Reversible CO_2 Activation by a *N*-Phosphinoamidinato Digermyne

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Supporting Information

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S1. Experimental Procedure

General procedure. All operations were carried out under an inert atmosphere of argon gas by standard Schlenk techniques. Chemicals were purchased from Sigma-Aldrich and used directly without further purification. *N*-phosphinoamidine was prepared according to literature.[1] All solvents were dried over K metal or CaH_2 prior to use. The ^{1}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ and $^{31}P\{^{1}H\}$ NMR spectra were recorded on a JEOL ECA 400 or Bruker Avance III 400 (BBFO 400) spectrometer. The NMR spectra were recorded in deuterated solvents and the chemical shifts are relative to $SiMe_4$ for ^{1}H and ^{13}C; $BF_3{\cdot}Et_2O$ for ^{19}F, 85% H_3PO_4 for ^{31}P, respectively. The solid-state ^{31}P NMR experiment was completed on a 14.1 T Bruker Advance III HD 600 MHz spectrometer. The spectrum was processed using the Topspin software package and referenced to the unified scale using IUPAC recommended frequency ratios relative to the ^{13}C adamantane$_{(s)}$ methylene resonance (δ = 37.77 ppm).[2,3] The ^{31}P NMR decoupled one-pulse experiment was acquired using a 4 mm Bruker HXY probe at an MAS frequency of 14 kHz, utilising a $\pi/2$ pulse of 3.8 μs (determined on $(NH_4)H_2PO_{4(s)}$), high power proton decoupling and a recycle delay of 30 s (determined via a saturation recovery measurement). IR spectra were recorded on Bruker Apex FTIR spectrometer in solution IR cells fitted with KBr windows and a 0.1mm pathlength, at 2cm^{-1} resolution. HRMS spectra were obtained at the Mass Spectrometry Laboratory in the Division of Chemistry and Biological Chemistry, Nanyang Technological University. Melting points were measured with an OptiMelt Automated Melting Point System.

Synthesis of 2 and 3: A hexane solution of *n*BuLi (2.6 M, 0.4 mL, 1.05 mmol) was slowly added into a 100 mL Schlenk flask containing a stirring diethyl ether solution (40 mL) of *N*-phosphinoamidine (Ph: 0.34 g, 1 mmol, Dipp: 0.47 g, 1 mmol) at -78 ^{o}C. The solution was warmed to room temperature and stirred for 3 h. The resulting yellow solution was dried under vacuum to remove all volatiles to get the lithiated derivative. 40 mL of toluene was then added to the reaction flask containing the lithiated derivative and $GeCl_2$.dioxane (0.232 g, 1 mmol) at -78 °C. The reaction mixture was allowed to warm to room temperature and stirred for 6 hours. The reaction mixture was filtered to remove LiCl and the filtrate was concentrated to obtain colorless crystals of **2** and **3**, respectively. Yield: **2**: 0.398 g (75%); **3**: 0.326 g (73%).

2: **M.p.**: 181 ^{o}C. **^{1}H NMR (C_6D_6, 400 MHz, 25 °C):** δ 7.72-7.69 (m, 2 H, Ar-*H*), 7.11-7.04 (m, 3 H, Ar-*H*), 6.89-6.87 (m, 3 H, Ar-*H*), 3.49 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 3.38 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 1.52-1.46 (overlapping signals, 12 H, C(C*H*$_3$)$_3$ and CH(C*H*$_3$)$_2$), 1.40 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.26 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.15 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 16 Hz)), 0.50 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz). **^{13}C{^{1}H}**

(C_6D_6, 101 MHz, 25 °C): δ 174.3 (N*C*N), 146.4 (*C*-Ar), 144.3 (*C*-Ar), 139.1 (*C*-Ar), 136.8 (*C*-Ar), 130.6 (*C*-Ar), 129.8 (*C*-Ar), 127.5 (*C*-Ar), 127.4 (*C*-Ar), 125.6 (*C*-Ar), 124.3 (*C*-Ar), 40.5 (d, *C*(CH_3)$_3$, J_{PC} = 11 Hz), 36.2 (d, *C*(CH_3)$_3$, J_{PC} = 26 Hz), 29.5 (*C*H(CH_3)$_2$), 28.4 (*C*H(CH_3)$_2$), 28.1 (C(*C*H_3)$_3$), 27.6 (C(*C*H_3)$_3$), 26.4 (CH(*C*H_3)$_2$), 26.1 (CH(*C*H_3)$_2$), 24.5 (CH(*C*H_3)$_2$), 24.0 (CH(*C*H_3)$_2$). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**: δ 77.3. HRMS (ESI): *m/z* calcd for $C_{27}H_{41}{}^{74}GeN_2PCl$: 533.1908 [(*M* + *H*)]$^+$; found: 533.1907.

3: **M.p.**: 113 °C. **^{1}H NMR (C_6D_6, 400 MHz, 25 °C)**: δ 7.51-7.49 (m, 2 H, Ar-*H*), 7.18-7.12 (m, 2 H, Ar-*H*), 6.93-6.86 (m, 5 H, Ar-*H*), 6.78-6.74 (m, 1 H, Ar-*H*), 1.42 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 16 Hz), 1.12 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 16 Hz). **^{13}C{^{1}H} (C_6D_6, 101 MHz, 25 °C)**: δ 176.1 (N*C*N), 145.5 (*C*-Ar), 137.1 (*C*-Ar), 129.9 (*C*-Ar), 129.3 (*C*-Ar), 129.0 (*C*-Ar), 127.7 (*C*-Ar), 127.5 (*C*-Ar), 124.9 (*C*-Ar), 39.3 (d, *C*(CH_3)$_3$, J_{PC} = 13 Hz), 37.4 (d, *C*(CH_3)$_3$, J_{PC} = 13 Hz), 28.3 (C(*C*H_3)$_3$), 27.3 (C(*C*H_3)$_3$). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**: δ 80.5. HRMS (ESI): *m/z* calcd for $C_{21}H_{28}{}^{74}GeN_2PClNa$: 471.0788 [(*M* + *Na*)]$^+$; found: 471.0787.

Synthesis of 4 and 5: 60 mL of toluene was added to a 100 mL Schlenk flask containing the chlorogermylene (**2:** 0.532 g, 1 mmol; **3:** 0.448 g, 1 mmol) and excess potassium graphite (0.311 g, 2.3 mmol). Upon addition of toluene, a red suspension was observed, and the reaction mixture was stirred for 6 hours at room temperature. The reaction mixture was then filtered to give a red solution. All volatiles were removed under vacuum and gave compounds **4** and **5** as a red solid. Dark red crystals of **4** were obtained from a saturated hexane solution. Dark orange crystals of **5** were obtained from a saturated toluene solution. Yield: **4**: 0.238g (48%); **5**: 0.247 g (60%).

4: **M.p.**: 193 °C. **^{1}H NMR (C_6D_6, 400 MHz, 25 °C)**: δ 7.61 (d, 4 H, Ar*H*, J_{HH} = 8 Hz), 7.06-7.00 (m, 4 H, Ar*H*), 6.93-6.86 (m, 8 H, Ar*H*), 4.19 (sep, 2 H, C*H*Me$_2$, J_{HH} = 8 Hz), 3.34 (sep, 2 H, C*H*Me$_2$, J_{HH} = 8 Hz), 1.52 (d, 6 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.38 (d, 6 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.32-1.20 (overlapping signals, 42 H, CH(C*H*$_3$)$_2$ and C(C*H*$_3$)$_3$), 0.49 (d, 6 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz). **^{13}C{^{1}H} (C_6D_6, 101 MHz, 25 °C)**: δ 169.2 (N*C*N), 144.6 (*C*-Ar), 144.5 (*C*-Ar), 143.8 (*C*-Ar), 137.8 (*C*-Ar), 131.0 (*C*-Ar), 128.5 (*C*-Ar), 127.2 (*C*-Ar), 126.6 (*C*-Ar), 125.5 (*C*-Ar), 124.6 (*C*-Ar), 40.2 (*C*(CH_3)$_3$), 37.1 (*C*(CH_3)$_3$), 29.9 C(*C*H_3)$_3$, 29.1-28.6 (overlapping signals, CH(*C*H_3)$_2$, C(*C*H_3)$_3$), 26.8 (CH(*C*H_3)$_2$), 25.1 (CH(*C*H_3)$_2$), 23.4 (CH(*C*H_3)$_2$). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**: δ 100.9. HRMS (ESI): *m/z* calcd for $C_{54}H_{81}{}^{73}Ge_2N_4P_2$: 993.4406 [(*M* + *H*)]$^+$; found: 993.4391.

5: **M.p.**: 144 °C. **^{1}H NMR (C_6D_6, 400 MHz, 25 °C)**: δ 7.81-7.78 (m, 2 H, Ar-*H*), 7.51 (d, 2 H, Ar-*H*, J_{HH} = 4 Hz), 7.28 (d, 2 H, Ar-*H*, J_{HH} = 8 Hz), 7.12 (d, 2 H, Ar-*H*, J_{HH} = 8 Hz), 6.96-6.86 (m, 10 H, Ar-*H*), 6.70 (q, 2 H, Ar-*H*, J_{HH} = 8 Hz), 1.46 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 12 Hz), 1.43 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 12 Hz), 1.34 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 8 Hz),

1.30 (d, 9 H, C(C*H*$_3$)$_3$, J_{PH} = 8 Hz). **^{13}C{^{1}H} (C$_6$D$_6$, 101 MHz, 25 °C)**: δ 171.7 (NC*N*), 171.0 (NC*N*), 147.8 (*C*-Ar), 147.5 (*C*-Ar), 138.3 (*C*-Ar), 137.5 (*C*-Ar), 130.7 (*C*-Ar), 129.9 (*C*-Ar), 128.9 (*C*-Ar), 128.8 (*C*-Ar), 128.7 (*C*-Ar), 128.6 (*C*-Ar), 127.6 (*C*-Ar), 127.5 (*C*-Ar), 127.4 (*C*-Ar), 124.5 (*C*-Ar), 124.0 (*C*-Ar), 40.0 (*C*(CH$_3$)$_3$), 39.8 (*C*(CH$_3$)$_3$), 37.6 (*C*(CH$_3$)$_3$), 37.4 (*C*(CH$_3$)$_3$), 29.5 (C(*C*H$_3$)$_3$), 29.1 (C(*C*H$_3$)$_3$), 27.7 (C(*C*H$_3$)$_3$), 27.6 (C(*C*H$_3$)$_3$). **^{31}P{^{1}H} (C$_6$D$_6$, 162 MHz, 25 °C)**: δ 99.3, 99.1. HRMS (ESI): *m/z* calcd for $C_{42}H_{57}{}^{73}Ge_2N_4P_2$: 825.2528 [(*M* + *H*)]$^+$; found: 825.2509.

Synthesis of 6: 40 mL of toluene was added to a 100 mL Schlenk flask containing **4** (0.496 g, 0.5 mmol). The reaction mixture was degassed using a freeze−pump−thaw method. CO_2 (1 bar) was introduced. The dark red reaction mixture was stirred at room temperature for 4 hours to give an orange solution. The solution was filtered and concentrated to afford **6** as orange crystals. Yield: 0.316 g (61%).

M.p.: 138 ºC. **^{1}H NMR (C$_6$D$_6$, 400 MHz, 25 °C):** δ 7.80-7.75 (m, 4 H, Ar*H*), 7.09-7.05 (m, 3 H, Ar*H*), 6.96-6.86 (m, 9 H, Ar*H*), 3.87 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 3.74 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 3.53 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 3.27 (sep, 1 H, C*H*Me$_2$, J_{HH} = 8 Hz), 1.67 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.62 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.59 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.45 (d, *J* = 4 Hz, 3H, CH(C*H*$_3$)$_2$), 1.36 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.33 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 1.31-1.25 (overlapping signals, 36 H, C(C*H*$_3$)$_3$), 0.53 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz), 0.49 (d, 3 H, CH(C*H*$_3$)$_2$, J_{HH} = 8 Hz). **^{13}C{^{1}H} (C$_6$D$_6$, 101 MHz, 25 °C):** δ 206.6 (O*C*O), 173.5 (NC*N*), 171.7 (NC*N*), 146.7 (*C*-Ar), 145.6 (*C*-Ar), 144.1 (*C*-Ar), 143.8 (*C*-Ar), 140.6 (*C*-Ar), 137.6 (*C*-Ar), 130.7 (*C*-Ar), 130.5 (*C*-Ar), 129.4 (*C*-Ar), 129.3 (*C*-Ar), 128.6 (*C*-Ar), 127.4 (*C*-Ar), 126.4 (*C*-Ar), 126.2 (*C*-Ar), 125.7 (*C*-Ar), 125.3 (*C*-Ar), 124.8 (*C*-Ar), 124.1 (*C*-Ar), 40.1 (d, *C*(CH$_3$)$_3$, J_{PC} = 9 Hz), 39.9 (d, *C*(CH$_3$)$_3$, J_{PC} = 11 Hz), 36.0 (d, *C*(CH$_3$)$_3$, J_{PC} = 13 Hz), 35.7 (d, *C*(CH$_3$)$_3$, J_{PC} = 7 Hz), 29.5 (C(*C*H$_3$)$_3$), 28.8 (CH(*C*H$_3$)$_2$), 28.3 (CH(*C*H$_3$)$_2$), 28.1 (CH(*C*H$_3$)$_2$), 27.9 (CH(*C*H$_3$)$_2$), 27.7 (C(*C*H$_3$)$_3$), 27.3 (C(*C*H$_3$)$_3$), 26.9 (C(*C*H$_3$)$_3$), 26.2 (CH(*C*H$_3$)$_2$), 25.7 (CH(*C*H$_3$)$_2$), 24.8 (CH(*C*H$_3$)$_2$), 24.7 (CH(*C*H$_3$)$_2$), 23.8 (CH(*C*H$_3$)$_2$). **^{31}P{^{1}H} (C$_6$D$_6$, 162 MHz, 25 °C):** δ 82.9, 73.4. IR (benzene, KBr) υ (cm^{-1}): 1581 (C=O), 1261 (C-O). HRMS (ESI): *m/z* calcd for $C_{55}H_{81}{}^{73}Ge_2N_4P_2O_2$: 1037.4304 [(*M* + *H*)]$^+$; found: 1037.4287.

Synthesis of 7: 5 (0.082 g, 0.1 mmol) and deuterated benzene (0.4 mL) were placed into a J-Young NMR tube. The solution was degassed using a freeze−pump−thaw method. Carbon dioxide (1 bar) was introduced and the color of the solution changed immediately from red to pale orange. The ^{1}H and ^{31}P{^{1}H} NMR spectroscopy showed that compound **5** was fully converted to compound **7**. Leaving compound **7** to stand for a few hours revealed the presence of a second set of signals. ^{13}C{^{1}H} NMR spectroscopy confirmed the presence of 2 conformers of compound **7**. CO_2 were removed under reduced pressure. The solution changed immediately from pale orange

to red. The $^{31}P\{^{1}H\}$ NMR spectroscopy showed that compound **7** was fully converted to compound **5**.

^{1}H NMR (C_6D_6, 400 MHz, 25 °C): δ 7.66-7.61 (m, 3 H, Ar*H*), 7.43-7.41(m, 2 H, Ar*H*), 7.31-7.23 (m, 3 H, Ar*H*), 6.97-6.87 (m, 10 H, Ar*H*), 6.78-6.67 (m, 2 H, Ar*H*), 1.45 (d, 9 H, C(CH_3)$_3$, J_{HH} = 14 Hz), 1.33 (d, 9 H, C(CH_3)$_3$, J_{HH} = 8 Hz), 1.29 (d, 9 H, C(CH_3)$_3$, J_{HH} = 8 Hz), 1.23 (d, 9 H, C(CH_3)$_3$, J_{HH} = 14 Hz). **^{13}C{^{1}H} (C_6D_6, 101 MHz, 25 °C)**: δ 209.2 (O*C*O), 207.6 (O*C*O), 175.3 (N*C*N), 175.1 (N*C*N), 174.9 (N*C*N), 174.2 (N*C*N), 147.5 (*C*-Ar), 147.4 (*C*-Ar), 147.3 (*C*-Ar), 147.2 (*C*-Ar), 147.1 (*C*-Ar), 147.0 (*C*-Ar), 146.7 (*C*-Ar), 146.6 (*C*-Ar), 138.2 (*C*-Ar), 138.0 (*C*-Ar), 138.0 (*C*-Ar), 137.9 (*C*-Ar), 137.7 (*C*-Ar), 130.3 (*C*-Ar), 130.2 (*C*-Ar), 130.0 (*C*-Ar), 129.0 (*C*-Ar), 128.7 (*C*-Ar), 128.6 (*C*-Ar), 128.5 (*C*-Ar), 128.2 (*C*-Ar), 127.9 (*C*-Ar), 127.9 (*C*-Ar), 127.7 (*C*-Ar), 127.6 (*C*-Ar), 126.8 (*C*-Ar), 124.8 (*C*-Ar), 124.4 (*C*-Ar), 124.0 (*C*-Ar), 124.0 (*C*-Ar), 123.9 (*C*-Ar), 121.8 (*C*-Ar), 39.3 (*C*(CH$_3$)$_3$), 38.8 (*C*(CH$_3$)$_3$), 38.7 (*C*(CH$_3$)$_3$), 38.3 (*C*(CH$_3$)$_3$), 37.1 (*C*(CH$_3$)$_3$), 36.9 (*C*(CH$_3$)$_3$), 36.9 (*C*(CH$_3$)$_3$), 36.7 (*C*(CH$_3$)$_3$), 28.4 (C(*C*H$_3$)$_3$), 28.1 (C(*C*H$_3$)$_3$), 27.9 (C(*C*H$_3$)$_3$), 27.8 (C(*C*H$_3$)$_3$), 27.7 (C(*C*H$_3$)$_3$), 27.4 (C(*C*H$_3$)$_3$). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**: δ 87.8, 77.8. IR (benzene, KBr) υ (cm^{-1}): 1593 (C=O), 1260 (C-O). HRMS (ESI): *m/z* calcd for $C_{43}H_{56}{}^{74}Ge_2N_4P_2O_2Na$: 893.2200 $[(M + Na)]^+$; found: 893.2216.

Synthesis of 8 from 7: 40 mL of toluene was added to a 100 mL Schlenk flask containing compound **5** (0.412 g, 0.5 mmol). The solution was degassed using a freeze−pump−thaw method. CO_2 (1 bar) was then introduced. The color of the reaction solution changed immediately from red to yellow. The $^{31}P\{^{1}H\}$ NMR spectroscopy showed that compound **5** was fully converted to compound **7**. The diphenylacetylene (0.089 g, 0.5 mmol) was then added into the reaction and the mixture was stirred at 60 ^{o}C for 6 hours. The color of the solution changed from brown yellow to red to bright yellow. The reaction mixture was filtered and concentrated to give **8** as yellow crystals. Yield: 0.326 g (65%).

Synthesis of 8 from 5: 40 mL of toluene was added to a 100 mL Schlenk flask containing **5** (0.412 g, 0.5 mmol) and diphenylacetylene (0.0891 g, 0.5 mmol). The reaction mixture was stirred for 3 days at room temperature to give a yellow solution. The reaction mixture was filtered and concentrated to give **8** as yellow crystals. Yield: 0.341 g (68%).

M.p.: 118 ^{o}C. **^{1}H NMR (C_6D_6, 400 MHz, 25 °C)**: δ 7.70-7.68 (m, 4 H, Ar*H*), 7.53-7.50 (m, 2 H, Ar*H*), 7.41 (d, 4 H, Ar*H*, J_{HH} = 8 Hz), 7.00-6.89 (m, 10 H, Ar*H*), 6.77-6.73 (m, 4 H, Ar*H*), 6.65-6.61 (m, 2 H, Ar*H*), 6.38-6.35 (m, 4 H, Ar*H*), 1.75 (d, 18 H, C(CH_3)$_3$, J_{HH} = 12 Hz), 1.44 (d, 18 H, C(CH_3)$_3$, J_{HH} = 12 Hz). **^{13}C{^{1}H} (C_6D_6, 101 MHz, 25 °C)**: δ 174.5 (N*C*N), 170.6 (*C*-Ar), 147.5 (*C*-Ar), 145.4 (*C*-Ar), 137.4 (*C*-Ar), 131.9 (*C*-Ar), 131.5 (*C*-Ar), 130.6 (*C*-Ar), 129.5 (*C*-Ar), 129.3 (*C*-Ar), 128.3 (*C*-Ar),

127.5 (*C*-Ar), 125.6 (*C*-Ar), 124.7 (*C*-Ar), 123.1 (*C*-Ar), 90.2 (Ph*C*=*C*Ph), 38.6 (d, *C*(CH_3)$_3$, J_{PC} = 20 Hz), 37.8 (d, *C*(CH_3)$_3$, J_{PC} = 16 Hz), 29.4 (C(*C*H_3)$_3$), 27.9 (C(*C*H_3)$_3$). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**: δ 80.9. HRMS (ESI): *m/z* calcd for $C_{56}H_{67}{}^{73}Ge_2N_4P_2$: 1003.3310 [(*M* + *H*)]$^+$; found: 1003.3298.

Synthesis of 9 and 10 from 7: 40 mL of toluene was added to a 100 mL Schlenk flask containing **5** (0.412 g, 0.5 mmol). The solution was degassed using a freeze−pump−thaw method. CO_2 (1 bar) was then introduced. The color of the reaction solution changed immediately from red to yellow. The ^{31}P{^{1}H} NMR spectroscopy showed that compound **5** was fully converted to compound **7**. The hexafluorobenzene (0.372 g, 2 mmol) was then added into the reaction and the mixture was stirred at 80 °C for 4 hours. The color of the solution changed from brown yellow to red to brown. Volatiles were removed under reduced pressure to give a mixture of compounds **9** and **10** as a brown solid.

Synthesis of 9 and 10 from 5: 40 mL of toluene was added to a 100 mL Schlenk flask containing **5** (0.412 g, 0.5 mmol) and hexafluorobenzene (0.372 g, 2 mmol). The reaction mixture was stirred at 90 °C for 7 hours to give a brown solution. Volatiles were removed under reduced pressure to give a mixture of compounds **9** and **10** as a brown solid.

