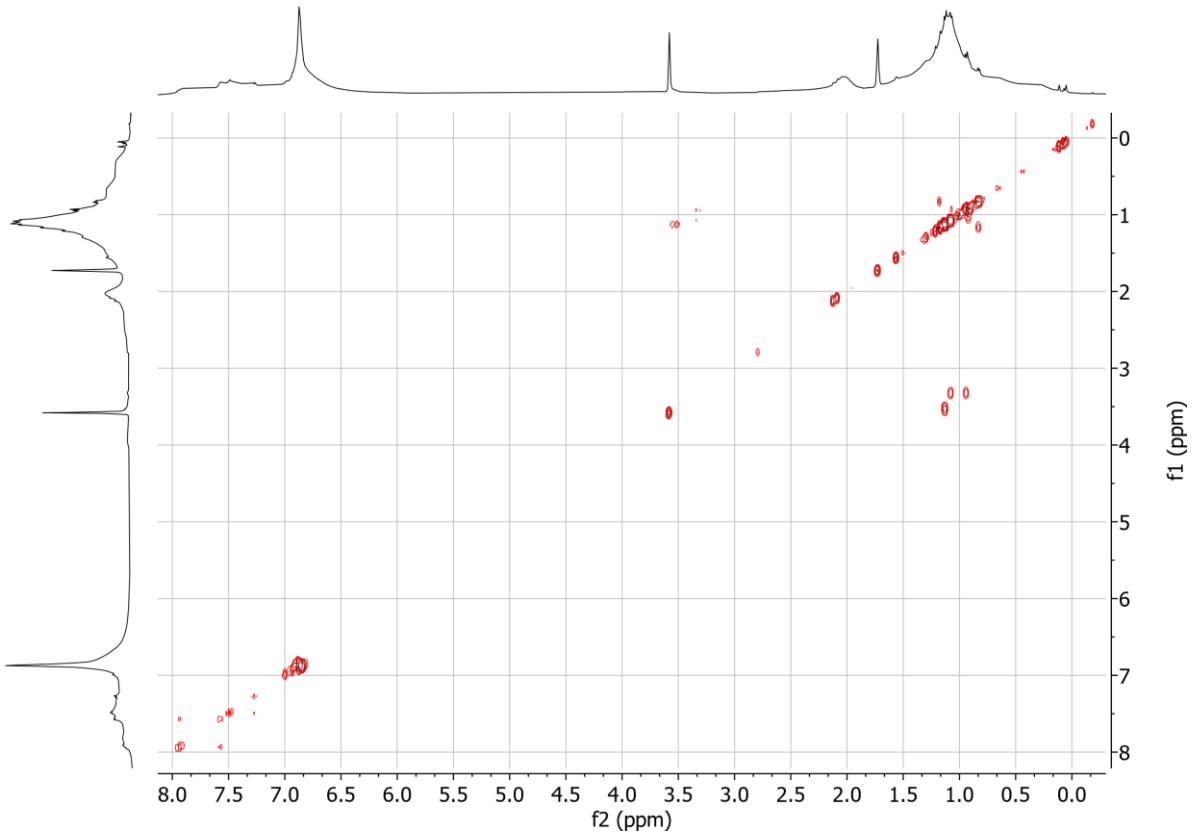


Figure S32. COSY-NMR-spectrum (400 MHz, THF-d_8, 298 K) of **4**.

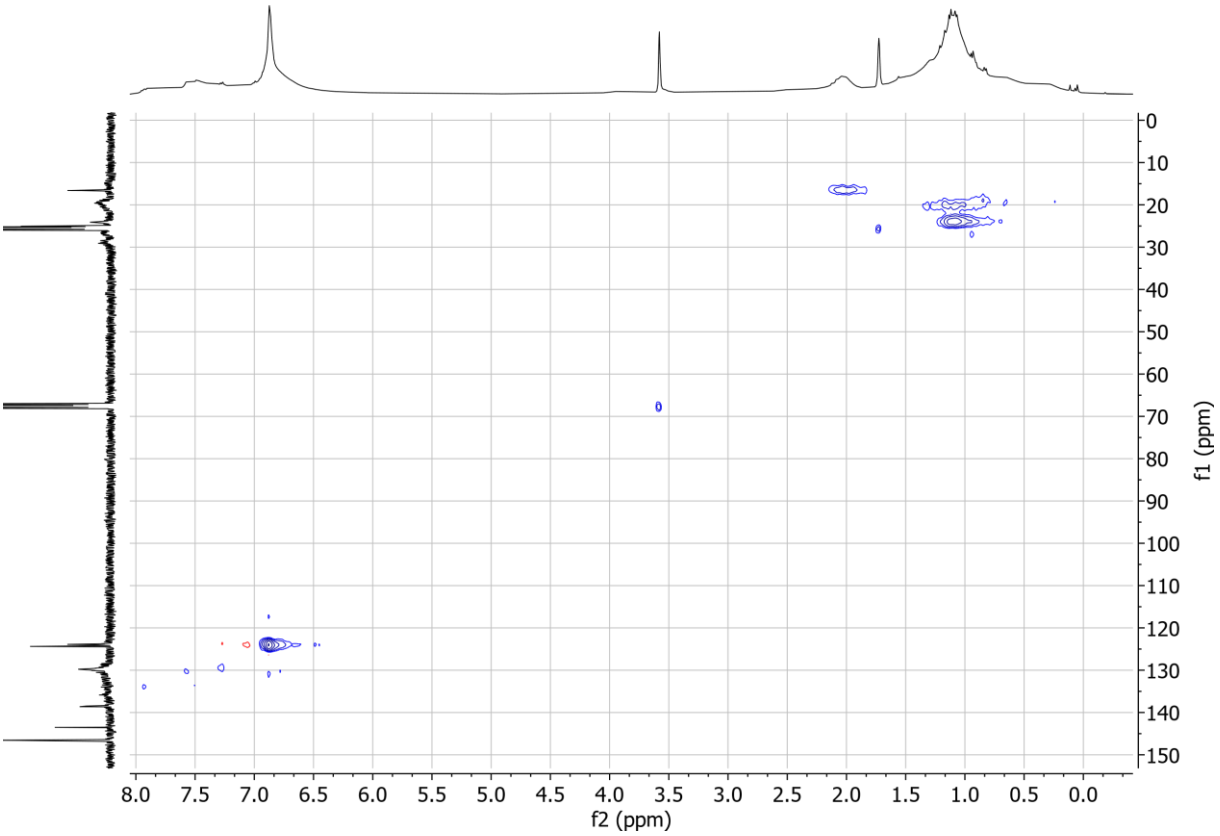


Figure S33. HSQC-NMR-spectrum (400/101 MHz, THF-d_8, 298 K) of **4**.

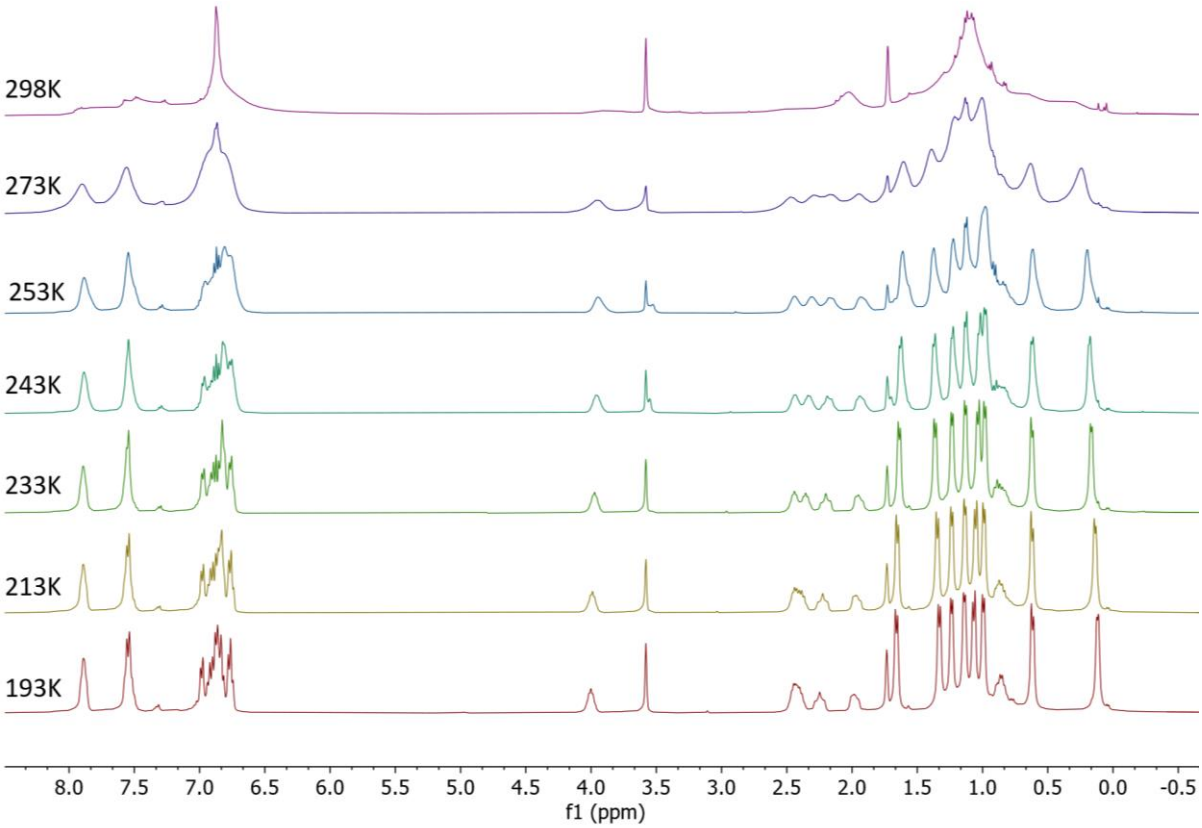


Figure S34. ^{1}H-NMR-spectrum (400 MHz, THF-d_8) of **4** from 2 193 - 298K, from bottom to top.

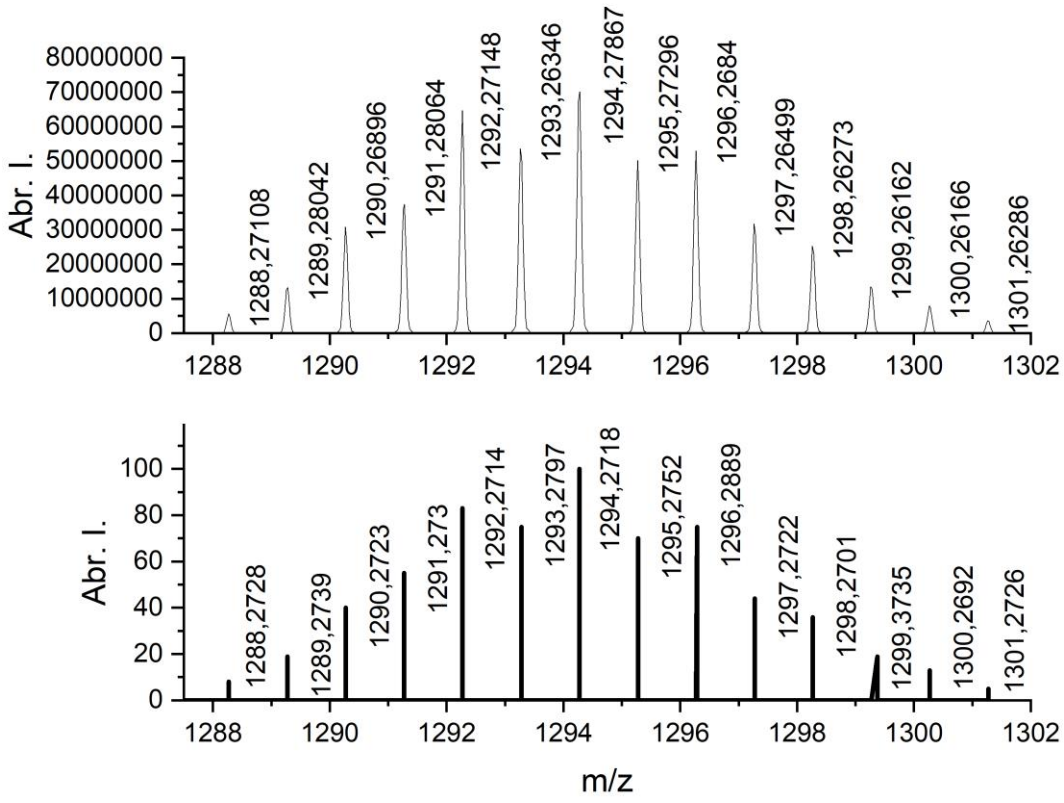


Figure S35. Cutout from LIFDI/MS of **4**, Top: found MS for [(^{PhiP}DippNGaCl)$_2$Pd]+; Bottom: Calculated MS spectrum of [(^{PhiP}DippNGaCl)$_2$Pd]+.

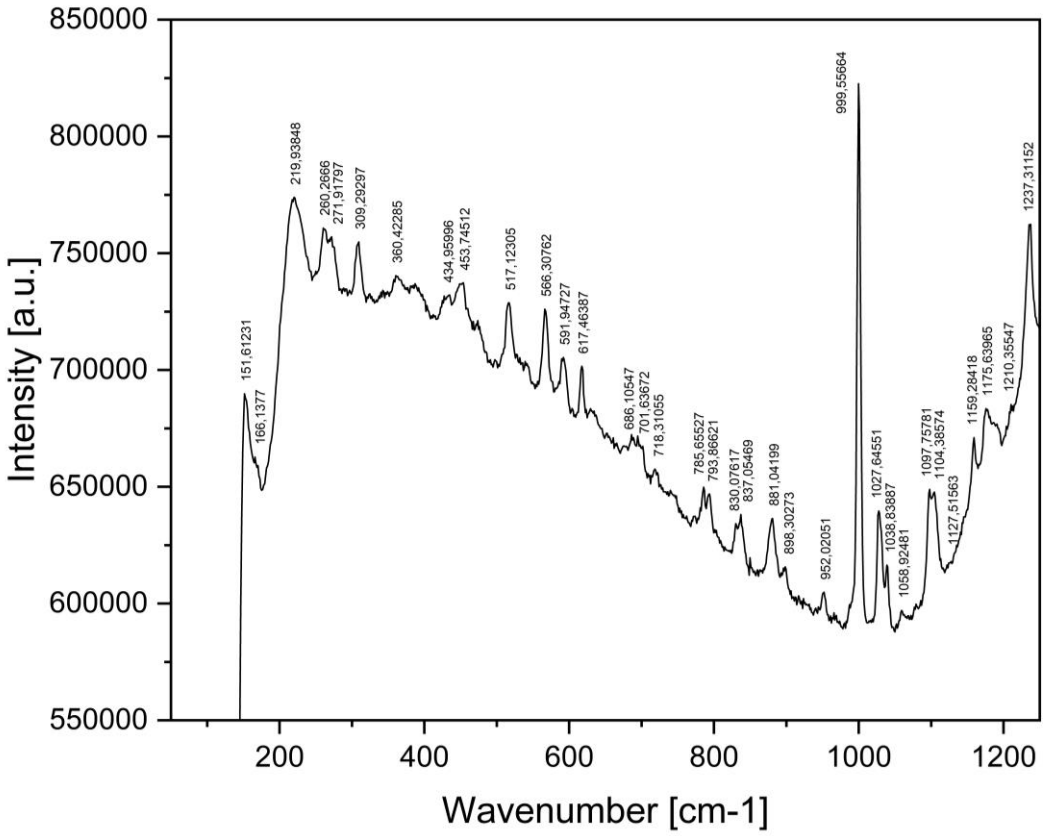


Figure S36. Raman-Spectra of **4**.

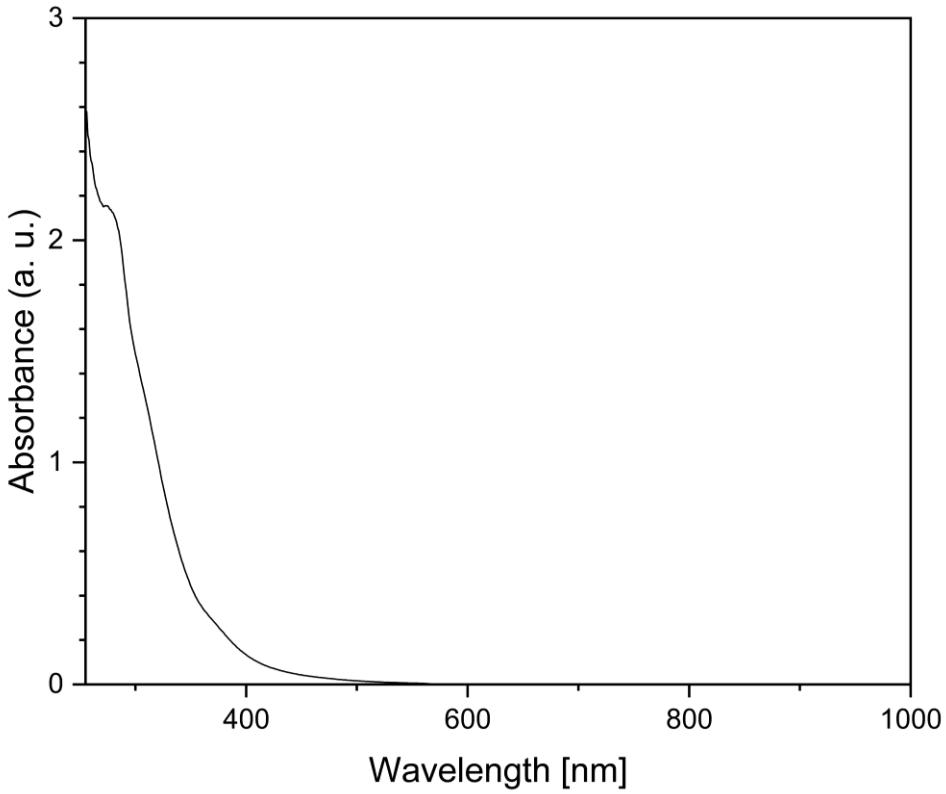


Figure S37. UV/Vis spectrum of a 3.125x10^{-6} M solution of **4**. in THF at ambient temperature.

