

Supporting Information

**Reversible and Irreversible [2+2] Cycloaddition Reactions of
Heteroallenes to a Gallaphosphene**

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Supporting Information

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6. References

1. Experimental Section

General procedure. All experiments and manipulations were carried out under a dry argon atmosphere using either standard Schlenk or glovebox techniques. Toluene, benzene, and *n*-hexane were dried using an MBraun solvent drying system (SPS), degassed, and stored over 4Å molecular sieve. Deuterated solvents (C_6D_6 , toluene- d_8) were dried by refluxing over NaK alloy, distilled prior to use, and stored over 4Å molecular sieve. Commercial reagents were purchased from Aldrich, Acros, or Alfa-Aesar Chemical Co. and used as received. LGa(Cl)PLGa **1** ($L = HC[C(Me)N(Ar)]_2$, $Ar = 2,6\text{-}iPr_2\text{-}C_6H_3$), was prepared by literature method.^[1] NMR spectra (δ in ppm) were recorded using a Bruker Avance DPX 300 (1H 300 MHz, $^{13}C\{^1H\}$ 75 MHz, $^{31}P\{^1H\}$ 121 MHz), a Bruker Avance II 500 (1H 500 MHz, $^{13}C\{^1H\}$ 126 MHz, $^{31}P\{^1H\}$ 202 MHz), or a Bruker Avance III HD 600 (1H 600 MHz, $^{13}C\{^1H\}$ 151 MHz, $^{31}P\{^1H\}$ 243 MHz) spectrometer and were referenced to internal C_6D_5H (1H $\delta = 7.16$; ^{13}C $\delta = 128.06$) or C_7D_7H (1H $\delta = 2.08, 6.97, 7.01, 7.09$; ^{13}C $\delta = 137.48, 128.87, 127.96, 125.13, 20.43$), the ^{31}P NMR spectra are referenced to internal C_6D_5H (1H $\delta = 7.16$) or C_7D_7H (1H $\delta = 2.08, 6.97, 7.01, 7.09$) using chi-values (χ).^[2] Elemental analyses were performed at the *Elementaranalyse Labor* of the University of Duisburg-Essen. IR spectra were recorded by a Bruker ALPHA-T FT-IR spectrometer equipped with a single-reflection ATR sampling module.

Synthesis of 2: *N,N'*-diisopropylcarbodiimide (45 mg, 0.29 mmol) was added to a toluene solution (10 mL) of **1** (300 mg, 0.29 mmol). After shaking the reaction mixture at ambient temperature for one minute, all volatiles were removed under vacuum to yield a colorless crystalline solid. Yield: 99% (330 mg). M.p. 91 °C (dec.). Single crystals suitable for X-ray diffraction were grown by cooling a toluene solution of **2** at -30 °C for 12 h. Anal. calcd. (%) for $C_{65}H_{96}ClGa_2N_6P$ (1164.56): C, 66.88; H, 8.29; N, 7.20. Found: C, 66.95; H, 8.37; N, 7.31. 1H NMR (600 MHz, C_6D_6 , 298 K) $\delta = 0.85$ (d, $^3J_{HH} = 6.7$ Hz, 6H, $CH(CH_3)_2$), 0.91 (d, $^3J_{HH} = 6.8$ Hz, 6H, $CH(CH_3)_2$), 0.98 (d, $^3J_{HH} = 6.7$ Hz, 6H, $CH(CH_3)_2$), 1.06 (d, $^3J_{HH} = 6.8$ Hz, 6H, $CH(CH_3)_2$), 1.22 (d, $^3J_{HH} = 6.7$ Hz, 6H, $CH(CH_3)_2$), 1.24 (d, $^3J_{HH} = 6.8$ Hz, 6H, $CH(CH_3)_2$), 1.31 (s, 6H, CCH_3), 1.39 (d, $^3J_{HH} = 6.0$ Hz, 6H, $NCH(CH_3)_2$), 1.50 (d, $^3J_{HH} = 6.7$ Hz, 6H, $CH(CH_3)_2$), 1.52 (s, 6H, CCH_3), 1.54 (d, $^3J_{HH} = 6.7$ Hz, 6H, $CH(CH_3)_2$), 1.61 (d, $^3J_{HH} = 6.4$ Hz, 6H, $NCH(CH_3)_2$), 2.98 (sept, $^3J_{HH} = 6.0$ Hz, 1H, $NCH(CH_3)_2$), 3.04 (sept, $^3J_{HH} = 6.7$ Hz, 2H, $CH(CH_3)_2$), 3.25 (sept, $^3J_{HH} = 6.7$ Hz, 2H, $CH(CH_3)_2$), 3.49 (sept, $^3J_{HH} = 6.8$ Hz, 2H, $CH(CH_3)_2$), 3.54 (sept, $^3J_{HH} = 6.8$ Hz, 2H, $CH(CH_3)_2$), 4.23 (sept, $^3J_{HH} = 6.3$ Hz, 1H, $NCH(CH_3)_2$), 4.71 (s, 1H, CH), 4.76 (s, 1H, CH), 6.90 (t, $^3J_{HH} = 7.6$ Hz, 2H, C_6H_3), 6.99-7.02 (m, 3H, C_6H_3), 7.12-7.14 (m, 2H, C_6H_3), 7.16-7.17 (m, 3H, C_6H_3), 7.19 (t, $^3J_{HH} = 7.6$ Hz, 2H, C_6H_3). $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6 , 298 K) $\delta = 21.6, 24.5, 24.8, 24.9, 25.0, 25.4, 25.6, 25.7, 25.9, 26.6, 27.1$

(CH(CH₃)₂); 28.1, 28.3, 28.4, 28.6, 29.4, 29.6 (CH(CH₃)₂); 48.7 (d, ³J_{PC} = 5.4 Hz, NCH(CH₃)₂), 62.3 (d, ³J_{PC} = 13.8 Hz, NCH(CH₃)₂); 98.1, 98.2 (CH); 124.0, 125.0, 125.8, 127.3, 128.8, 129.5, 138.0, 143.4, 144.0, 144.4, 144.8, 145.9 (C₆H₃); 166.8 (d, ¹J_{PC} = 38.7 Hz, CNCH(CH₃)₂); 170.1, 171.5 (C₆H₃). ³¹P{¹H} (243 MHz, C₆D₆, 298 K) δ = -108.6 ppm. ATR-IR: ν 2960, 2921, 2864, 1573, 1524, 1463, 1386, 1314, 1254, 1209, 1168, 1106, 1018, 938, 859, 793, 757, 729, 695, 620, 581, 527 cm⁻¹.

Synthesis of 3: Compound **3** was synthesized by following the similar protocols used for **2** using *N,N*-dicyclohexylcarbodiimide (59 mg, 0.29 mmol), **1** (300 mg, 0.29 mmol), and toluene (10 mL). Yield: 99% (358 mg, colorless solid). M.p. 93 °C (dec.). Anal. calcd. (%) for C₇₁H₁₀₄ClGa₂N₆P (1244.63): C, 68.36; H, 8.40; N, 6.74. Found: C, 68.47; H, 8.51; N, 6.89. ¹H NMR (600 MHz, toluene-d₈, 298 K) δ = 0.89 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 0.95 (d, ³J_{HH} = 6.6 Hz, 12H, CH(CH₃)₂), 1.01 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.10 (d, ³J_{HH} = 6.7 Hz, 2H, CyH), 1.15 (d, ³J_{HH} = 6.7 Hz, 2H, CyH), 1.18 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 1.25 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.31 (d, ³J_{HH} = 12.4 Hz, 3H, CyH), 1.36 (s, 6H, CCH₃), 1.42 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 1.45 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 1.49-1.52 (m, 3H, CyH), 1.57 (s, 6H, CCH₃), 1.61 (d, ³J_{HH} = 9.4 Hz, 1H, CyH), 1.76 (s, 1H, CyH), 1.88-1.94 (m, 6H, CyH), 2.69 (bs, 1H, CyH), 2.81 (d, ³J_{HH} = 11.1 Hz, 2H, CyH), 2.96 (sept, ³J_{HH} = 6.6 Hz, 2H, CH(CH₃)₂), 3.15 (sept, ³J_{HH} = 6.6 Hz, 2H, CH(CH₃)₂), 3.50 (sept, ³J_{HH} = 6.8 Hz, 4H, CH(CH₃)₂), 3.69 (t, ³J_{HH} = 10.93 Hz, 1H, CyH), 4.79 (s, 1H, CH), 4.81 (s, 1H, CH), 6.93 (t, ³J_{HH} = 7.3 Hz, 2H, C₆H₃), 7.00 (t, ³J_{HH} = 6.7 Hz, 2H, C₆H₃), 7.06-7.13 (m, 6H, C₆H₃), 7.16 (t, ³J_{HH} = 6.7 Hz, 2H, C₆H₃). ¹³C{¹H} NMR (151 MHz, C₆D₆, 298 K) δ = 23.8, 24.0, 24.4, 24.5, 24.7, 25.0, 25.1, 25.2, 25.3, 26.3, 26.5, 26.8, 27.3, 27.6 (CH(CH₃)₂, Cy); 28.0, 28.9, 29.0, 34.2, 36.0 (CH(CH₃)₂, Cy); 57.5 (d, ³J_{PC} = 3.6 Hz, NCH(CH₃)₂), 67.7 (d, ³J_{PC} = 14.4 Hz, NCH(CH₃)₂); 97.0, 97.8 (CH); 123.3, 124.1, 124.4, 126.8, 127.1, 140.4, 143.0, 143.3, 143.8, 144.3, 145.2 (C₆H₃); 165.5 (d, ¹J_{PC} = 41.5 Hz, CNCH(CH₃)₂); 169.2, 170.6 (C₆H₃). ³¹P{¹H} (243 MHz, C₆D₆, 298 K) δ = -105.3 ppm. ATR-IR: ν 2957, 2908, 2848, 1547, 1433, 1386, 1367, 1313, 1252, 1205, 1172, 1103, 1022, 936, 860, 795, 628, 556 cm⁻¹.

Synthesis of 4: Ethylisocyanate (31 μL, 0.38 mmol) was added to a toluene solution (15 mL) of **1** (400 mg, 0.38 mmol) at ambient temperature. After shaking the reaction mixture at this temperature for one minute, all volatiles were removed under vacuum to yield a colorless crystalline solid. Yield: 99% (420 mg). M.p. 141 °C (dec.). Anal. calcd. (%) for C₆₁H₈₇ClGa₂N₅OP (1109.48): C, 65.87; H, 7.88; N, 6.30. Found: C, 65.97; H, 7.93; N, 6.37. ¹H NMR (300 MHz, toluene-d₈, 298 K) δ = 0.91 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 0.98 (t, ³J_{HH} = 7.5 Hz, 6H, CH(CH₃)₂), 1.03-1.06 (m, 18H, CH(CH₃)₂), 1.08-1.10 (m, 9H, CH(CH₃)₂, NCH₂CH₃), 1.17 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.23

(d, $^3J_{\text{HH}} = 6.7$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.38 (s, 6H, CCH_3), 1.50 (s, 6H, CCH_3), 2.85 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.15 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 3.36 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.48 (sept, $^3J_{\text{HH}} = 6.7$ Hz, 2H, NCH_2CH_3), 4.73 (s, 1H, CH), 4.83 (s, 1H, CH), 7.00-7.03 (m, 4H, C_6H_3), 7.10-7.17 (m, 6H, C_6H_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, toluene- d_8 , 298 K) $\delta = 14.3, 15.4$ (NCH_2CH_3); 21.3, 23.1, 24.1, 24.3, 24.4, 24.5, 24.9, 25.3, 26.0 ($\text{CH}(\text{CH}_3)_2$); 27.8, 28.1, 28.3, 28.8, 29.7, 32.0 ($\text{CH}(\text{CH}_3)_2$); 39.3 (d, $^3J_{\text{PC}} = 2.6$ Hz, NCH_2CH_3); 97.4, 98.1 (CH); 123.9, 124.4, 124.5, 125.6, 127.4, 137.7, 141.2, 142.1, 142.3, 143.3, 145.2, 145.4, 169.2, 170.8 (C_6H_3); 179.7 (d, $^1J_{\text{PC}} = 13.8$ Hz, NCO). $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, C_6D_6 , 298 K) $\delta = -112.0$ ppm. ATR-IR: ν 2964, 2925, 2865, 1605, 1527, 1438, 1381, 1315, 1261, 1225, 1178, 1099, 1021, 935, 867, 795, 757, 727, 633, 531 cm^{-1} .