^{1}H NMR (C_6D_6, 400 MHz, 25 °C): δ 7.62-7.60 (m, 2 H, Ar*H*), 7.55-7.53 (m, 2 H, Ar*H*), 7.28-7.22 (m, 1 H, Ar*H*), 7.03-7.01 (m, 2 H, Ar*H*), 6.93-6.88 (m, 11 H, Ar*H*), 6.77-6.72 (m, 2 H, Ar*H*), 1.35 (d, 9 H, C(C*H*$_3$)$_3$, J_{HH} = 16 Hz), 1.21 (d, 9 H, C(C*H*$_3$)$_3$, J_{HH} = 12 Hz), 1.14 (d, 9 H, C(C*H*$_3$)$_3$, J_{HH} = 16 Hz), 0.98 (d, 18 H, C(C*H*$_3$)$_3$, J_{HH} = 12 Hz). **^{13}C{^{1}H} (C_6D_6, 101 MHz, 25 °C)**: δ 176.2 (N*C*N), 175.6 (N*C*N), 146.2 (*C*-Ar), 145.9 (*C*-Ar), 137.1 (*C*-Ar), 136.7 (*C*-Ar), 129.8 (*C*-Ar), 129.7 (*C*-Ar), 129.1 (*C*-Ar), 128.9 (*C*-Ar), 128.7 (*C*-Ar), 128.6 (*C*-Ar), 126.8 (*C*-Ar), 126.0 (*C*-Ar), 124.2 (*C*-Ar), 124.0 (*C*-Ar), 121.5 (*C*-Ar), 37.3 (d, *C*(CH_3)$_3$, J_{PC} = 24 Hz), 36.1 (d, *C*(CH_3)$_3$, J_{PC} = 20 Hz), 27.7 (C(*C*H_3)$_3$), 27.5 (C(*C*H_3)$_3$), 26.9 (C(*C*H_3)$_3$), 26.7 (C(*C*H_3)$_3$). **^{19}F{^{1}H} NMR (376 MHz, 25 °C, C_6D_6)**, **9**: -148.1 (d, 1 F, J_{PF} = 7 Hz); **10**: δ -127.4 (dd, 1 F, J_{FF} = 7, 7 Hz), -154.3 (dt, 2 F, J_{FF} = 22, 4 Hz), -161.2 (m, 2 F). **^{31}P{^{1}H} (C_6D_6, 162 MHz, 25 °C)**, **9**: δ 76.7 (d, J_{PF} = 6 Hz); **10**: δ 85.3. HRMS (ESI), **9**: *m/z* calcd for $C_{21}H_{29}{}^{74}GeN_2PF$: 433.1264 [(*M* + *H*)]$^+$; found: 433.1268; **10**: *m/z* calcd for $C_{27}H_{29}{}^{74}GeN_2PF_5$: 581.1200 [(*M* + *H*)]$^+$; found: 581.1207.

S2. Selected NMR Spectra

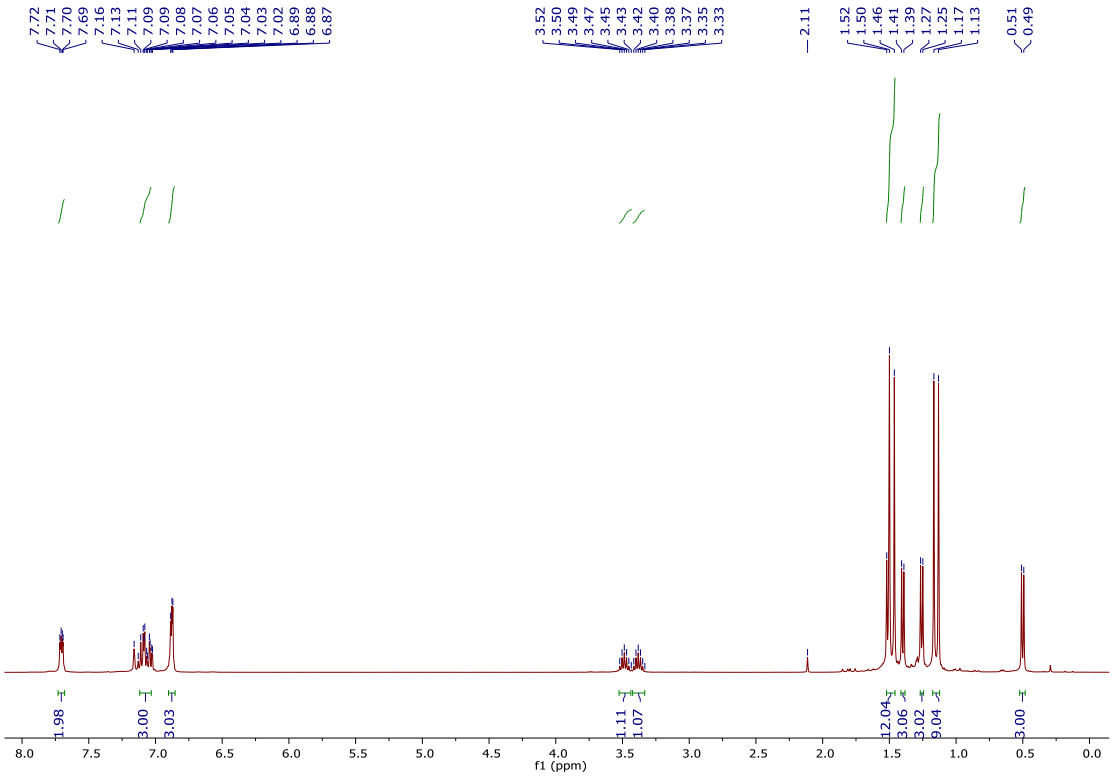


Figure S1. ^{1}H NMR spectrum of compound **2** (in C_6D_6).

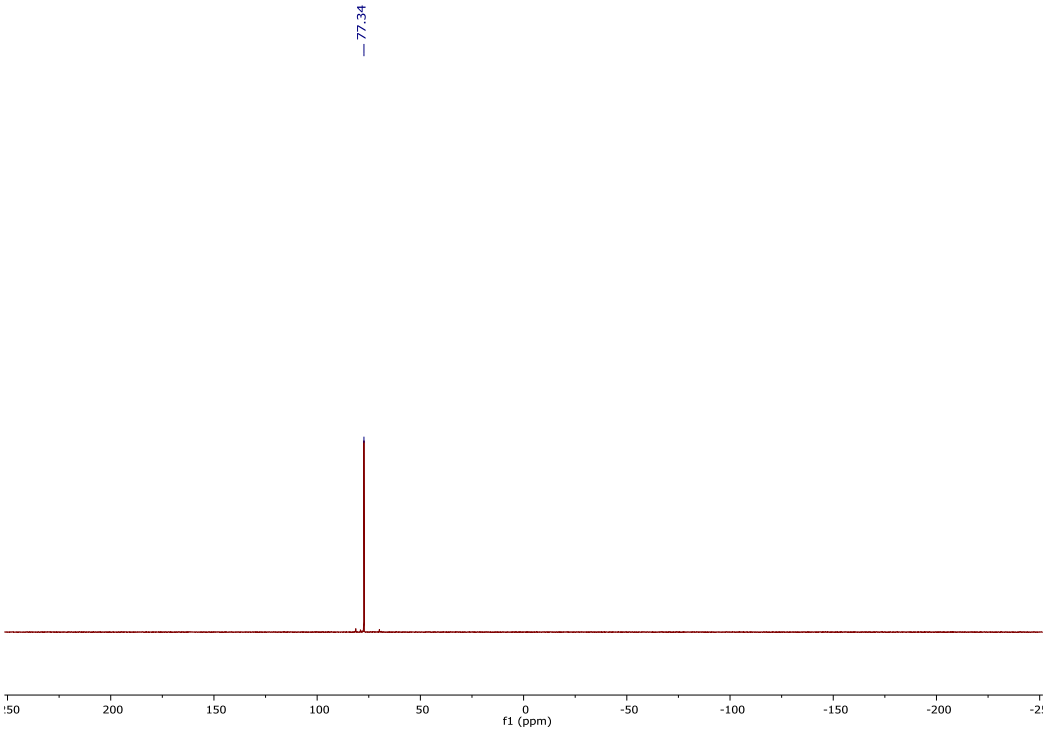


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of compound **2** (in C_6D_6).

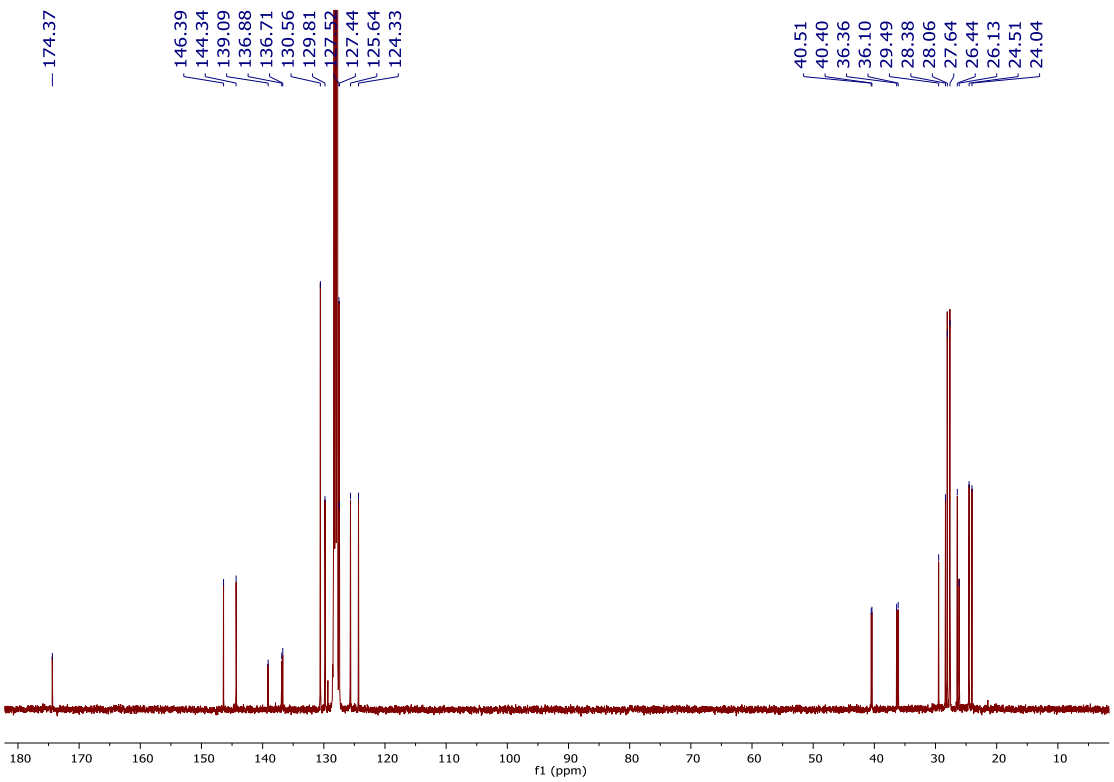


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2** (in C_6D_6).

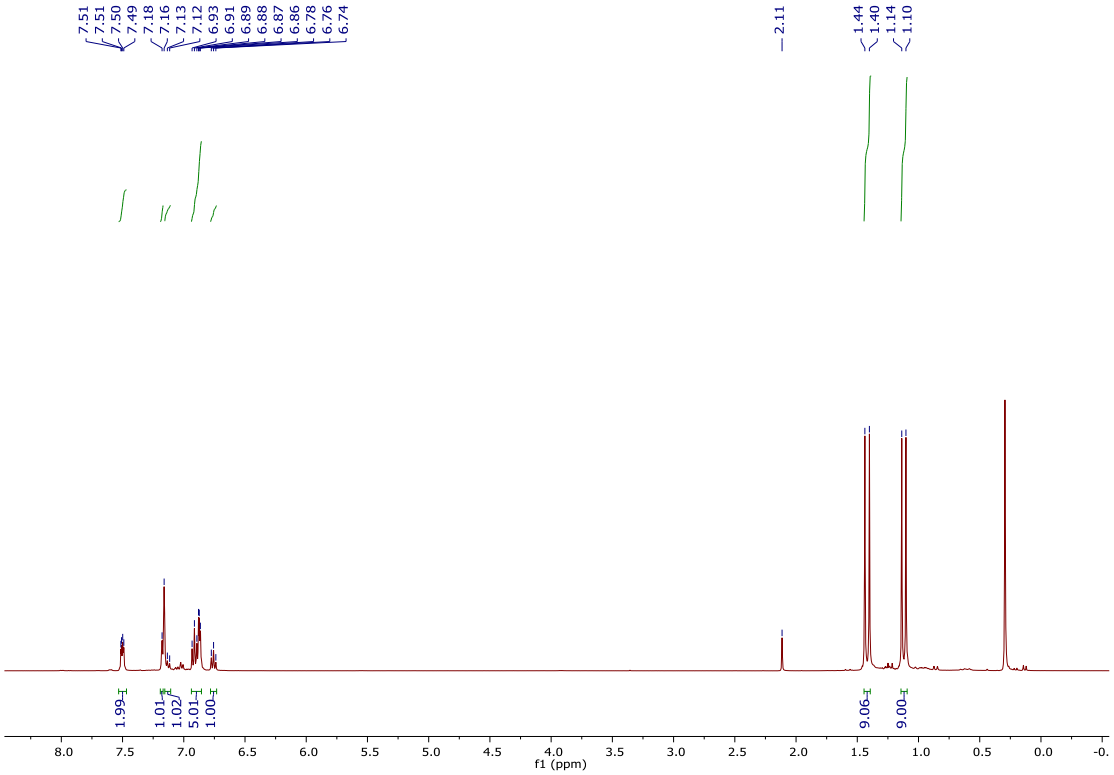


Figure S4. ^{1}H NMR spectrum of compound **3** (in C_6D_6).

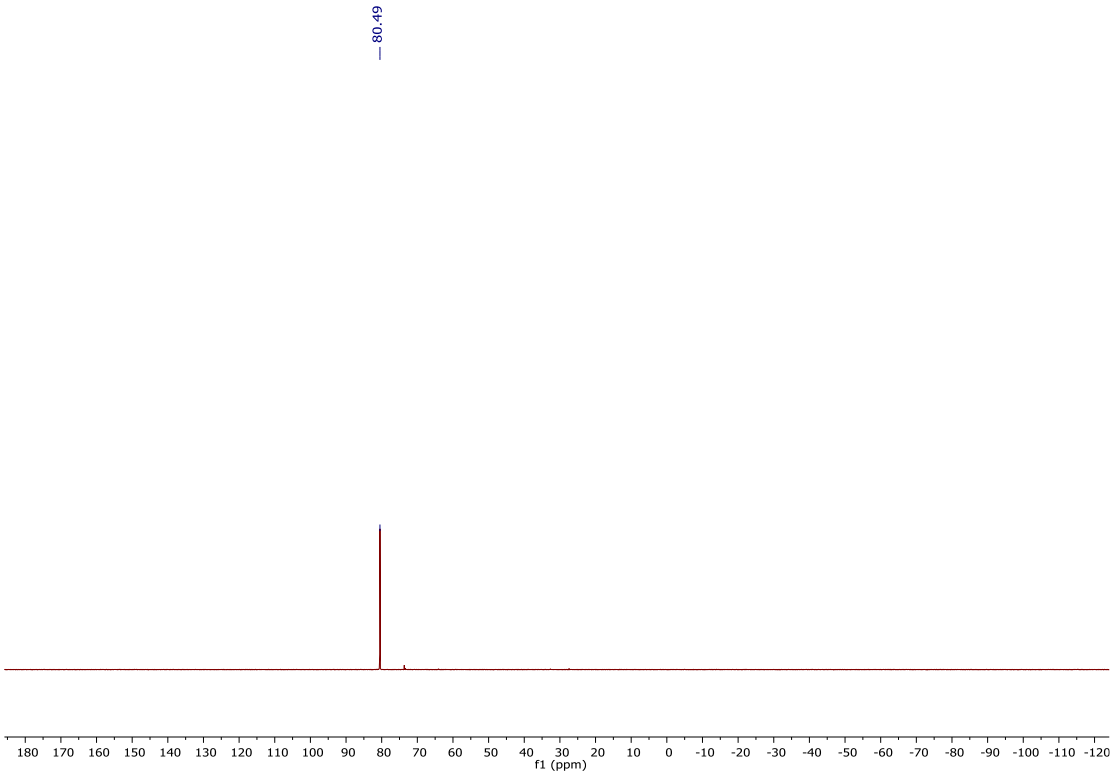


Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of compound **3** (in C_6D_6).

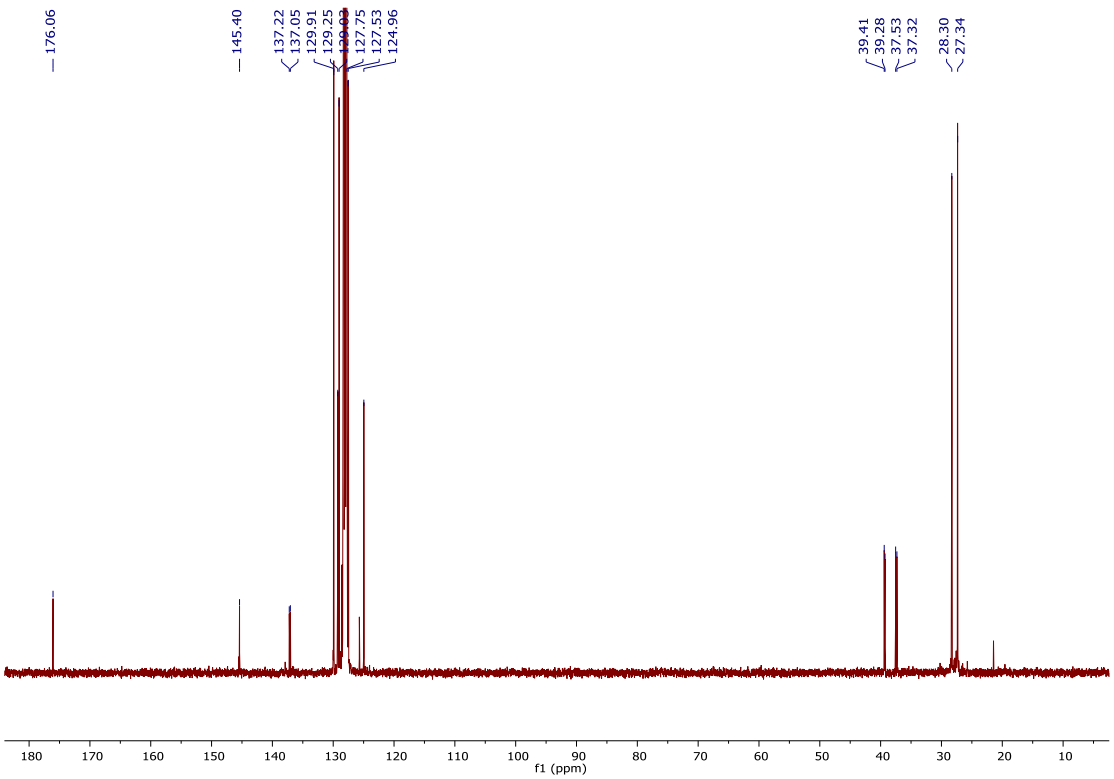


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** (in C_6D_6).

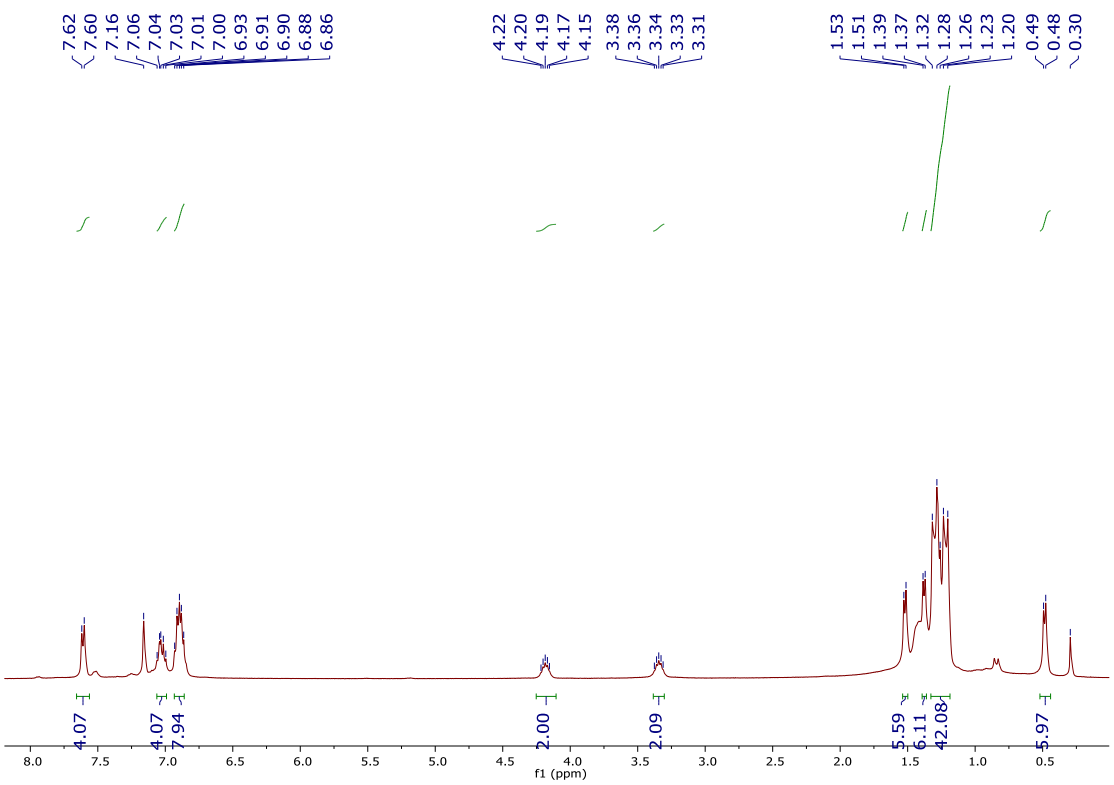


Figure S7. ^{1}H NMR spectrum of compound **4** (in C_6D_6).