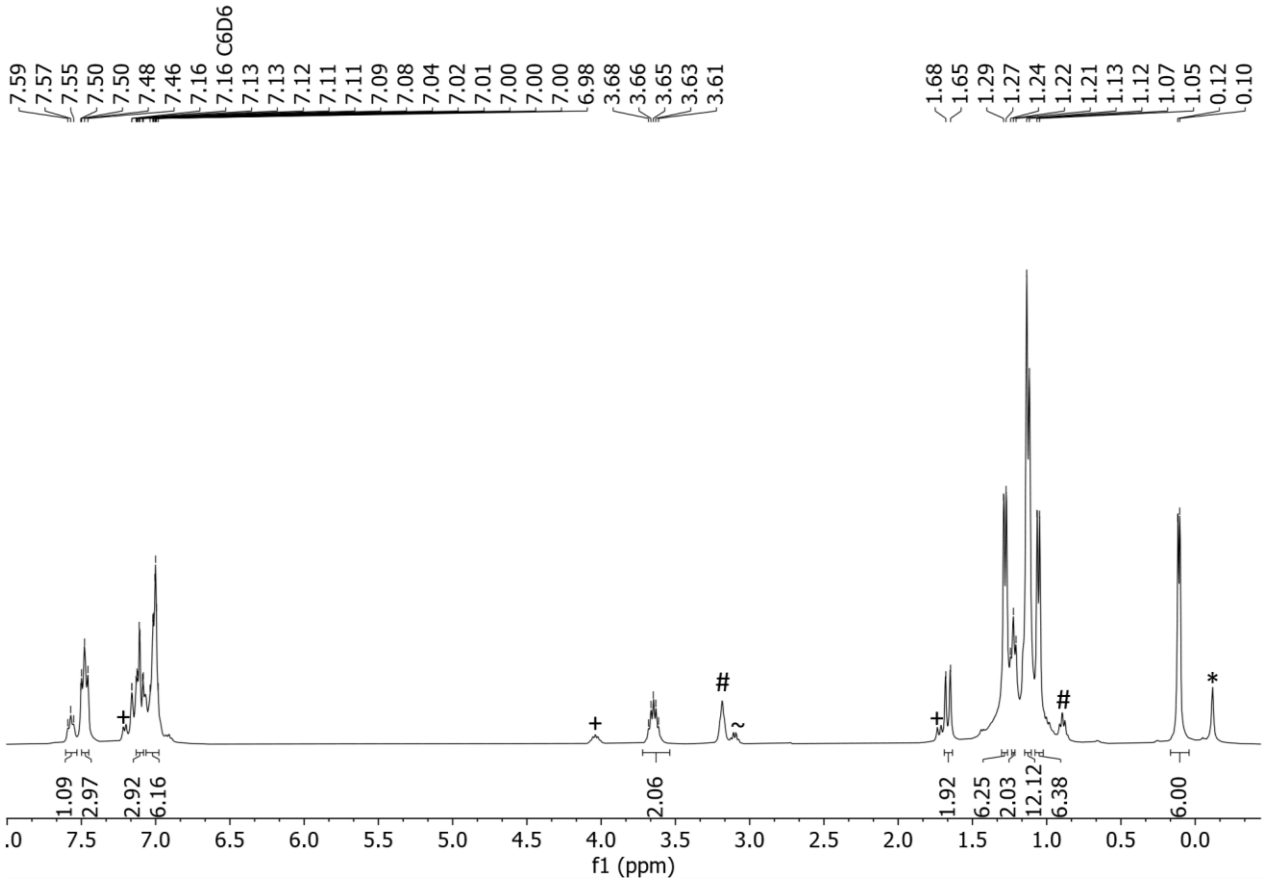


Figure S38. ^{1}H-NMR-spectrum (400 MHz, C_6D_6, 298 K) of **6**. * Denotes minor amounts of MeLi. # denotes minor amounts of coordinated diethyl-ether. ~ denotes minor amounts of uncoordinated diethyl-ether. + denotes minor amounts of ^{PhiP}DippNH.

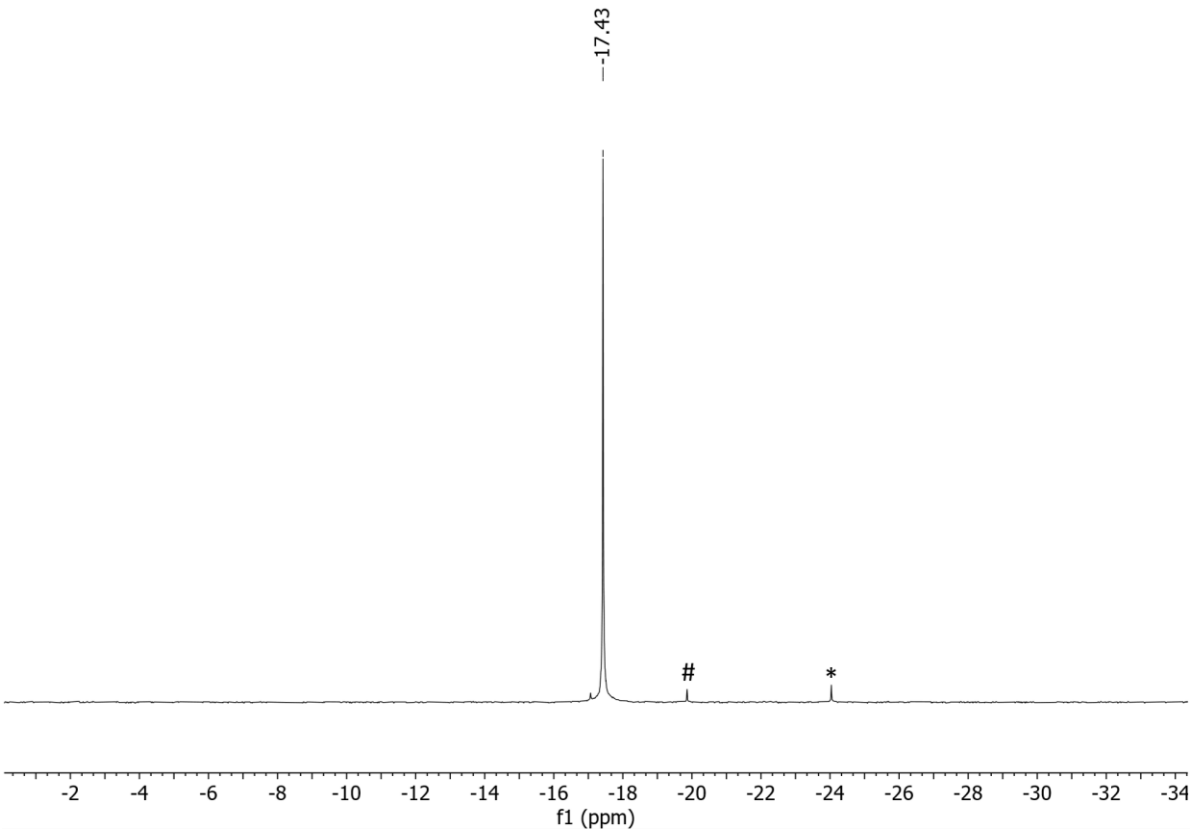


Figure S39. $^{31}P\{^{1}H\}$-NMR-spectrum (162 MHz, C_6D_6, 298 K) of **6**. * Denotes minor amounts of ^{PhiP}DippNH and # denotes minor amounts of ^{PhiP}DippNGaCl$_2$.

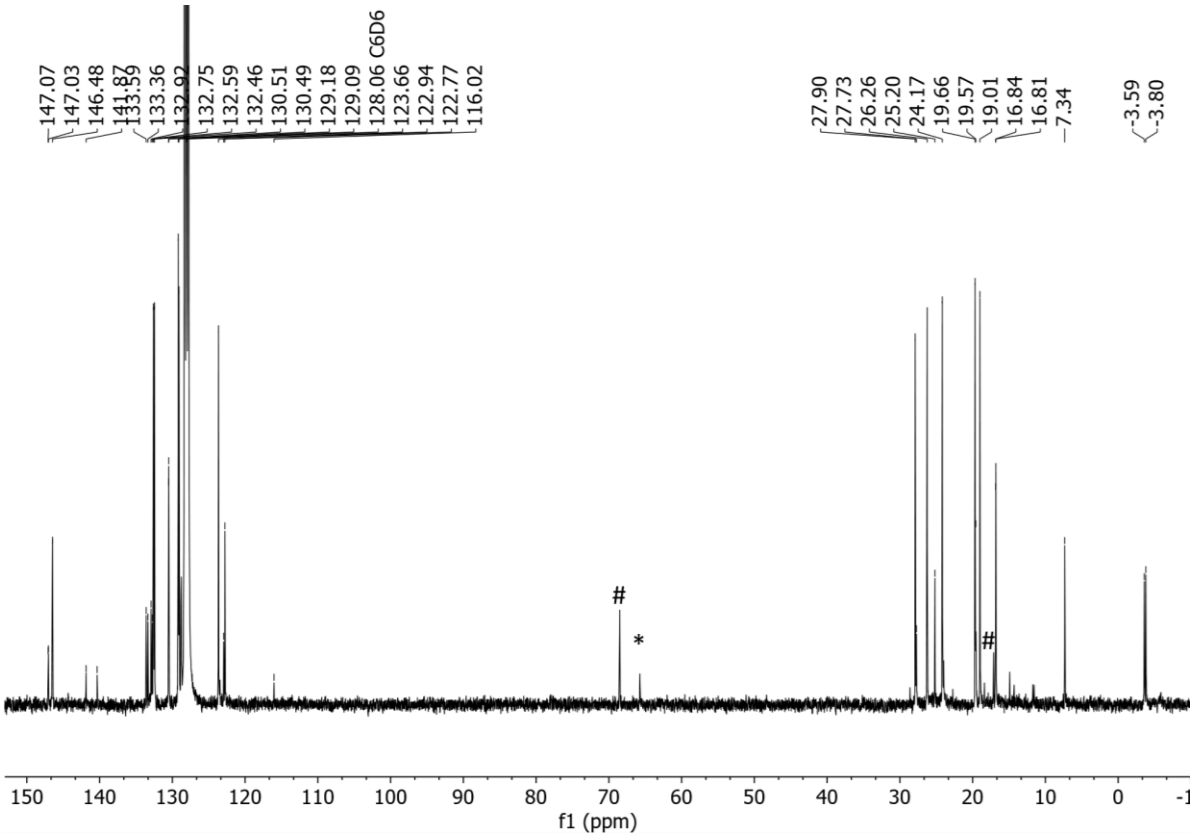


Figure S40. ^{13}C NMR-spectrum (101 MHz, C_6D_6, 298 K) of **6**. * Denotes minor amounts of uncoordinated diethyl-ether and # denotes minor amounts of coordinated diethyl-ether.

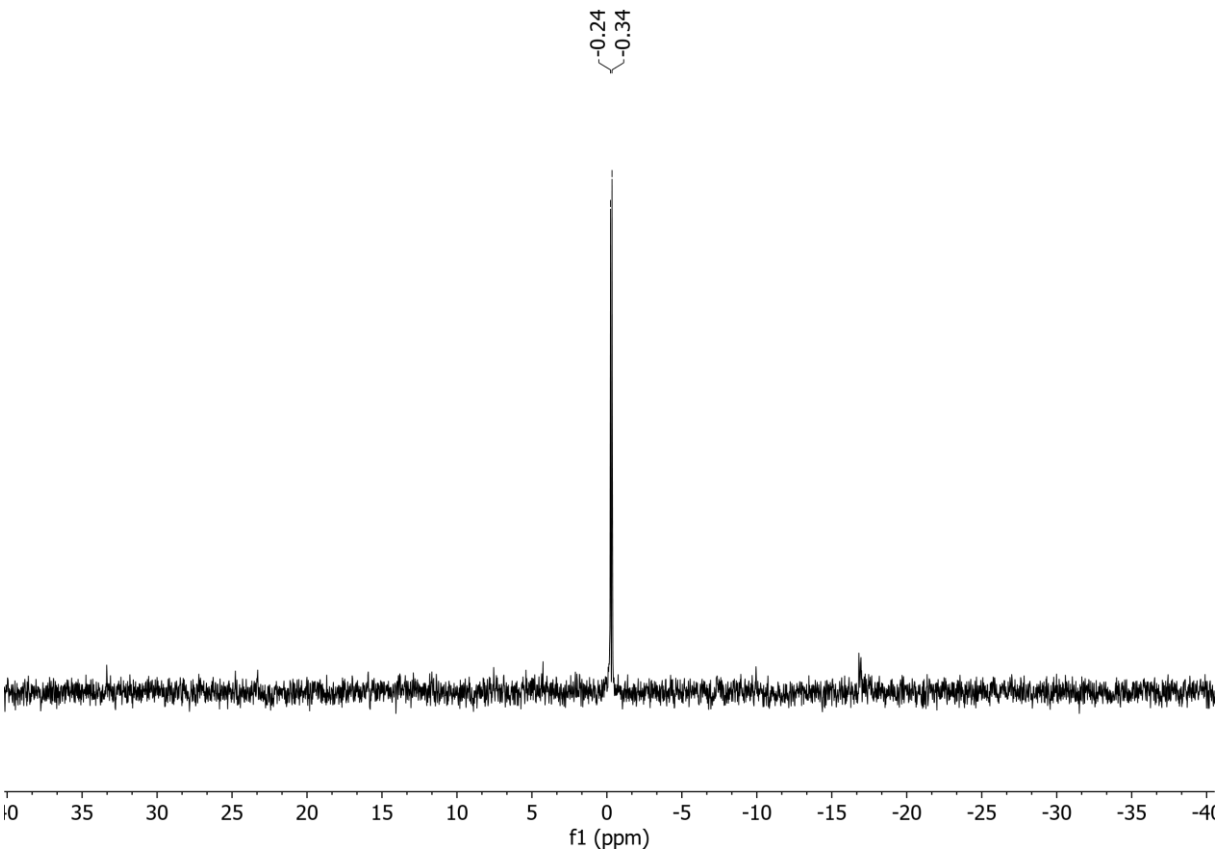


Figure S41. $^{29}Si\{^{1}H\}$-NMR-spectrum (99 MHz, C_6D_6, 298 K) of **6**.