Synthesis of 5: Compound **5** was synthesized by following the similar protocols used for **4** using isopropylisocyanate (29 μL , 0.29 mmol), **1** (300 mg, 0.29 mmol), and toluene (10 mL). Yield: 99% (496mg, colorless solid). M.p. 147 $^\circ\text{C}$ (dec.). Anal. calcd. (%) for $\text{C}_{62}\text{H}_{89}\text{ClGa}_2\text{N}_5\text{OP}$ (1123.50): C, 66.12; H, 7.96; N, 6.22. Found: C, 66.20; H, 7.99; N, 6.33. ^1H NMR (600 MHz, C_6D_6 , 298 K) $\delta = 0.95$ (d, $^3J_{\text{HH}} = 6.6$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.06-1.08 (m, 18H, $\text{CH}(\text{CH}_3)_2$), 1.13 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.18 (d, $^3J_{\text{HH}} = 6.6$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.24 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.31 (d, $^3J_{\text{HH}} = 6.7$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.33 (s, 6H, CCH_3), 1.43 (d, $^3J_{\text{HH}} = 6.7$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.50 (s, 6H, CCH_3), 2.86 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.38 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.42 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.58 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.67 (sept, $^3J_{\text{HH}} = 6.5$ Hz, 2H, $\text{NCH}(\text{CH}_3)_2$), 4.76 (s, 1H, CH), 4.88 (s, 1H, CH), 7.01-7.03 (m, 4H, C_6H_3), 7.11-7.14 (m, 4H, C_6H_3), 7.16-7.18 (m, 4H, C_6H_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, C_6D_6 , 298 K) $\delta = 21.4$ ($\text{NCH}(\text{CH}_3)_2$); 24.0, 24.2, 24.3, 24.5, 24.6, 25.1, 25.3, 25.7, 26.5 ($\text{CH}(\text{CH}_3)_2$); 27.9, 28.1, 28.3, 28.7, 29.6 ($\text{CH}(\text{CH}_3)_2$); 46.6 ($\text{NCH}(\text{CH}_3)_2$); 98.3, 98.8 (CH); 124.0, 124.5, 125.0, 125.7, 127.2, 128.5, 129.3, 137.9, 141.6, 142.2, 142.7, 143.3, 145.4, 145.5, 169.3, 170.8 (C_6H_3); 180.4 (d, $^1J_{\text{PC}} = 14.9$ Hz, NCO). $^{31}\text{P}\{^1\text{H}\}$ (243 MHz, C_6D_6 , 298 K) $\delta = -114.8$ ppm. ATR-IR: ν 2963, 2924, 2865, 1623, 1517, 1462, 1435, 1380, 1317, 1254, 1203, 1175, 1101, 1021, 935, 864, 795, 760, 542, 531 cm^{-1} .

Synthesis of 6: Compound **6** was synthesized by following the similar protocols used for **4** using cyclohexylisocyanate (37 μL , 0.29 mmol), **1** (300 mg, 0.29 mmol), and toluene (10 mL). Yield: 98% (330 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown by cooling an *n*-hexane solution of **6** at -30 $^\circ\text{C}$ for 12 h. M.p. 143 $^\circ\text{C}$ (dec.). Anal. calcd. (%) for $\text{C}_{65}\text{H}_{93}\text{ClGa}_2\text{N}_5\text{OP}$ (1163.53): C, 66.94; H, 8.04; N, 6.00. Found: C, 67.03; H, 8.11; N, 6.03. ^1H NMR (600 MHz, C_6D_6 , 298 K) $\delta = 0.87$ (t, $^3J_{\text{HH}} = 7.1$ Hz, 3H, $\text{CH}(\text{CH}_3)_2$), 0.92 (d, $^3J_{\text{HH}} = 6.6$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.04-1.06 (m, 18H, $\text{CH}(\text{CH}_3)_2$, CH_2), 1.15 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.21 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H,

CH(CH₃)₂), 1.23-1.26 (m, 2H, CH₂), 1.30 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.31 (s, 6H, CCH₃), 1.42 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.47 (s, 6H, CCH₃), 1.73 (d, ³J_{HH} = 11.3 Hz, 2H, CH₂), 2.29 (d, ³J_{HH} = 11.3 Hz, 2H, CH₂), 2.85 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 3.29 (m, 1H, CH), 3.40 (sept, ³J_{HH} = 6.8 Hz, 4H, CH(CH₃)₂), 3.56 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 4.81 (s, 1H, CH), 4.86 (s, 1H, CH), 7.01 (dd, ³J_{HH} = 2.3, 6.8 Hz, 2H, C₆H₃), 7.08-7.11 (m, 3H, C₆H₃), 7.12-7.14 (m, 6H, C₆H₃), 7.18 (d, ³J_{HH} = 7.7 Hz, 1H, C₆H₃). ¹³C{¹H} NMR (151 MHz, C₆D₆, 298 K) δ = 14.5, 23.2, 24.4, 24.5, 24.7, 25.4, 25.5, 25.8, 26.6, 26.7 (CH(CH₃)₂); 27.4, 28.1, 28.3, 28.5, 28.8, 29.8 (CH(CH₃)₂, Cy); 32.1, 34.4, 56.2 (Cy); 98.5, 98.9 (CH); 124.2, 124.7, 125.2, 127.4, 141.9, 142.3, 142.9, 143.5, 145.6, 169.5, 170.0 (C₆H₃); 180.4 (d, ¹J_{PC} = 15.0 Hz, NCO). ³¹P{¹H} (243 MHz, C₆D₆, 298 K) δ = -115.4 ppm. ATR-IR: ν 2955, 2921, 2862, 1608, 1519, 1436, 1386, 1318, 1318, 1255, 1205, 1177, 1098, 1016, 935, 864, 795, 759, 637, 541 cm⁻¹.

Reaction of 2 with CO₂: A toluene solution (5 mL) of **2** (150 mg, 0.13 mmol) in a *J*-Young Schlenk flask was degassed using the freeze pump-thaw method. CO₂ (1 bar) gas was added, and the solution was stirred at ambient temperature for 1 h. All volatiles were then removed in *vacuo* to yield a colorless crystalline powder. The ³¹P{¹H} NMR spectrum at 25 °C shows two sharp singlets, which were assigned to the mono and double^[1] CO₂ addition products. Unfortunately, due to the similar solubility of these two products, we failed to isolate a pure sample of the mono CO₂ addition product. The crude ¹H and ³¹P{¹H} NMR spectra of the mixture are provided to confirm the bulk material's constitutions match (Figures S29-S30).

Reaction of 3 with CO₂: Compound **3** also led to the mono and double^[1] CO₂ addition products at room temperature, when exposed to CO₂ gas (1 bar) in toluene similar to compound **2**. Again, we failed to isolate a sample of the pure mono CO₂ addition product due to the similar solubility of these two products. The ¹H and ³¹P{¹H} NMR spectra of this mixture are provided to confirm the bulk material's constitutions match (Figures S30-S31).

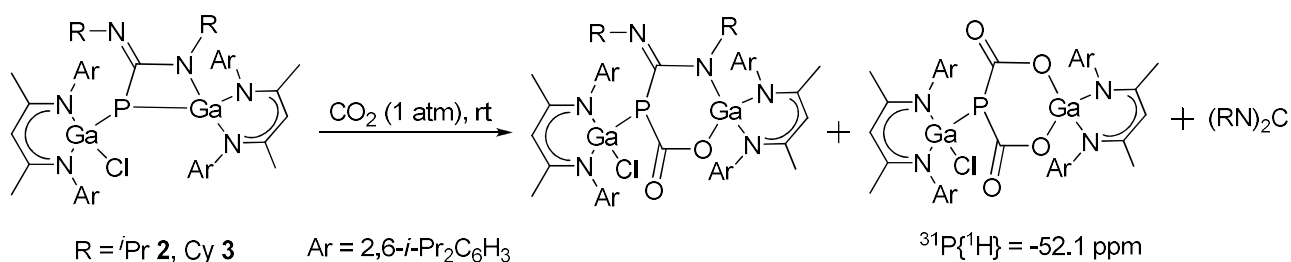
Synthesis of 7: A toluene solution (5 mL) of **4** (150 g, 0.13 mmol) in a *J*-Young Schlenk flask was degassed using the freeze pump-thaw method. CO₂ (1 bar) gas was added and the solution was stirred at room temperature for 1 h. All volatiles were then removed in *vacuo* to yield a colorless crystalline powder of **7**. Yield: 97% (150 mg). M.p. 93 °C (dec.). Anal. calcd. (%) for C₆₂H₈₇ClGa₂N₅O₃P (1153.47): C, 64.40; H, 7.58; N, 6.06. Found: C, 64.47; H, 7.66; N, 6.11. ¹H NMR (500 MHz, toluene-d₈, 298 K) δ = 0.79 (t, ³J_{HH} = 7.3 Hz, 3H, CH₂CH₃), 0.99 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.04 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.10 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.14 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.22 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.26 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.29 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.40 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂),

1.42 (s, 6H, CCH₃), 1.60 (s, 6H, CCH₃), 2.92 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 3.01 (sept, ³J_{HH} = 6.7 Hz, 2H, CH(CH₃)₂), 3.14 (q, ³J_{HH} = 7.3 Hz, 2H, CH₂CH₃), 3.32 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 3.67 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 4.72 (s, 1H, CH), 4.86 (s, 1H, CH), 7.07-7.20 (m, 12H, C₆H₃). ¹³C{¹H} NMR (126 MHz, toluene-d₈, 298 K) δ = 14.3, 21.3 (NCH₂CH₃); 23.6, 24.3, 24.4, 24.7, 24.8, 24.9 (CH(CH₃)₂); 26.2, 28.2, 28.8, 29.5 (CH(CH₃)₂); 32.0, 40.0 (CH₂); 97.5, 97.6 (CH); 123.1, 124.5, 125.6, 126.9, 138.8, 142.2, 142.5, 143.8, 144.7, 146.1, 169.6, 172.0 (C₆H₃); 174.6 (d, ¹J_{CP} = 28.4 Hz, OCO); 179.8 (d, ¹J_{CP} = 15.6 Hz, NCO). ³¹P{¹H} (121 MHz, C₆D₆, 298 K) δ = -40.0 ppm. ATR-IR: ν 2964, 2925, 2863, 1943, 1667, 1521, 1436, 1383, 1315, 1251, 1174, 1097, 1018, 940, 867, 795, 757, 710, 636, 541 cm⁻¹.