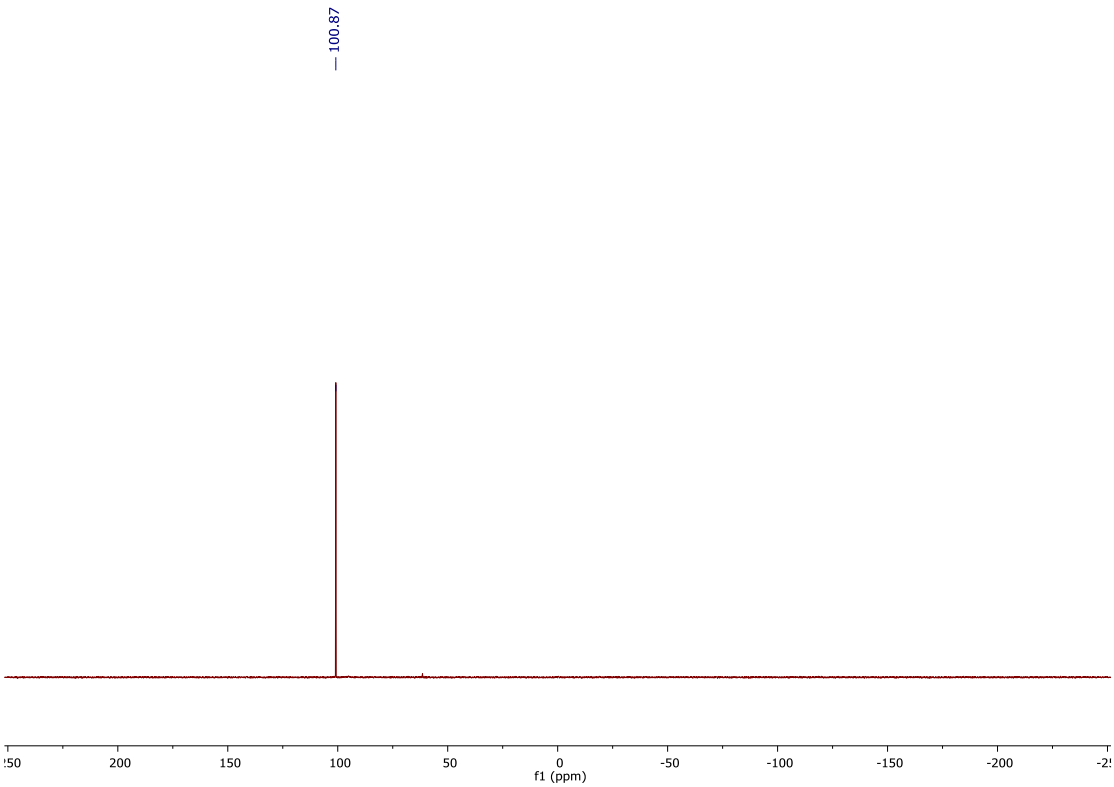


Figure S8. ^{31}P{^{1}H} NMR spectrum of compound **4** (in C_6D_6).

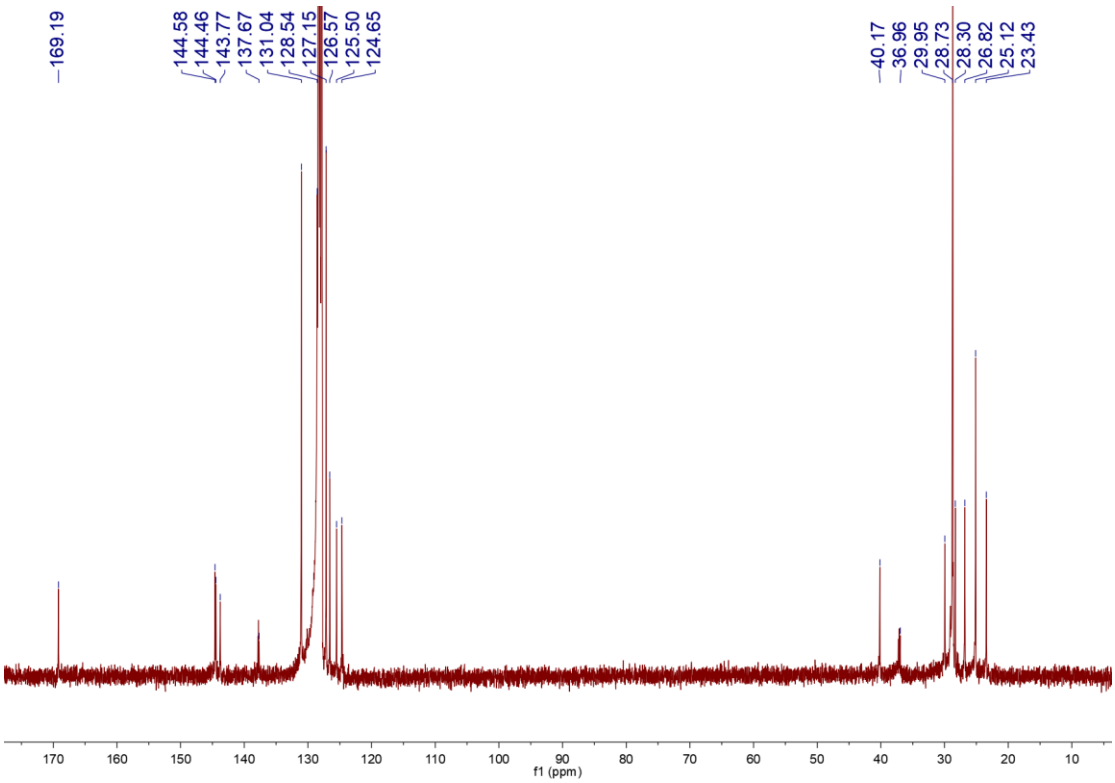


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** (in C_6D_6).

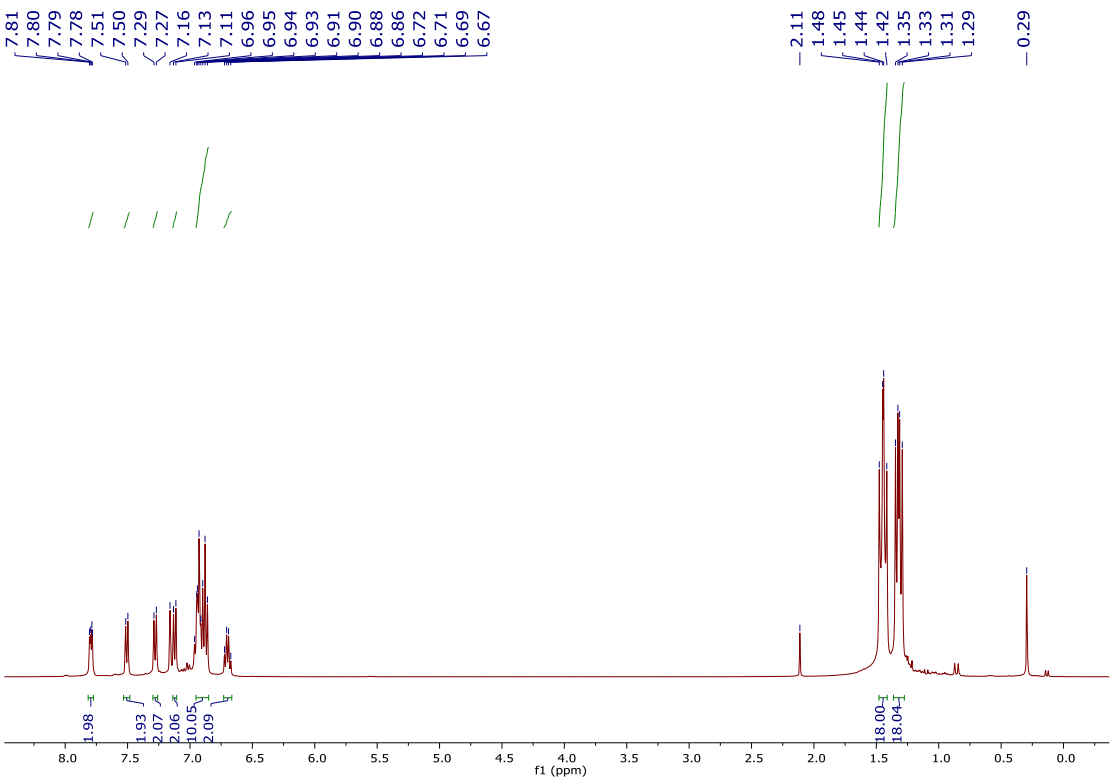


Figure S10. ^{1}H NMR spectrum of compound **5** (in C_6D_6).

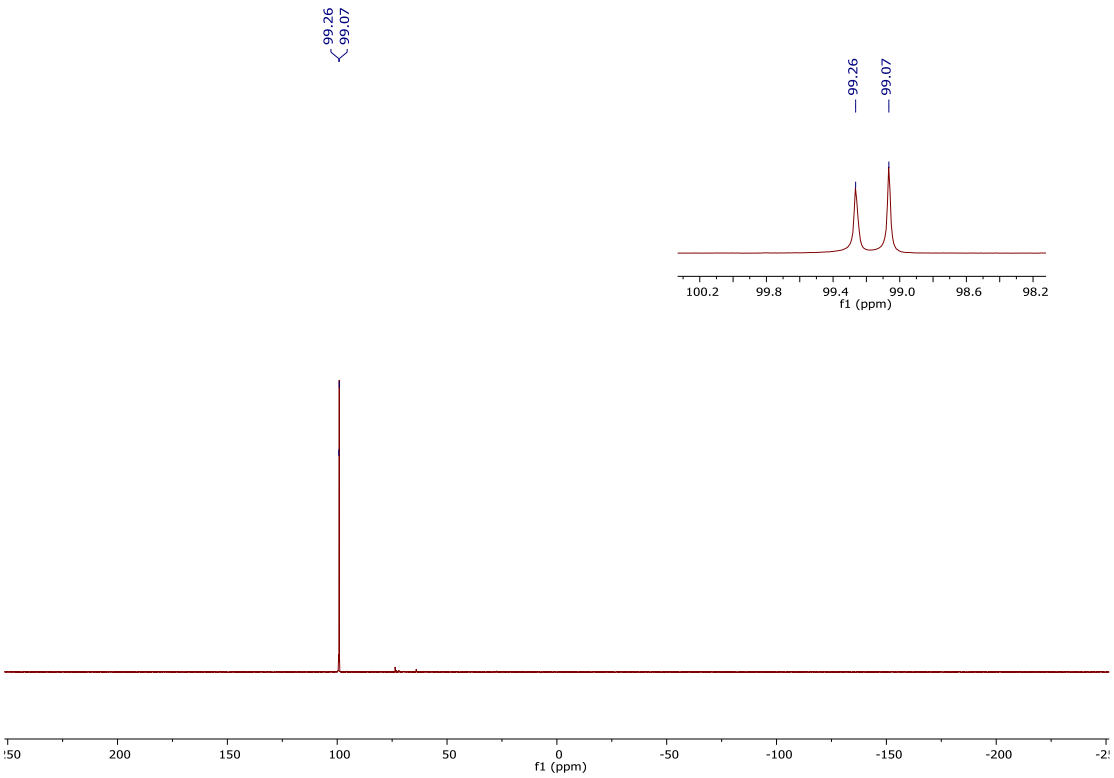


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of compound **5** (in C_6D_6).

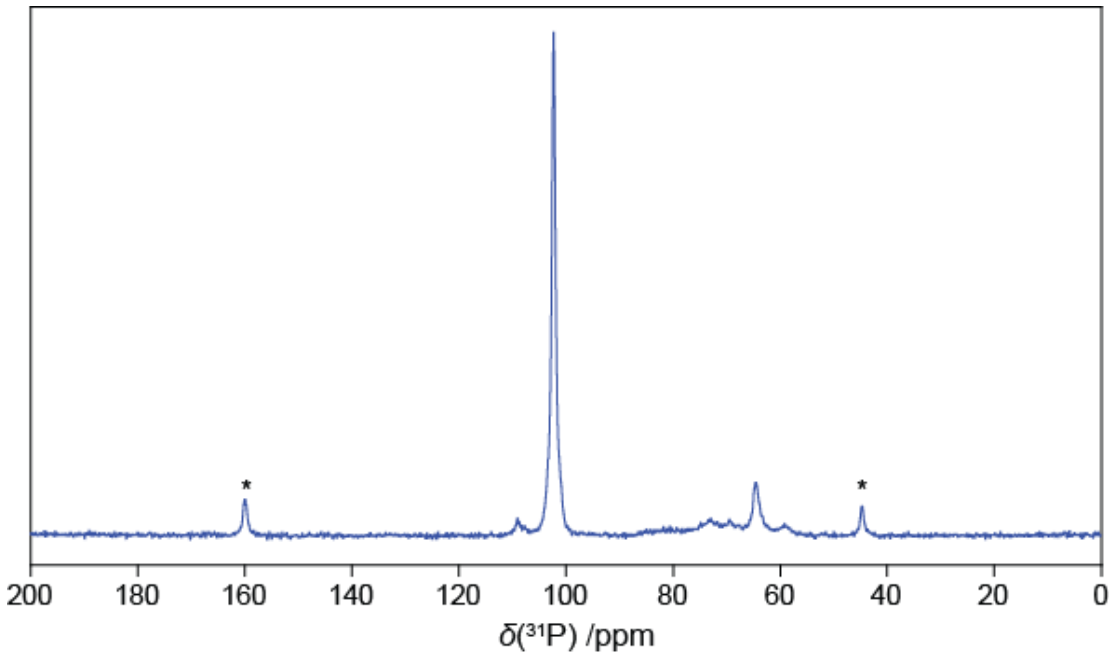


Figure S12. Solid state $^{31}P\{^{1}H\}$ CPMAS NMR of compound **5**. (*: MAS spinning sidebands; 65ppm: free ligand).

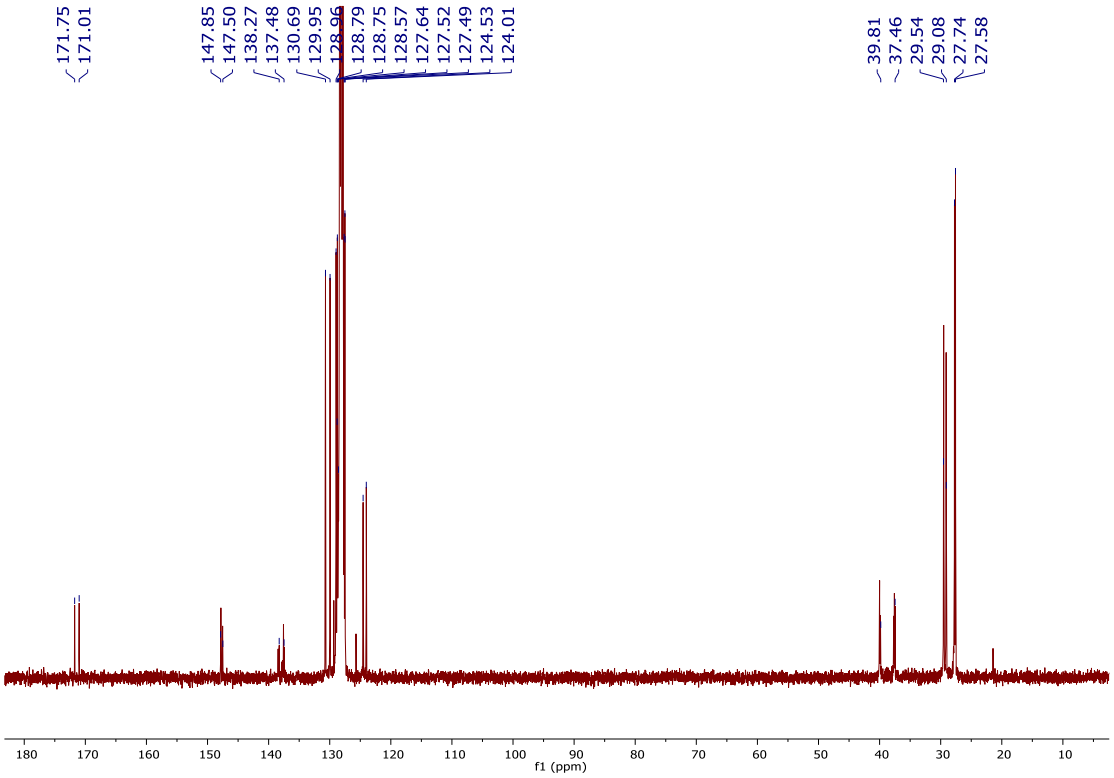


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5** (in C_6D_6).

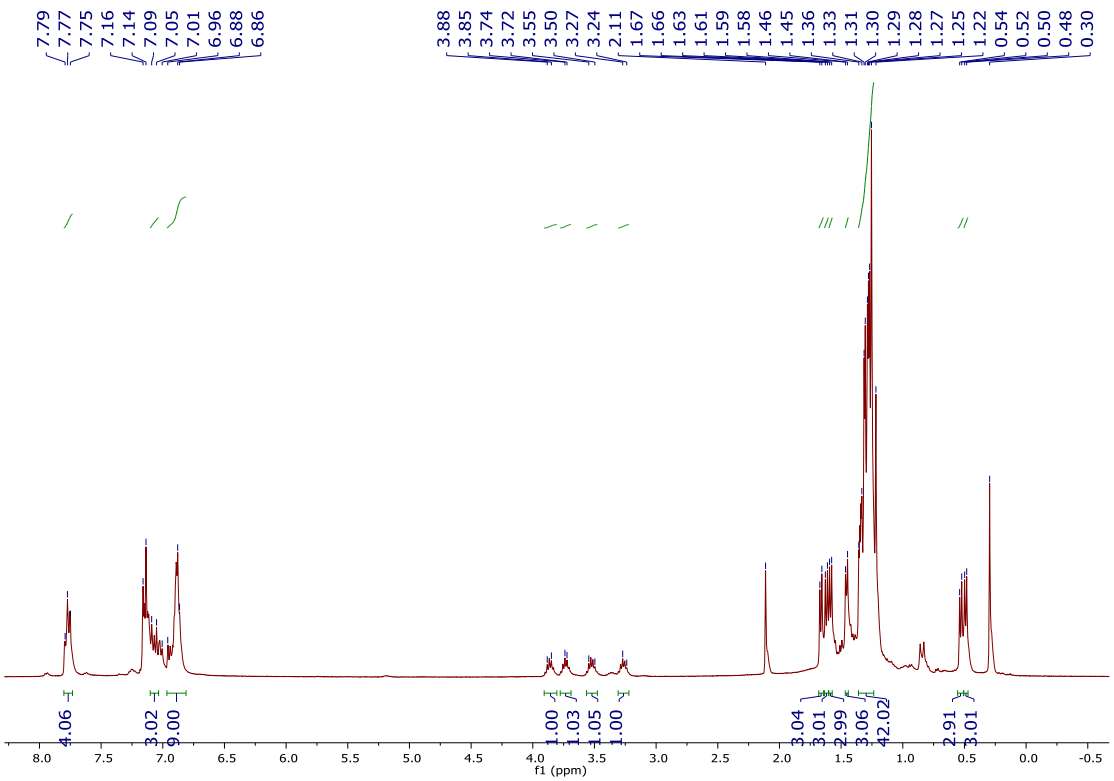


Figure S14. ^{1}H NMR spectrum of compound **6** (in C_6D_6).

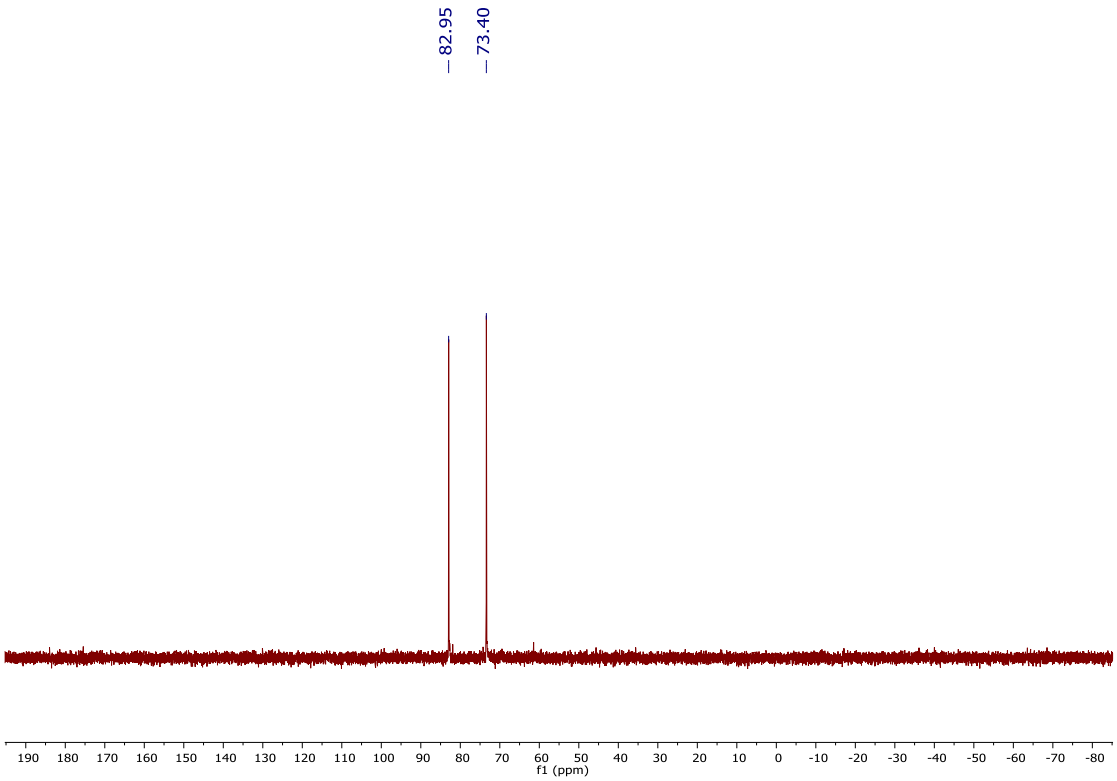


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of compound **6** (in C_6D_6).