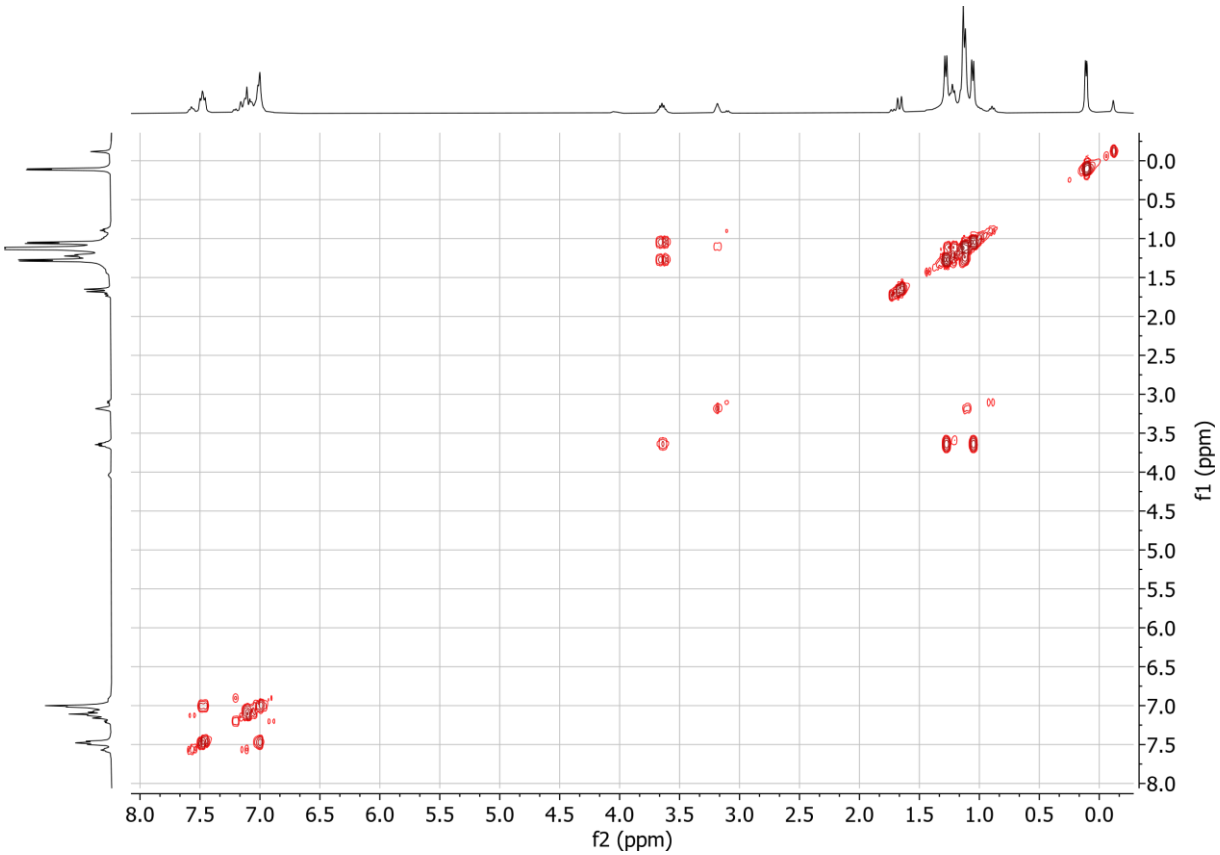


Figure S42. COSY-NMR-spectrum (400 MHz, C_6D_6, 298 K) of **6**.

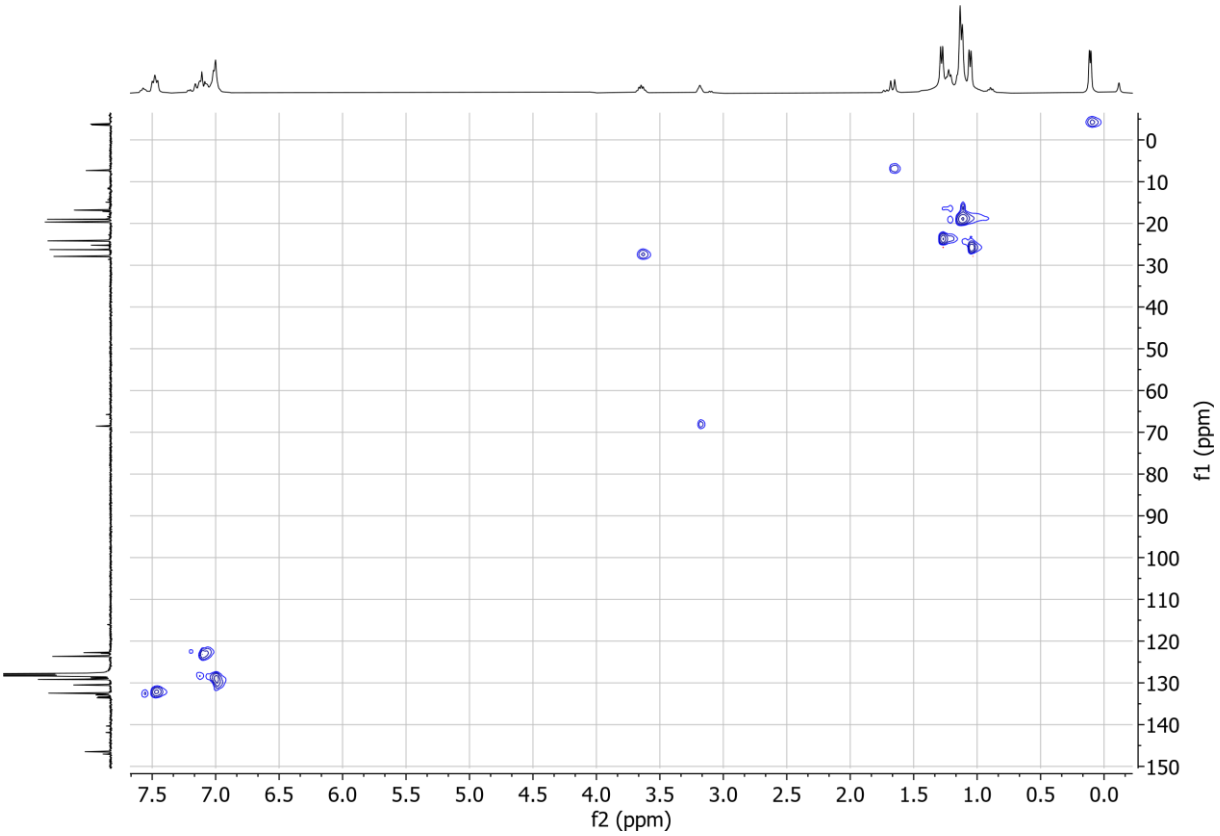


Figure S43. HSQC-NMR-spectrum (400/101 MHz, C_6D_6, 298 K) of **6**.

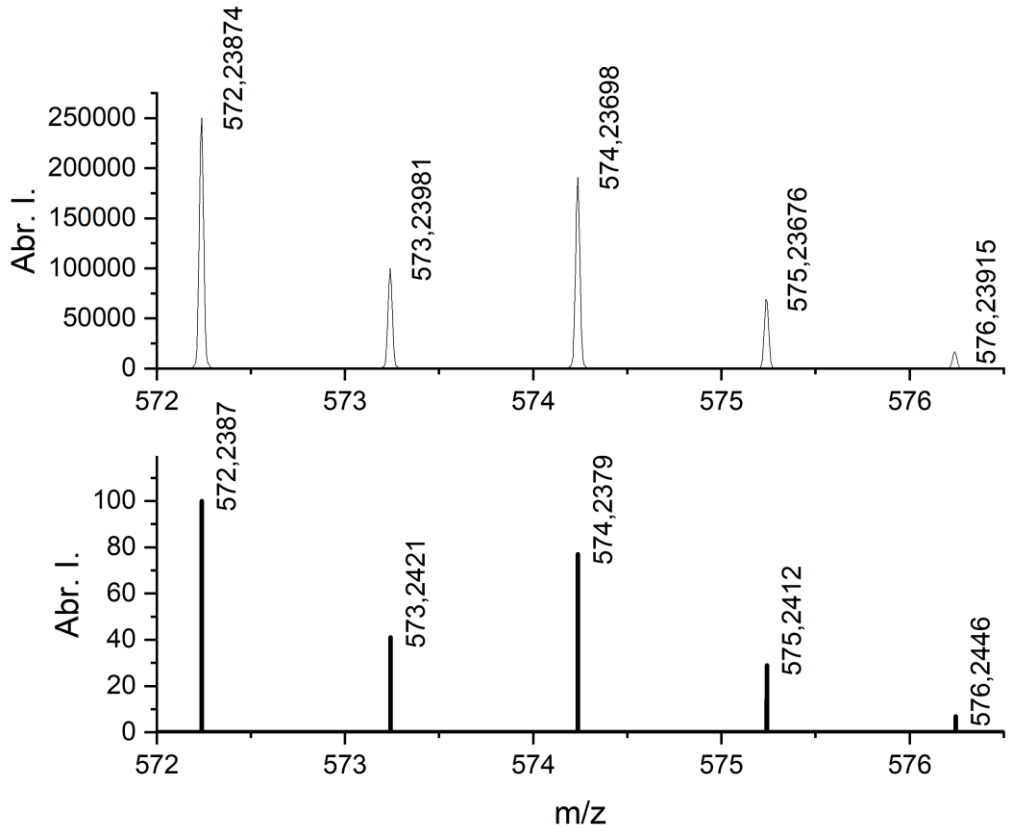


Figure S44. Cutout from LIFDI/MS of **6**, Top: found MS for $[M\text{-}CH_3]^+$; Bottom: Calculated MS spectrum of $[M\text{-}CH_3]^+$.

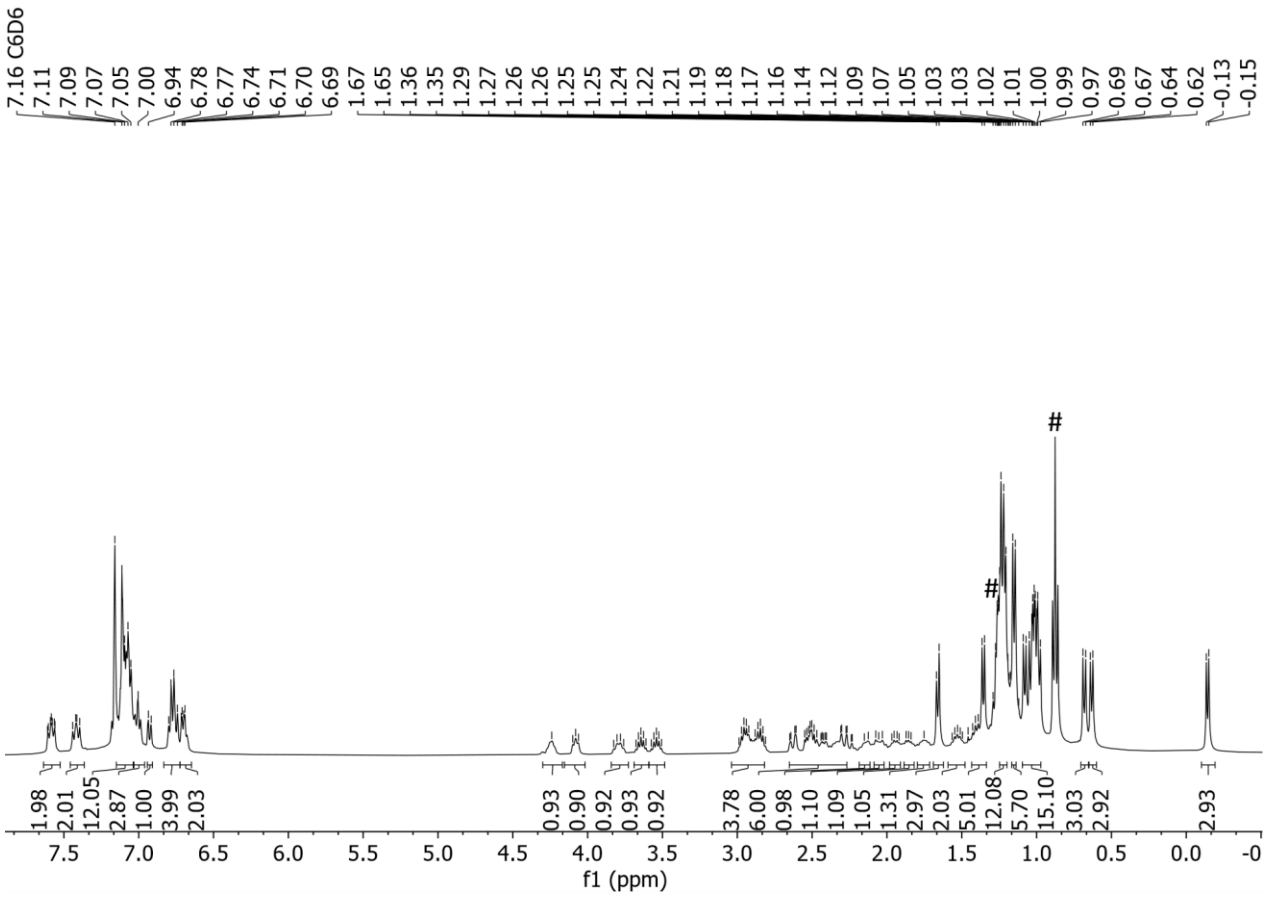


Figure S45. ^{1}H-NMR-spectrum (400 MHz, C_6D_6, 298 K) of **7**. # denotes minor amounts of pentane.

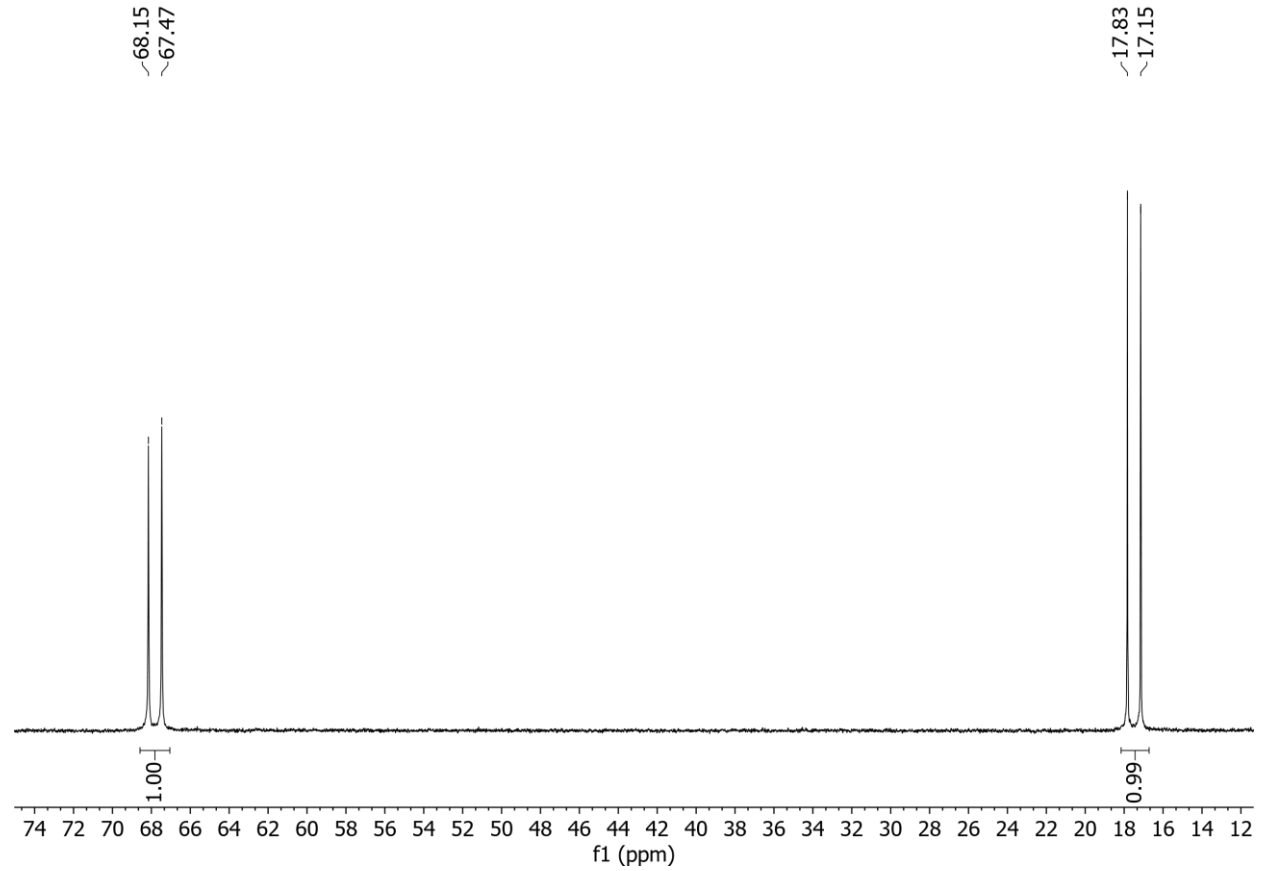


Figure S46. ^{31}P{^{1}H}-NMR-spectrum (162 MHz, C_6D_6, 298 K) of **7**.