Synthesis of 8: Compound **8** was synthesized by following the similar protocols used for **7** using compound **5** (200 mg, 0.18 mmol), CO₂ gas (1 bar), and toluene (10 mL). Yield: 98% (200 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown upon storage of saturated toluene solution of **8** at ambient temperature. M.p. 95 °C (dec.). Anal. calcd. (%) for C₆₃H₈₉ClGa₂N₅O₃P (1167.49): C, 64.66; H, 7.67; N, 5.98. Found: C, 64.71; H, 7.73; N, 5.98. ¹H NMR (600 MHz, toluene-d₈, 298 K) δ = 1.01 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.05 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.07 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.10 (d, ³J_{HH} = 6.7 Hz, 6H, CH(CH₃)₂), 1.17 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.21 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.25 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.29 (d, ³J_{HH} = 6.8 Hz, 6H, CH(CH₃)₂), 1.39 (s, 6H, CCH₃), 1.44 (d, ³J_{HH} = 6.6 Hz, 6H, CH(CH₃)₂), 1.60 (s, 6H, CCH₃), 2.98 (sept, ³J_{HH} = 6.7 Hz, 2H, CH(CH₃)₂), 3.03 (sept, ³J_{HH} = 6.7 Hz, 2H, CH(CH₃)₂), 3.32 (sept, ³J_{HH} = 6.8 Hz, 2H, CH(CH₃)₂), 3.61 (sept, ³J_{HH} = 6.5 Hz, 1H, NCH(CH₃)₂), 3.69 (sept, ³J_{HH} = 6.7 Hz, 2H, CH(CH₃)₂), 4.79 (s, 1H, CH), 4.86 (s, 1H, CH), 7.01-7.03 (m, 5H, C₆H₃), 7.08 (t, ³J_{HH} = 7.6 Hz, 3H, C₆H₃), 7.13 (t, ³J_{HH} = 6.7 Hz, 2H, C₆H₃), 7.17 (d, ³J_{HH} = 6.7 Hz, 2H, C₆H₃). ¹³C{¹H} NMR (151 MHz, toluene-d₈, 298 K) δ = 22.7, 23.9, 24.3, 24.4, 24.6, 24.7, 24.9, 25.1, 25.2, 25.7, 26.4 (CH(CH₃)₂); 28.2, 28.5, 28.8, 29.4 (CH(CH₃)₂); 48.3 (NCH(CH₃)₂); 97.5, 98.8 (CH); 123.1, 124.5, 126.9, 139.3, 142.1, 142.5, 143.6, 144.9, 146.0, 169.5, 171.9 (C₆H₃); 174.4 (d, ¹J_{CP} = 27.4 Hz, OCO); 180.6 (d, ¹J_{CP} = 15.3 Hz, NCO). ³¹P{¹H} (121 MHz, toluene-d₈, 298 K) δ = -34.5 ppm. ATR-IR: ν 2963, 2925, 2861, 1671, 1577, 1522, 1439, 1384, 1314, 1238, 1173, 1149, 1103, 1018, 937, 864, 795, 757, 730, 695, 642, 531 cm⁻¹.

Synthesis of 9: Compound **9** was synthesized by following the similar protocols used for **7** using compound **7** (200 mg, 0.17 mmol), CO₂ gas (1 bar), and toluene (10 mL). Yield: 98% (200 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown upon storage of saturated toluene solution of **9** at ambient temperature. M.p. 93 °C (dec.). Anal. calcd. (%) for C₆₆H₉₃ClGa₂N₅O₃P (1207.52): C, 65.49; H, 7.74; N, 5.79. Found: C, 65.57; H, 7.82; N, 5.83. ¹H

NMR (600 MHz, toluene- d_8 , 298 K) δ = 1.00 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.10 (td, $^3J_{\text{HH}} = 7.2$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.22 (td, $^3J_{\text{HH}} = 6.7$ Hz, 12H, $\text{CH}(\text{CH}_3)_2$), 1.25 (d, $^3J_{\text{HH}} = 6.7$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.29 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.39 (s, 6H, CCH_3), 1.40 (d, $^3J_{\text{HH}} = 6.8$ Hz, 6H, $\text{CH}(\text{CH}_3)_2$), 1.43-1.54 (m, 5H, CH_2), 1.59 (s, 6H, CCH_3), 1.66 (m, 1H, CH_2), 1.74 (br, 2H, CH_2), 1.94 (br, 1H, CH_2), 2.96 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.08 (sept, $^3J_{\text{HH}} = 6.7$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.32 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 3.39 (br, 1H, CH), 3.70 (sept, $^3J_{\text{HH}} = 6.8$ Hz, 2H, $\text{CH}(\text{CH}_3)_2$), 4.85 (s, 2H, CH), 7.00-7.04 (m, 4H, C_6H_3), 7.07-7.12 (m, 6H, C_6H_3), 7.16 (d, $^3J_{\text{HH}} = 6.4$ Hz, 2H, C_6H_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, toluene- d_8 , 298 K) δ = 23.9, 24.3, 24.4, 24.6, 24.9, 25.2, 25.4, 25.6, 26.3, 26.8, 27.0 ($\text{CH}(\text{CH}_3)_2$); 28.2, 28.6, 29.4 ($\text{CH}(\text{CH}_3)_2$); 32.7, 57.1 (NCy); 97.5, 98.8 (CH); 123.2, 124.6, 124.7, 124.8, 125.4, 126.9, 139.2, 142.2, 142.5, 143.8, 144.7, 146.1, 169.5, 171.7 (C_6H_3); 174.1 (d, $^1J_{\text{CP}} = 28.3$ Hz, OCO); 181.1 (d, $^1J_{\text{CP}} = 14.7$ Hz, NCO). $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, toluene- d_8 , 298 K) δ = -35.0 ppm. ATR-IR: ν 2958, 2925, 2865, 1663, 1577, 1518, 1436, 1384, 1317, 1251, 1235, 1176, 1098, 1024, 938, 864, 795, 757, 734, 695, 649, 531 cm^{-1} .



Scheme S1. Reactions of compounds **2** and **3** with CO_2 .

2. Spectroscopic Characterization

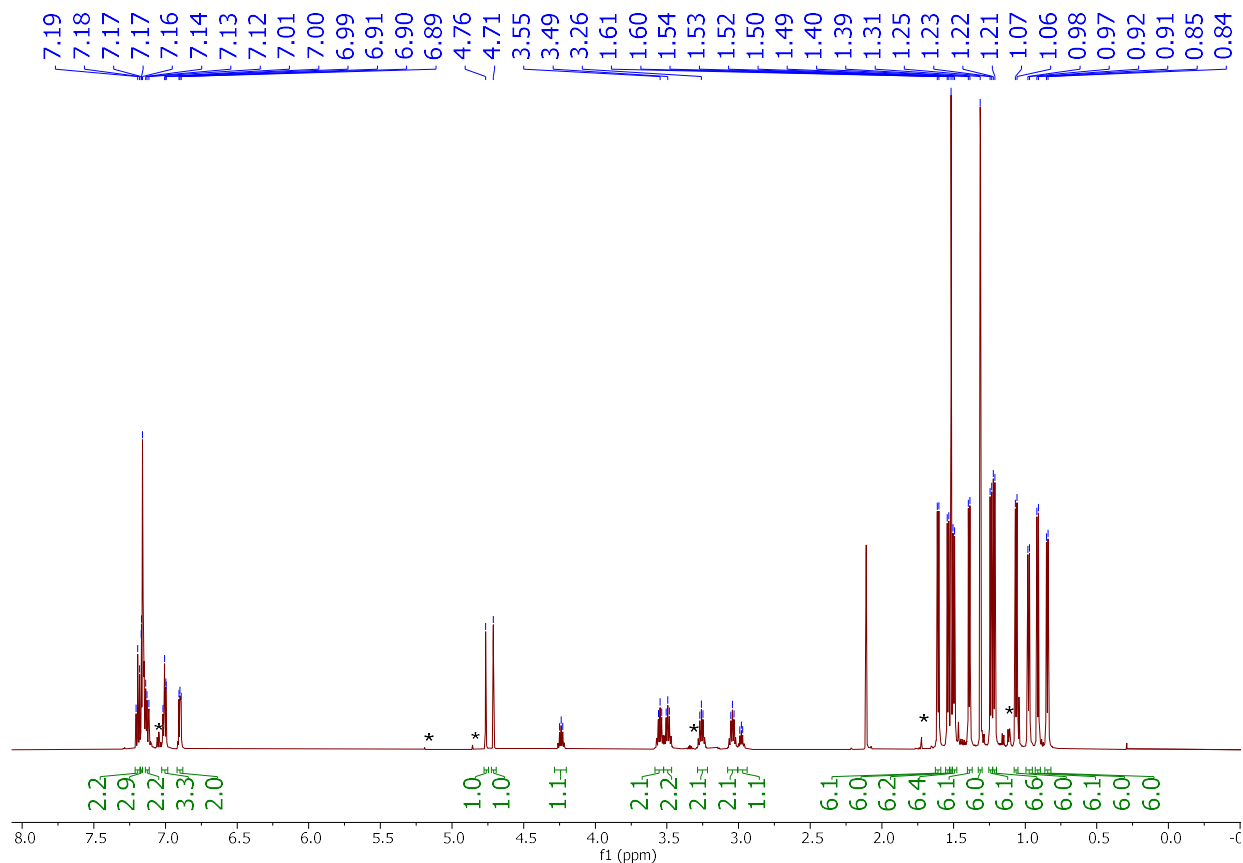


Figure S1. ¹H NMR (600 MHz, C₆D₆, 298 K) spectrum of compound 2. *trace impurities.

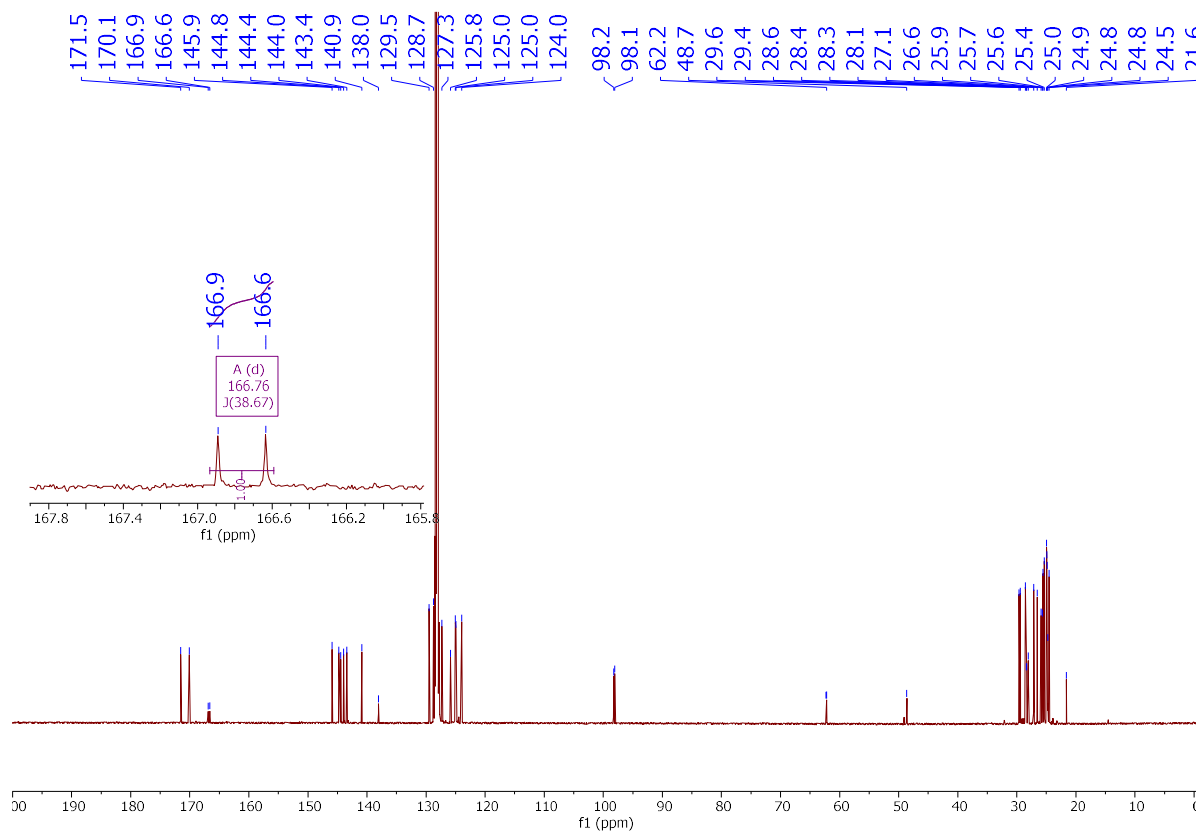


Figure S2. ¹³C{¹H} NMR (151 MHz, C₆D₆, 298 K) spectrum of compound 2.