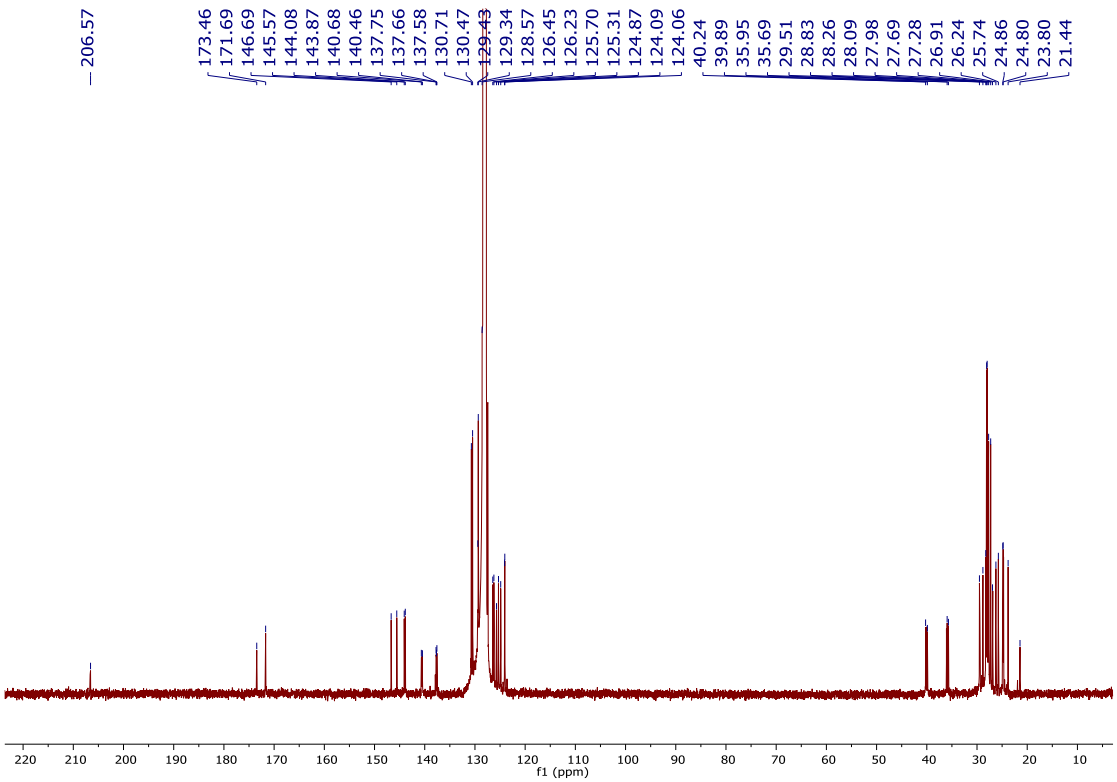


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** (in C_6D_6).

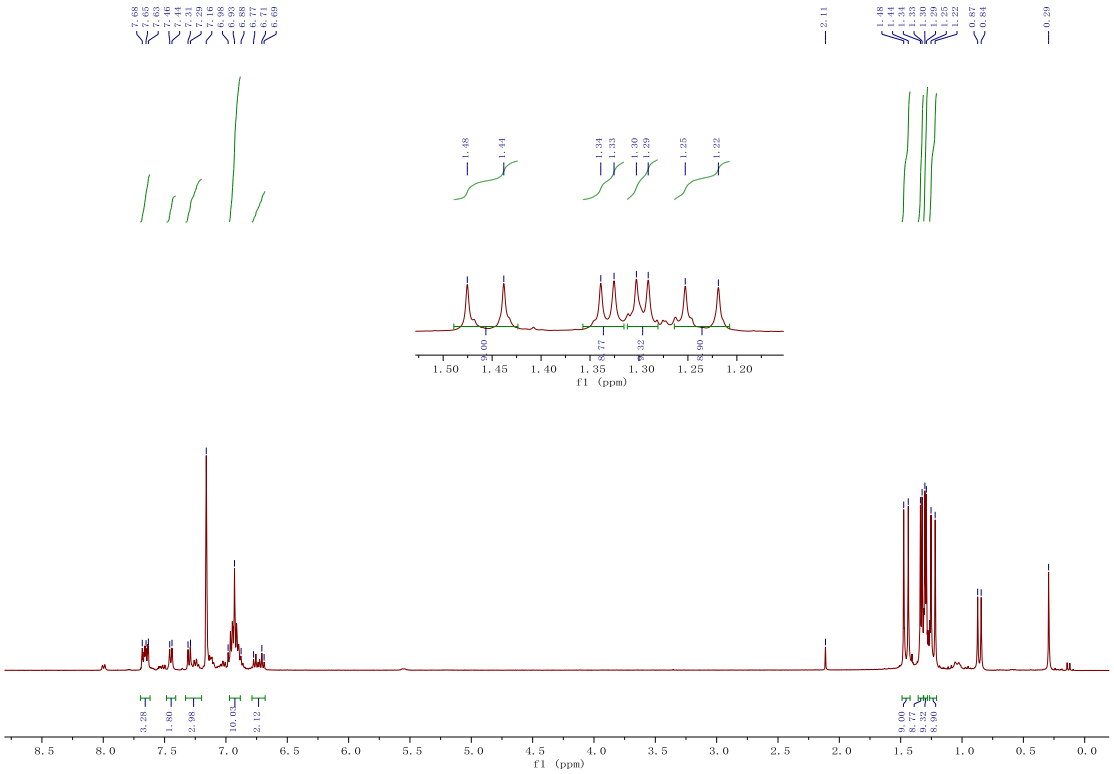


Figure S17. ^{1}H NMR of compound **7** in C_6D_6.

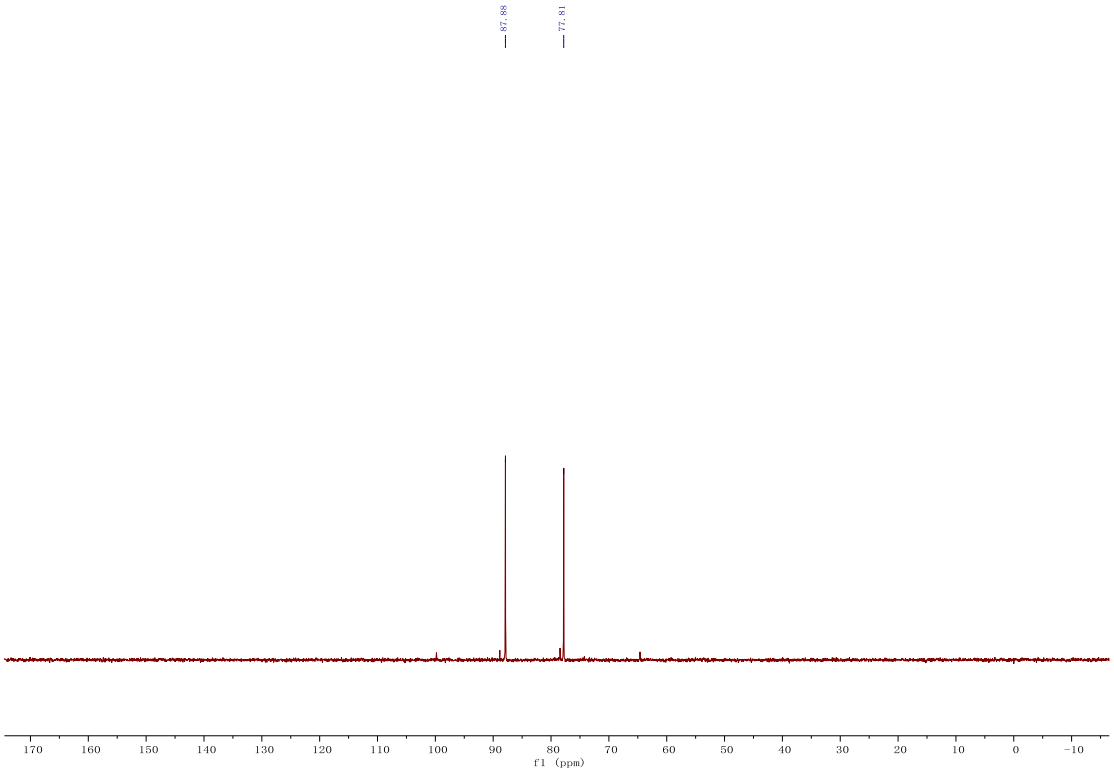


Figure S18. ^{31}P{^{1}H} NMR spectrum of compound **7** (in C_6D_6).

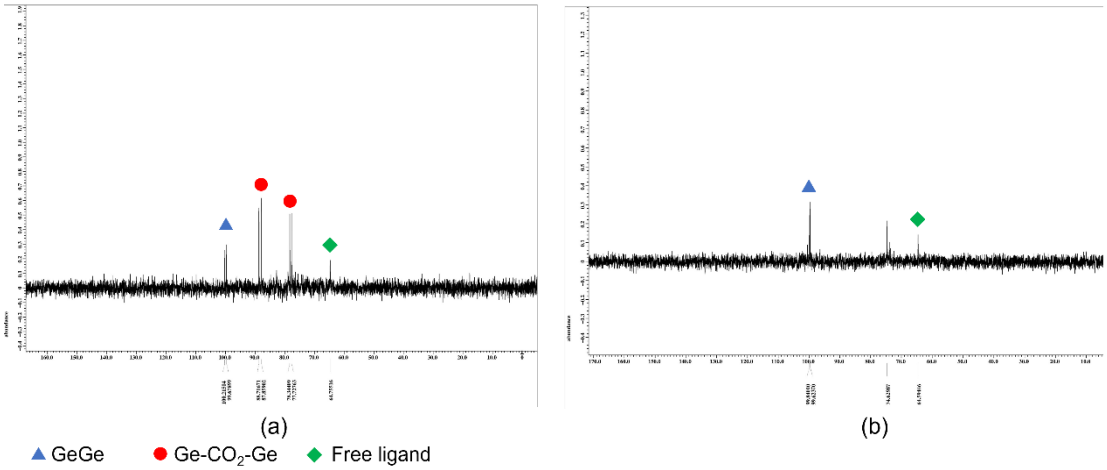


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum of compound **7** *after CO_2 was removed* (C_6D_6). (a): 2 h. (b): 5 h.

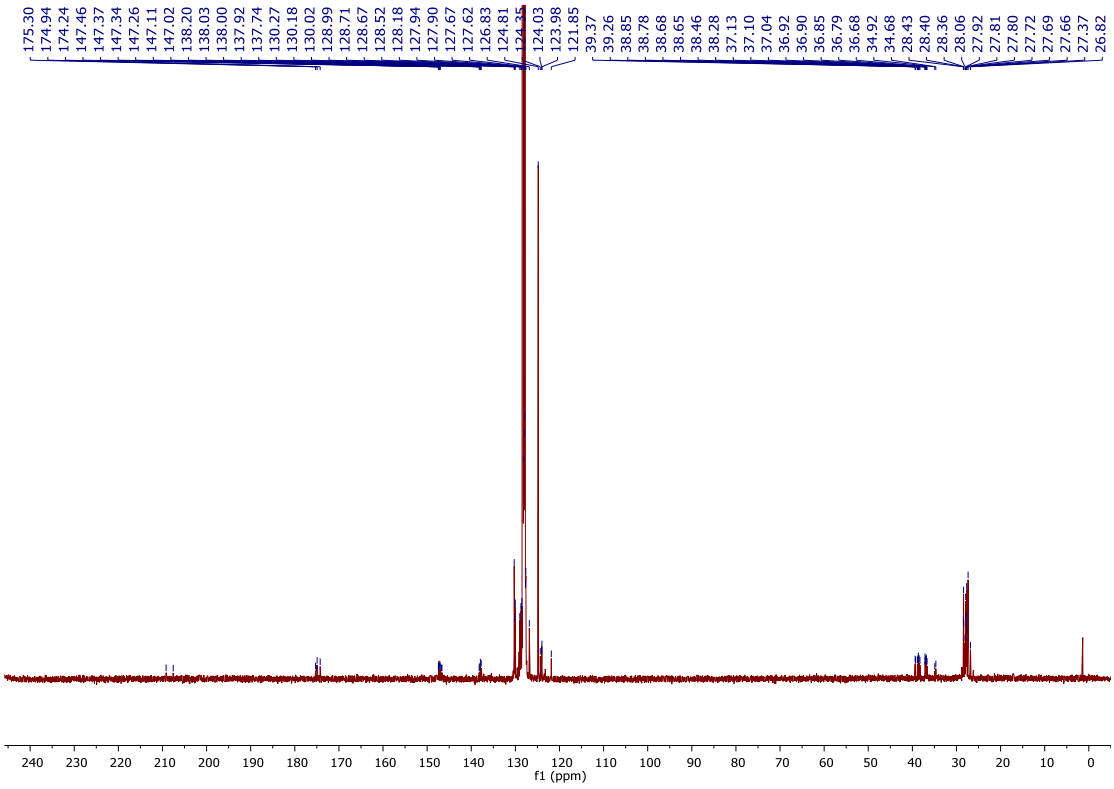


Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of compound 7 (in C_6D_6).

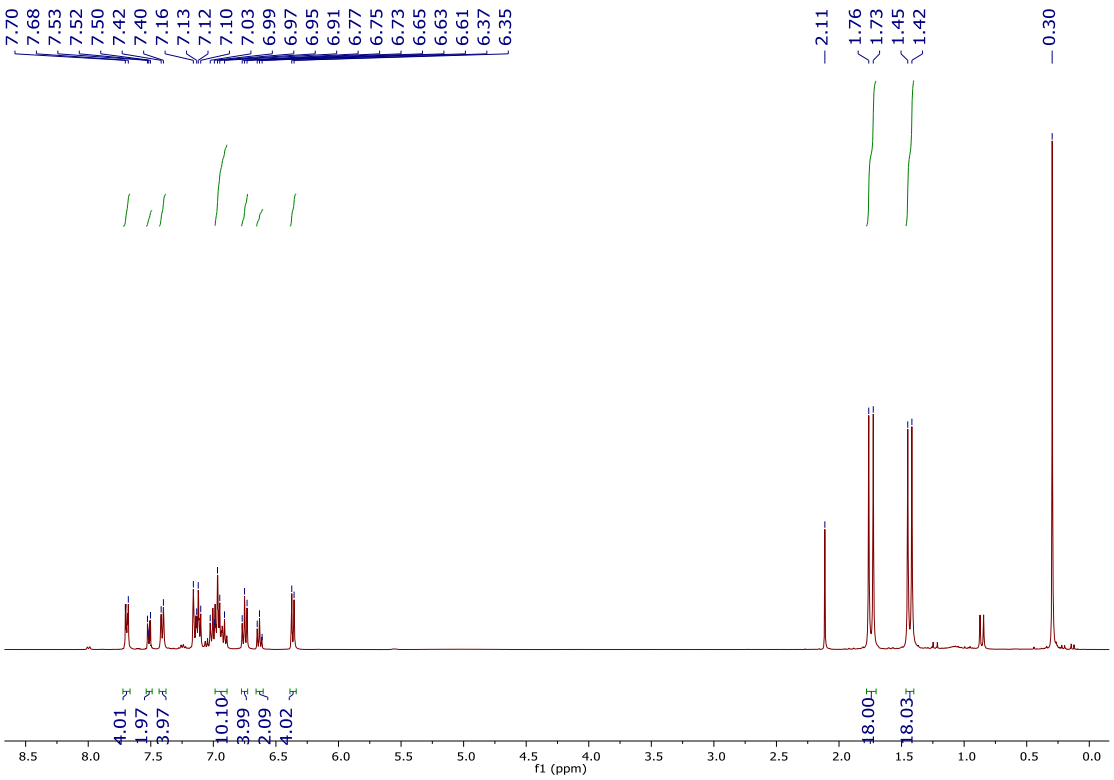


Figure S21. ^{1}H NMR spectrum of compound **8** (in C_6D_6).

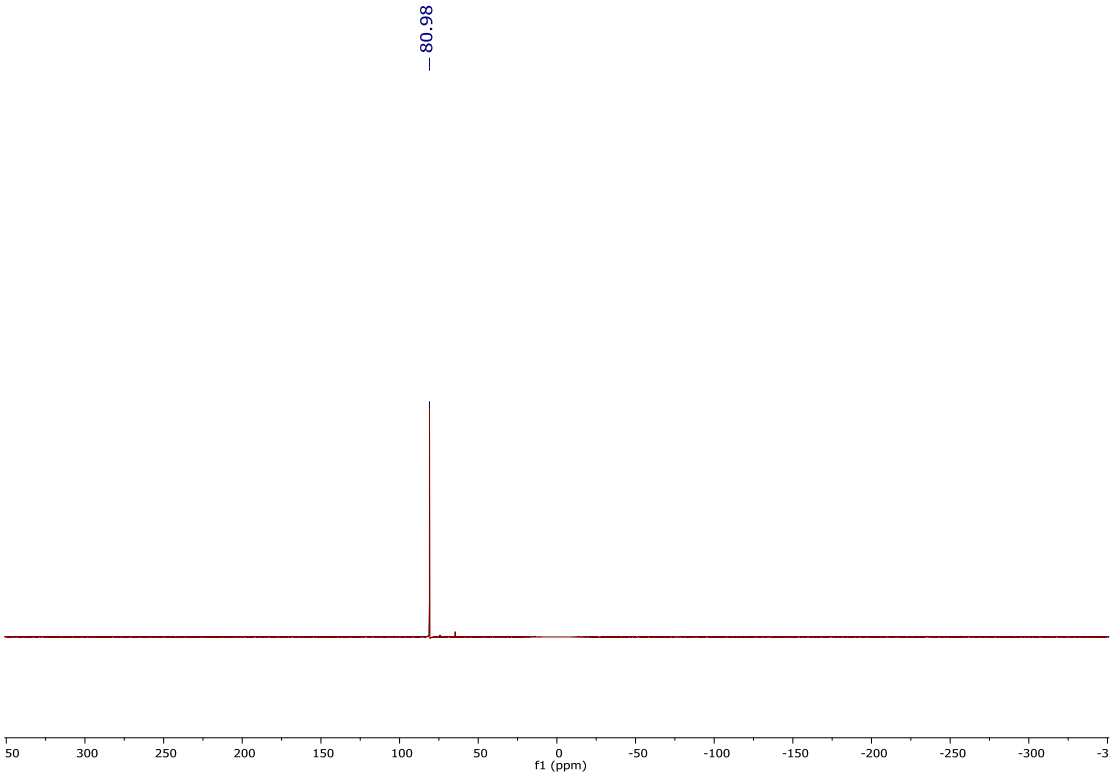


Figure S22. $^{31}P\{^{1}H\}$ NMR spectrum of compound **8** (in C_6D_6).

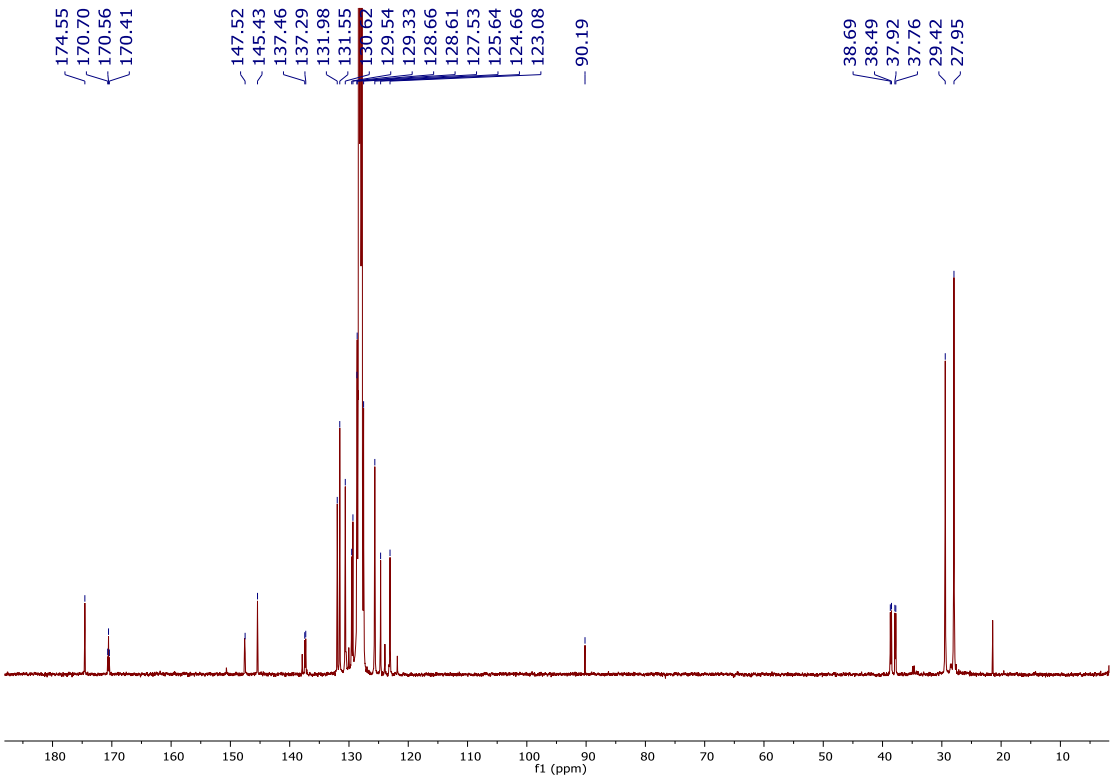


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8** (in C_6D_6).