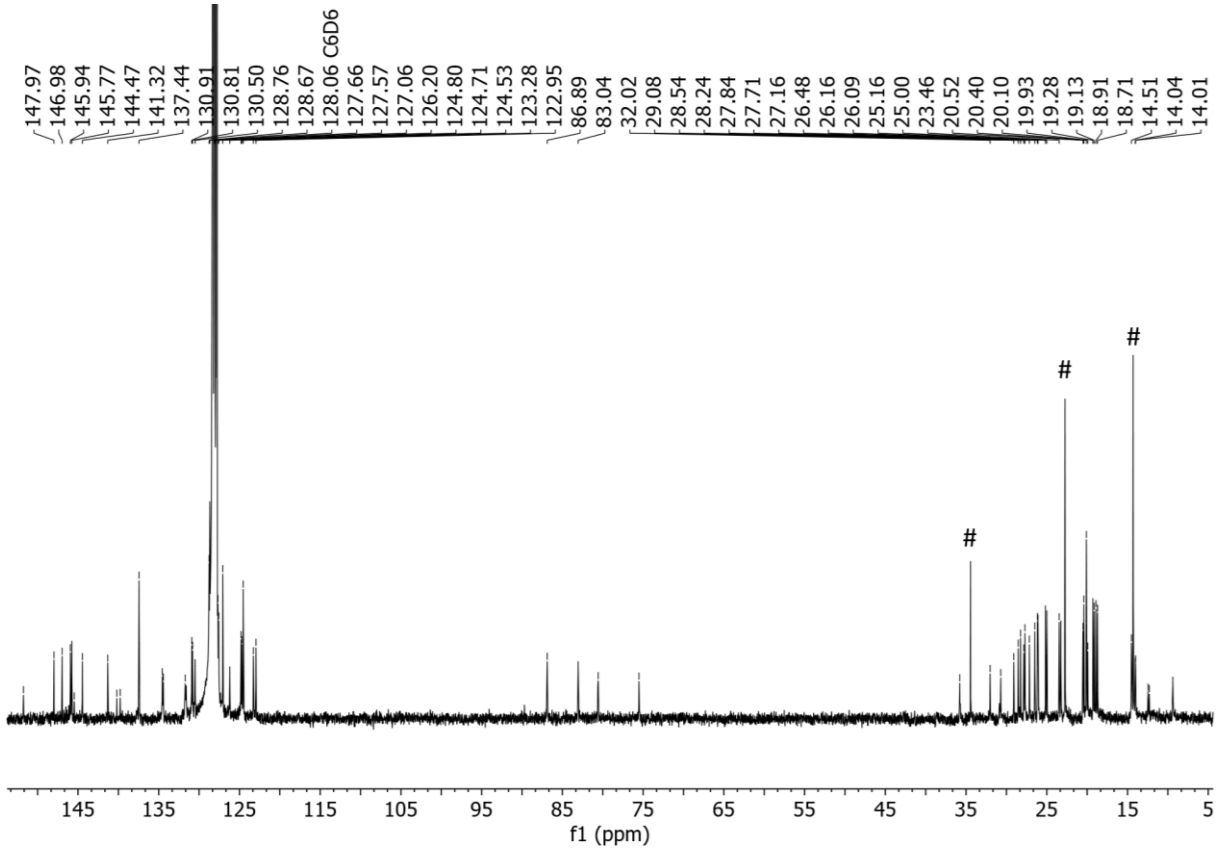


Figure S47. ^{13}C-NMR-spectrum (101 MHz, C_6D_6, 298 K) of **7**. # denotes minor amounts of pentane.

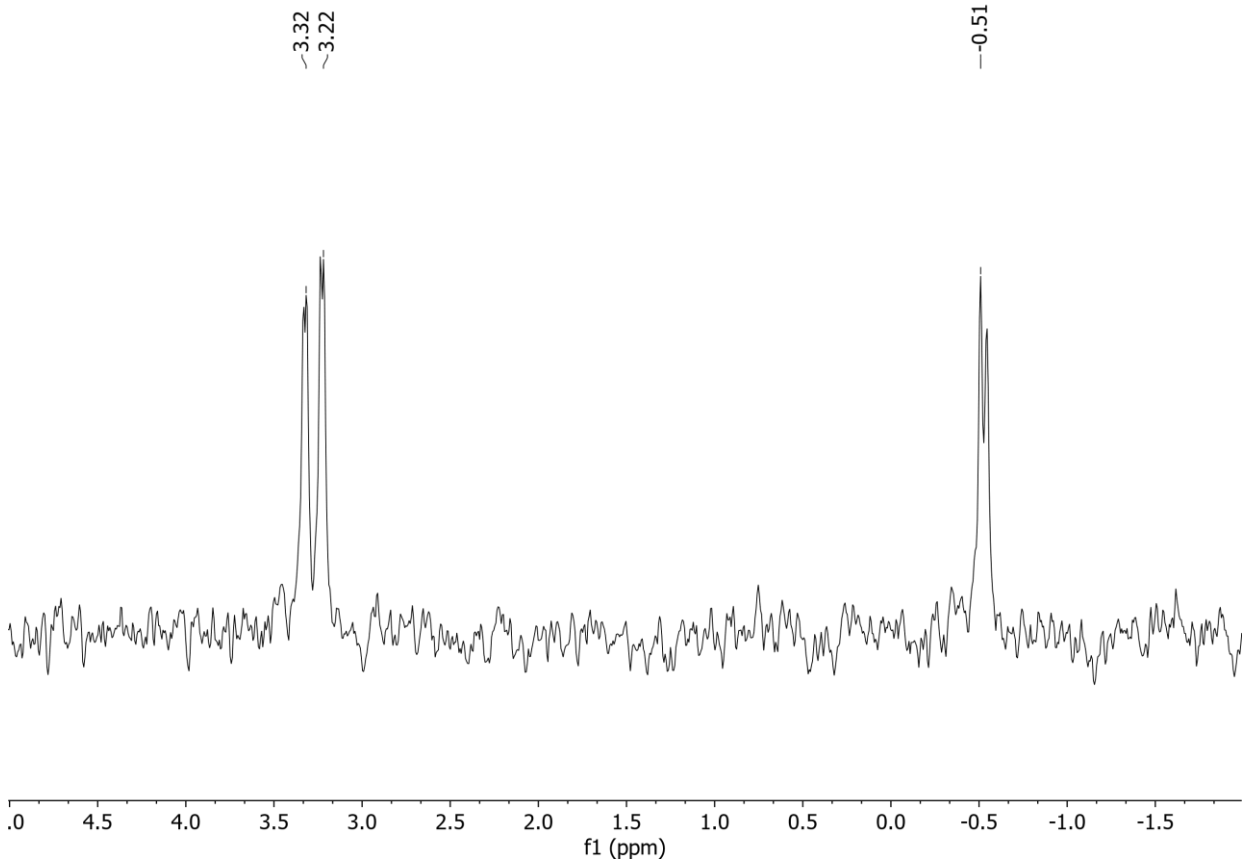


Figure S48. ^{29}Si{^{1}H}-NMR-spectrum (99 MHz, C_6D_6, 298 K) of **7**.

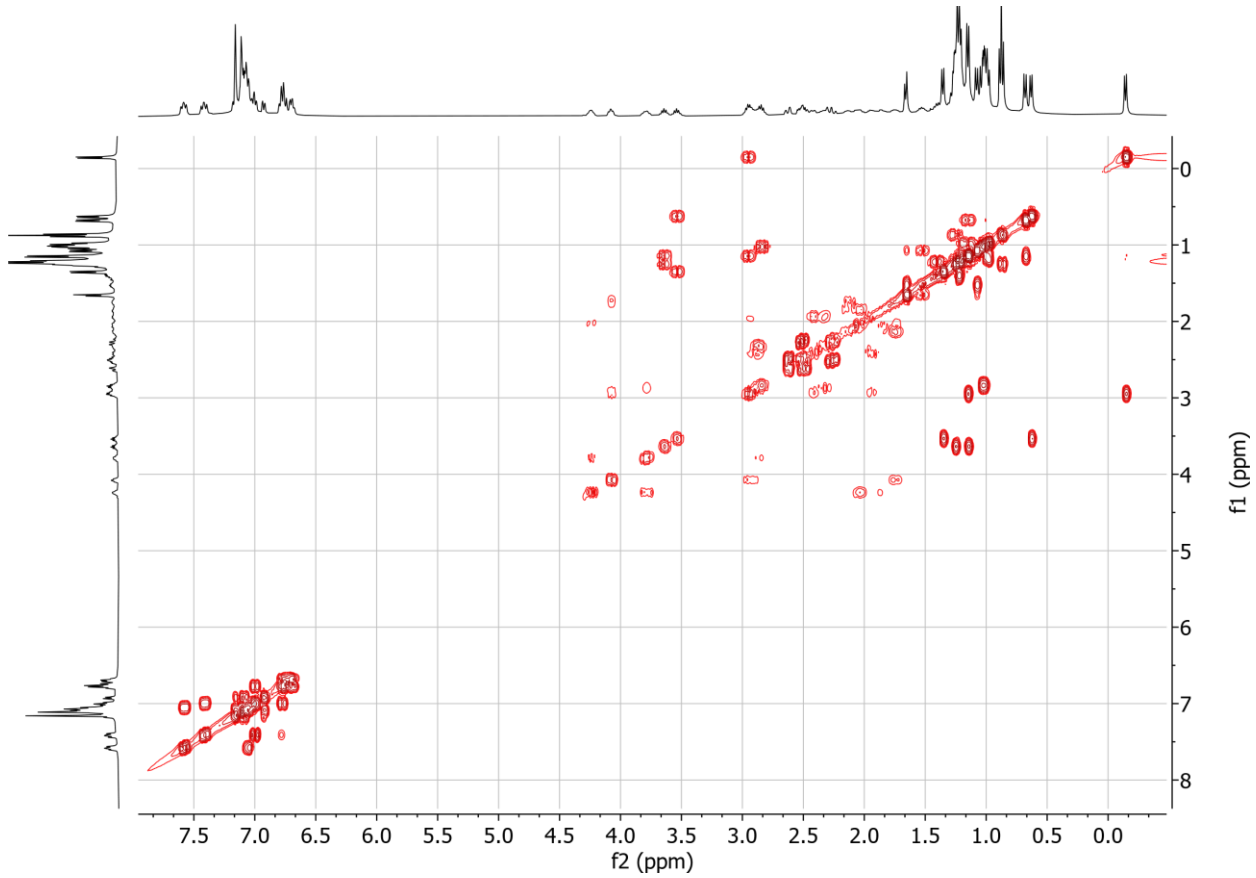


Figure S49. COSY-NMR-spectrum (400 MHz, C_6D_6, 298 K) of **7**.

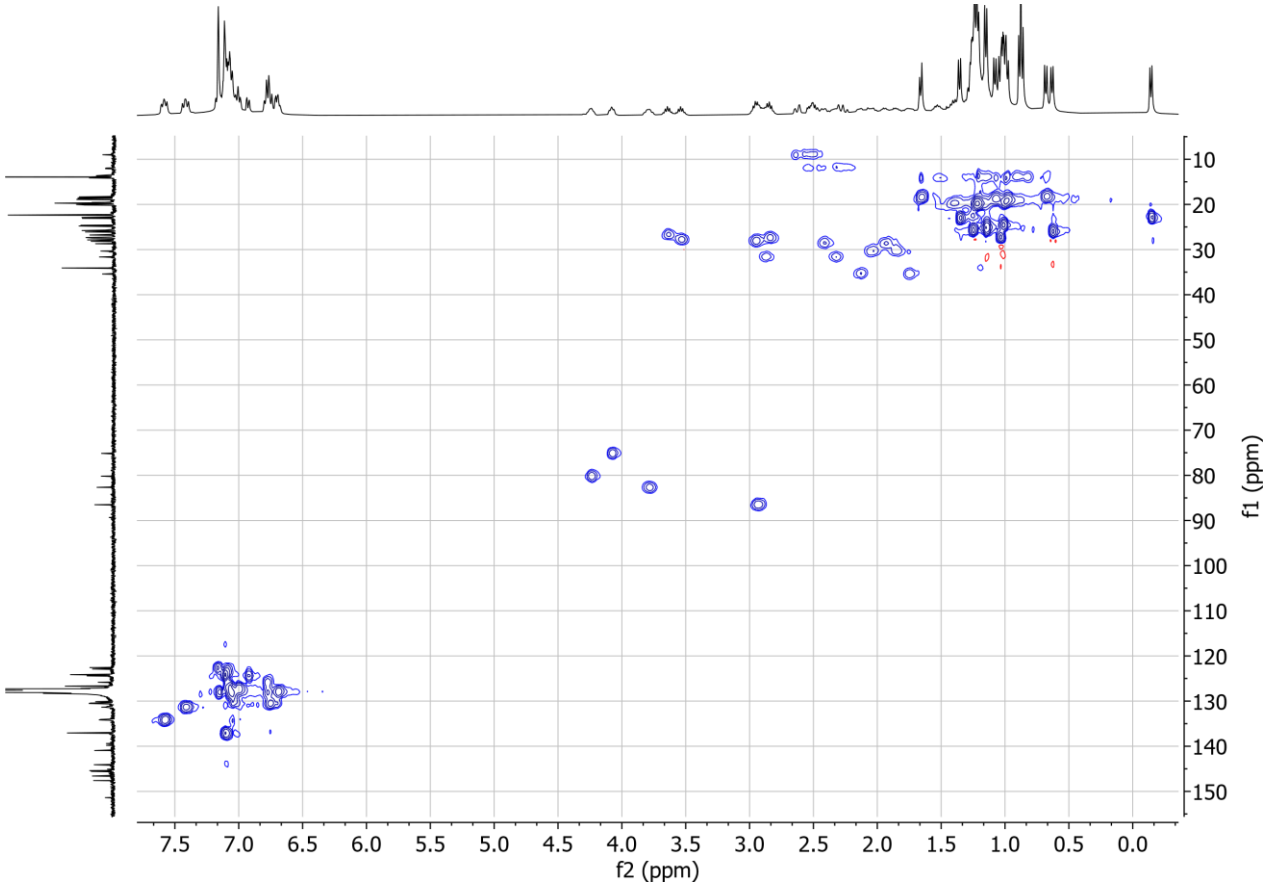


Figure S50. COSY-NMR-spectrum (400/ 101 MHz, C_6D_6, 298 K) of **7**.

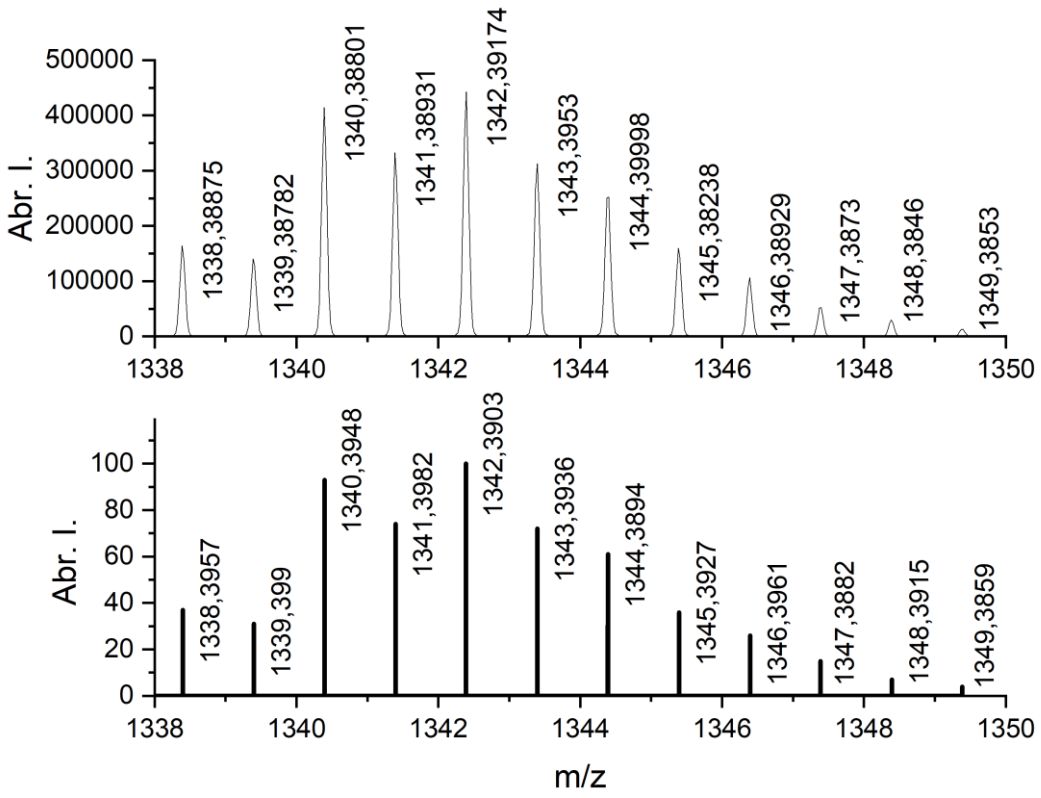


Figure S51. Cutout from LIFDI/MS of **7**, Top: found MS for [(^{PhiP}DippNGa)(^{PhiP}DippNGaPh)(Ni)((Ni(COD))]+ Bottom: Calculated MS spectrum of [(^{PhiP}DippNGa)(^{PhiP}DippNGaPh)(Ni)((Ni(COD))]+.