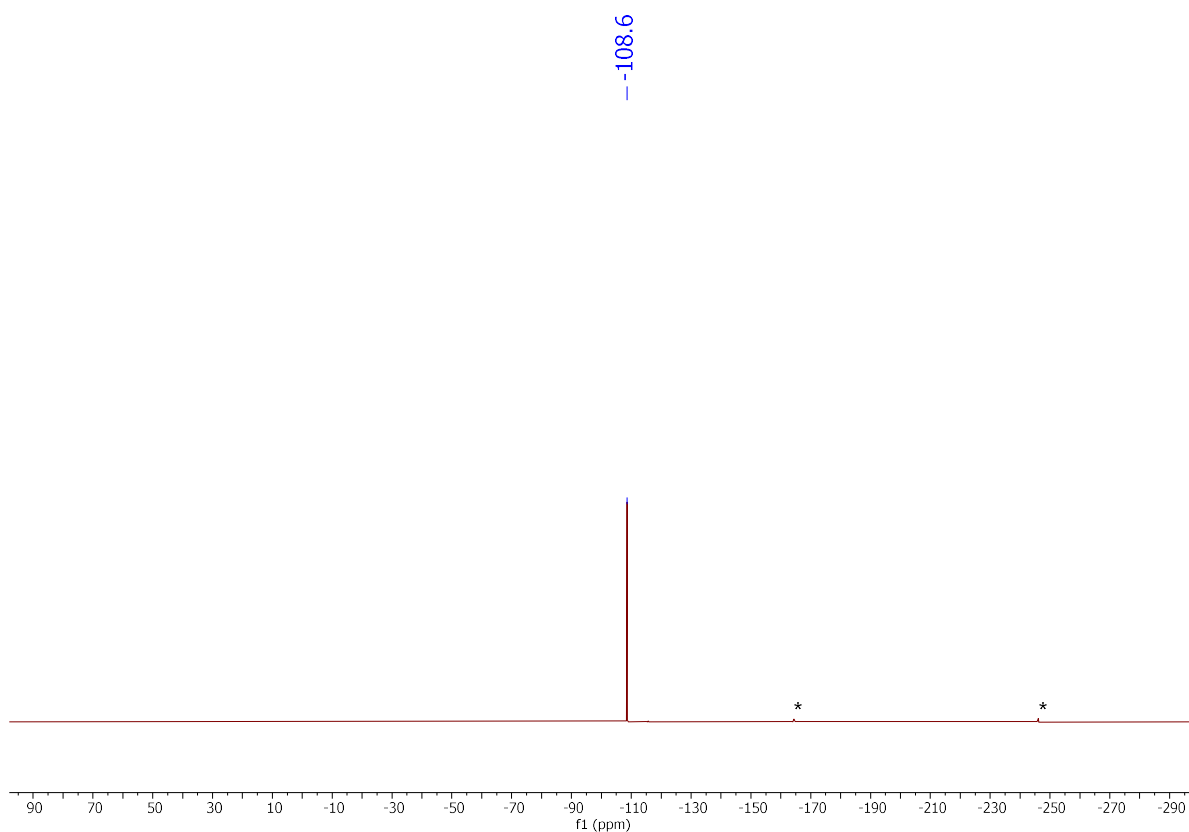


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR (243 MHz, C_6D_6 , 298 K) spectrum of compound **2**. *trace impurities.

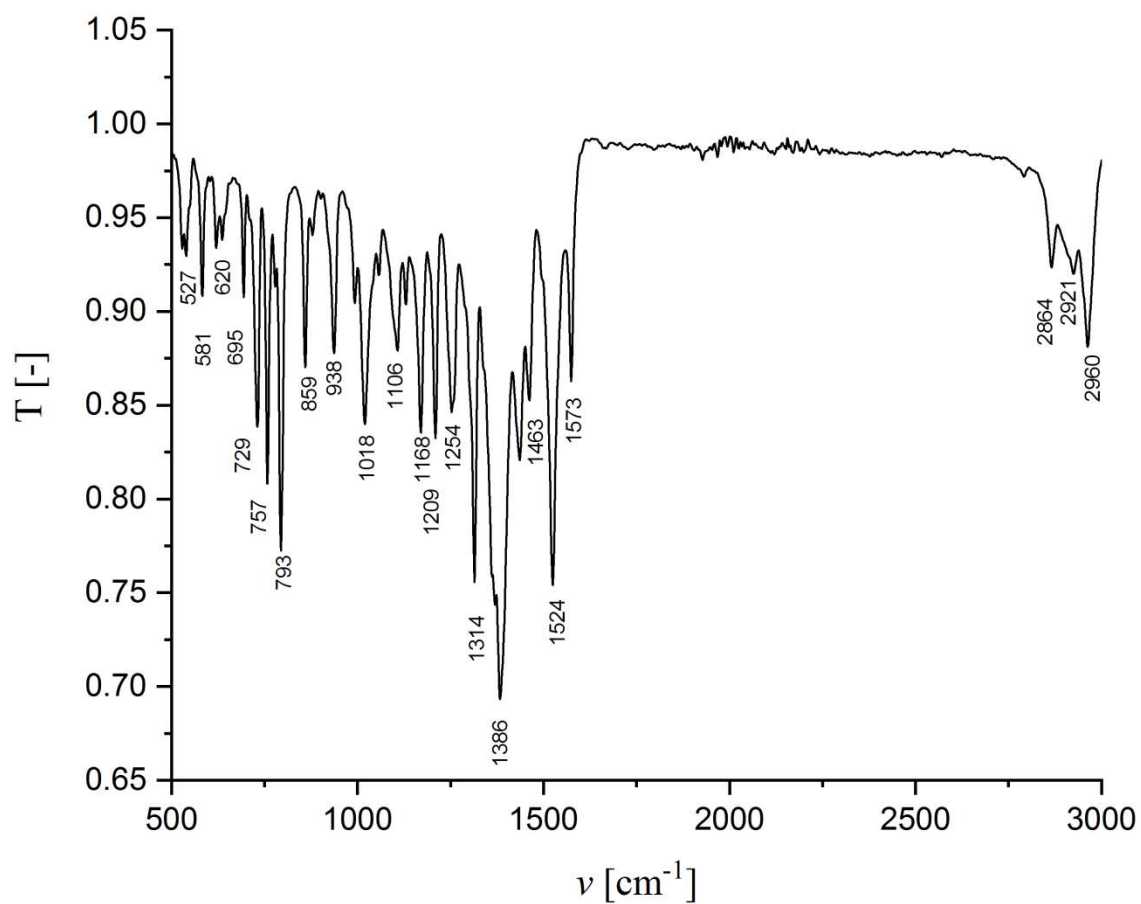


Figure S4. ATR-IR spectrum of **2**.

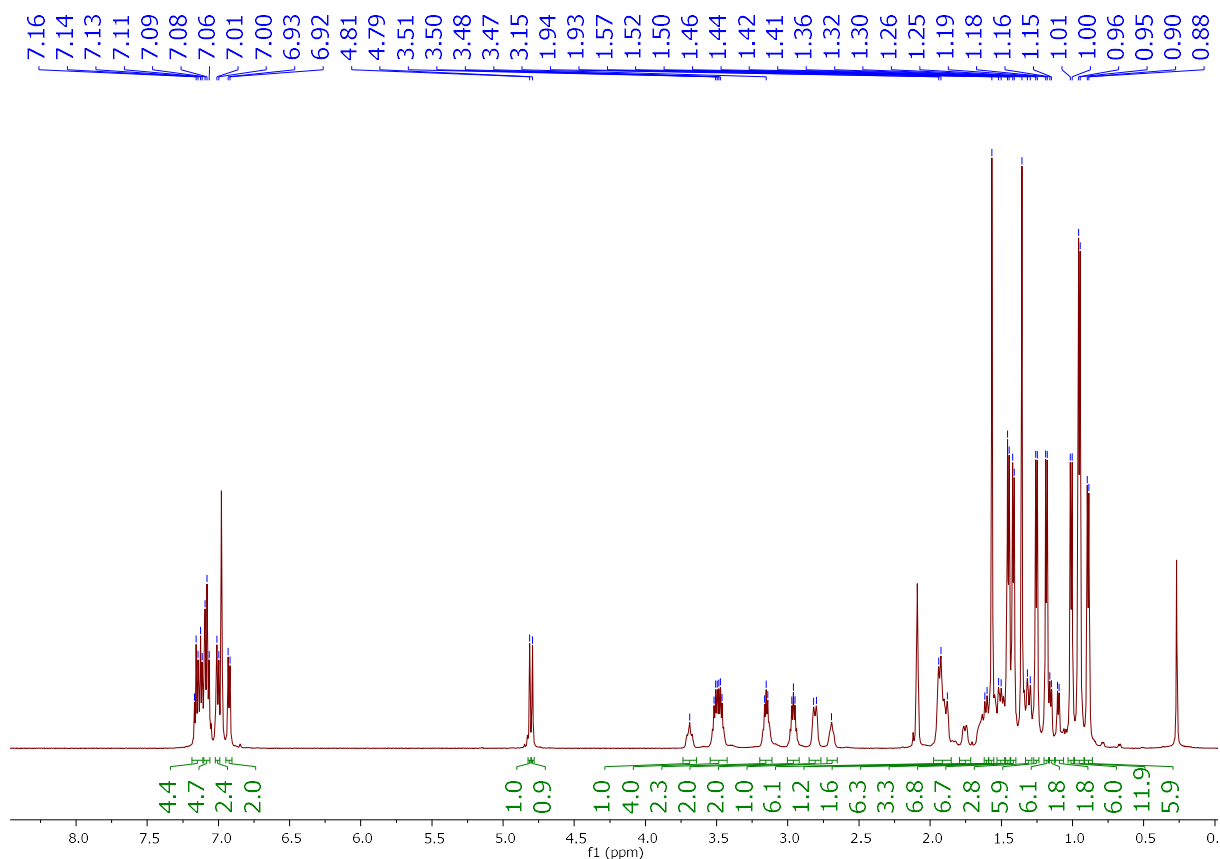


Figure S5. ^1H NMR (600 MHz, toluene- d_8 , 298 K) spectrum of compound **3**.