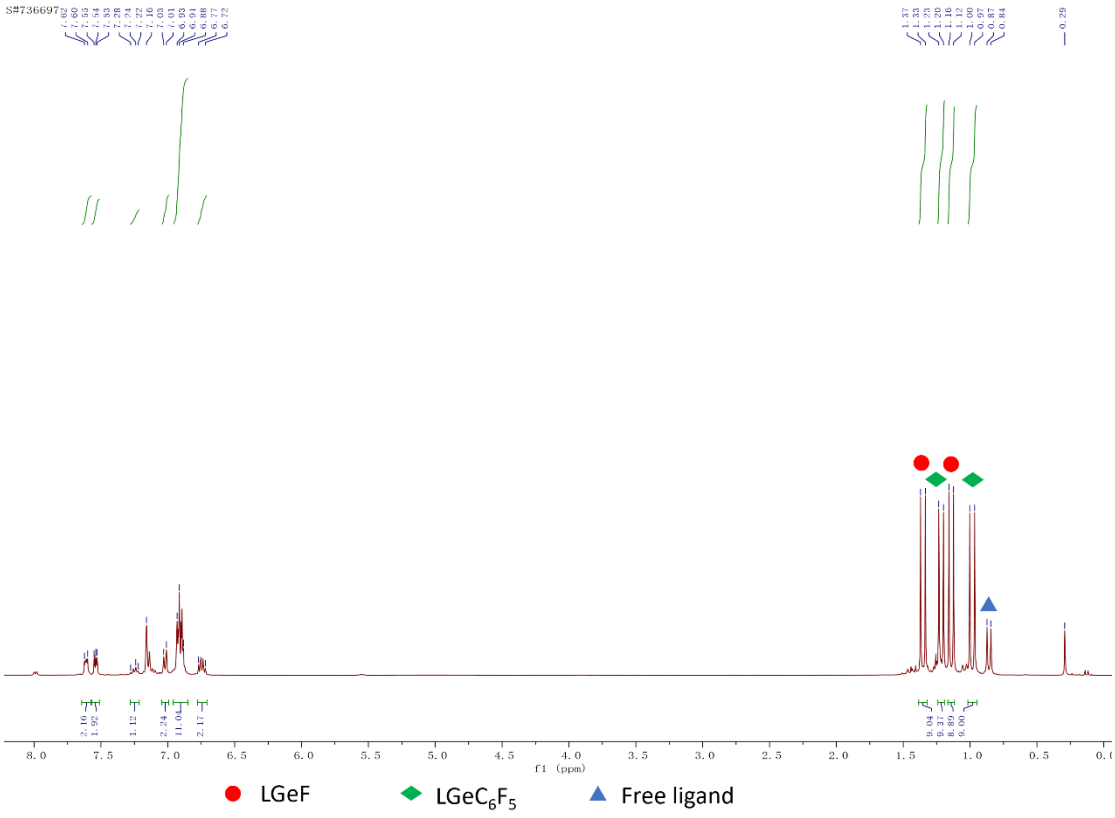


Figure S24. ^{1}H NMR spectrum of compound **9** (LGeF) and **10** ($LGeC_6F_5$) (in C_6D_6).

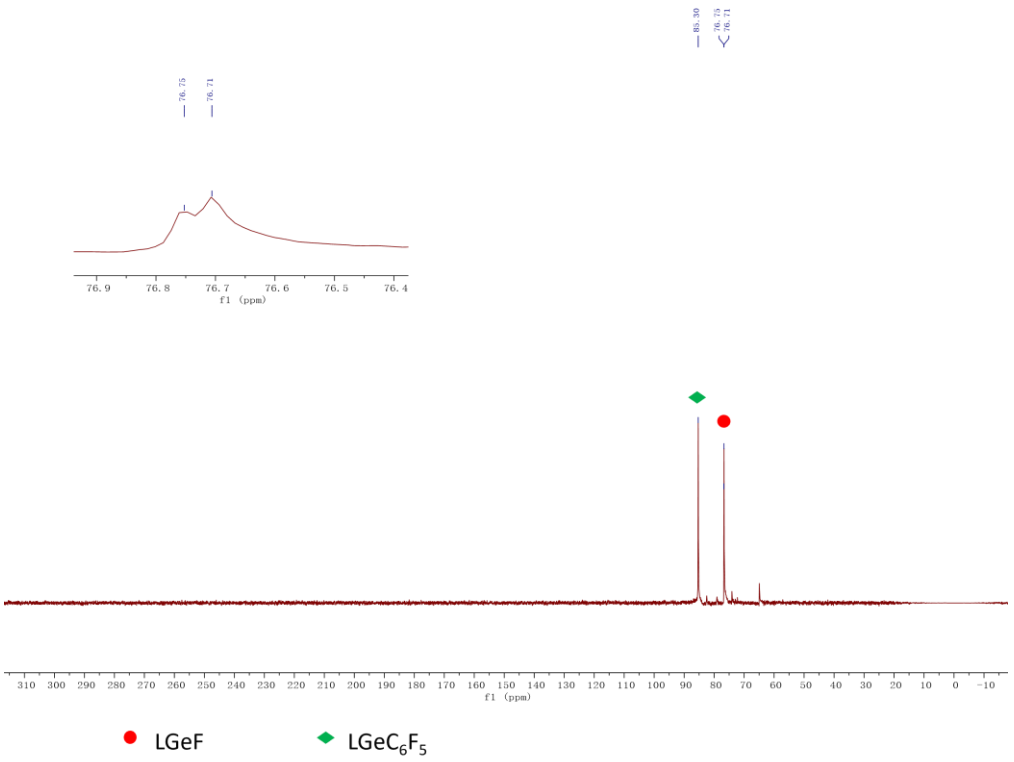


Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum of compound **9** (LGeF) and **10** ($LGeC_6F_5$) (in C_6D_6).

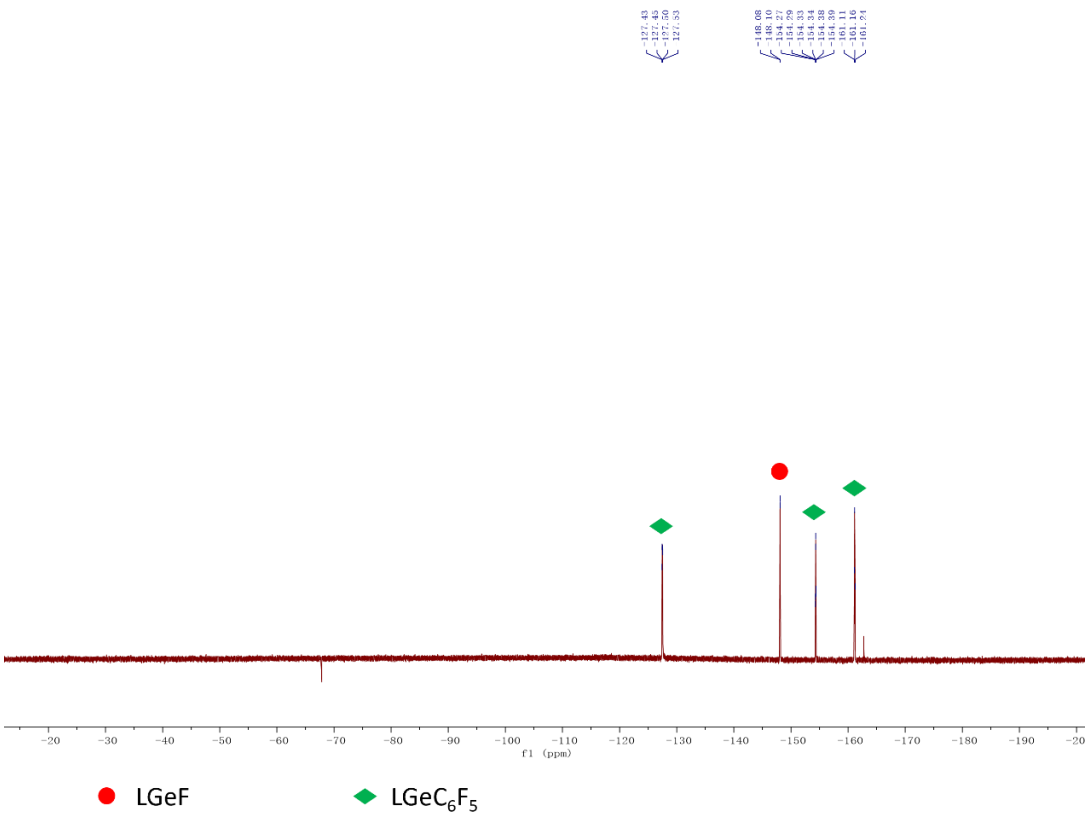


Figure S26. $^{19}F\{^{1}H\}$ NMR spectrum of compound **9 (**LGeF) and **10** ($LGeC_6F_5$) (in C_6D_6).

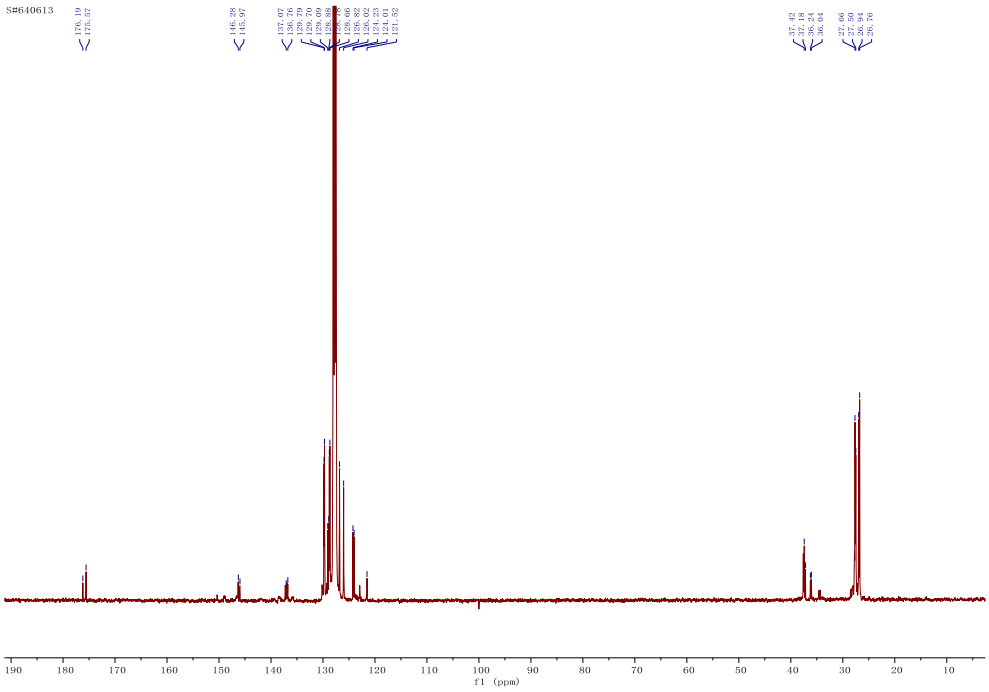


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** (LGeF) and **10** ($LGeC_6F_5$) (in C_6D_6).

S3. IR Spectra

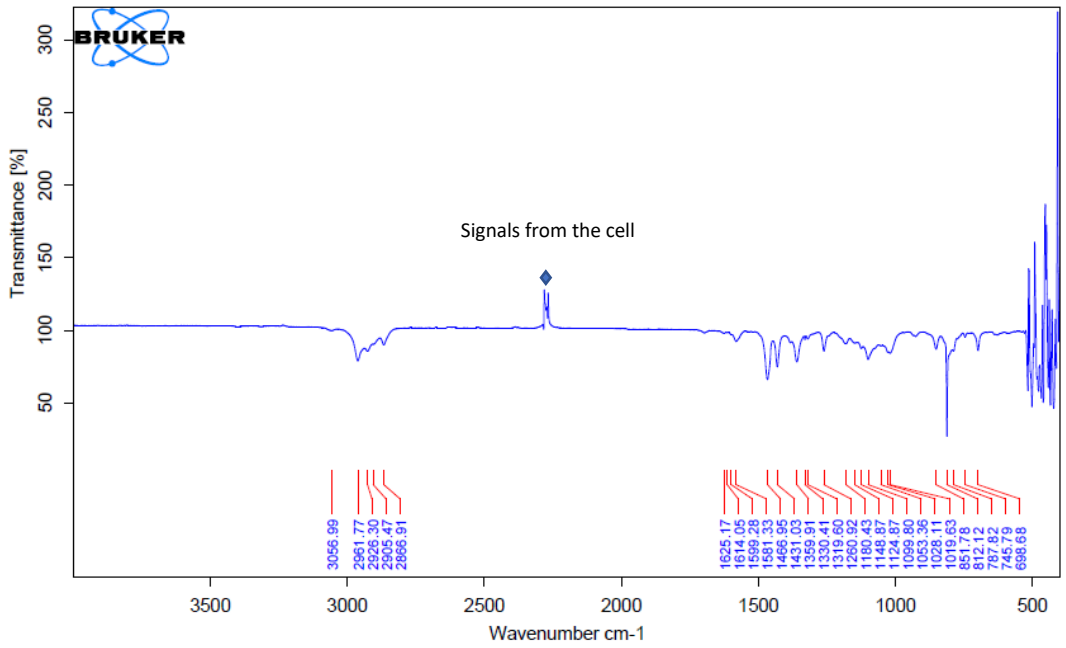


Figure S28. FTIR of compound **6 (**in benzene).

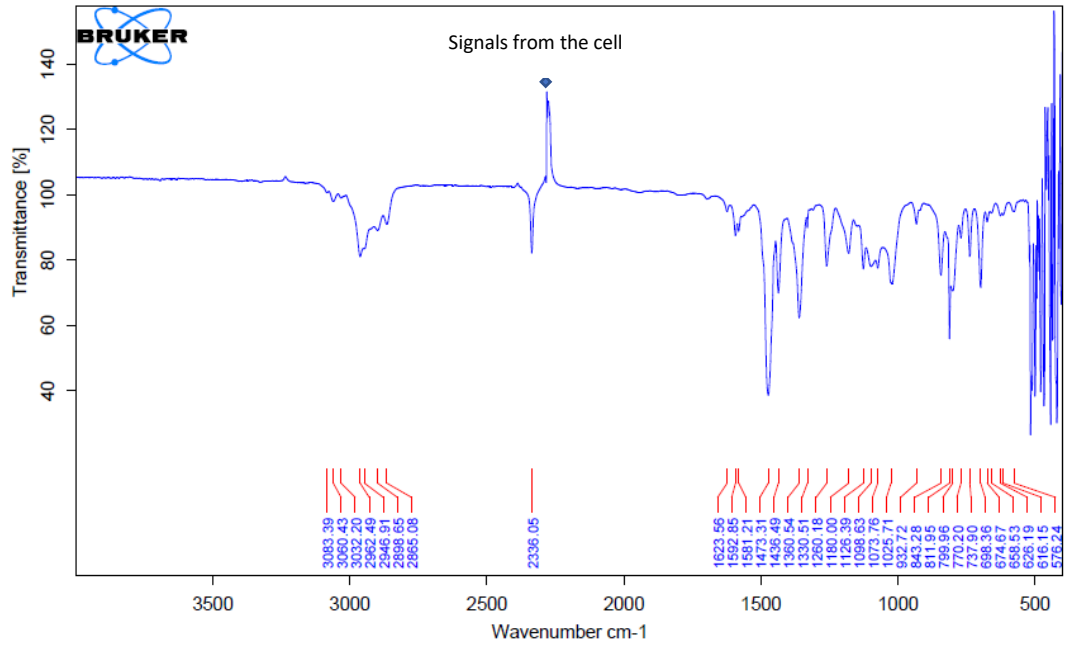


Figure S29. FTIR of compound **7 (**in benzene).

S4. VT-NMR studies for 5

Interconversion of the conformers for 5

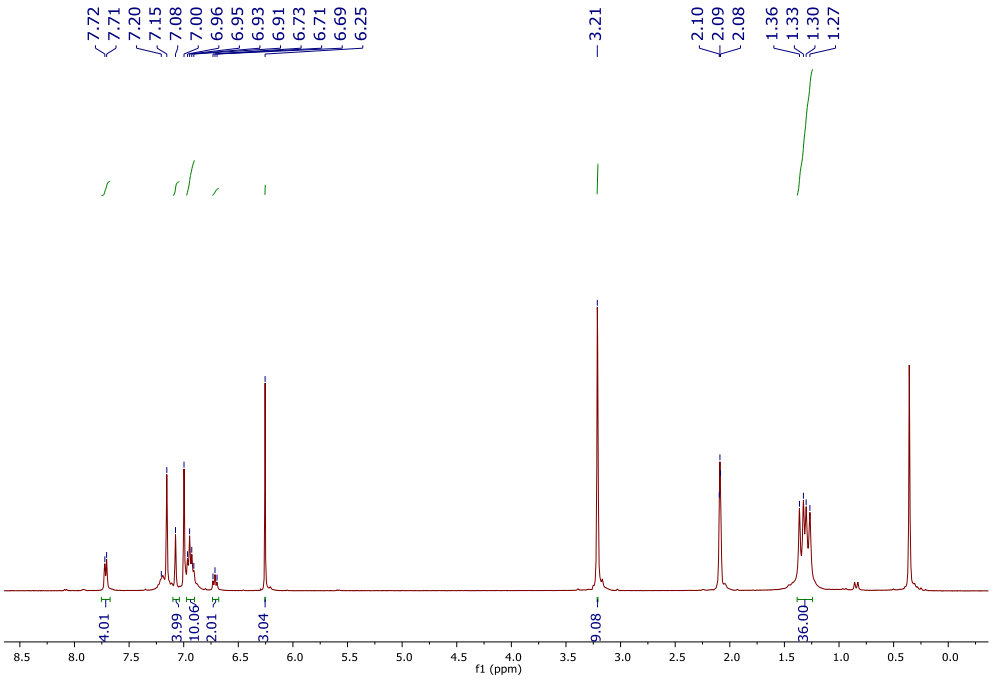


Figure S30. ^{1}H NMR of **5** at -70°C in C_7D_8, where only 1 conformer is observed

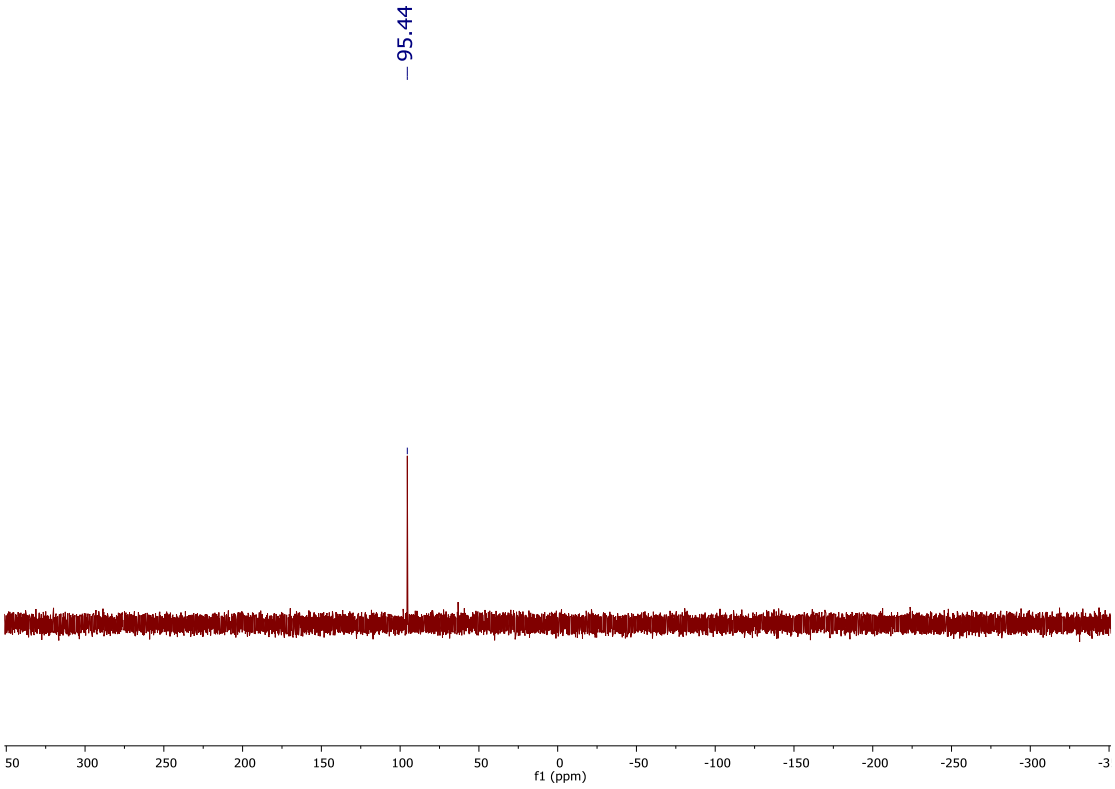
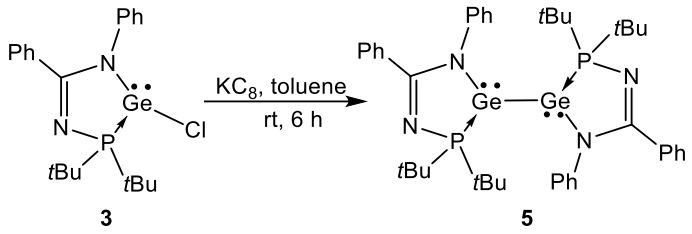


Figure S31. **^{31}P{**^{1}H} NMR of **5** at -70°C in C_7D_8, where only 1 conformer is observed



3 5

Table S1. ^{1}H NMR data and concentration of Conformer **A** and Conformer **B** at 25°C in C_7D_8.