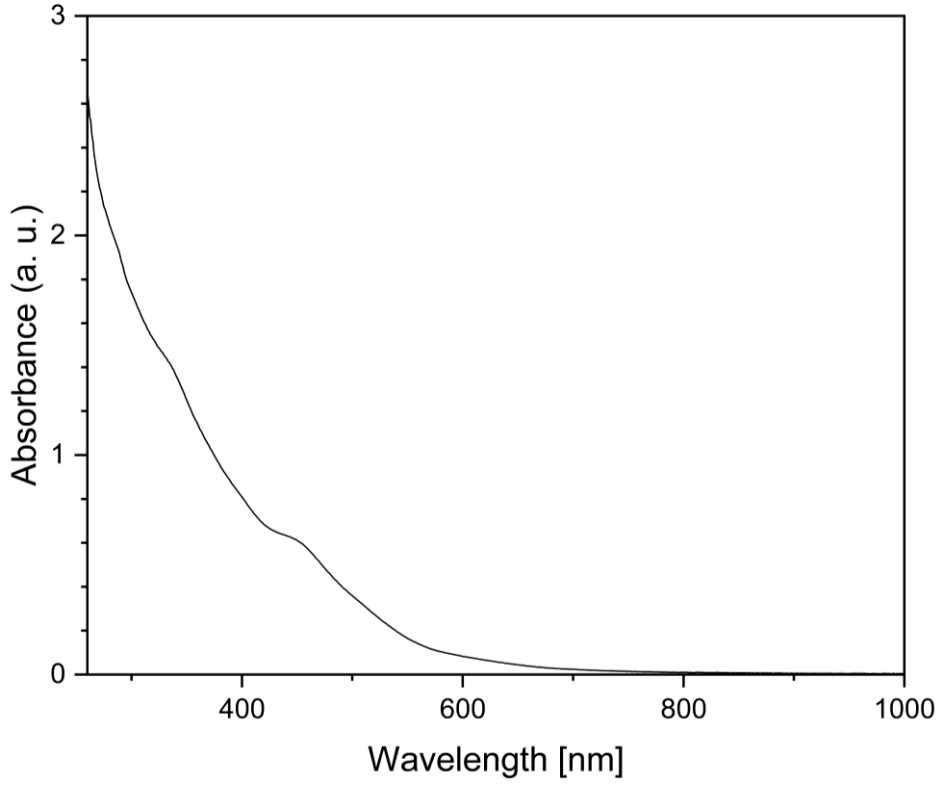


Figure S52. UV/Vis spectrum of a 3.125x10^{-6} M solution of **7** in THF at ambient temperature.

2. X-ray Crystallographic Details

Single crystals of **1**-**4**, **6**, and **7** suitable for X-ray structural analysis were mounted in perfluoroalkyl ether oil on a nylon loop and positioned in a 150 K cold N_2 gas stream. Data collection was performed with a STOE StadiVari diffractometer (MoKα radiation) equipped with a DECTRIS PILATUS 300K detector. Structures were solved by Direct Methods (SHELXS-97)[8] and refined by full-matrix least-squares calculations against F^2 (SHELXL-2018).[9] All non-hydrogen atoms were treated with anisotropic displacement parameters. Crystal data, details of data collections, and refinements for all structures can be found in their CIF files, which are available free of charge via www.ccdc.cam.ac.uk/data_request/cif, and are summarized in Tables S1.

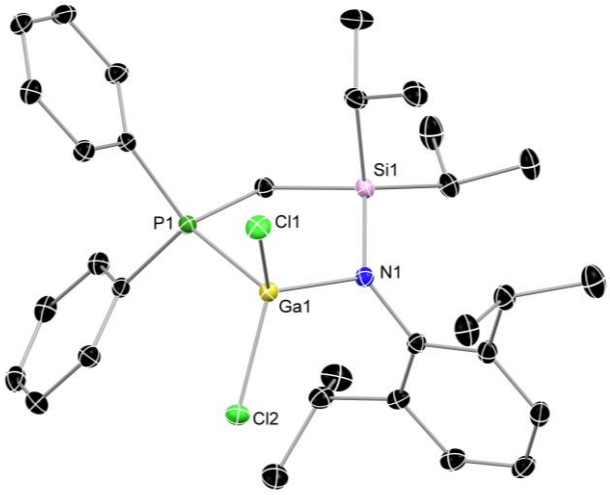


Figure S53. The molecular structure of **1**, with thermal ellipsoids at 30% probability, and hydrogen atoms omitted for clarity. Selected bond distances (Å) and angle (°) for **1**: Ga1-P1 2.431(1); Ga1-N1 1.886(2); Ga1-Cl1 2.185(1); Ga1-Cl2 2.168(1); N1-Ga1-P1 93.83(6); Cl1-Ga1-Cl2 105.97(3).

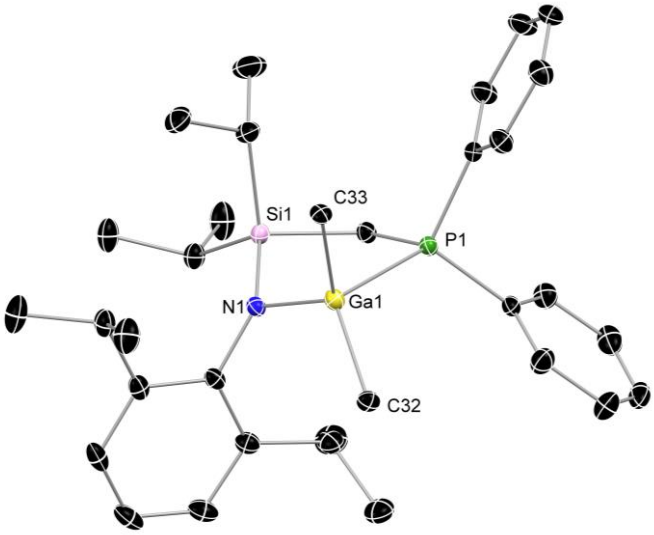


Figure S54. The molecular structure of **6**, with thermal ellipsoids at 30% probability, and hydrogen atoms omitted for clarity. Selected bond distances (Å) and angle (°) for **6**: Ga1-P1 2.5175(9); Ga1-N1 1.934(2); Ga1-C32 1.993(2); Ga1-C33 2.017(2); N1-Ga1-P1 89.03(5); C32-Ga1-C33 113.27(8).

Table S1. Summary of X-ray crystallographic data for **1**-**4**, **6**, and **7**.

	1	**2**	**3**	**4**	**6**	**7**
empirical form.	$C_{31}H_{43}Cl_2GaNPSi$	$C_{62}H_{86}Cl_2Ga_2N_2P_2Si_2$, $0.5(C_4H_{10}O)$	$C_{62}H_{86}Cl_2Ga_2N_2NiP_2Si_2$, C_9H_{20}	$C_{62}H_{86}Cl_2Ga_2N_2P_2PdSi_2$	$C_{33}H_{49}GaNPSi$	$C_{70}H_{98}Ga_2N_2Ni_2P_2Si_2$
formula wt	629.34	2449.69	1374.74	1294.18	588.51	1342.48
crystal syst.	triclinic	monoclinic	orthorhombic	orthorhombic	triclinic	monoclinic
space group	*P-1*	*P2₁/c*	*Pnna*	*Pnna*	*P-1*	*C2/c*
a (Å)	9.860(2)	23.090(5)	15.629(3)	15.714(3)	10.009(2)	25.060(5)
b (Å)	9.920(2)	27.340(6)	22.820(5)	22.937(5)	10.011(2)	15.840(3)
c (Å)	18.120(4)	22.520(5)	20.425(4)	20.691(4)	18.111(4)	39.860(8)
α (deg.)	81.90(3)	90	90	90	85.20(3)	90
β (δεγ)	84.70(3)	111.90(3)	90	90	82.22(3)	106.50(3)
γ (deg.)	67.40(3)	90	90	90	67.29(3)	90
vol ($Å^3$)	1618.5(7)	13191(5)	7285(3)	7457(3)	1657.6(7)	15171(6)
Z	2	4	4	4	2	8
ρ(calc) ($g.cm^{-3}$)	1.291	1.234	1.253	1.153	1.179	1.176
μ (mm^{-1})	1.122	1.022	1.180	1.135	0.935	1.302
F(000)	660	5176	2912	2688	628	5664
T (K)	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)
reflns collect.	21256	85103	26641	95573	22347	53768
unique reflns	6369	25618	7142	7330	6520	14835
R_{int}	0.0306	0.1513	0.0828	0.0211	0.0261	0.0409
R1 [$I>2\sigma(I)$]	0.0346	0.0523	0.0489	0.0354	0.0295	0.0357
*w*R2 (all data)	0.0970	0.1230	0.1382	0.0940	0.0765	0.1006
CCDC No.						

3. Computational Methods and Details

The geometry ptimization of all reported structures and frequency calculations were performed with the Gaussian 16 program.[10] The calculations were carried out for all molecules using the BP86[11,12] functional in conjunction with def2-TZVPP and def2-SVP basis sets[13-15] and with dispersion correction by Grimme with Becke-Johnson damping D3(BJ)[16]. The calculation of Pd employed a relativistic effective core potential (ECP) where 28 core electrons replaced by an ECP.[17] Vibrational frequency calculations were performed for all stationary points to identify whether they were local minima (no imaginary frequencies) or transition structures (only one imaginary frequency). Partial charges (q) and Wiberg bond order (P) were obtained at the BP86-D3(BJ)/def2-TZVPP level using NBO 7.0[18] as implemented with Gaussian 16 program. The Laplacian of the electron density was estimated by the Bader's quantum theory of atoms-in-molecules (QTAIM) method with the AIMALL program[19]. All presented structures were visualized with CYLView software[20].

The bonding situation was analyzed by means of an energy decomposition analysis (EDA)[21,22] together with the natural orbitals for chemical valence (NOCV)[23,24] method using the ADF 2019.103 program package[25,26]. The EDA-NOCV calculations were carried out at the BP86-(D3BJ)/DZ2P+ZORA level[27,28] using the BP86-(D3BJ)/def2-SVP optimized geometries. In this analysis, the intrinsic interaction energy (ΔEint) between two fragments can be divided into four energy components as follows:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp} \quad (1)$$

While the electrostatic ΔE_{elstat} term represents the quasiclassical electrostatic interaction between the unperturbed charge distributions of the prepared fragments, the Pauli repulsion ΔE_{Pauli} corresponds to the energy change associated with the transformation from the superposition of the unperturbed electron densities of the isolated fragments to the wavefunction[29], which properly obeys the Pauli principle through explicit antisymmetrization and renormalization of the production wavefunction. The orbital term ΔEorb can be further decomposed into contributions from each irreducible representation of the point group of the interacting system as follows:

$$\Delta E_{orb} = \sum_{r} \Delta E_{r} \quad (2)$$

The addition of ΔE_{prep} to the intrinsic interaction energy ΔEint gives the total energy ΔE, which has opposite sign compared with the bond dissociation energy De [Eq. (3)].

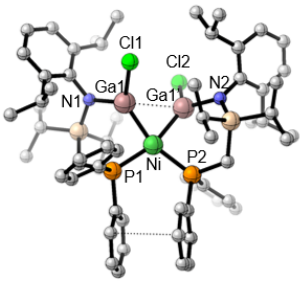
$$\Delta E(-D_e) = \Delta E_{int} + \Delta E_{prep} \quad (3)$$

The combination of the EDA with NOCV enables the partition of the total orbital interactions into pairwise contributions of the orbital interactions which is very vital to get a complete picture of the bonding. The charge deformation $\Delta\rho_{k(r)}$, resulting from the mixing of the orbital pairs $\psi_{k(r)}$ and $\psi_{-k(r)}$ of the interacting fragments presents the amount and the shape of the charge flow due to the orbital interactions [Eq. (4)], and the associated energy term ΔEorb provides with the size of stabilizing orbital energy originated from such interaction [Eq. (5)].

$$\Delta\rho_{orb}(r) = \sum_{k}\Delta\rho_{k}(r) = \nu_{k}\,[-\psi 2\ -k(r) + \psi 2\ k(r)] \quad (4)$$

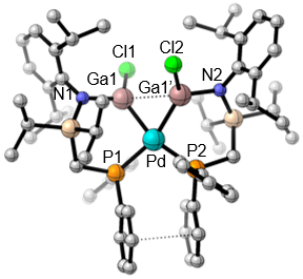
$$\Delta E_{orb} = \sum_{k}\Delta E k\ orb = \sum_{k=1}^{N/2} \nu_{k}[FTS\ \ -k,-k + FTS\ k,k] \quad (5)$$

More details about the EDA-NOCV method and its application are given in recent reviews articles[30-33].



(a) compound 3

	BP86-(D3BJ)/ def2-SVP	BP86-(D3BJ)/ def2-TZVPP	Experimental
Ga1-Ga1'	2.807	2.813	2.771
Ga1-Ni	2.311	2.331	2.300
P1-Ni	2.196	2.190	2.208
N1-Ga1	1.888	1.887	1.866
Ga1-Ni-Ga1'	74.78	74.25	74.08
P1-Ni-P1'	107.05	108.42	109.23
Ni1-Ga1-Ga1'	52.61	52.87	52.96

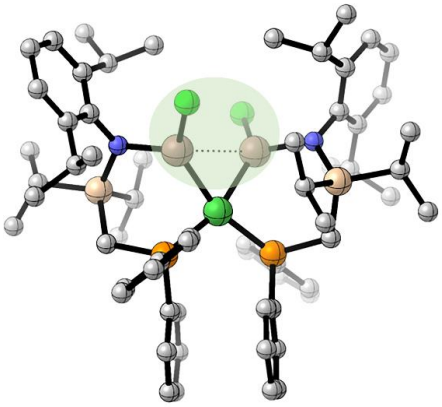


(b) compound 4

	BP86-(D3BJ)/ def2-SVP	BP86-(D3BJ)/ def2-TZVPP	Experimental
Ga1-Ga1'	2.897	2.924	2.856
Ga1-Pd	2.397	2.400	2.386
P1-Pd	2.341	2.326	2.351
N1-Ga1	1.886	1.887	1.859
Ga1-Pd-Ga1'	74.35	75.05	73.53
P1-Pd-P1'	106.53	106.96	109.58
Pd-Ga1-Ga1'	52.83	52.48	53.24

Figure **S55.** Optimized geometries of (a) **3** and (b) **4** and the most important bond lengths and angles at BP86-D3(BJ)/def2-SVP and BP86-D3(BJ)/def2-TZVPP

Table S2. EDA-NOCV results of **compound 3** by using the Ga_2Cl_2 and [Ni] as interacting fragments at the BP86-D3(BJ)/TZ2P+ZORA//BP86-D3(BJ)/def2-SVP level of theory. Fragments are given in various electronic states (i.e., singlet (S), doublet (D), and triplet (T)). Energy values are given in kcal/mol.

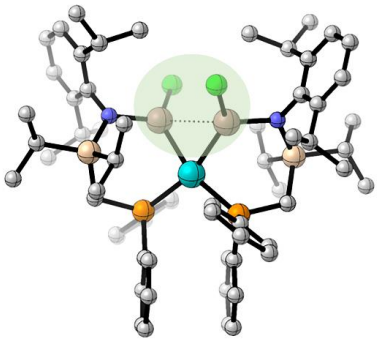


Fragments	Ga_2Cl_2 (**S**) + [Ni] (**S**)	Ga_2Cl_2 **(T) +** [Ni] **(T)**	$Ga_2Cl_2^{1+}$ **(D) +** $[Ni]^{1-}$**(D)**	$Ga_2Cl_2^{2+}$**(S) +** $[Ni]^{2-}$**(S)**	$Ga_2Cl_2^{1-}$**(D) +** $[Ni]^{1+}$**(D)**	$Ga_2Cl_2^{2-}$**(S) +** $[Ni]^{2+}$**(S)**
ΔE_{int}	-231.2	-295.2	-341.6	-680.5	-300.2	-625.3
ΔE_{Pauli}	570.2	592.4	636.2	487.4	885.2	957.5
ΔE_{disp}[a]	-50.5(6.3%)	-50.5(5.7%)	-50.5(5.2%)	-50.5(4.3%)	-50.5(4.3%)	-50.5(3.2%)
ΔE_{elstat}[a]	-369.2(46.1%)	-400.5(45.1%)	-455.5(46.6%)	-620.0(53.1%)	-541.2(45.6%)	-819.1(51.7%)
ΔE_{orb}[a]	-381.7(46.6%)	-436.7(49.2%)	-471.9(48.2%)	-497.3(42.6%)	-593.6(50.1%)	-713.3(45.1%)
ΔE_{orb1}[b]	-193.2(50.6%)					
ΔE_{orb2}[b]	-70.4(18.4%)					
ΔE_{orb3}[b]	-30.4(8.0%)					
ΔE_{orb4}[b]	-17.4(4.6%)					
ΔE_{rest}	-70.3(18.4%)					

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

Table S3. EDA-NOCV results of **compound 4** by using [Ga_2Cl_2] and [Pd] as interacting fragments at the BP86-D3(BJ)/TZ2P+ZORA //BP86-D3(BJ)/def2-SVP level of theory. Fragments are given in various electronic states (i.e., singlet (S), doublet (D), and triplet (T)). Energy values are given in kcal/mol.