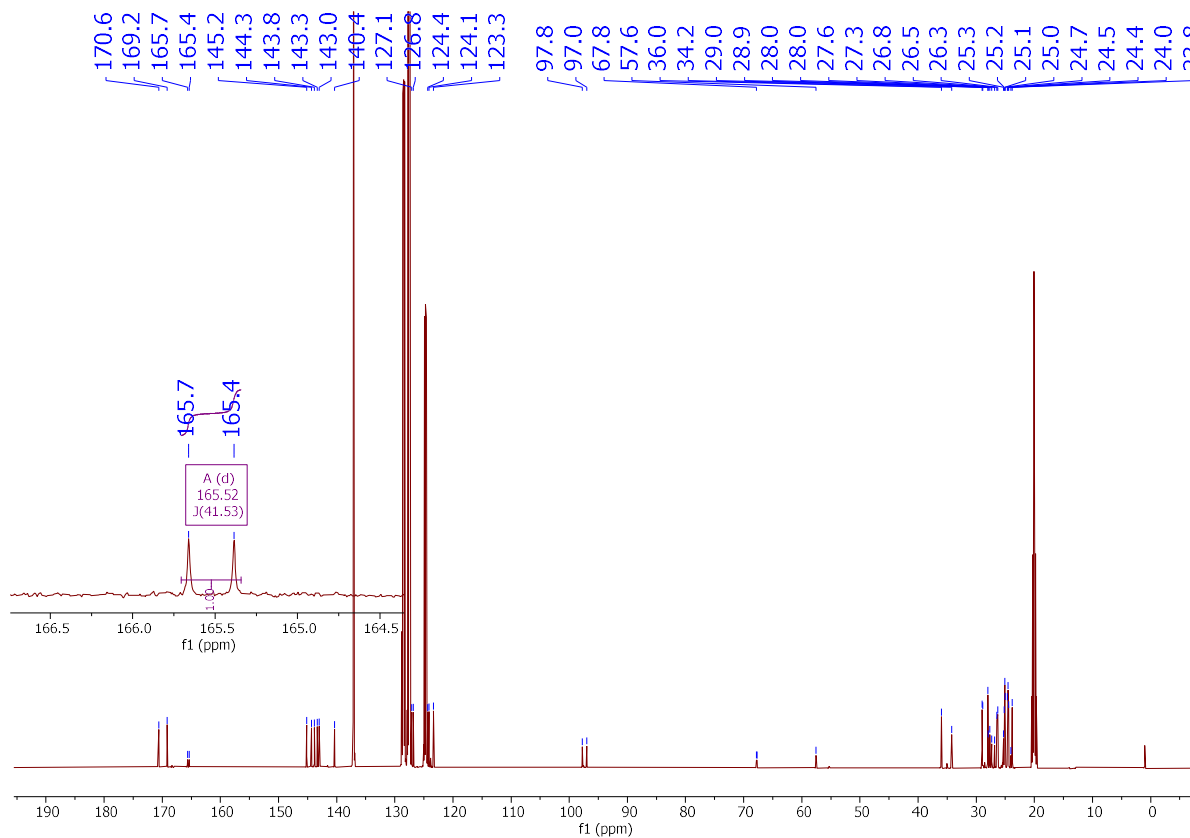


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, toluene- d_8 , 298 K) spectrum of compound **3**.

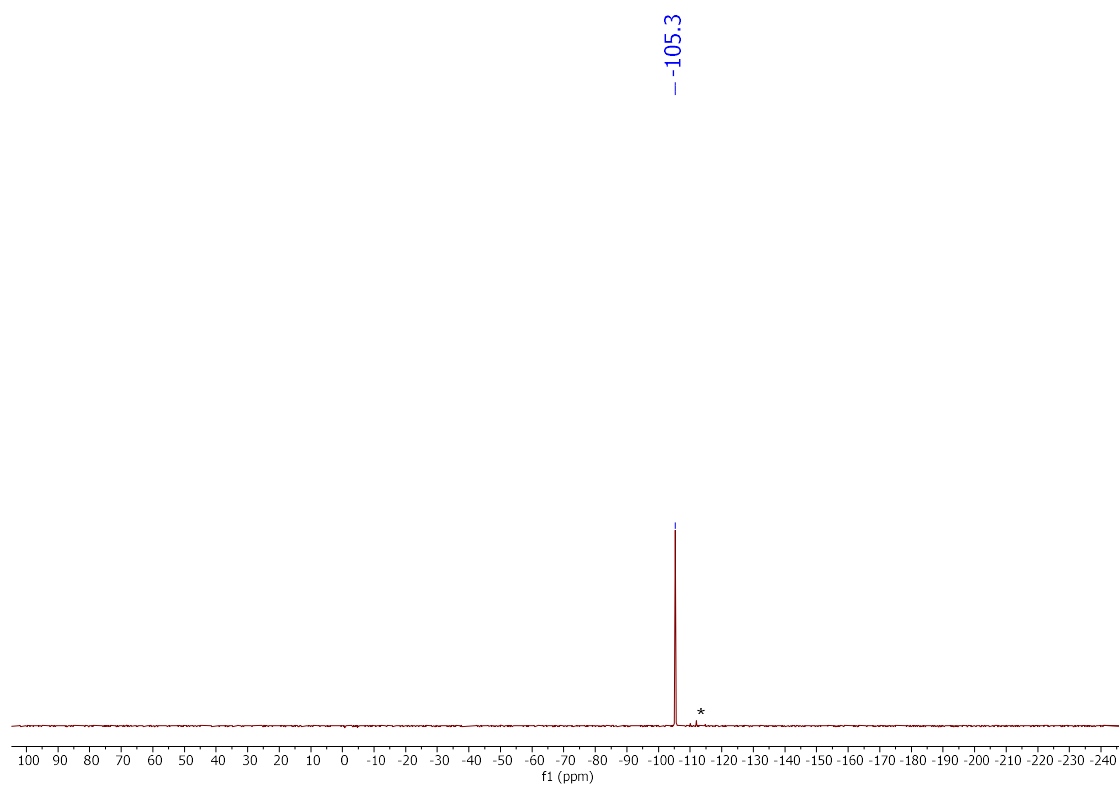


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8 , 298 K) spectrum of compound **3**. *trace impurity.

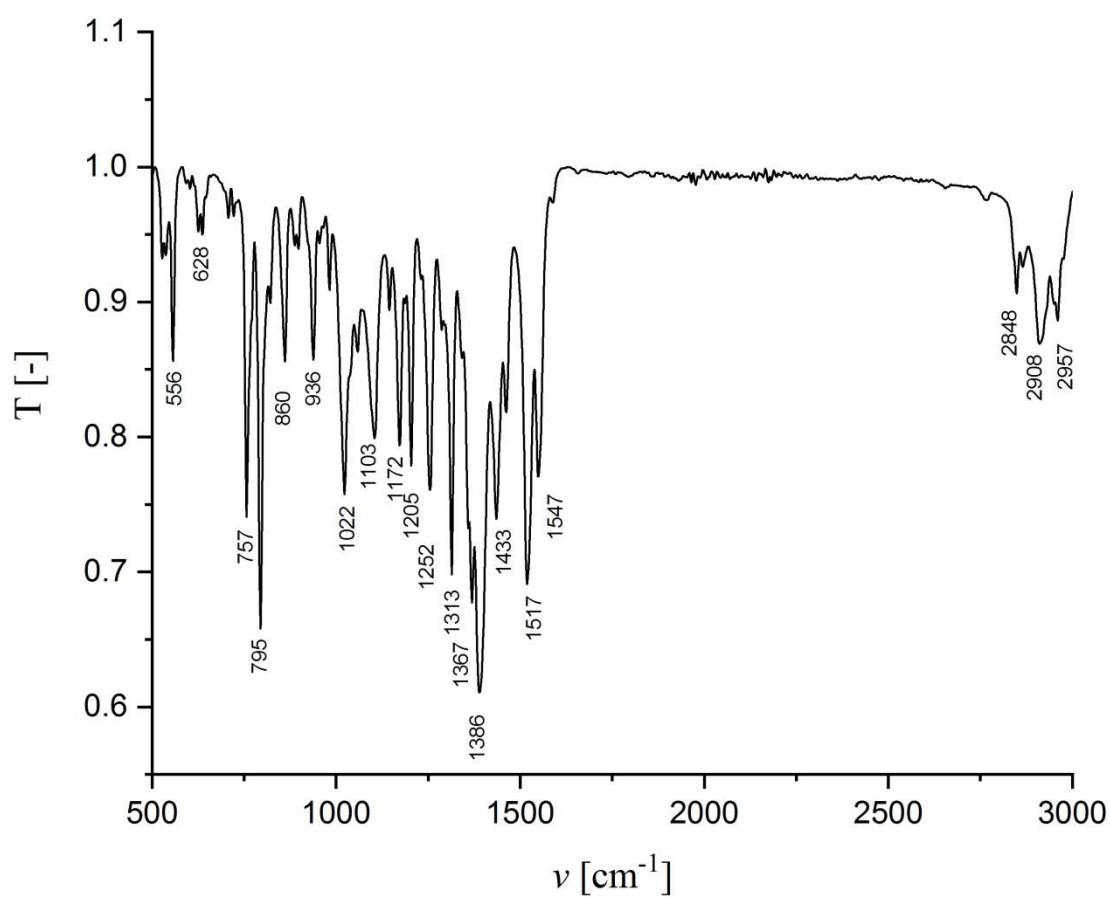


Figure S8. ATR-IR spectrum of **3**.

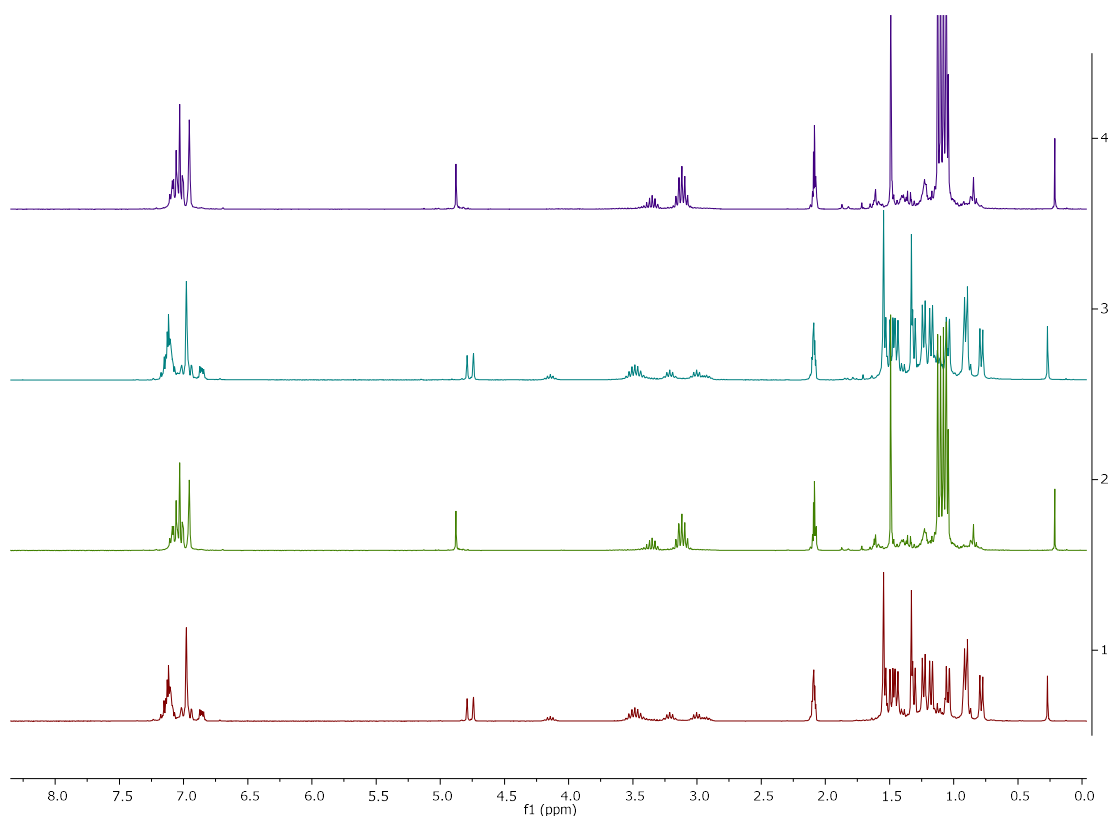


Figure S9. ^1H NMR (300 MHz, toluene- d_8) spectra of the temperature-dependent reversible reaction of DIC and gallaphosphene **1**; 1) compound **2**; 2) compound **2** after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.