Int (A)	Int (B)	Int (IS)	Time (min)	[A]/ mmol/L	[B]/ mmol/L
23.3	12.7	3.00	0	10.9	5.94
20.7	15.3	2.99	15	9.71	7.19
19.7	16.3	3.00	30	9.23	7.61
19.1	16.9	3.05	45	8.80	7.77
18.7	17.3	3.03	60	8.69	7.99
18.4	17.6	3.05	75	8.46	8.11
18.0	18.0	3.01	90	8.40	8.39

Conditions: C_7D_8 (0.6 mL), 1,3,5-trimethoxybenzene (internal standard: 0.0017g, 0.0168 mol/L), concentration of **5**: 0.0166 mol/L, under argon, 25°C (Int: integration; [**A**] and [**B**]: concentration of conformers **A** and **B**)

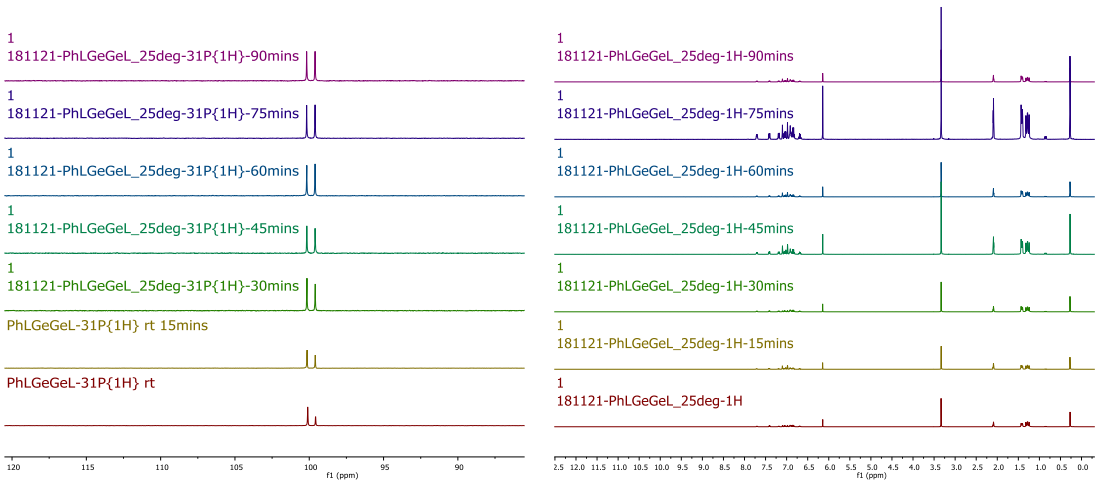


Figure S32. Stacked ^{1}H NMR and ^{31}P{^{1}H} spectra of the interconversion of the conformers for **5** at 25°C

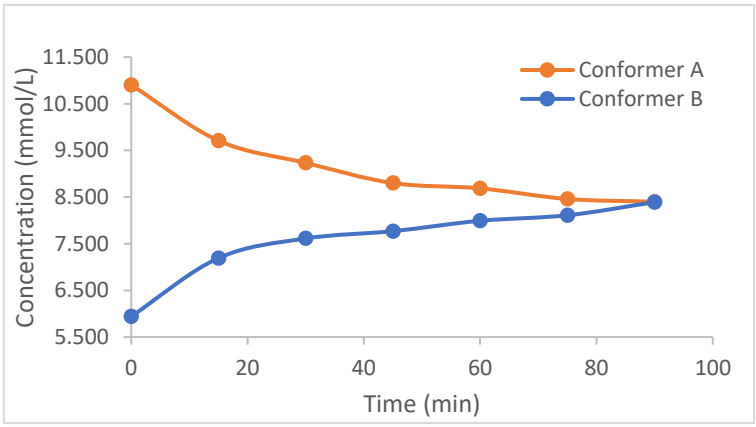


Figure S33. Concentration versus time plot of the interconversion of conformers **A** and **B** at 25°C

Table S2. Variable Temperature ^{1}H NMR data and Reaction Equilibrium Constant ***K*** of the above interconversion.

Int (**A**)	Int (**B**)	Int (IS)	T (K)	1/T (K^{-1})	[**A**]/ mmol/L	[**B**]/ mmol/L	*K*	ln*K*
34.2	1.78	3.00	263	0.00380	16.0	0.833	0.0520	-2.96
34.1	1.86	3.01	273	0.00366	15.9	0.867	0.0545	-2.91
32.2	3.83	2.99	283	0.00353	15.1	1.798	0.1191	-2.13
27.2	8.81	3.02	293	0.00341	12.6	4.095	0.3240	-1.13
23.3	12.70	3.00	298	0.00336	10.9	5.943	0.5451	-0.61

Condition: C_7D_8 (0.6 mL), 1,3,5-trimethoxybenzene (internal standard: 0.0017g, 0.0168 mol/L), concentration of **5**: 0.0166 mol/L, under argon, 25°C (Int: integration; [**A**] and [**B**]: concentration of conformers **A** and **B**; *K*: reaction equilibrium constant).

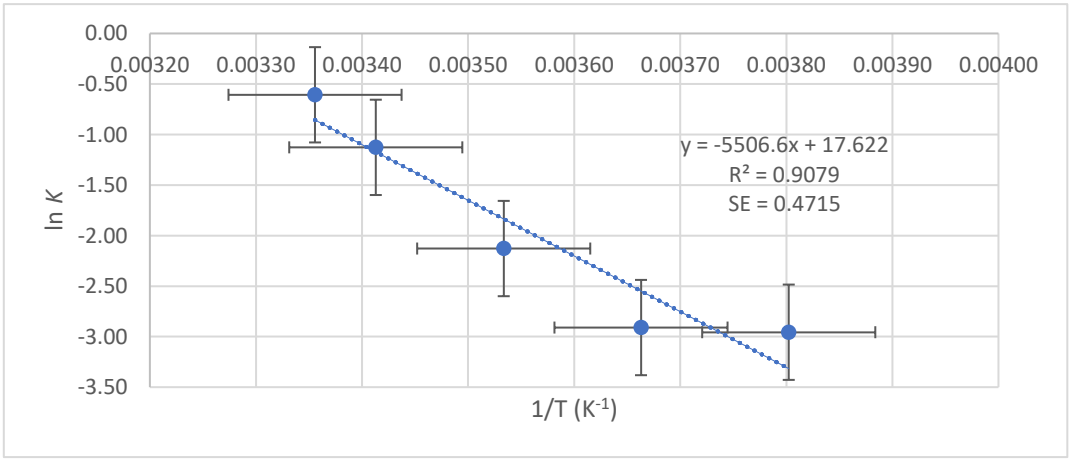


Figure S34. Plot of ln *K* versus T^{-1} for the interconversion

From the obtained linear equation, $\Delta H = 45.78\ \text{kJ/mol}, \Delta S = 146.52\ \text{J/mol.K}$
At 298.13K, $\Delta G = \Delta H - T\Delta S = 2.10\ \text{kJ/mol} = 0.50\ \text{kcal/mol}$

S4. Reversible Activation of Carbon Dioxide

The Reversible Activation of Carbon Dioxide by Compound 4.

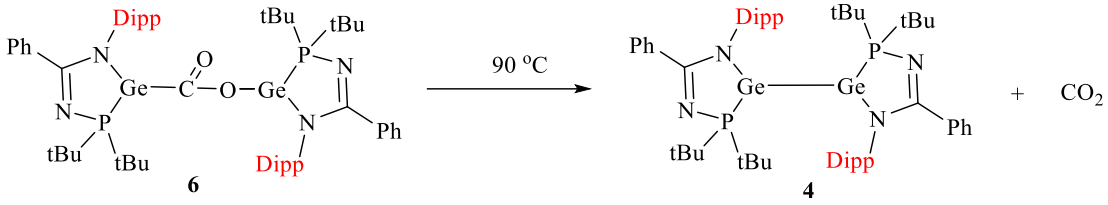


Table S3. ^{1}H NMR data and concentration of **4** [GeGe] and **6** [Ge-CO_2-Ge] at 90 °C in C_6D_6.

Int(Ge-CO_2-Ge)	Int(GeGe)	Int(Tol)	Time(min)	[GeGe]/mmol/L	[Ge-CO_2-Ge]/mmol/L
0.35	0.29	3	30	1.97	2.38
0.24	0.4	3	60	2.72	1.63
0.19	0.43	3	90	2.92	1.29
0.17	0.45	3	120	3.06	1.16
0.16	0.45	3	240	3.06	1.09
0.16	0.46	3	360	3.12	1.09

Condition: C_6D_6 (0.4 mL), Toluene (internal standard: 0.0010 g, 0.027 mol/L), concentration of Ge-CO_2-Ge (**6**): 4.58 mmol/L, under argon, 90 °C. (Int: integration; [GeGe] and [Ge-CO_2-Ge]: concentration of **4** and **6**).

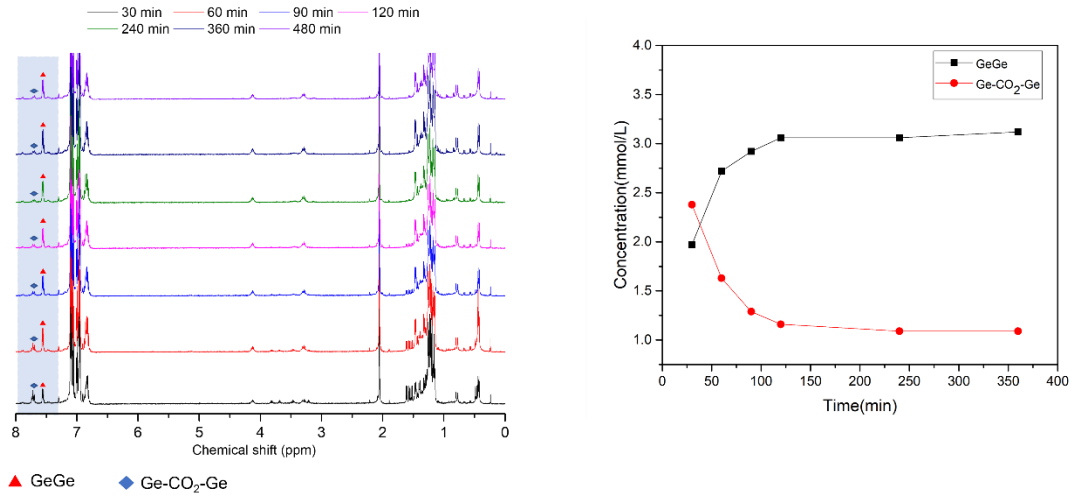


Figure S35. Stacked ^{1}H NMR spectrum and concentration versus time plot of the reversible activation of carbon dioxide by **4** at 90 °C in C_6D_6.

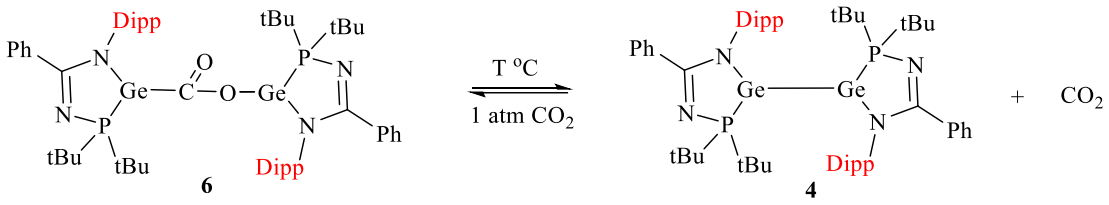


Table S4. Variable Temperature ^{1}H NMR data and Reaction Equilibrium Constant ***K*** of the above reversible reaction.

Int(Ge-CO_2-Ge)	Int(GeGe)	Int(Tol)	T °C/K	1/T K^{-1}	[GeGe]/mmol/L	[Ge-CO_2-Ge]/mmol/L	K	LnK
0.97	0.12	3	80/353	$2.83*10^{-3}$	1.67	13.31	0.125	-2.079
0.87	0.21	3	85/358	$2.79*10^{-3}$	2.86	12.02	0.24	-1.427
0.72	0.37	3	90/363	$2.75*10^{-3}$	5.02	9.83	0.51	-0.673
0.58	0.50	3	95/368	$2.72*10^{-3}$	6.83	8.03	0.85	-0.162
0.46	0.60	3	100/373	$2.68*10^{-3}$	8.31	6.29	1.32	0.277
0.34	0.71	3	105/378	$2.64*10^{-3}$	9.75	4.68	2.08	0.732

Condition: C_6D_6 (0.4 mL), Toluene (internal standard, 2 mg, 0.022 mmol, 55 mmol/L), Ge-CO_2-Ge (**6**, 6 mg, 0.006 mmol, 15 mmol/L), 1 atm CO_2. (Int: integration; [GeGe] and [Ge-CO_2-Ge]: concentration of **4** and **6**; *K*: reaction equilibrium constant).

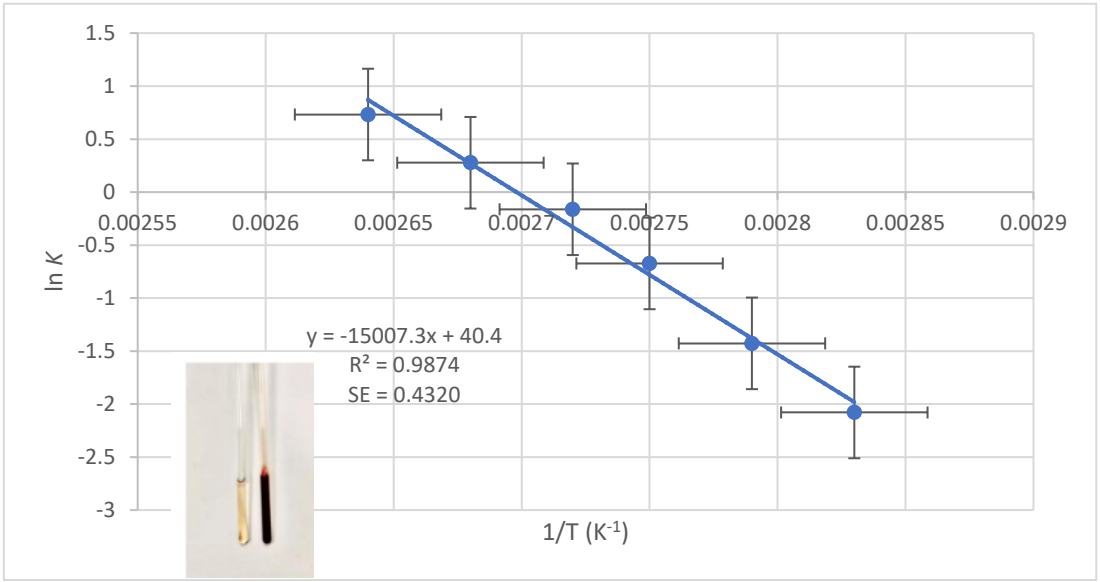


Figure S36. Plot of ln *K* versus T^{-1} for the above reversible reaction.

Y = aX + b; a = -15007.3, b = 40.4; ΔH = 124.8 kJ/mol, ΔS = 335.8 J/(mol*K)

At 298.15 K, $\Delta G = \Delta H - T\Delta S$ = 24.7 kJ/mol.

The Reaction of Compound 7 with Diphenylacetylene or C_6F_6

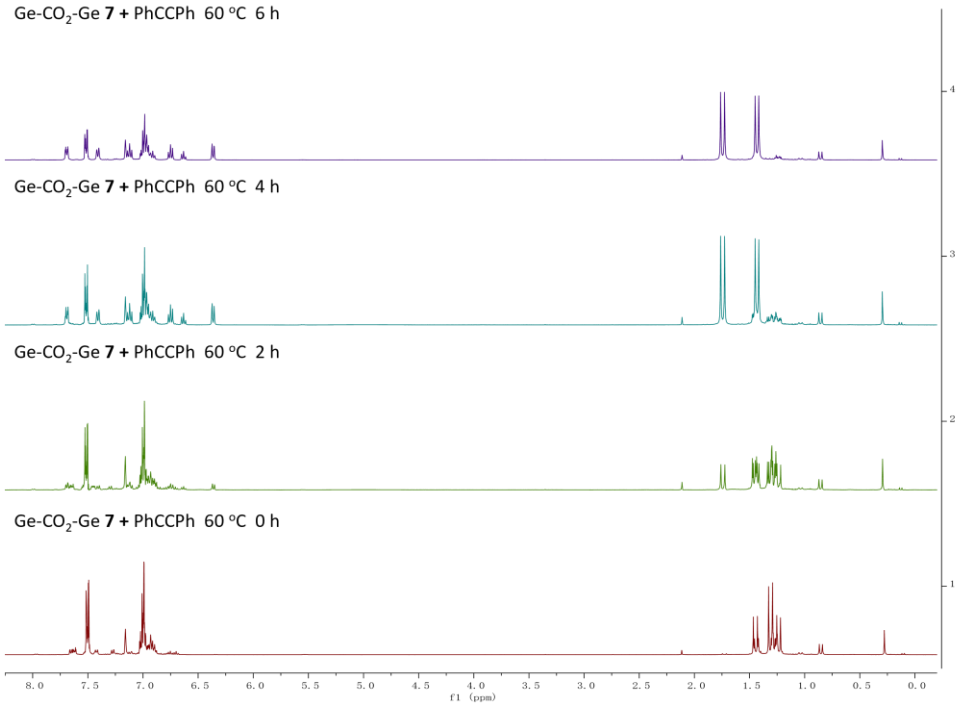


Figure S37. Stacked ^{1}H NMR spectrum of the reaction of compound **7** with diphenylacetylene.

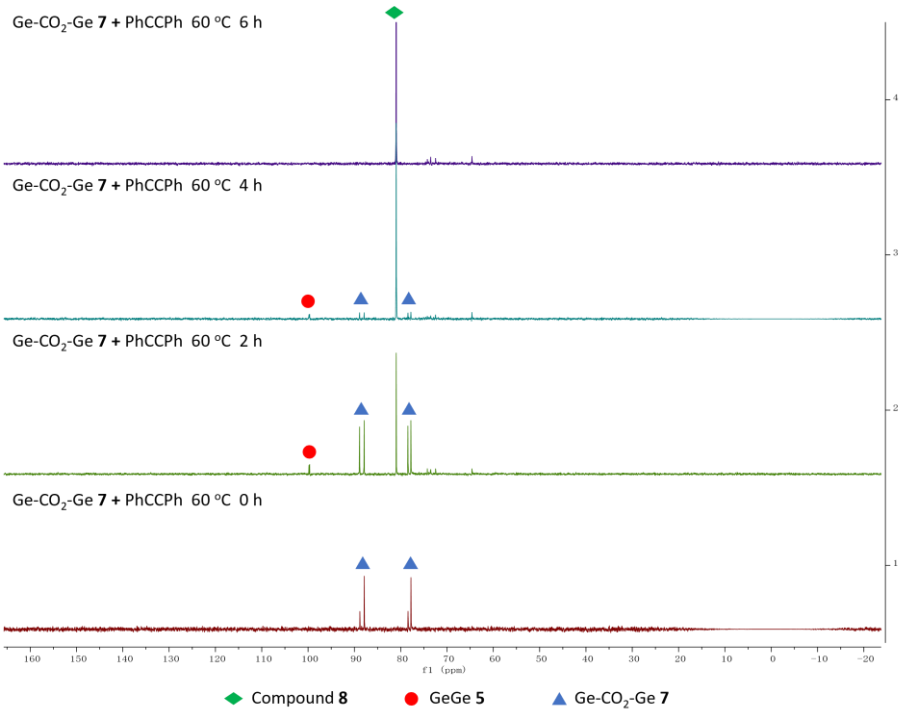


Figure S38. Stacked ^{31}P NMR spectrum of the reaction of compound **7** with diphenylacetylene.

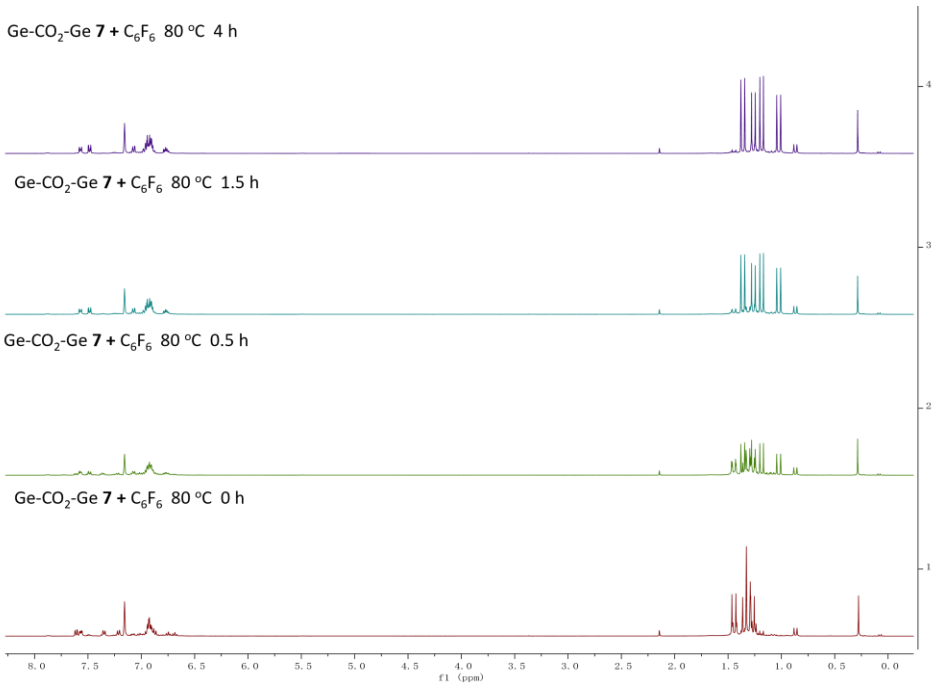


Figure S39. Stacked ^{1}H NMR spectrum of the reaction of compound **7** with C_6F_6