Fragments	Ga_2Cl_2 **(S)** + [Pd] **(S)**	Ga_2Cl_2 **(T)** + [Pd] **(T)**	$Ga_2Cl_2^{1+}$ **(D)** + $[Pd]^{1-}$**(D)**	$Ga_2Cl_2^{2+}$**(S)** + $[Pd]^{2-}$**(S)**	$Ga_2Cl_2^{1-}$**(D)** + $[Pd]^{1+}$**(D)**	$Ga_2Cl_2^{2-}$**(S)** + $[Pd]]^{2+}$**(S)**
ΔE_{int}	-221.1	-296.2	-350.3	-671.9	-332.6	-574.2
ΔE_{Pauli}	692.9	601.5	611.8	507.9	844.1	1073.0
ΔE_{disp}[a]	-48.6(5.3%)	-48.6(5.4%)	-48.6(5.1%)	-48.6(4.1%)	-48.6(4.1%)	-48.6(3.0%)
ΔE_{elstat}[a]	-442.3(48.4%)	-415.8(46.3%)	-446.8(46.4%)	-644.0(54.6%)	-537.7(45.7%)	-885.6(53.8%)
ΔE_{orb}[a]	-423.1(46.3%)	-433.3(48.3%)	-466.6(48.5%)	-487.1(41.3%)	-590.3(50.2%)	-713.0(43.2%)
ΔE_{orb1}[b]	-239.0(56.5%)					
ΔE_{orb2}[b]	-72.4(17.1%)					
ΔE_{orb3}[b]	-34.9(8.2%)					
ΔE_{orb4}[b]	-15.2(3.6%)					
ΔE_{rest}	-61.6(14.6%)					

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

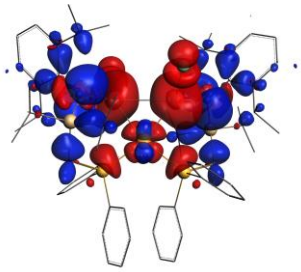
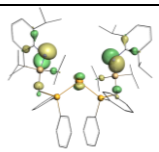
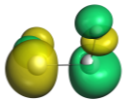
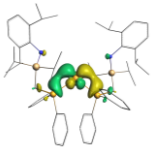
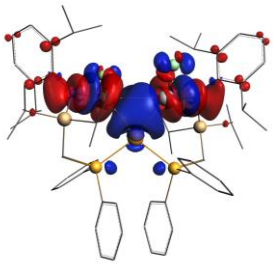
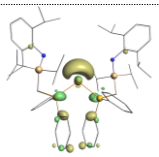
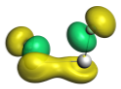
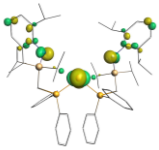
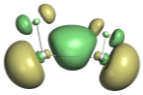
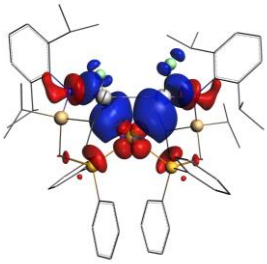
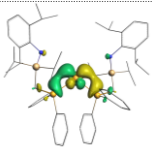
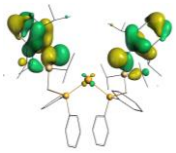
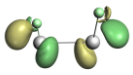
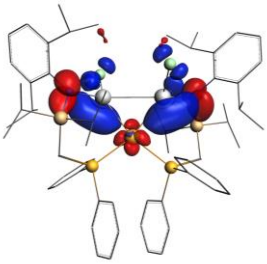
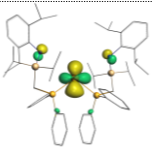
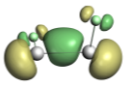
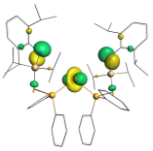
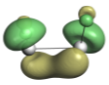
Δρ	[Pd] (Orbital)		Ga_2Cl_2 (Orbital)
		←	
ΔE_{orb1} = -239.0 kcal/mol |ν1| =1.999	[Pd] (LUMO); ν = 1.899		Ga_2Cl_2 (HOMO); ν = -1.012
		→	
	[Pd] (HOMO); ν = -0.290		Ga_2Cl_2 (LUMO+2); ν = 0.038
		←	
ΔE_{orb2} = -72.4 kcal/mol |ν2| = 0.790	[Pd] (LUMO+9); ν = 0.205		Ga_2Cl_2 (HOMO-1); ν = -0.191
		→	
	[Pd] (HOMO-3); ν = -0.126		Ga_2Cl_2 (LUMO); ν = 0.249
		→	
ΔE_{orb3} = -34.9 kcal/mol |ν3| = 0.543	[Pd] (HOMO); ν = -0.179		Ga_2Cl_2 (LUMO+2); ν = 0.203
		←	
	[Pd] (HOMO-2); ν = -0.023		Ga_2Cl_2 (LUMO+4); ν = 0.055
		→	
ΔE_{orb4} = -15.2 kcal/mol |ν4| = 0.470	[Pd] (HOMO-7); ν = -0.071		Ga_2Cl_2 (LUMO); ν = 0.124
		→	
	[Pd] (HOMO-4);ν = -0.059		Ga_2Cl_2 (LUMO+1); ν = 0.076

Figure S56. Plot of deformation densities Δρ of the pairwise orbital interactions ΔE_{orb1} - ΔE_{orb4} and the shape of the most important interacting MOs of the two fragments [Pd] and Ga_2Cl_2 in the singlet states in **4**. The direction of the charge flow is red→blue. The isosurface value of the plot of deformation densities is 0.001 and the isosurface value of the orbital diagram is 0.05.

Table S4. Coordinates and energies (in hartrees) of the calculated structures at the BP86-D3(BJ)/def2-SVP level

Compound 2

Energy= -8554.21091275

Ga	-1.141677	0.316667	0.359819
Ga	1.168523	0.223774	-0.427420
Cl	-0.801355	1.812281	2.083918
Cl	1.251224	1.846377	-2.079050
P	-2.413277	1.648047	-1.244218
P	2.537565	1.611201	1.051981
Si	4.306483	-0.363830	-0.528795
Si	-4.343595	0.136054	0.684029
N	2.648532	-0.962580	-0.744055
N	-2.755459	-0.651823	0.785935
C	-2.667807	-2.031662	1.158590
C	-2.577628	-2.668858	-1.330017
H	-2.980584	-1.639225	-1.394854
C	2.375701	-2.323328	-1.101983
C	2.885962	0.914141	2.704686
C	-2.672935	-2.417430	2.534350
C	-2.365689	3.970571	-2.860833
H	-2.920154	3.383264	-3.609180
C	-2.578834	-3.037886	0.146590
C	-2.774261	-1.381453	3.646477
H	-2.991491	-0.416732	3.154671
C	2.353044	-2.720028	-2.475860
C	2.098094	-3.296751	-0.092938
C	-1.962646	3.370940	-1.649162
C	-2.657189	0.789300	-2.838712
C	-2.584252	-3.783108	2.866951
H	-2.585998	-4.077879	3.928801
C	-1.778968	0.115225	-5.009526
H	-0.964732	0.130621	-5.749427
C	-4.047333	1.692496	-0.415321
H	-4.861581	1.900803	-1.139195
H	-3.990213	2.567651	0.265809
C	-1.618007	0.800587	-3.795832
H	-0.680694	1.337042	-3.578800
C	-5.090056	0.834139	2.313084
H	-5.168099	-0.035658	3.000840
C	2.010402	-0.045897	3.245359
H	1.100226	-0.317467	2.694664
C	-2.479609	-4.389544	0.528072
H	-2.399459	-5.162292	-0.252253
C	-1.238772	4.115441	-0.693370
H	-0.908540	3.641209	0.245087
C	2.569418	-1.702776	-3.585872
H	2.989706	-0.803935	-3.104178
C	-5.583917	-1.107967	-0.097954
H	-4.964914	-1.651641	-0.843924
C	2.072660	-4.059719	-2.805844
H	2.053667	-4.357359	-3.866411
C	-3.478083	-3.579678	-2.180043
H	-3.074617	-4.611543	-2.252868
H	-3.550325	-3.182953	-3.213647
H	-4.503666	-3.648912	-1.760829
C	-2.961021	-0.597465	-5.275845
H	-3.077344	-1.139858	-6.227070
C	-1.441989	-1.189361	4.390977
H	-1.088582	-2.139417	4.846664
H	-1.550600	-0.437347	5.200406
H	-0.661197	-0.816091	3.703239
C	2.055805	-2.927317	1.382540
H	2.491894	-1.912577	1.469325
C	1.841760	3.897602	2.551912
H	1.673988	3.202853	3.387928
C	4.036671	1.296810	3.427798
H	4.711813	2.067726	3.023850
C	4.104293	1.429697	0.124809

H	4.980576	1.770373	0.711695
H	4.011142	2.086890	-0.763395
C	2.293270	-0.641520	4.484851
H	1.601706	-1.391598	4.897453
C	2.270051	3.402161	1.301796
C	-0.943475	5.463720	-0.946852
H	-0.383202	6.038994	-0.195733
C	-2.485451	-4.769561	1.877132
H	-2.410484	-5.832490	2.155804
C	1.232805	-1.263520	-4.204125
H	0.708326	-2.112654	-4.692229
H	1.397156	-0.470007	-4.963577
H	0.558377	-0.849276	-3.432124
C	-4.215516	1.903321	2.987475
H	-4.173903	2.834673	2.381284
H	-3.165724	1.582169	3.132628
H	-4.633896	2.187505	3.978134
C	5.229332	-1.454441	0.747983
H	4.450876	-1.662553	1.514646
C	-3.844777	0.078985	-3.111760
H	-4.661321	0.059412	-2.380077
C	-3.916320	-1.696792	4.629042
H	-3.695258	-2.595625	5.243245
H	-4.870406	-1.889086	4.096257
H	-4.075430	-0.849494	5.328695
C	-6.776175	-0.488350	-0.851338
H	-7.354491	-1.275508	-1.383856
H	-6.471943	0.261130	-1.612247
H	-7.481475	0.023553	-0.166604
C	-1.342738	6.063434	-2.153621
H	-1.099403	7.119401	-2.351436
C	4.790728	0.947860	-3.050923
H	5.135203	1.933247	-2.668249
H	3.683711	0.999720	-3.103653
H	5.180806	0.854662	-4.087725
C	5.656080	-2.801196	0.128859
H	6.439123	-2.663945	-0.646817
H	4.807715	-3.331438	-0.349108
H	6.084276	-3.478444	0.901056
C	2.448372	4.290452	0.219117
H	2.724319	3.904457	-0.773369
C	-2.048989	5.314821	-3.112112
H	-2.358820	5.780826	-4.060795
C	5.315580	-0.192710	-2.155322
H	5.164082	-1.158925	-2.686302
C	1.625810	5.273661	2.723185
H	1.293914	5.654148	3.701805
C	-1.154318	-2.623321	-1.906646
H	-0.523658	-1.886280	-1.369163
H	-1.176437	-2.326796	-2.974149
H	-0.641264	-3.602962	-1.823411
C	3.449701	-0.273975	5.192463
H	3.674723	-0.743908	6.162653
C	-6.065663	-2.146710	0.936019
H	-6.688008	-1.676374	1.727228
H	-5.221032	-2.663659	1.433256
H	-6.692647	-2.926341	0.449639
C	-3.993641	-0.614102	-4.323517
H	-4.925718	-1.165610	-4.521116
C	6.397067	-0.765739	1.476539
H	6.831397	-1.443245	2.245016
H	6.070545	0.152093	2.005626
H	7.220337	-0.484453	0.788781
C	0.603427	-2.856269	1.871982
H	0.038656	-2.060972	1.345006
H	0.550577	-2.647867	2.958207
H	0.061254	-3.804154	1.685763
C	2.879297	-3.871916	2.275040
H	2.420461	-4.881258	2.339108
H	2.932888	-3.468032	3.307963
H	3.914167	-3.995512	1.900252
C	1.801867	-5.013527	-1.815870
H	1.578214	-6.056072	-2.091958
C	4.317019	0.701988	4.667142

H	5.218398	0.998887	5.225569
C	1.808846	-4.622519	-0.470959
H	1.582716	-5.364254	0.311494
C	6.828962	-0.018851	-1.924079
H	7.362311	0.106424	-2.892534
H	7.286227	-0.885758	-1.407628
H	7.049805	0.886582	-1.317633
C	-6.515370	1.377659	2.088155
H	-6.908709	1.840423	3.020222
H	-7.231357	0.586907	1.789088
H	-6.540784	2.166579	1.304446
C	3.552087	-2.181727	-4.666497
H	4.506867	-2.535060	-4.224582
H	3.784482	-1.356750	-5.372154
H	3.134915	-3.018443	-5.266453
C	1.834379	6.162112	1.653348
H	1.673859	7.242659	1.794353
C	2.240767	5.666419	0.401854
H	2.389559	6.353494	-0.445616

compound 3

Energy= -10062.7057400

Ga	0.341717	1.361036	-1.170508
Ni	0.000000	0.000000	0.665557
P	0.067219	1.764957	1.971301
Si	-1.905287	3.189079	-0.108830
Cl	2.115811	1.601906	-2.474160
N	-0.743025	2.888239	-1.402859
C	-0.358623	3.892174	-2.344245
C	0.000000	1.750870	4.876039
H	1.005795	2.194424	4.884968
C	-0.964491	3.269218	1.559255
H	-0.290799	4.147222	1.541548
H	-1.672364	3.424137	2.397541
C	-0.617288	1.416655	3.657725
C	-2.753404	4.873649	-0.399064
H	-1.937143	5.501567	-0.825531
C	1.751176	2.467129	2.221703
C	0.634476	4.862536	-2.019660
C	1.978899	3.625065	2.996975
H	1.134198	4.142993	3.477475
C	-1.883081	0.790861	3.674312
H	-2.345305	0.480360	2.727029
C	-3.870380	4.795191	-1.454767
H	-4.732304	4.194481	-1.093841
H	-3.515228	4.340495	-2.399926
H	-4.257196	5.808706	-1.699279
C	0.954820	5.851092	-2.971489
H	1.716193	6.608465	-2.723782
C	-3.243641	5.543202	0.897827
H	-3.694393	6.537116	0.682816
H	-2.421778	5.706335	1.625333
H	-4.022674	4.938035	1.408531
C	-0.611827	4.899918	-4.554890
H	-1.082539	4.913353	-5.549748
C	1.366112	4.849665	-0.681875
H	1.074732	3.912834	-0.164460
C	-1.935411	2.782906	-4.015803
H	-2.454952	2.492195	-3.081164
C	-0.658832	1.490079	6.090382
H	-0.161767	1.744825	7.039455
C	-0.966077	3.895133	-3.636399
C	-1.932261	0.897362	6.100546
H	-2.441234	0.697431	7.056305
C	-2.541076	0.538317	4.885313
H	-3.526099	0.046259	4.875247
C	-3.746171	1.165896	-1.167568
H	-4.315366	0.233461	-0.960659
H	-3.007452	0.912403	-1.949628
H	-4.458350	1.905841	-1.587715
C	-4.107219	1.924646	1.223684
H	-4.896854	2.629531	0.886605

H	-3.666057	2.341127	2.151536
H	-4.618989	0.976333	1.501236
C	3.281213	4.127316	3.150856
H	3.450509	5.029173	3.759745
C	-3.075893	1.694877	0.105177
H	-2.342359	0.910577	0.447377
C	2.840509	1.848150	1.574161
H	2.657639	0.971093	0.933714
C	0.334499	5.882110	-4.226360
H	0.597088	6.664539	-4.955809
C	2.895288	4.809878	-0.845557
H	3.199157	3.940744	-1.460848
H	3.383551	4.722316	0.146667
H	3.279934	5.732092	-1.330472
C	4.364929	3.488886	2.520547
H	5.383597	3.890514	2.636327
C	-3.002149	3.195402	-5.039768
H	-3.544706	4.110869	-4.724174
H	-3.745660	2.381368	-5.166247
H	-2.564211	3.392222	-6.041358
C	4.141042	2.354274	1.722789
H	4.977611	1.867224	1.198898
C	-1.166042	1.537333	-4.498361
H	-0.625113	1.751002	-5.444175
H	-1.847411	0.677582	-4.661012
H	-0.399411	1.222029	-3.762904
C	0.940643	6.029936	0.212001
H	1.237309	6.998809	-0.242829
H	1.424572	5.963463	1.209685
H	-0.158012	6.062894	0.359404
Ga	-0.341717	-1.361036	-1.170508
P	-0.067219	-1.764957	1.971301
Si	1.905287	-3.189079	-0.108830
Cl	-2.115811	-1.601906	-2.474160
N	0.743025	-2.888239	-1.402859
C	0.358623	-3.892174	-2.344245
C	0.000000	-1.750870	4.876039
H	-1.005795	-2.194424	4.884968
C	0.964491	-3.269218	1.559255
H	0.290799	-4.147222	1.541548
H	1.672364	-3.424137	2.397541
C	0.617288	-1.416655	3.657725
C	2.753404	-4.873649	-0.399064
H	1.937143	-5.501567	-0.825531
C	-1.751176	-2.467129	2.221703
C	-0.634476	-4.862536	-2.019660
C	-1.978899	-3.625065	2.996975
H	-1.134198	-4.142993	3.477475
C	1.883081	-0.790861	3.674312
H	2.345305	-0.480360	2.727029
C	3.870380	-4.795191	-1.454767
H	4.732304	-4.194481	-1.093841
H	3.515228	-4.340495	-2.399926
H	4.257196	-5.808706	-1.699279
C	-0.954820	-5.851092	-2.971489
H	-1.716193	-6.608465	-2.723782
C	3.243641	-5.543202	0.897827
H	3.694393	-6.537116	0.682816
H	2.421778	-5.706335	1.625333
H	4.022674	-4.938035	1.408531
C	0.611827	-4.899918	-4.554890
H	1.082539	-4.913353	-5.549748
C	-1.366112	-4.849665	-0.681875
H	-1.074732	-3.912834	-0.164460
C	1.935411	-2.782906	-4.015803
H	2.454952	-2.492195	-3.081164
C	0.658832	-1.490079	6.090382
H	0.161767	-1.744825	7.039455
C	0.966077	-3.895133	-3.636399
C	1.932261	-0.897362	6.100546
H	2.441234	-0.697431	7.056305
C	2.541076	-0.538317	4.885313
H	3.526099	-0.046259	4.875247
C	3.746171	-1.165896	-1.167568