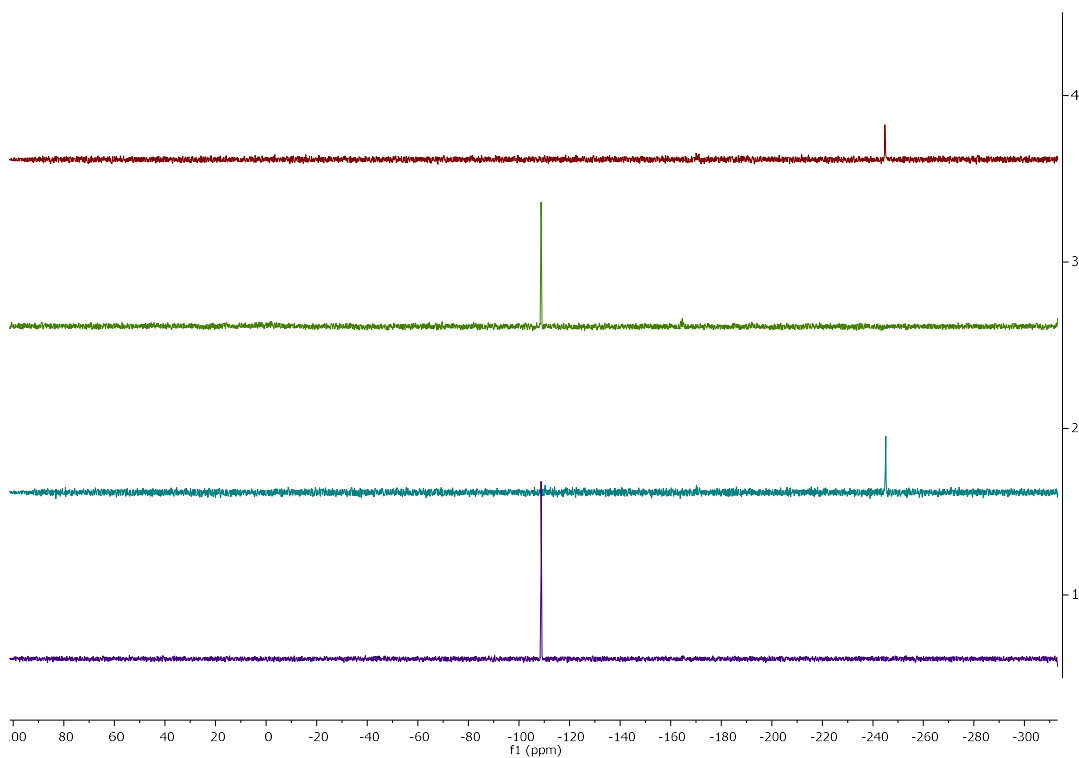


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8) spectra tracking the temperature dependent reversible reaction of DIC and gallaphosphene **1**; 1) compound **2**; 2) compound **2** after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.

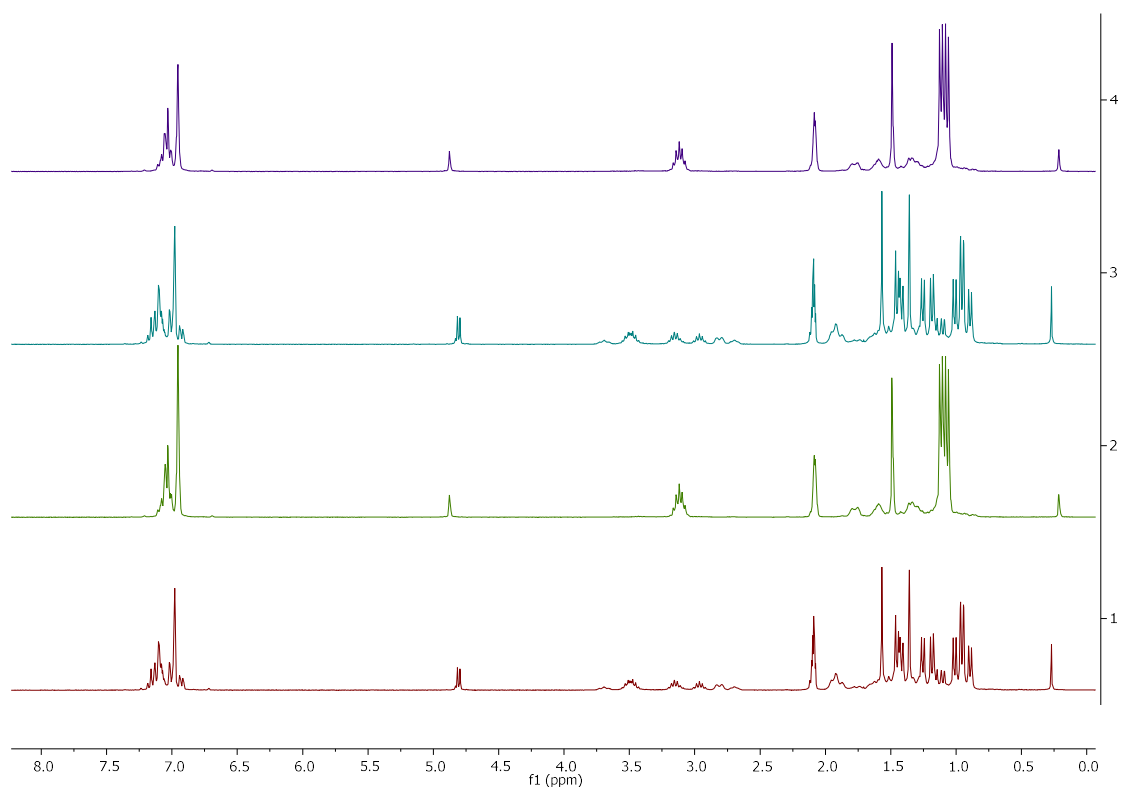


Figure S11. ^1H NMR (300 MHz, toluene- d_8) spectra of the temperature dependent reversible reaction of DCC and gallaphosphene **1**; 1) compound **3**; 2) compound **3** after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.

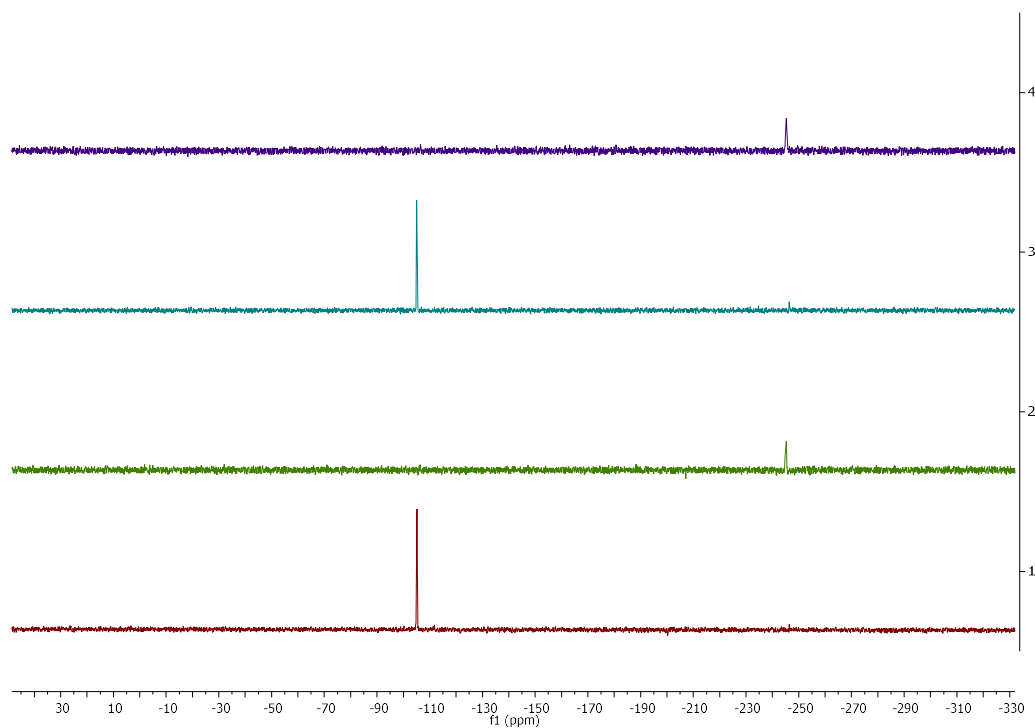


Figure S12. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8) spectra tracking the temperature dependent reversible reaction of DCC and gallaphosphene **1**; 1) compound **3**; 2) compound **3** after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.

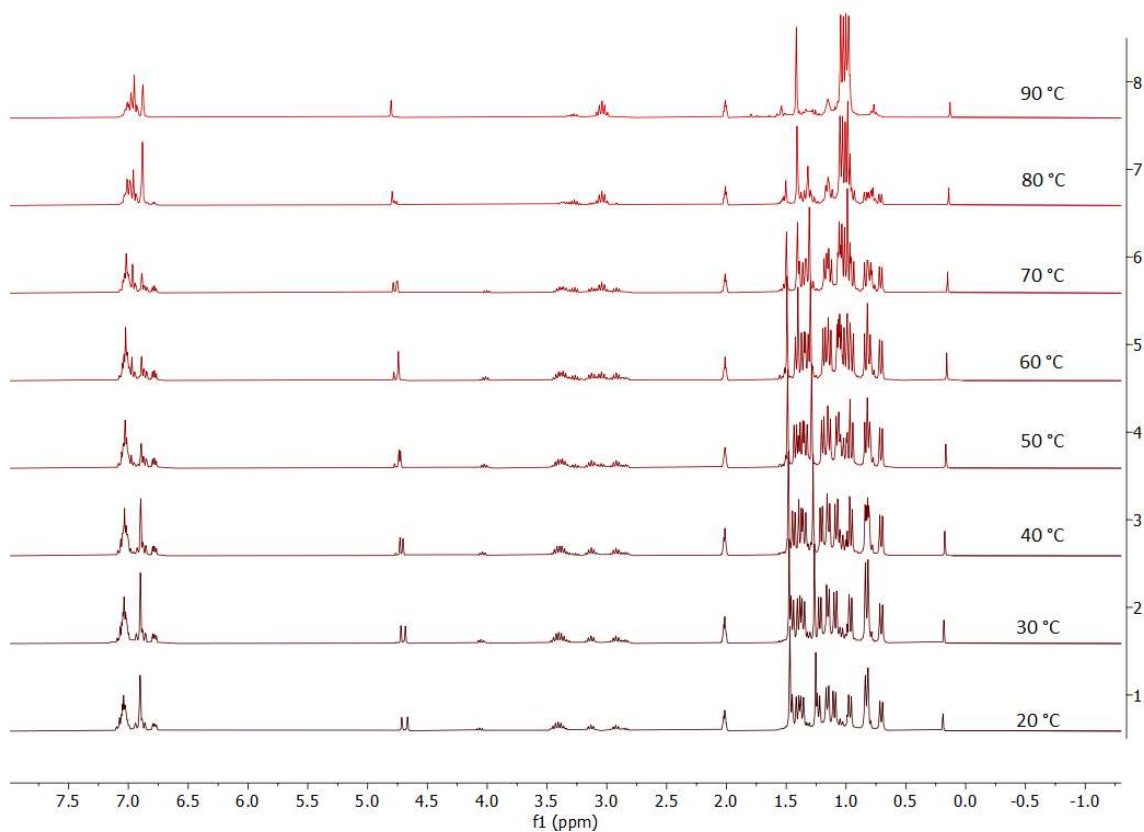


Figure S13. Stacked variable temperature (VT) ^1H NMR (300 MHz, toluene- d_8) spectra of compound **2**.