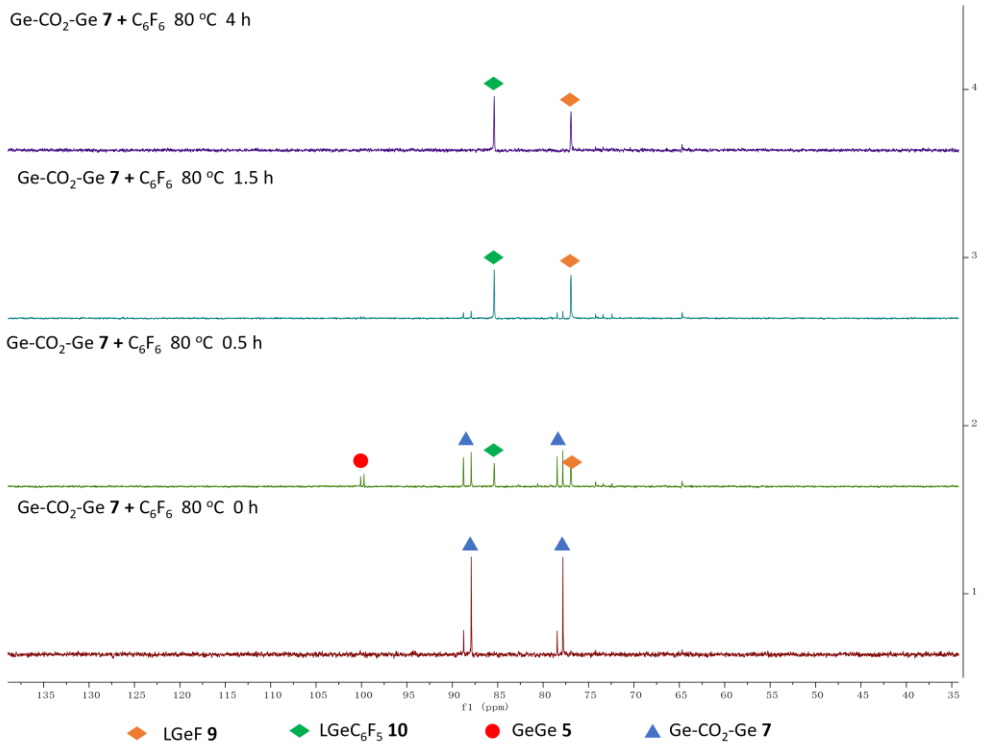
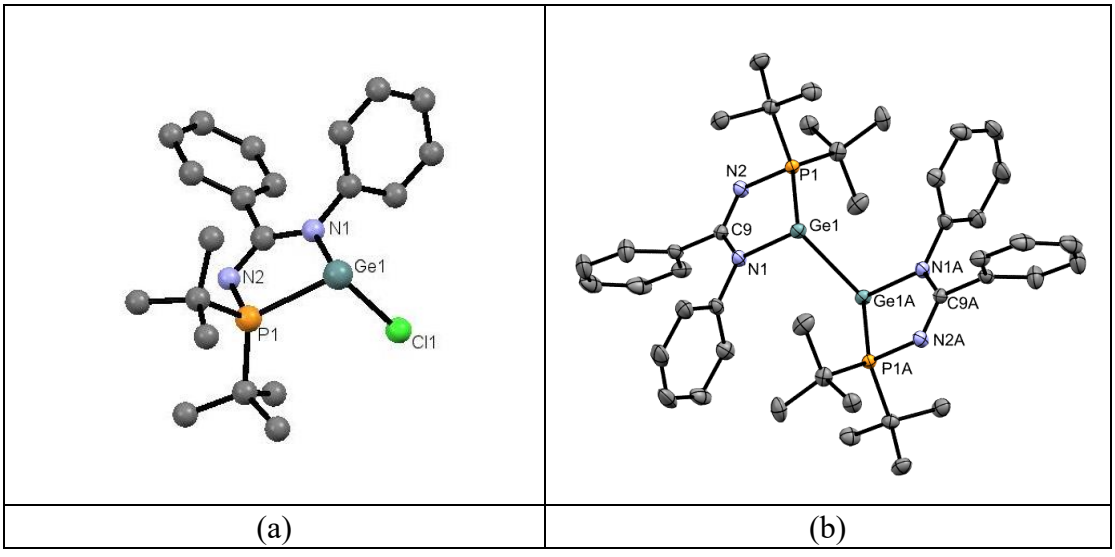


Figure S40. Stacked ^{31}P NMR spectrum of the reaction of compound **7** with C_6F_6

S5. X-ray Data Collection and Structural Refinement

X-ray data collection and structural refinement. The X-ray diffraction intensity data were measured at 100 K with a Bruker APEX II diffractometer equipped with a CCD detector, employing Mo K α radiation (λ = 0.71073 Å), with the SMART suite of programs.[4] All data were processed and corrected for Lorentz and polarization effects with SAINT and for absorption effects with SADABS. Structural solution and refinement were carried out with the SHELXTL suite of programs.[5] The structures were solved by direct methods to locate the heavy atoms, followed by difference maps for the light, non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic thermal parameters. The *R*1 ($I > 2\sigma(I)$) values of compounds **2**, **4** and **8** are larger than 0.07 probably due to crystal decomposition during the X-ray diffraction analysis. CCDC-2109346 **2**, CCDC-2109347 **3**, CCDC-2109348 **4**, CCDC- 2109349 **5**, CCDC-2109350 **6**, CCDC-2109351 **8** contain the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.



(a) (b)

Figure S41. Molecular structures of **3** and **5** obtained by X-ray crystallography. Thermal ellipsoids are shown at 30 % probability. All hydrogen atoms are removed for clarity. (a) Selected bond lengths (Å) and angles (deg) of **3**: Ge1-N1 1.997(4), Ge1-P1 2.4712(13), Ge1-Cl1 2.2914(12), P1-Ge1-N1 76.94(11), P1-Ge1-Cl1 100.57(4), N1-Ge1-Cl1 95.51(11). (b) Selected bond lengths (Å) and angles (deg) of **5**: Ge1-Ge1A 2.5854(5), Ge1-P1 2.4512(6), Ge1-N1 2.0217(19), P1-Ge1-N1 78.26(5), P1-Ge1-Ge1A 103.661(19), N1-Ge1-Ge1A 93.98(6).

Table S6. X-Ray crystallographic data for compounds **2 - 4.**

	2	**3**	**4**
Formula	$C_{27}H_{40}ClGeN_2P$	$C_{21}H_{28}ClGeN_2P$	$C_{54}H_{80}Ge_2N_4P_2$
Fw	531.62	447.46	992.34
T/K	100(2)	100(2)	100(2)
cryst system	orthorhombic	monoclinic	monoclinic
space group	*P n a* 21	*P* 1 21/*c* 1	*P* 1 21/*c* 1
a (Å)	15.8519(13)	14.931(2)	16.8440(6)
b (Å)	10.8312(8)	9.1937(13)	12.6688(6)
c (Å)	16.0462(12)	16.339(2)	25.5968(13)
α (deg)	90	90	90
β (deg)	90	107.054(5)	103.500(4)
γ (deg)	90	90	90
V (Å^3)	2755.1(4)	2144.3(5)	5311.3(4)
Z	4	4	4
d_{calcd} (g cm^{-3})	1.282	1.386	1.241
μ (mm^{-1})	1.284	1.635	2.240
F(000)	1120	928	2104
cryst size (mm)	0.12 x 0.22 x 0.24	0.02 x 0.16 x 0.20	0.01 x 0.04 x 0.10
2θ range (deg)	5.139< 2θ <56.21	5.141< 2θ <55.31	7.855< 2θ <132.9
index range	-	-	$-19 \le h \le 20$, $-14 \le k \le 15$, $-30 \le l \le 27$
no. of rflns collected	8578	6529	19270
no. of indep rflns	8578	6529	9112
*R*1, *wR*2 ($I > 2\sigma(I)$)	0.0891/0.2074	0.0594/0.1148	0.0888/0.2180
*R*1, *wR*2 (all data)	0.1342/0.2518	0.1112/0.1359	0.1434/0.2473
goodness of fit, F^2	0.993	1.013	1.076
no. of data/restraints/params	8578 / 1 / 300	6529 / 0 / 242	9112 / 0 / 579
largest diff peak and hole, eÅ^{-3}	1.278 and -1.638	0.764 and -1.232	2.064 and -1.161

Table S6. X-Ray data for compounds **5, 6** and **8.**

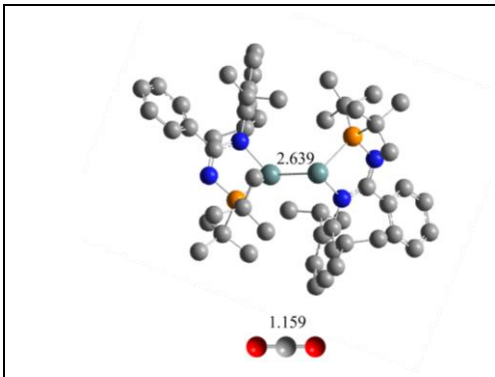
	5	**6**	**8**
Formula	$C_{42}H_{56}Ge_2N_4P_2$	$C_{55}H_{80}Ge_2N_4O_2P_2$	$C_{64.75}H_{76}Ge_2N_4P_2$
Fw	824.02	1036.35	1117.41
T/K	100(2)	100(2)	100(2)
cryst system	triclinic	monoclinic	triclinic
space group	*P* -1	*P* 1 *n* 1	*P* -1
a (Å)	9.0774(3)	13.5796(14)	12.3583(8)
b (Å)	10.8130(3)	13.6534(15)	19.8949(11)
c (Å)	12.0946(3)	15.0168(17)	24.9120(16)
α (deg)	66.6525(11)	90	102.273(3)
β (deg)	72.9065(10)	94.063(6)	98.169(4)
γ (deg)	80.3782(11)	90	89.971(3)
V (Å^3)	1040.04(5)	2777.2(5)	5921.5(6)
Z	1	2	4
d_{calcd} (g cm^{-3})	1.316	1.239	1.253
μ (mm^{-1})	1.555	2.192	1.111
F(000)	430	1096	2346
cryst size (mm)	0.14 x 0.20 x 0.24	0.10 x 0.12 x 0.20	0.04 x 0.20 x 0.24
2θ range (deg)	5.245< 2θ <60.69	8.485< 2θ <135.6	4.389< 2θ <52.03
index range	-13≤ *h* ≤13, -13≤ *k* ≤ 16, -15 ≤ *l* ≤18	-16 ≤ *h* ≤ 16, -16 ≤ *k* ≤ 16, -17 ≤ *l* ≤ 17	-
no. of rflns collected	29235	33072	25276
no. of indep rflns	7538	9654	25276
*R*1, *wR*2 (*I* > 2σ(*I*))	0.0499/0.0881	0.0582/0.1489	0.0921/0.1906
*R*1, *wR*2 (all data)	0.0877/0.1031	0.0643/0.1575	0.1420/0.2150
goodness of fit, F^2	1.050	1.030	1.060
no. of data/restraints/params	7538 / 0 / 232	9654 / 141 / 586	25276 / 2229 / 1242
largest diff peak and hole, eÅ^{-3}	1.467 and -0.710	0.755 and -0.768	1.569 and -1.780

S7. Theoretical Studies

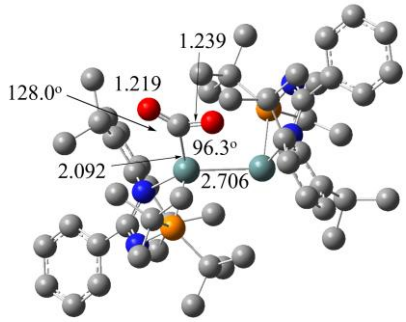
All geometry optimization and MO analysis were computed using the B3LYP-D3(BJ) functional with def2-TZVPP basis set as implemented in the Gaussian 09 package of programs.[6] The potential energy was refined by single point calculation with larger basis sets (def2-TZVPP). The vibrational frequency calculations were performed to establish the nature of stationary points. The local minima were confirmed by zero imaginary frequencies, and transition states were characterized by an imaginary frequency. In the free energy profile, the Gibbs free energy (ΔG) was calculated at 298.15 K and 1 atm.

List of colour coded atom used in optimised structures

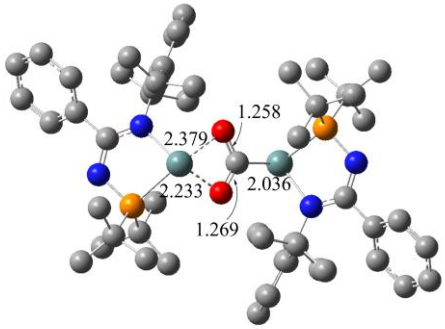
Abbreviation	Definition
Grey	Carbon
Blue	Nitrogen
Orange	Phosphorus
Red	Oxygen
Green	Germanium



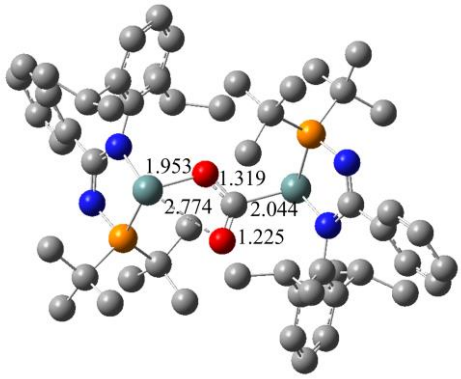
Compound **4** +CO_2



Int



TS



6

Figure S42. Optimised geometries of the minimal and transition states at (B3LYP-

D3(BJ)/ def2-TZVPP). Hydrogen atoms are omitted for clarity. The bond lengths displayed are measured in Angstroms (Å).

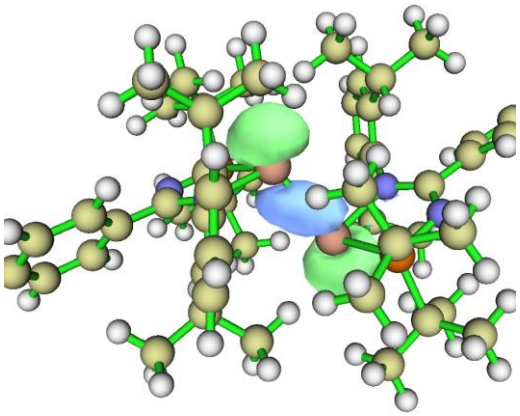
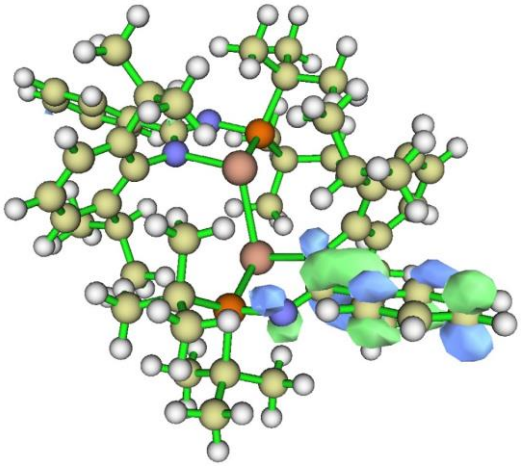
	
HOMO: -3.93 eV	LUMO: -1.05 eV

Figure S43. HOMO and LUMO of compound **4**.

Table S7

B3LYP-D3(BJ)/def2-TZVPP

Compound **4**

Sum of electronic and thermal Free Energies = -7163.189334 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	3.50979100	7.28081000	6.66780500
C	4.88364100	7.46026400	6.94607200
C	5.68468500	8.02287900	5.95625500
H	6.73894000	8.16334500	6.14125900
C	5.16171500	8.40021300	4.72787200
H	5.80757200	8.82779200	3.97254800
C	3.81078100	8.23887300	4.47853600
H	3.40569900	8.54843100	3.52541600
C	2.96317300	7.68773700	5.43625400
C	1.47971800	7.55927800	5.13754300
H	1.05557600	6.84909600	5.83763200
C	0.76609500	8.89007200	5.38500400
H	0.92383800	9.22535600	6.40900200
H	-0.30877300	8.78952100	5.22692500
H	1.13727400	9.66716500	4.71549600
C	1.19522300	7.02270900	3.73280700
H	1.48186100	7.73523500	2.95815100
H	0.12750300	6.83021000	3.61838600
H	1.72857200	6.09032300	3.55389500
C	5.49373700	7.01811200	8.27052800
H	4.80968100	7.33545100	9.05989100
C	5.60998800	5.49189100	8.38930400
H	4.64441000	5.00119000	8.30607100
H	6.03211100	5.22819000	9.36008900
H	6.26950500	5.08991000	7.61757100
C	6.84719600	7.65824600	8.57881900
H	7.63431800	7.28977000	7.91813200
H	7.13922700	7.40943500	9.59944500
H	6.81465400	8.74344900	8.49565300
C	2.11253900	5.44828800	7.41227000
C	2.41344100	4.63557200	6.18762200
C	3.66425900	4.55813800	5.57313500
H	4.50377100	5.09848700	5.97131300
C	3.84778300	3.78045900	4.43696600
H	4.82759300	3.73161700	3.98158600

C	2.78555800	3.07739700	3.88462900
H	2.92994200	2.48234100	2.99291000
C	1.53570300	3.14269400	4.49056100
H	0.69951200	2.59813900	4.07294100
C	1.35670700	3.90465800	5.63412900
H	0.39321300	3.94869200	6.11769200
C	1.01911700	4.75298600	11.04292100
C	2.47110200	4.26332600	10.91987500
H	2.73055100	3.71112300	11.82570300
H	3.16769200	5.09427400	10.81707500
H	2.59348400	3.60578600	10.06143100
C	0.10448900	3.53293500	11.17233300
H	0.09995900	2.93364400	10.26315500
H	-0.91813300	3.81376000	11.41457800
H	0.47096200	2.90477100	11.98761800
C	0.89308900	5.64982100	12.27813200
H	-0.12185700	6.00706400	12.43432300
H	1.54581700	6.51780600	12.21302600
H	1.18524700	5.08695600	13.16691700
C	-1.14771300	6.00068100	9.15449700
C	-1.84158200	4.67156400	8.82950300
H	-2.01913500	4.06511100	9.71176400
H	-1.25658600	4.08805900	8.12067500
C	-1.83404700	6.71696300	10.31519800
H	-2.85114200	6.99352100	10.02860300
H	-1.30789900	7.63138000	10.58089700
H	-1.89976200	6.08709500	11.20087700
C	-1.20842200	6.88093800	7.89686300
H	-0.73751100	6.38603800	7.04959000
H	-0.73084400	7.84610600	8.04937700
C	1.33376200	9.58085300	12.38666600
C	2.45372000	9.04192000	13.05477200
C	2.24242300	8.33304300	14.23764800
H	3.09414400	7.92646100	14.76509000
C	0.97429900	8.13892400	14.74816700
H	0.83444400	7.58669500	15.66786800
C	-0.12285800	8.64594300	14.06710800
H	-1.10996100	8.48223200	14.47160800
C	0.02536700	9.36908400	12.88801500
C	-1.20137000	9.96380000	12.20569000
H	-1.08411600	9.80205400	11.13179800
C	-1.31791600	11.48278200	12.40198100
H	-2.20516300	11.85335900	11.88636400

H	-0.46003400	12.01650500	12.00562600
H	-1.41871000	11.73097500	13.46023300
C	-2.51902800	9.30766200	12.62320400
H	-2.47861000	8.22179600	12.56129400
H	-2.79844200	9.57748300	13.64339100
C	3.89060600	9.22175800	12.58706800
H	3.87035800	9.75324200	11.63749700
C	4.59452200	7.87763600	12.35405200
H	4.69527900	7.31936500	13.28587800
H	5.59882000	8.04927100	11.96194800
H	4.05323400	7.26599900	11.63636400
C	4.71730100	10.04051200	13.59159300
H	4.24972000	10.98562200	13.84397100
H	5.70614100	10.24767500	13.17923800
H	4.85764400	9.47828200	14.51626000
C	2.06027600	11.59565000	11.23332200
C	3.58733900	11.26666000	6.34619800
H	4.58764900	11.16331600	5.92337900
H	3.05641700	12.01801900	5.76324800
H	3.08857400	10.30966600	6.21849100
C	4.51643800	10.60429900	8.57344500
H	5.51117700	10.55080100	8.13032400
H	4.06761400	9.61694800	8.50991300
H	4.62239000	10.86549300	9.62559400
Ge	2.34936000	7.55203000	9.47854200
Ge	0.77209400	9.66653100	9.37979100
N	2.66827800	6.66027000	7.63431100
N	1.23214200	4.90392700	8.22213400
N	1.49691100	10.37120300	11.20882100
N	2.31766500	12.28273500	10.14209200
P	0.68996100	5.79123000	9.51624700
P	2.01053800	11.62243400	8.65565900
H	-2.25525700	7.06172500	7.64392800
H	-2.81233600	4.88563700	8.37571500
C	2.45936300	12.29775400	12.49796600
C	1.80421500	12.16595500	13.72394000
C	3.55318800	13.16795100	12.42431600
C	2.23738100	12.87238200	14.83866900
H	0.95728200	11.51366300	13.82739000
C	3.99538200	13.85945300	13.54016900
H	4.05147700	13.28464300	11.47518900
C	3.33825700	13.71391300	14.75708800
H	1.71131600	12.75445800	15.77625000

H	4.85387400	14.51268700	13.46039200
H	3.67999400	14.25229800	15.63082400
C	3.69431600	11.65629000	7.81809800
C	4.39938500	13.01010100	7.97832000
H	5.45306000	12.88368200	7.71841600
H	3.99030700	13.77378600	7.32465300
H	4.34100000	13.36511900	9.00501800
H	-3.31910800	9.65208500	11.96739800
C	-0.31907700	13.05043100	8.90580800
C	0.76751300	12.78596600	7.85141700
H	-0.78538400	12.12463500	9.24058400
H	0.09047800	13.56336200	9.77327500
H	-1.09185800	13.68031500	8.45953300
C	1.38261900	14.12677300	7.44226300
C	0.12742900	12.10381500	6.63873800
H	2.06082200	14.02569800	6.59770900
H	0.58015300	14.80271600	7.13760200
H	1.91630400	14.59126300	8.26970900
H	-0.63520500	12.76310700	6.21830300
H	0.84938100	11.88883500	5.85424000
H	-0.35953200	11.17142200	6.92225000

Table S8

B3LYP-D3(BJ)/def2-TZVPP

CO_2

Sum of electronic and thermal Free Energies = -188.6715805 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	0.00000000	0.00000300	-0.00000500
O	1.15982400	-0.00000100	0.00000200
O	-1.15982400	-0.00000100	0.00000200

Table S9

B3LYP-D3(BJ)/def2-TZVPP

Int

Sum of electronic and thermal Free Energies = -7351.86604375 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.37946900	1.47156300	0.32679200
C	-3.59320500	2.31938100	-0.78292900
C	-3.96667200	3.64842400	-0.54502500
H	-4.13823500	4.31805200	-1.39008000
C	-4.12475100	4.12671800	0.75355500
H	-4.41917100	5.16548500	0.92207100
C	-3.90337300	3.27963900	1.83979600
H	-4.02966600	3.66564200	2.85172000
C	-3.52689500	1.94298100	1.65631300
C	-3.32492800	1.01454100	2.84612900
H	-2.46910000	0.36572100	2.63036400
C	-2.97776000	1.74061900	4.14808700
H	-2.17043700	2.47282000	4.00192100
H	-2.62768300	1.00491600	4.88659400
H	-3.84510000	2.26908600	4.57810900
C	-4.51920400	0.07258300	3.07320900
H	-5.44369100	0.63711700	3.28145400
H	-4.31494500	-0.57801900	3.93759300
H	-4.70301200	-0.58060200	2.21004200