H	4.315366	-0.233461	-0.960659
H	3.007452	-0.912403	-1.949628
H	4.458350	-1.905841	-1.587715
C	4.107219	-1.924646	1.223684
H	4.896854	-2.629531	0.886605
H	3.666057	-2.341127	2.151536
H	4.618989	-0.976333	1.501236
C	-3.281213	-4.127316	3.150856
H	-3.450509	-5.029173	3.759745
C	3.075893	-1.694877	0.105177
H	2.342359	-0.910577	0.447377
C	-2.840509	-1.848150	1.574161
H	-2.657639	-0.971093	0.933714
C	-0.334499	-5.882110	-4.226360
H	-0.597088	-6.664539	-4.955809
C	-2.895288	-4.809878	-0.845557
H	-3.199157	-3.940744	-1.460848
H	-3.383551	-4.722316	0.146667
H	-3.279934	-5.732092	-1.330472
C	-4.364929	-3.488886	2.520547
H	-5.383597	-3.890514	2.636327
C	3.002149	-3.195402	-5.039768
H	3.544706	-4.110869	-4.724174
H	3.745660	-2.381368	-5.166247
H	2.564211	-3.392222	-6.041358
C	-4.141042	-2.354274	1.722789
H	-4.977611	-1.867224	1.198898
C	1.166042	-1.537333	-4.498361
H	0.625113	-1.751002	-5.444175
H	1.847411	-0.677582	-4.661012
H	0.399411	-1.222029	-3.762904
C	-0.940643	-6.029936	0.212001
H	-1.237309	-6.998809	-0.242829
H	-1.424572	-5.963463	1.209685
H	0.158012	-6.062894	0.359404

compound 4

Energy= -8682.33738607

Pd	0.000000	0.000000	0.609374
Ga	-0.291233	1.419017	-1.300949
P	-0.051045	1.875075	2.009440
Si	1.930264	3.227581	-0.109224
Cl	-2.055705	1.667958	-2.616303
N	0.784664	2.962197	-1.428300
C	0.418773	3.981567	-2.359956
C	-1.733766	2.569170	2.254816
C	-0.575303	4.949318	-2.032666
C	1.035088	3.993523	-3.647767
C	0.997567	3.351488	1.568048
H	1.722338	3.503582	2.392832
H	0.341624	4.243043	1.548299
C	0.623028	1.481205	3.683563
C	-1.966938	3.741306	3.006971
H	-1.123900	4.274637	3.473853
C	0.000000	1.805278	4.902268
H	-0.994760	2.273922	4.908073
C	1.873371	0.823725	3.700576
H	2.339680	0.517219	2.753582
C	3.068617	1.707435	0.108221
H	2.335092	0.938986	0.482279
C	-1.311757	4.921596	-0.697939
H	-1.006988	3.987736	-0.183079
C	0.640379	1.508274	6.118184
H	0.139469	1.756599	7.066898
C	2.013443	2.888329	-4.027466
H	2.524595	2.591450	-3.089845
C	0.684530	5.004789	-4.560704
H	1.160233	5.026464	-5.553046
C	3.692670	1.143659	-1.174005
H	4.401295	1.863013	-1.634177
H	2.927464	0.883640	-1.928911
H	4.256363	0.208407	-0.964287

C	3.297462	5.567680	0.906030
H	4.050362	4.950143	1.440720
H	2.465084	5.761382	1.613631
H	3.777548	6.547242	0.688563
C	-3.272686	4.236246	3.154831
H	-3.447567	5.150404	3.743447
C	-0.890991	5.945087	-2.978312
H	-1.653999	6.700473	-2.729292
C	2.818586	4.894669	-0.393367
H	2.023012	5.534823	-0.840629
C	4.131122	1.936470	1.197797
H	4.640944	0.984823	1.467688
H	3.714107	2.359108	2.134542
H	4.919014	2.634018	0.841937
C	2.513500	0.537719	4.913838
H	3.487033	0.023308	4.905219
C	-0.264568	5.983883	-4.230099
H	-0.524053	6.770673	-4.955962
C	-2.820357	1.921928	1.630162
H	-2.627655	1.032546	1.008282
C	3.955543	4.787476	-1.425102
H	4.367899	5.791494	-1.667142
H	3.612699	4.333777	-2.374958
H	4.797453	4.171964	-1.042562
C	1.901064	0.889501	6.129404
H	2.396465	0.661886	7.086103
C	1.262927	1.640087	-4.532132
H	0.502080	1.295260	-3.802932
H	1.957821	0.794347	-4.710461
H	0.716231	1.861101	-5.472827
C	-4.353385	3.573487	2.544509
H	-5.374808	3.969583	2.655196
C	-4.124629	2.420305	1.774832
H	-4.960654	1.912891	1.269681
C	-2.839465	4.856150	-0.868307
H	-3.238197	5.774531	-1.349236
H	-3.330849	4.752809	0.121135
H	-3.124949	3.986351	-1.491688
C	3.088480	3.318899	-5.035723
H	2.660060	3.521016	-6.040301
H	3.840589	2.512612	-5.161003
H	3.618848	4.236313	-4.705675
C	-0.905808	6.105672	0.199615
H	0.192337	6.152934	0.348975
H	-1.391125	6.030172	1.195980
H	-1.214739	7.071740	-0.253015
Ga	0.291233	-1.419017	-1.300949
P	0.051045	-1.875075	2.009440
Si	-1.930264	-3.227581	-0.109224
Cl	2.055705	-1.667958	-2.616303
N	-0.784664	-2.962197	-1.428300
C	-0.418773	-3.981567	-2.359956
C	1.733766	-2.569170	2.254816
C	0.575303	-4.949318	-2.032666
C	-1.035088	-3.993523	-3.647767
C	-0.997567	-3.351488	1.568048
H	-1.722338	-3.503582	2.392832
H	-0.341624	-4.243043	1.548299
C	-0.623028	-1.481205	3.683563
C	1.966938	-3.741306	3.006971
H	1.123900	-4.274637	3.473853
C	0.000000	-1.805278	4.902268
H	0.994760	-2.273922	4.908073
C	-1.873371	-0.823725	3.700576
H	-2.339680	-0.517219	2.753582
C	-3.068617	-1.707435	0.108221
H	-2.335092	-0.938986	0.482279
C	1.311757	-4.921596	-0.697939
H	1.006988	-3.987736	-0.183079
C	-0.640379	-1.508274	6.118184
H	-0.139469	-1.756599	7.066898
C	-2.013443	-2.888329	-4.027466
H	-2.524595	-2.591450	-3.089845
C	-0.684530	-5.004789	-4.560704

H	-1.160233	-5.026464	-5.553046
C	-3.692670	-1.143659	-1.174005
H	-4.401295	-1.863013	-1.634177
H	-2.927464	-0.883640	-1.928911
H	-4.256363	-0.208407	-0.964287
C	-3.297462	-5.567680	0.906030
H	-4.050362	-4.950143	1.440720
H	-2.465084	-5.761382	1.613631
H	-3.777548	-6.547242	0.688563
C	3.272686	-4.236246	3.154831
H	3.447567	-5.150404	3.743447
C	0.890991	-5.945087	-2.978312
H	1.653999	-6.700473	-2.729292
C	-2.818586	-4.894669	-0.393367
H	-2.023012	-5.534823	-0.840629
C	-4.131122	-1.936470	1.197797
H	-4.640944	-0.984823	1.467688
H	-3.714107	-2.359108	2.134542
H	-4.919014	-2.634018	0.841937
C	-2.513500	-0.537719	4.913838
H	-3.487033	-0.023308	4.905219
C	0.264568	-5.983883	-4.230099
H	0.524053	-6.770673	-4.955962
C	2.820357	-1.921928	1.630162
H	2.627655	-1.032546	1.008282
C	-3.955543	-4.787476	-1.425102
H	-4.367899	-5.791494	-1.667142
H	-3.612699	-4.333777	-2.374958
H	-4.797453	-4.171964	-1.042562
C	-1.901064	-0.889501	6.129404
H	-2.396465	-0.661886	7.086103
C	-1.262927	-1.640087	-4.532132
H	-0.502080	-1.295260	-3.802932
H	-1.957821	-0.794347	-4.710461
H	-0.716231	-1.861101	-5.472827
C	4.353385	-3.573487	2.544509
H	5.374808	-3.969583	2.655196
C	4.124629	-2.420305	1.774832
H	4.960654	-1.912891	1.269681
C	2.839465	-4.856150	-0.868307
H	3.238197	-5.774531	-1.349236
H	3.330849	-4.752809	0.121135
H	3.124949	-3.986351	-1.491688
C	-3.088480	-3.318899	-5.035723
H	-2.660060	-3.521016	-6.040301
H	-3.840589	-2.512612	-5.161003
H	-3.618848	-4.236313	-4.705675
C	0.905808	-6.105672	0.199615
H	-0.192337	-6.152934	0.348975
H	1.391125	-6.030172	1.195980
H	1.214739	-7.071740	-0.253015

compound 7

Energy= -10962.7127948

Ga	2.163788	-0.484709	-0.315856
Ga	-2.165552	0.280768	0.596218
Ni	-0.147138	-0.105658	-0.398970
Ni	1.079819	-2.322755	-0.919795
P	-0.895334	-2.145967	-0.110182
P	0.426931	1.954913	-0.463902
Si	-3.386454	-1.247194	-1.727124
Si	3.246130	1.971901	1.331606
N	3.587919	0.421708	0.558922
N	-3.743783	-0.177218	-0.375849
C	1.367186	2.373572	-1.993292
C	-2.524216	1.235730	2.292925
C	4.885101	-0.136919	0.309272
C	-5.931442	0.952506	-0.266660
C	-1.169482	3.973417	-1.723117
H	-0.736864	3.623402	-2.671063
C	1.197534	1.537000	-3.115324
H	0.627164	0.600621	-2.999058

C	-2.142513	-0.370634	-2.893143	H	1.239601	-4.030077	1.064939
H	-1.224348	-0.358038	-2.227205	C	-5.554958	1.775666	-1.487625
C	-0.813420	3.346089	-0.509442	H	-4.879189	1.140954	-2.094519
C	-2.406745	-2.732649	-1.004460	C	-1.802384	-1.190325	-4.146247
H	-3.075865	-3.265458	-0.299841	H	-2.594913	-1.082916	-4.916554
H	-2.103979	-3.455759	-1.789293	H	-1.697750	-2.274693	-3.937870
C	4.867709	0.884909	-2.073239	H	-0.849306	-0.852202	-4.609897
H	3.988905	1.404319	-1.640805	C	-5.004740	-1.891918	-2.529757
C	5.506472	0.052683	-0.966596	H	-5.770237	-1.710966	-1.738488
C	-5.353238	-0.747323	1.424211	C	6.734217	-0.581824	-1.241437
C	-5.009905	-0.012091	0.247434	H	7.199894	-0.438570	-2.229533
C	-1.006106	-2.759980	1.610494	C	1.912042	-2.832822	-2.800063
C	0.688439	-3.486698	-2.567515	H	1.877771	-1.951346	-3.462769
H	-0.194149	-3.083950	-3.089990	C	-7.467001	0.482842	1.580326
C	5.544111	-0.954418	1.283245	H	-8.415234	0.681964	2.104071
C	2.133255	3.550671	-2.112333	C	4.992110	-1.145359	2.689564
H	2.256169	4.218844	-1.247396	H	3.998774	-0.660776	2.703752
C	-2.451647	1.091128	-3.230221	C	-7.143992	1.183211	0.408750
H	-1.614062	1.554119	-3.797148	H	-7.846671	1.933897	0.015209
H	-2.607877	1.693817	-2.315597	C	4.075403	4.753534	0.895999
H	-3.361984	1.184422	-3.858877	H	4.073592	5.033591	1.969148
C	3.280261	1.850828	3.246266	H	3.063131	4.985169	0.502758
H	4.287432	1.458328	3.495405	H	4.787789	5.437015	0.383423
C	-6.574653	-0.477612	2.071807	C	-2.053848	5.063448	-1.726454
H	-6.829628	-1.037669	2.985707	H	-2.313154	5.548114	-2.680914
C	-0.306173	-2.048043	2.611367	C	2.719644	3.888136	-3.341961
H	0.190184	-1.103050	2.332232	H	3.325819	4.803599	-3.425873
C	-4.455620	-1.847373	1.972592	C	-4.170517	-1.722484	3.477680
H	-3.478877	-1.768968	1.451403	H	-3.771017	-0.719552	3.724284
C	-1.375527	3.822375	0.696113	H	-3.420152	-2.477850	3.787900
H	-1.119912	3.353719	1.655773	H	-5.085451	-1.887578	4.085535
C	1.441330	2.507791	0.976306	C	2.825284	-3.160422	-0.099521
H	0.839864	2.180504	1.850357	H	3.197847	-2.667867	0.814860
H	1.429263	3.617930	1.005302	C	3.274047	-3.497426	-2.611580
C	4.480005	3.284262	0.683361	H	3.986500	-3.086606	-3.356044
H	4.495795	3.097156	-0.413748	H	3.181812	-4.577274	-2.854720
C	1.702149	-4.010738	0.063674	C	6.767786	-1.569974	0.957349

H	7.262063	-2.204192	1.710744
C	-1.517376	1.253957	3.283545
H	-0.605425	0.655785	3.136784
C	3.116528	3.206613	3.956954
H	2.171971	3.715599	3.665544
H	3.951868	3.900513	3.735139
H	3.083866	3.076228	5.061472
C	1.754173	1.894605	-4.353968
H	1.600104	1.245503	-5.229888
C	0.530109	-4.901761	-2.036348
H	0.689654	-5.650188	-2.850716
H	-0.529435	-5.020217	-1.723385
C	2.517400	3.069133	-4.468383
H	2.964596	3.344450	-5.436343
C	-1.592826	-3.998922	1.946443
H	-2.109769	-4.588510	1.173148
C	-3.689622	2.005014	2.517085
H	-4.501859	2.010540	1.775352
C	-0.227314	-2.535855	3.921515
H	0.309150	-1.954597	4.688039
C	-0.833943	-3.762360	4.254112
H	-0.776267	-4.149627	5.283042
C	-2.269062	4.905283	0.686554
H	-2.702083	5.251492	1.637493
C	-6.747729	2.173989	-2.367876
H	-7.373352	1.296440	-2.631132
H	-6.391759	2.638949	-3.311104
H	-7.403761	2.918467	-1.868697
C	1.441457	-5.224007	-0.824438
H	0.967454	-6.023287	-0.217983
H	2.408876	-5.644284	-1.172264
C	-5.437189	-1.118333	-3.789362
H	-4.736098	-1.292060	-4.632659
H	-5.488568	-0.025206	-3.620387
H	-6.443476	-1.446789	-4.130958
C	4.351803	-0.029193	-3.199908
H	5.154044	-0.701095	-3.570774
H	3.972443	0.565923	-4.052769
H	3.518917	-0.665427	-2.835572
C	3.872703	-3.320870	-1.191672
H	4.548298	-4.175151	-0.947589
H	4.520221	-2.421180	-1.177322
C	-2.604102	5.535608	-0.522573
H	-3.300024	6.388823	-0.528989
C	5.901566	-0.441413	3.718890
H	6.877381	-0.964925	3.805746
H	5.433987	-0.432115	4.726263
H	6.120233	0.605450	3.426066
C	7.367155	-1.396004	-0.295802
H	8.321990	-1.890569	-0.532878
C	2.230578	0.844560	3.754124
H	2.439549	0.525452	4.798080
H	2.173293	-0.072231	3.129219
H	1.219767	1.301468	3.755098
C	5.823209	1.961685	-2.618030
H	6.222367	2.598785	-1.802567
H	5.291348	2.614988	-3.339273
H	6.690944	1.514897	-3.147461
C	-4.731005	3.004571	-1.072612
H	-5.319744	3.675994	-0.412488
H	-4.409706	3.589084	-1.957819
H	-3.817591	2.708988	-0.519470
C	-5.047011	-3.226449	1.621558
H	-6.034314	-3.367450	2.110509
H	-4.378339	-4.044213	1.960478
H	-5.206216	-3.331037	0.527941
C	5.896665	3.013870	1.229907
H	6.642031	3.698538	0.767824
H	6.231848	1.975955	1.031189
H	5.944021	3.178408	2.328239
C	-1.508236	-4.492823	3.259640
H	-1.974908	-5.459421	3.507713
C	4.795069	-2.620792	3.084685
H	5.759453	-3.170886	3.110568