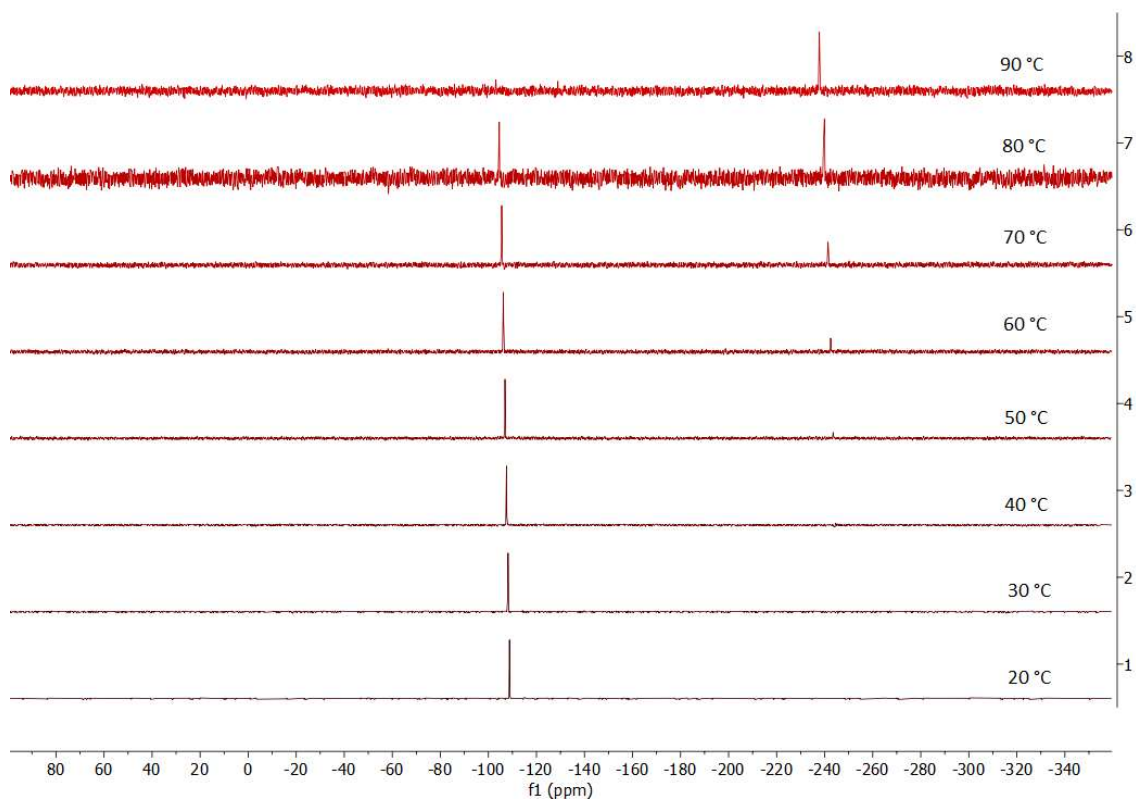


Figure S14. Stacked variable temperature (VT) ^{31}P NMR (121 MHz, toluene- d_8) spectra of compound **2**.

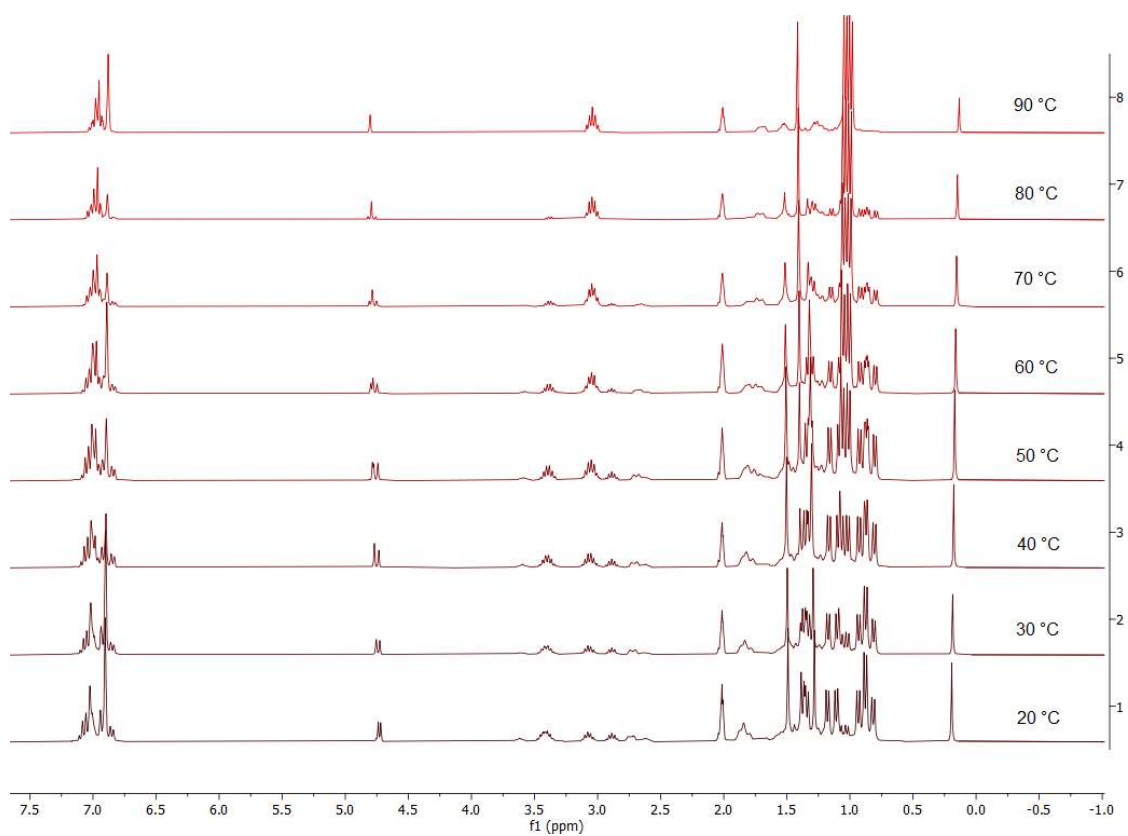


Figure S15. Stacked variable temperature (VT) ^1H NMR (300 MHz, toluene- d_8) spectra of compound **3**.

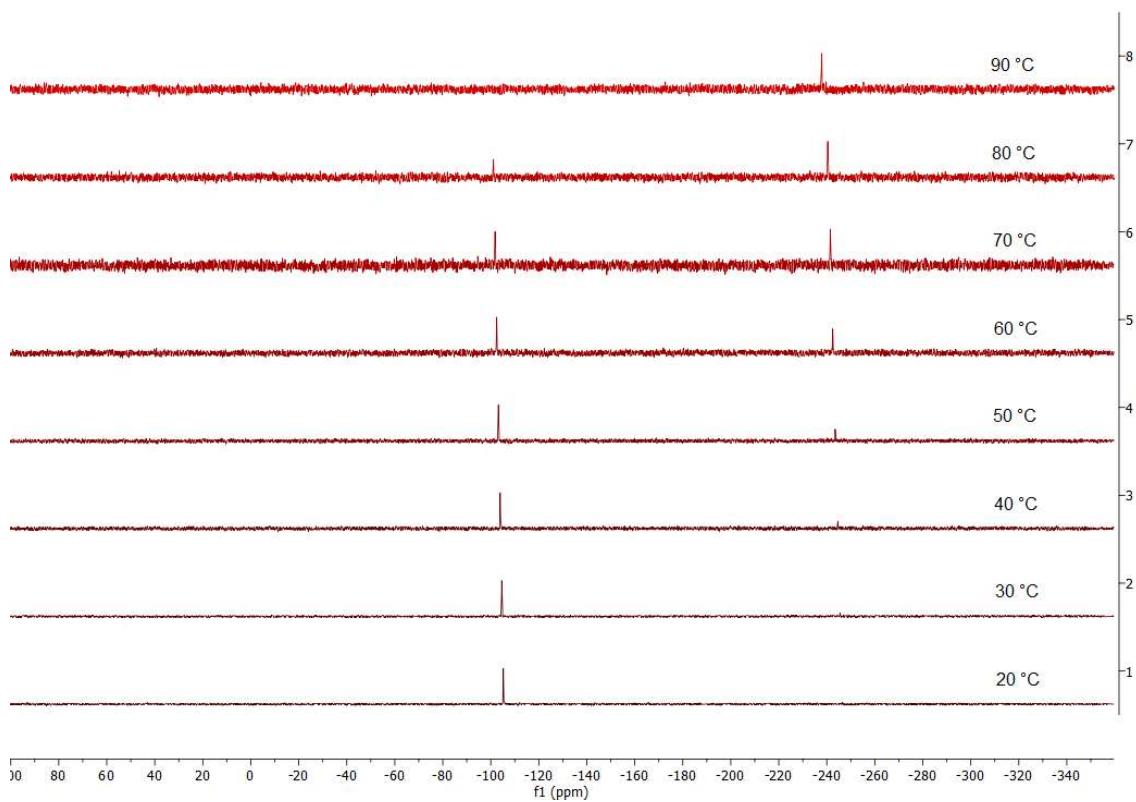


Figure S16. Stacked variable temperature (VT) ^{31}P NMR (121 MHz, toluene- d_8) spectra of compound **3**.