C	-3.40517200	1.82088600	-2.20831900
H	-3.40477400	0.72587300	-2.18544200
C	-4.54539000	2.23990400	-3.14330600
H	-5.51971400	1.92888500	-2.73766900
H	-4.42029100	1.76806200	-4.13084800
H	-4.57120100	3.32972700	-3.30266000
C	-2.03172300	2.24467500	-2.74151200
H	-1.94132600	3.34132800	-2.78578200
H	-1.85450200	1.84398500	-3.75260300
H	-1.22911000	1.87088000	-2.08732000
C	-3.82914100	-0.82907000	-0.39786300
C	-5.25513400	-0.51857800	-0.76584300
C	-6.08483600	0.38050800	-0.07551100
H	-5.72469700	0.90334400	0.80397400
C	-7.39458400	0.60972700	-0.50274900
H	-8.02350400	1.30689100	0.05545300
C	-7.89656500	-0.03949200	-1.63227300
H	-8.91849200	0.15131700	-1.96875700
C	-7.08167000	-0.93940200	-2.32576800
H	-7.46271900	-1.45761200	-3.20894000
C	-5.78054600	-1.18296600	-1.88976600
H	-5.14266800	-1.89275500	-2.41544500
C	-1.23559300	-2.92007200	-2.17182500
C	-1.33452000	-1.62582500	-3.00176800
H	-1.01737000	-1.83829000	-4.03534800
H	-0.68538200	-0.82823300	-2.61556400
H	-2.36845100	-1.25243800	-3.03356600
C	-2.16024900	-3.96756200	-2.81209900
H	-3.21510300	-3.67302300	-2.72091300
H	-2.03735800	-4.96286700	-2.36992900
H	-1.91327500	-4.04800100	-3.88367500
C	0.21173800	-3.41772700	-2.11053600
H	0.28526600	-4.40473400	-1.63436200
H	0.87165600	-2.73127500	-1.56136300
H	0.61543500	-3.51178700	-3.13036200
C	-1.78437000	-3.83839000	0.81831300
C	-2.45098300	-5.11226200	0.28152500
H	-1.83836700	-5.61246100	-0.48052900
H	-3.44488500	-4.90127400	-0.13922900
C	-0.32967000	-4.10905300	1.23502900
H	-0.32416200	-4.76025400	2.12390600
H	0.21271000	-3.19040100	1.49423400
H	0.23988200	-4.61927200	0.44673600

C	-2.60377500	-3.31714500	2.01572700
H	-3.64259800	-3.11156600	1.72113300
H	-2.17269200	-2.41501000	2.46879700
C	3.33255500	-1.48081400	-0.19920100
C	3.53934300	-1.98677500	-1.51597000
C	3.70986800	-3.36359900	-1.70500200
H	3.84671300	-3.75000500	-2.71752500
C	3.72423300	-4.24118200	-0.62675600
H	3.84152800	-5.31583000	-0.78654800
C	3.63855000	-3.72663400	0.66322800
H	3.71794300	-4.40807800	1.51178100
C	3.46734000	-2.35814000	0.91926100
C	3.57176300	-1.92028200	2.37895600
H	3.25287900	-0.87513100	2.44763600
C	5.03323300	-2.04394200	2.85597800
H	5.14295100	-1.60348600	3.85961700
H	5.74377700	-1.54776200	2.18773100
H	5.32604100	-3.10470300	2.92318400
C	2.68800200	-2.72974200	3.34140100
H	1.63813500	-2.72114200	3.03817300
H	3.03385500	-3.77271200	3.42966000
C	3.70106500	-1.08223200	-2.73772600
H	3.59150800	-0.04479400	-2.39616300
C	2.65323200	-1.32852700	-3.83177600
H	2.71703600	-2.35735000	-4.22139500
H	2.81529400	-0.64197700	-4.67859500
H	1.63504000	-1.16461300	-3.45761400
C	5.11119700	-1.22083700	-3.34236900
H	5.90261400	-1.06248100	-2.59590200
H	5.25577000	-0.48424800	-4.14922900
H	5.26427100	-2.22229200	-3.77436500
C	3.61824100	0.87190400	0.53267700
C	1.07321300	3.88298000	-2.40037100
H	1.39773800	4.50485700	-3.25133800
H	0.23207100	4.39461500	-1.91471600
H	0.70675400	2.92959700	-2.80729500
C	3.36293500	2.89723100	-2.20425600
H	3.68575700	3.49729200	-3.07067200
H	2.99938300	1.93249600	-2.58777600
H	4.23629900	2.71450500	-1.56357700
Ge	-1.02796600	-0.34497500	0.42246400
Ge	1.13276900	0.40389100	-1.02426400
N	-2.99347100	0.11477800	0.11284900

N	-3.43725000	-2.05618300	-0.67062600
N	2.91638400	-0.11258000	-0.07234900
N	3.16696200	2.09865200	0.71703000
P	-1.82120600	-2.44665500	-0.44465600
P	1.72694500	2.55079300	-0.00553000
H	-2.61469200	-4.09902700	2.79255000
H	-2.57790400	-5.82074100	1.11655900
C	5.03499300	0.67985100	0.97704900
C	5.97607400	0.01994200	0.17711800
C	5.45690500	1.27207500	2.17791400
C	7.31386300	-0.05573700	0.57270700
H	5.66553200	-0.43277300	-0.75983200
C	6.78647400	1.17590800	2.58392700
H	4.72347200	1.80261800	2.78570300
C	7.72169800	0.51308700	1.78099300
H	8.03681600	-0.56905100	-0.06566900
H	7.09823300	1.62391200	3.53041300
H	8.76515000	0.44249200	2.09726200
C	2.25973900	3.66307100	-1.45287900
C	2.83400700	5.00236200	-0.97598700
H	3.28026200	5.52701100	-1.83743800
H	2.06054000	5.66061900	-0.55777300
H	3.62160200	4.85363800	-0.22371400
H	2.74260000	-2.28573100	4.34781900
C	0.32977600	2.41825000	2.33739400
C	0.78931500	3.48957800	1.33863500
H	1.14424600	1.74347600	2.63383900
H	-0.06062500	2.91125400	3.24068800
H	-0.48095700	1.80950600	1.92148000
C	-0.43325400	4.20761800	0.75710900
C	1.72741200	4.46313800	2.07203900
H	-0.15517800	5.05950500	0.11979100
H	-1.07489300	3.52695700	0.17692000
H	-1.05150100	4.59737700	1.58087500
H	2.64844500	3.95467800	2.38842200
H	2.00066100	5.33272900	1.46457600
H	1.20746900	4.83450400	2.97036800
C	-0.22938500	-0.73977100	2.31607500
O	0.94814100	-0.85487500	1.94640300
O	-0.82041200	-0.81889900	3.37931800

Table S10

B3LYP-D3(BJ)/def2-TZVPP

TS

Sum of electronic and thermal Free Energies = -7351.85820575 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-3.47275800	1.61584900	0.22916700
C	-3.37554400	2.16650800	-1.06401800
C	-3.36990300	3.55130300	-1.20113900
H	-3.29501700	3.98092600	-2.19091500
C	-3.44132200	4.38930200	-0.10112000
H	-3.42594400	5.46336100	-0.23009500
C	-3.53298400	3.83821500	1.16524300
H	-3.59301000	4.49125200	2.02547300
C	-3.55477200	2.45878700	1.35490600
C	-3.68102800	1.92857100	2.77366000
H	-3.72354200	0.84153700	2.72325600
C	-2.46137400	2.31150700	3.62162800
H	-2.39939600	3.39365200	3.74811700
H	-1.53775800	1.97411200	3.15401000
H	-2.52625200	1.85993400	4.61309400
C	-4.97518600	2.39794800	3.45189000
H	-5.05545700	1.96757800	4.45152400
H	-5.85746300	2.09764400	2.88678000
H	-4.99968600	3.48351400	3.55428200
C	-3.26028600	1.32079100	-2.31804700
H	-3.28978500	0.27601000	-2.02493300
C	-4.43095400	1.57232700	-3.27784300
H	-5.39085400	1.44526000	-2.78255600
H	-4.38659000	0.87833200	-4.11903600
H	-4.39170600	2.58489300	-3.68243300
C	-1.92200900	1.54790300	-3.03195300
H	-1.82380900	0.86742600	-3.87953300
H	-1.08847200	1.38307900	-2.35543300
H	-1.84888000	2.56752200	-3.41401000
C	-4.29908000	-0.68281300	-0.04269800
C	-5.63749100	-0.23860600	-0.53547300
C	-6.33118700	0.83666500	0.01835700
H	-5.89933400	1.39817600	0.82835300
C	-7.58137300	1.19465200	-0.46839600
H	-8.10729100	2.02896400	-0.02454400

C	-8.15047900	0.49096000	-1.52221200
H	-9.11881200	0.77933100	-1.90856600
C	-7.46980800	-0.58911000	-2.07447600
H	-7.90667000	-1.14479000	-2.89321900
C	-6.22937600	-0.95650400	-1.57738100
H	-5.69694600	-1.80023700	-1.98884000
C	-2.92691700	-3.72378500	1.79979200
C	-3.86138500	-2.96601100	2.75818300
H	-4.81817400	-2.74954300	2.28783000
H	-3.42347600	-2.02591900	3.09718600
H	-4.03607800	-3.58377200	3.64140100
C	-1.60058200	-4.01398800	2.51666500
H	-1.11528800	-3.09758900	2.85295700
H	-0.89760200	-4.55155400	1.88460500
H	-1.79654100	-4.62902400	3.39777900
C	-3.60658000	-5.02906000	1.37992000
H	-3.92088200	-5.57096300	2.27519900
H	-2.93062100	-5.67750700	0.82687500
H	-4.49019200	-4.84227400	0.77139400
C	-1.87331400	-3.35676400	-1.14328900
C	-2.83912600	-4.37327100	-1.76625200
H	-2.47580000	-4.63088700	-2.76383400
H	-3.84007100	-3.95627100	-1.86639000
H	-2.90272400	-5.29308700	-1.19276000
C	-0.51995700	-3.99846900	-0.82537300
H	-0.62729400	-4.88426500	-0.20063800
H	0.15658200	-3.30006900	-0.33784200
H	-0.04809800	-4.31415900	-1.75788900
C	-1.67584700	-2.21197100	-2.15173900
H	-1.01155200	-1.44443600	-1.76919400
H	-2.62707700	-1.75693600	-2.42095400
H	-1.22989100	-2.62253100	-3.05963100
C	0.30570800	0.26451900	-0.17945900
O	-0.59732800	1.11381900	0.03501800
O	0.15174500	-0.92412300	0.23953900
C	3.32833700	-1.61406200	-0.43936400
C	3.33996600	-2.35855400	-1.63745100
C	3.20126000	-3.74228300	-1.57245000
H	3.20712500	-4.31664100	-2.48897100
C	3.06736200	-4.39696900	-0.36068700
H	2.96046000	-5.47300900	-0.32890900
C	3.07285300	-3.65937100	0.81030200
H	2.97211500	-4.17003300	1.75828600

C	3.19597500	-2.27242600	0.80172200
C	3.19871400	-1.55274300	2.13812400
H	3.29206600	-0.48780700	1.94935300
C	1.88920700	-1.76002300	2.90836000
H	1.03715400	-1.44974500	2.31206900
H	1.90045900	-1.17944400	3.83248200
H	1.75372800	-2.80875200	3.17817000
C	4.39276400	-1.98687400	3.00084600
H	4.45103700	-1.37375000	3.90168100
H	5.33428400	-1.89478000	2.46556800
H	4.28414100	-3.02638100	3.31428800
C	3.53160400	-1.71920600	-3.00297900
H	3.66758000	-0.64928600	-2.85834400
C	4.78899600	-2.24378200	-3.70974900
H	5.68509600	-2.08008800	-3.11118800
H	4.92562400	-1.73175000	-4.66360800
H	4.71645400	-3.31283800	-3.91344400
C	2.29575900	-1.91560100	-3.88948200
H	2.13052200	-2.97328300	-4.10170200
H	2.42026200	-1.39599300	-4.84082900
H	1.40118000	-1.52390400	-3.40731000
C	4.32006000	0.58635600	0.05609000
C	5.62867000	0.01929000	0.49350000
C	6.27569400	0.60145300	1.58580100
H	5.80315600	1.43704600	2.07904500
C	7.49468800	0.11238600	2.02808900
H	7.97575300	0.56357400	2.88538100
C	8.09748500	-0.95568800	1.37175300
H	9.04868400	-1.33904200	1.71570500
C	7.47342000	-1.52422700	0.26834100
H	7.93963900	-2.34722500	-0.25603600
C	6.24537400	-1.04345000	-0.16567900
H	5.76988500	-1.49847600	-1.01729700
C	2.02065300	3.24584500	1.45226200
C	3.02804800	4.13869900	2.19110900
H	2.67486500	4.28312600	3.21462800
H	3.12920500	5.11955400	1.73859400
H	4.01115600	3.67214500	2.23535000
C	1.76932800	2.01174700	2.33327600
H	2.69847000	1.48647500	2.54512500
H	1.06646200	1.31722300	1.88794400
H	1.34833000	2.34667600	3.28310400
C	0.70106700	3.98345200	1.20195900

H	0.24339900	4.22649200	2.16344400
H	-0.00570700	3.37042900	0.64507600
H	0.85762200	4.92117800	0.67072600
C	3.12657200	3.93286400	-1.40786200
C	1.82994100	4.34096200	-2.12145900
H	1.11398300	4.80617500	-1.44749600
H	1.34546700	3.48492600	-2.59148000
H	2.06697900	5.06171100	-2.90702100
C	3.80988600	5.16176400	-0.80279400
H	4.15929300	5.80520700	-1.61339000
H	4.67244400	4.88541700	-0.19830200
H	3.12637900	5.74877500	-0.19363200
C	4.08418900	3.29415200	-2.42725600
H	4.29211200	4.02262800	-3.21362000
H	3.64791700	2.41254300	-2.89672700
H	5.02310400	3.00648000	-1.95875300
Ge	-1.70527600	-0.48774500	1.40164200
Ge	1.82363300	0.76911300	-1.44050000
N	-3.38844900	0.20241600	0.42050500
N	-4.09319400	-1.98284500	-0.10097200
N	3.37009900	-0.18754900	-0.50700900
N	4.18027800	1.88382400	0.24967500
P	-2.60222600	-2.54663900	0.38148600
P	2.73209000	2.59067100	-0.15951200

Table S11

B3LYP-D3(BJ)/def2-TZVPP

Compound **6**

Sum of electronic and thermal Free Energies = -7351.8680856 Hartree

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	3.54029300	-1.55621300	0.32198400
C	3.38578500	-2.12581500	-0.95805300
C	3.34894500	-3.51337100	-1.06946900
H	3.22969200	-3.95873600	-2.04794400
C	3.45306700	-4.33277500	0.04199900
H	3.41549100	-5.40841100	-0.06726700
C	3.60684500	-3.76265700	1.29442100
H	3.69448800	-4.40250400	2.16218500
C	3.65586000	-2.38115100	1.45997100
C	3.85935300	-1.82140100	2.85863100
H	3.91603100	-0.73706900	2.77800800
C	2.67965700	-2.16172400	3.77776700
H	2.59049600	-3.24049100	3.91719900
H	1.74176500	-1.79355300	3.36466100
H	2.81672900	-1.70669500	4.76011000
C	5.17745600	-2.30147900	3.48169800
H	5.31892000	-1.84496200	4.46266600
H	6.03586900	-2.03861000	2.86378800
H	5.18331600	-3.38397900	3.61481100
C	3.25761800	-1.29538400	-2.22119400
H	3.32870800	-0.24800200	-1.94669600
C	4.39076400	-1.59742100	-3.21037300
H	5.36808300	-1.48946100	-2.74469900
H	4.34102600	-0.91512000	-4.06049600
H	4.31150800	-2.61438300	-3.59764300
C	1.89038200	-1.48821000	-2.88354700
H	1.79164100	-0.83452000	-3.75171200
H	1.09218800	-1.25190300	-2.18496300
H	1.75936400	-2.51618600	-3.22327500
C	4.36280300	0.73669200	-0.03982700
C	5.68587100	0.28336100	-0.56199000
C	6.39724100	-0.77509600	0.00194600
H	5.99405300	-1.30679100	0.84622300
C	7.62852800	-1.15273400	-0.51673200
H	8.16911600	-1.97325300	-0.06461400

C	8.16064100	-0.48490500	-1.61265400
H	9.11442200	-0.78792800	-2.02321200
C	7.46228200	0.57834500	-2.17575800
H	7.87104800	1.10603300	-3.02694700
C	6.24043800	0.96489700	-1.64783500
H	5.69409300	1.79513100	-2.06873800
C	2.94850600	3.78656400	1.74357900
C	3.89696900	3.05477800	2.70854800
H	4.85357600	2.84064900	2.23649500
H	3.47132800	2.11725900	3.06841500
H	4.07055400	3.69076600	3.57881000
C	1.61780000	4.06556500	2.45750500
H	1.13604400	3.14597800	2.78884900
H	0.91299000	4.59913400	1.82468900
H	1.80929500	4.68081300	3.33938800
C	3.60890800	5.09672200	1.30792200
H	3.89787300	5.66113400	2.19765700
H	2.92954500	5.72133100	0.73188400
H	4.50605600	4.91588000	0.71760900
C	1.92918100	3.41268100	-1.20148500
C	2.94745800	4.35785000	-1.85482000
H	2.58225200	4.62209200	-2.85001300
H	3.91853800	3.87751600	-1.96324500
H	3.07843900	5.28023800	-1.29670000
C	0.62173600	4.14669600	-0.88758000
H	0.79557800	5.04134200	-0.29090900
H	-0.09084000	3.50817800	-0.36847500
H	0.16474100	4.46644100	-1.82667100
C	1.65851300	2.25983200	-2.18279100
H	0.97660700	1.51932900	-1.78021600
H	2.58339600	1.75646300	-2.45923600
H	1.21520800	2.67136100	-3.09106300
C	-0.50531000	0.44088700	-0.03571400
O	0.66487700	-0.16891300	-0.00597600
O	-0.69714500	1.47126700	0.59914600
C	-3.81412400	1.50324200	-0.26580100
C	-3.95314700	2.35070900	-1.38449700
C	-4.10786100	3.71894700	-1.17805400
H	-4.21005300	4.37394000	-2.03300300
C	-4.14820300	4.25380200	0.09765700
H	-4.27062300	5.31919900	0.24066900
C	-4.03914300	3.40942500	1.18921600
H	-4.07820800	3.82614700	2.18635300

C	-3.86517300	2.03663500	1.03974000
C	-3.75901900	1.19513800	2.29934600
H	-3.60310400	0.16140900	2.00571200
C	-2.56522700	1.59790500	3.17510000
H	-1.63623900	1.55331000	2.61492000
H	-2.49425100	0.92957800	4.03573400
H	-2.68521600	2.61341200	3.55673300
C	-5.05774500	1.26262400	3.11760300
H	-5.01625300	0.55982800	3.95173200
H	-5.93115600	1.02431800	2.51555800
H	-5.19822400	2.26194700	3.53286600
C	-3.97925400	1.83268400	-2.81359400
H	-3.87898800	0.74948900	-2.78176900
C	-5.31274300	2.14368500	-3.50788000
H	-6.15821700	1.72686400	-2.96041600
H	-5.32277700	1.71913600	-4.51315800
H	-5.47386700	3.21866800	-3.59835600
C	-2.80714600	2.38466900	-3.63461100
H	-2.87612800	3.46907600	-3.73599400
H	-2.80410700	1.95183100	-4.63639200
H	-1.85331700	2.14912100	-3.16367700
C	-4.28101400	-0.90146500	-0.01710400
C	-5.69719600	-0.69883900	0.40496400
C	-6.22143500	-1.52052900	1.40521200
H	-5.58003700	-2.26790700	1.84662000
C	-7.53430100	-1.37372700	1.82440400
H	-7.92128500	-2.00663400	2.61167300
C	-8.35168900	-0.41481700	1.23507900
H	-9.37646700	-0.29834400	1.56140300
C	-7.84577800	0.38993200	0.22170400
H	-8.47659200	1.13085800	-0.25027700
C	-6.52629600	0.25246400	-0.18790900
H	-6.14441400	0.88806100	-0.96811800
C	-1.43602900	-3.09044500	1.20514900
C	-2.22007800	-4.24600500	1.84335400
H	-1.84353800	-4.40041800	2.85705900
H	-2.10204900	-5.18022600	1.30461200
H	-3.28183200	-4.01290500	1.90878500
C	-1.46138000	-1.91671000	2.19614600
H	-2.48273700	-1.63034100	2.43869700
H	-0.93908100	-1.04203300	1.82547600
H	-0.97121800	-2.23158800	3.11917500
C	0.01119000	-3.49518700	0.91415300

H	0.51908300	-3.71533300	1.85421000
H	0.56689000	-2.69962400	0.42091600
H	0.06855900	-4.39110400	0.29884200
C	-2.35645400	-3.73262300	-1.72752700
C	-1.00896800	-3.77537900	-2.45868900
H	-0.19278600	-4.09519900	-1.81432700
H	-0.75184100	-2.80071600	-2.87006800
H	-1.07553900	-4.48098900	-3.28987300
C	-2.74538200	-5.13211200	-1.24403100
H	-2.95151500	-5.75957400	-2.11415200
H	-3.64179700	-5.11008800	-0.62613700
H	-1.94263900	-5.60680100	-0.68403000
C	-3.43793400	-3.23276700	-2.69960900
H	-3.47461900	-3.90821300	-3.55679800
H	-3.21633800	-2.23271500	-3.07245900
H	-4.41667700	-3.21473300	-2.22505900
Ge	1.79427800	0.56008500	1.41200600
Ge	-1.78161500	-0.35154100	-1.42318500
N	3.48356100	-0.14041600	0.49289600
N	4.13220700	2.02861700	-0.14188200
N	-3.53060700	0.11845600	-0.47684800
N	-3.84184300	-2.14226400	0.07591200
P	2.63883100	2.59850500	0.33204400
P	-2.26901500	-2.45816300	-0.35391800

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