H	4.126562	-3.154068	2.380678
H	4.345883	-2.692226	4.097471
C	-3.829406	2.776459	3.683927
H	-4.744329	3.371211	3.837471
C	-4.962243	-3.405871	-2.812056
H	-5.930801	-3.758773	-3.230323
H	-4.760764	-4.001644	-1.898626
H	-4.175519	-3.662480	-3.554632
C	-1.651523	2.017455	4.455943
H	-0.852001	2.011155	5.214795
C	-2.810806	2.788551	4.654421
H	-2.923396	3.393870	5.568163

Table S5. Coordinates and energies (in hartrees) of the calculated structures at the BP86-D3(BJ)/def2-TZVPP level

Compound 2

Energy= -8558.18738700

Ga	1.152625	0.331041	-0.364792
Ga	-1.178630	0.252505	0.405851
Cl	0.846904	1.811217	-2.096154
Cl	-1.236307	1.874722	2.044576
P	2.447650	1.662956	1.211112
P	-2.568281	1.603931	-1.077620
Si	-4.301818	-0.331936	0.560640
Si	4.333551	0.105704	-0.695532
N	-2.663711	-0.922630	0.766799
N	2.758437	-0.660439	-0.789028
C	2.655749	-2.047167	-1.131520
C	2.543470	-2.634491	1.361216
H	2.917071	-1.604062	1.418368
C	-2.397433	-2.285256	1.121690
C	-2.910363	0.879210	-2.707643
C	2.663552	-2.461024	-2.490450
C	2.429206	3.970728	2.819615
H	2.994886	3.388076	3.547582
C	2.549572	-3.024864	-0.104995
C	2.777285	-1.458813	-3.625517
H	3.004422	-0.490309	-3.168971
C	-2.376849	-2.682577	2.486741
C	-2.128767	-3.252177	0.115849
C	2.006255	3.376093	1.621122
C	2.709374	0.815708	2.796250
C	2.561928	-3.824915	-2.792114
H	2.566638	-4.139744	-3.837574
C	1.832835	0.107543	4.942804
H	1.013593	0.083741	5.661435
C	4.047367	1.691915	0.347068
H	4.871737	1.927470	1.034504
H	3.965855	2.533894	-0.357517
C	1.661696	0.779293	3.732453
H	0.714848	1.271818	3.504805
C	5.099486	0.736662	-2.330199
H	5.168541	-0.143640	-2.989273
C	-2.007506	-0.042545	-3.250966
H	-1.090363	-0.273521	-2.711991
C	2.436171	-4.375617	-0.455811
H	2.342327	-5.123396	0.333216
C	1.259807	4.117637	0.692120
H	0.910631	3.647562	-0.229039
C	-2.593655	-1.676160	3.600737
H	-3.001612	-0.775650	3.133781
C	5.557228	-1.105546	0.137338
H	4.947902	-1.601217	0.909867
C	-2.106995	-4.017652	2.811054
H	-2.089907	-4.316030	3.860926
C	3.462443	-3.515480	2.219045
H	3.086450	-4.546558	2.291449
H	3.517998	-3.112311	3.240147
H	4.481259	-3.559328	1.807647
C	3.036947	-0.543506	5.228439
H	3.161475	-1.074594	6.172968
C	1.448100	-1.283106	-4.374126
H	1.097405	-2.239080	-4.792818
H	1.561781	-0.564339	-5.199001
H	0.677030	-0.892374	-3.700411
C	-2.092303	-2.889058	-1.356697
H	-2.491010	-1.870178	-1.448063
C	-1.840131	3.839805	-2.606590
H	-1.674406	3.133415	-3.419300
C	-4.075926	1.209188	-3.417871
H	-4.772225	1.945356	-3.013459
C	-4.112242	1.437327	-0.138962

H	-4.986378	1.749988	-0.725540
H	-4.022061	2.115488	0.721399
C	-2.274145	-0.648003	-4.480292
H	-1.563294	-1.363778	-4.893744
C	-2.289927	3.377178	-1.360046
C	0.961258	5.454499	0.957078
H	0.381267	6.023777	0.231417
C	2.445979	-4.783444	-1.788165
H	2.361639	-5.841280	-2.041837
C	-1.261197	-1.262343	4.239446
H	-0.752637	-2.124103	4.698155
H	-1.429428	-0.501577	5.016836
H	-0.587259	-0.830872	3.490499
C	4.257711	1.802598	-3.045945
H	4.239196	2.745370	-2.476350
H	3.212161	1.505084	-3.190259
H	4.690869	2.035736	-4.032210
C	-5.246635	-1.442024	-0.667058
H	-4.494470	-1.678675	-1.437304
C	3.917174	0.166447	3.089534
H	4.736063	0.181629	2.375415
C	3.907561	-1.816569	-4.602492
H	3.671711	-2.724162	-5.178224
H	4.853924	-1.999605	-4.074086
H	4.065389	-0.999743	-5.322149
C	6.770704	-0.475898	0.844286
H	7.293286	-1.232395	1.452061
H	6.505407	0.354475	1.515505
H	7.500281	-0.079622	0.126100
C	1.382883	6.048211	2.150175
H	1.138050	7.091063	2.357582
C	-4.755556	1.032663	3.052748
H	-5.078718	2.005086	2.648548
H	-3.659093	1.063472	3.114122
H	-5.154649	0.965195	4.077248
C	-5.678803	-2.766735	-0.009883
H	-6.435005	-2.599382	0.771420
H	-4.835117	-3.294612	0.454923
H	-6.129336	-3.443819	-0.754438
C	-2.470375	4.286445	-0.305109
H	-2.772685	3.930963	0.679514
C	2.112518	5.304277	3.083120
H	2.436680	5.762989	4.018359
C	-5.294356	-0.115687	2.179758
H	-5.165687	-1.062148	2.730646
C	-1.598416	5.200241	-2.800995
H	-1.249294	5.551864	-3.772638
C	1.121152	-2.630766	1.933890
H	0.471924	-1.934417	1.384953
H	1.131515	-2.321892	2.987546
H	0.654388	-3.623077	1.864604
C	-3.444580	-0.331999	-5.173870
H	-3.657191	-0.809022	-6.131508
C	6.024774	-2.199753	-0.842331
H	6.626680	-1.773872	-1.659614
H	5.182375	-2.741704	-1.291139
H	6.657574	-2.938354	-0.323542
C	4.078558	-0.513426	4.298190
H	5.021848	-1.018521	4.509005
C	-6.424683	-0.773414	-1.393851
H	-6.862332	-1.468418	-2.129430
H	-6.109755	0.122778	-1.945549
H	-7.228845	-0.479622	-0.705723
C	-0.648493	-2.876595	-1.865736
H	-0.047064	-2.120497	-1.342602
H	-0.609843	-2.661048	-2.941320
H	-0.155300	-3.843042	-1.698727
C	-2.953346	-3.813538	-2.230450
H	-2.535065	-4.830043	-2.274475
H	-2.991244	-3.426163	-3.259536
H	-3.981396	-3.889842	-1.853756
C	-1.844750	-4.965846	1.824540
H	-1.630452	-6.000815	2.095489
C	-4.342640	0.602250	-4.644887

H	-5.252865	0.856314	-5.189406
C	-1.850059	-4.573330	0.488530
H	-1.631658	-5.307920	-0.288711
C	-6.803136	0.087958	1.953728
H	-7.315853	0.251359	2.915957
H	-7.279813	-0.773624	1.469373
H	-7.001258	0.974207	1.330376
C	6.530779	1.266397	-2.121616
H	6.915235	1.702193	-3.058239
H	7.230520	0.478329	-1.816215
H	6.567652	2.061515	-1.359832
C	-3.583190	-2.162983	4.668065
H	-4.526863	-2.504782	4.219438
H	-3.812116	-1.350464	5.373189
H	-3.173026	-2.999952	5.252931
C	-1.803120	6.107608	-1.756943
H	-1.621501	7.171818	-1.914276
C	-2.235881	5.646878	-0.509671
H	-2.385674	6.346988	0.313213

compound 3

Energy= -10066.9003109

Ga	0.442440	1.335352	-1.169913
Ni	0.000000	0.000000	0.688351
P	0.212105	1.763693	1.969165
Si	-1.591181	3.374497	-0.115803
Cl	2.217961	1.364983	-2.478097
N	-0.484140	2.962696	-1.402489
C	0.000000	3.924408	-2.342383
C	0.195883	1.742386	4.853264
H	1.241336	2.046728	4.838622
C	-0.663568	3.348405	1.551148
H	0.083821	4.152008	1.556671
H	-1.361461	3.558296	2.372808
C	-0.483203	1.497987	3.655034
C	-2.256672	5.130783	-0.396928
H	-1.395321	5.675809	-0.822137
C	1.948904	2.292523	2.212310
C	1.071626	4.791235	-2.012179
C	2.290142	3.420603	2.976775
H	1.507516	4.018610	3.445743
C	-1.814665	1.051019	3.702898
H	-2.338381	0.814982	2.776985
C	-3.381756	5.173933	-1.443505
H	-4.286958	4.663249	-1.082169
H	-3.082331	4.699308	-2.386622
H	-3.661524	6.215283	-1.670226
C	1.487526	5.741978	-2.954059
H	2.307299	6.417553	-2.701453
C	-2.677723	5.842551	0.899098
H	-3.012846	6.870199	0.684424
H	-1.853480	5.909383	1.623682
H	-3.512916	5.325649	1.395263
C	-0.143474	4.951141	-4.538537
H	-0.602878	5.012242	-5.525744
C	1.792251	4.712451	-0.676253
H	1.414240	3.822584	-0.153634
C	-1.666190	2.986106	-4.022388
H	-2.202411	2.722285	-3.101109
C	-0.459565	1.574624	6.076796
H	0.083848	1.758671	7.004563
C	-0.594960	3.988207	-3.629764
C	-1.793072	1.161869	6.117153
H	-2.298446	1.034069	7.075204
C	-2.468187	0.889888	4.923054
H	-3.501683	0.541187	4.938657
C	-3.630535	1.570542	-1.176846
H	-4.309066	0.728745	-0.964119
H	-2.926069	1.221311	-1.939197
H	-4.234502	2.381469	-1.608617
C	-3.933703	2.382798	1.192768
H	-4.614888	3.173425	0.844109
H	-3.467189	2.734761	2.123195

H	-4.557147	1.509859	1.447828
C	3.628206	3.785208	3.135131
H	3.883496	4.661581	3.732412
C	-2.915506	2.028132	0.096979
H	-2.299992	1.169806	0.456971
C	2.967935	1.563012	1.583315
H	2.700157	0.713508	0.951760
C	0.884331	5.833732	-4.205270
H	1.220432	6.582195	-4.924531
C	3.307498	4.523343	-0.841313
H	3.523617	3.632423	-1.444130
H	3.780861	4.400971	0.143149
H	3.769564	5.392617	-1.332240
C	4.638743	3.036548	2.521266
H	5.682661	3.329266	2.640104
C	-2.692549	3.523790	-5.026252
H	-3.137332	4.470578	-4.687324
H	-3.502696	2.792627	-5.160025
H	-2.245678	3.697590	-6.016561
C	4.305880	1.930239	1.735933
H	5.084093	1.361034	1.226852
C	-1.022172	1.693121	-4.553841
H	-0.484267	1.889825	-5.493323
H	-1.780548	0.918687	-4.735242
H	-0.286361	1.285109	-3.847883
C	1.494823	5.938297	0.203067
H	1.878555	6.855436	-0.268325
H	1.979197	5.836456	1.186196
H	0.416188	6.078971	0.359804
Ga	-0.442440	-1.335352	-1.169913
P	-0.212105	-1.763693	1.969165
Si	1.591181	-3.374497	-0.115803
Cl	-2.217961	-1.364983	-2.478097
N	0.484140	-2.962696	-1.402489
C	0.000000	-3.924408	-2.342383
C	-0.195883	-1.742386	4.853264
H	-1.241336	-2.046728	4.838622
C	0.663568	-3.348405	1.551148
H	-0.083821	-4.152008	1.556671
H	1.361461	-3.558296	2.372808
C	0.483203	-1.497987	3.655034
C	2.256672	-5.130783	-0.396928
H	1.395321	-5.675809	-0.822137
C	-1.948904	-2.292523	2.212310
C	-1.071626	-4.791235	-2.012179
C	-2.290142	-3.420603	2.976775
H	-1.507516	-4.018610	3.445743
C	1.814665	-1.051019	3.702898
H	2.338381	-0.814982	2.776985
C	3.381756	-5.173933	-1.443505
H	4.286958	-4.663249	-1.082169
H	3.082331	-4.699308	-2.386622
H	3.661524	-6.215283	-1.670226
C	-1.487526	-5.741978	-2.954059
H	-2.307299	-6.417553	-2.701453
C	2.677723	-5.842551	0.899098
H	3.012846	-6.870199	0.684424
H	1.853480	-5.909383	1.623682
H	3.512916	-5.325649	1.395263
C	0.143474	-4.951141	-4.538537
H	0.602878	-5.012242	-5.525744
C	-1.792251	-4.712451	-0.676253
H	-1.414240	-3.822584	-0.153634
C	1.666190	-2.986106	-4.022388
H	2.202411	-2.722285	-3.101109
C	0.459565	-1.574624	6.076796
H	-0.083848	-1.758671	7.004563
C	0.594960	-3.988207	-3.629764
C	1.793072	-1.161869	6.117153
H	2.298446	-1.034069	7.075204
C	2.468187	-0.889888	4.923054
H	3.501683	-0.541187	4.938657
C	3.630535	-1.570542	-1.176846
H	4.309066	-0.728745	-0.964119

H	2.926069	-1.221311	-1.939197
H	4.234502	-2.381469	-1.608617
C	3.933703	-2.382798	1.192768
H	4.614888	-3.173425	0.844109
H	3.467189	-2.734761	2.123195
H	4.557147	-1.509859	1.447828
C	-3.628206	-3.785208	3.135131
H	-3.883496	-4.661581	3.732412
C	2.915506	-2.028132	0.096979
H	2.299992	-1.169806	0.456971
C	-2.967935	-1.563012	1.583315
H	-2.700157	-0.713508	0.951760
C	-0.884331	-5.833732	-4.205270
H	-1.220432	-6.582195	-4.924531
C	-3.307498	-4.523343	-0.841313
H	-3.523617	-3.632423	-1.444130
H	-3.780861	-4.400971	0.143149
H	-3.769564	-5.392617	-1.332240
C	-4.638743	-3.036548	2.521266
H	-5.682661	-3.329266	2.640104
C	2.692549	-3.523790	-5.026252
H	3.137332	-4.470578	-4.687324
H	3.502696	-2.792627	-5.160025
H	2.245678	-3.697590	-6.016561
C	-4.305880	-1.930239	1.735933
H	-5.084093	-1.361034	1.226852
C	1.022172	-1.693121	-4.553841
H	0.484267	-1.889825	-5.493323
H	1.780548	-0.918687	-4.735242
H	0.286361	-1.285109	-3.847883
C	-1.494823	-5.938297	0.203067
H	-1.878555	-6.855436	-0.268325
H	-1.979197	-5.836456	1.186196
H	-0.416188	-6.078971	0.359804

compound 4

Energy= -8686.3513358

Pd	0.000000	0.000000	0.617443
Ga	-0.283925	1.434153	-1.286291
P	-0.031486	1.869019	2.001581
Si	1.942933	3.213112	-0.119915
Cl	-2.019484	1.673937	-2.622240
N	0.812884	2.962463	-1.428223
C	0.453475	3.989351	-2.354204
C	-1.698164	2.574402	2.247202
C	-0.522934	4.959910	-2.019332
C	1.064603	4.005780	-3.635430
C	1.023898	3.322998	1.554758
H	1.754931	3.454609	2.364320
H	0.385416	4.215844	1.556652
C	0.634052	1.491209	3.670975
C	-1.917789	3.744295	2.993151
H	-1.075150	4.266820	3.448473
C	0.000000	1.804596	4.878046
H	-0.994266	2.249493	4.875126
C	1.892367	0.865670	3.701370
H	2.370880	0.572466	2.767300
C	3.077437	1.701908	0.090738
H	2.362339	0.934117	0.470062
C	-1.256176	4.937249	-0.688215
H	-0.967067	4.009812	-0.174070
C	0.633601	1.529078	6.093689
H	0.125232	1.768552	7.028625
C	2.036224	2.906059	-4.029243
H	2.538437	2.585845	-3.106306
C	0.722232	5.020772	-4.535348
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compound 7

Energy= -10967.1420189

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