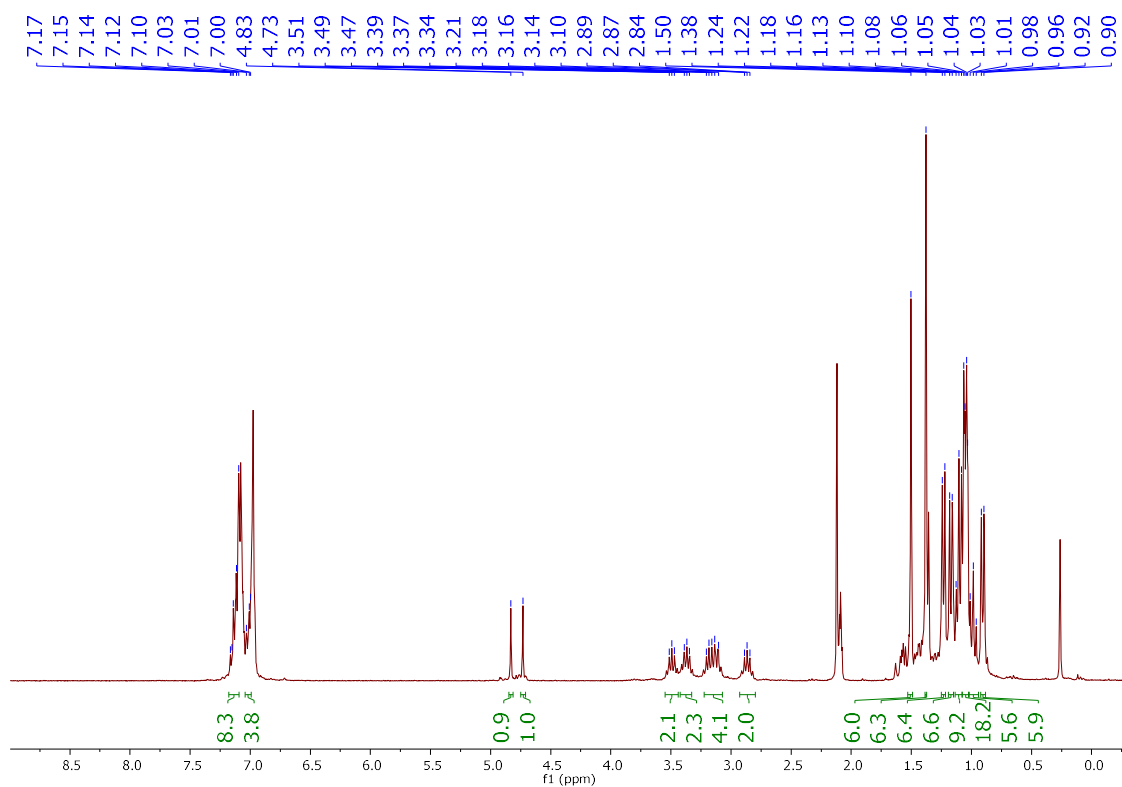


Figure S17. ^1H NMR (600 MHz, toluene- d_8 , 298 K) spectrum of compound 4.

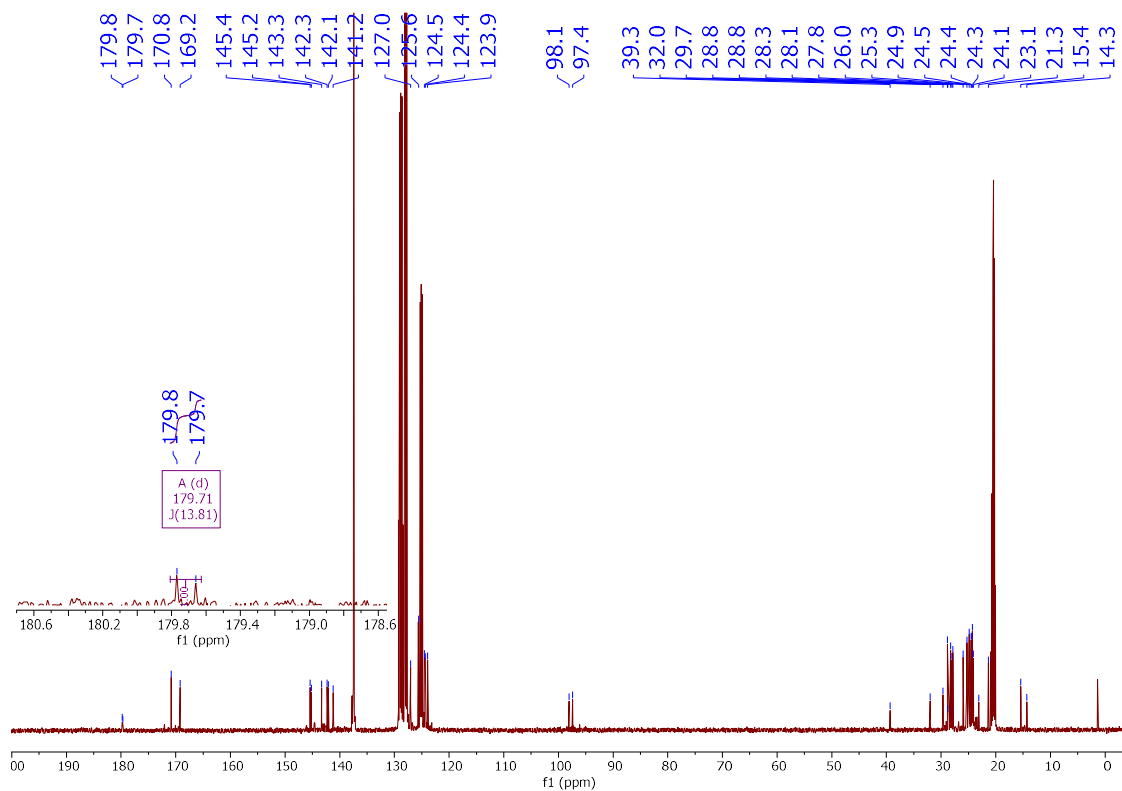


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, toluene- d_8 , 298 K) spectrum of compound 4.

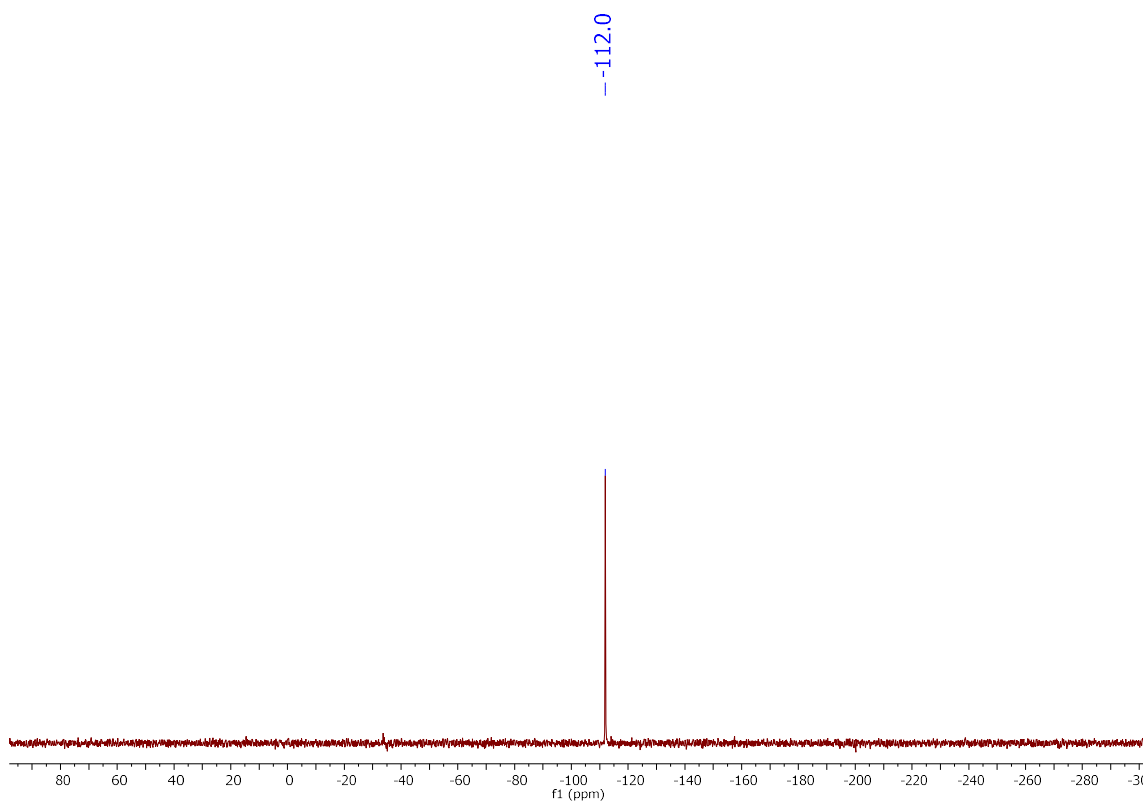


Figure S19. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, C_6D_6 , 298 K) spectrum of compound **4**.

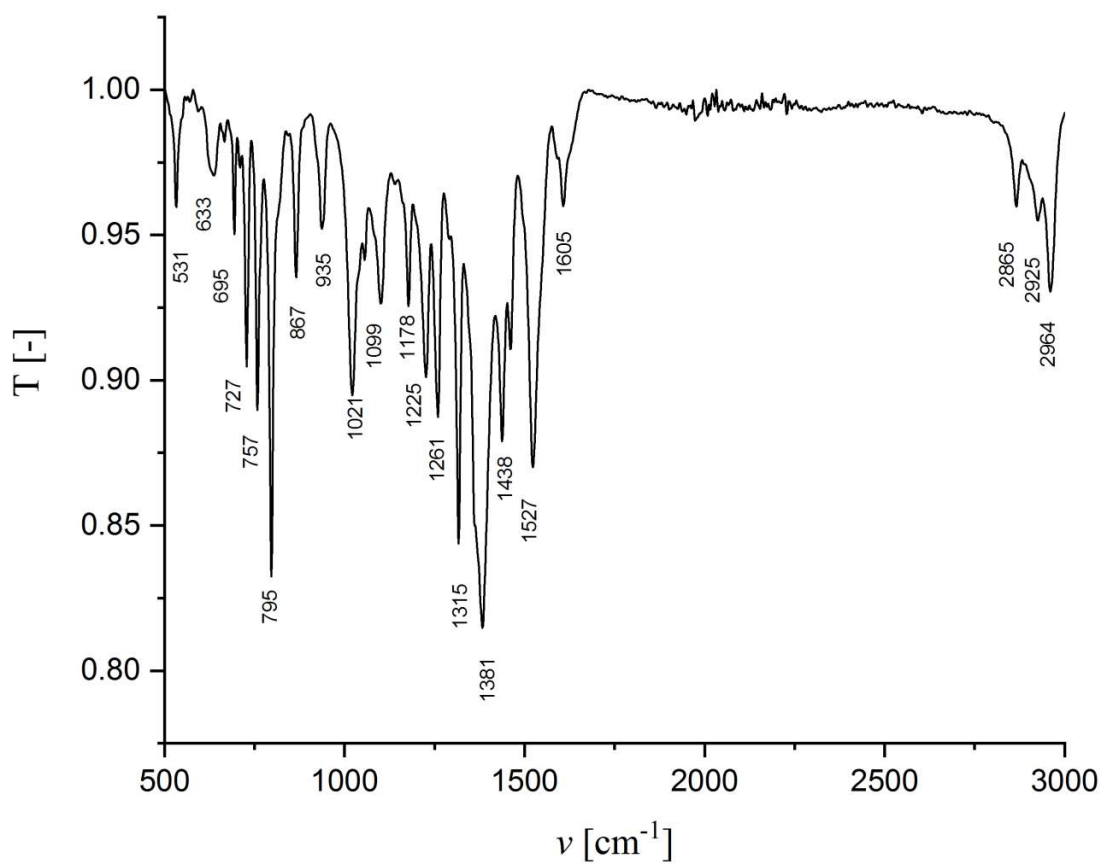


Figure S20. ATR-IR spectrum of **4**.

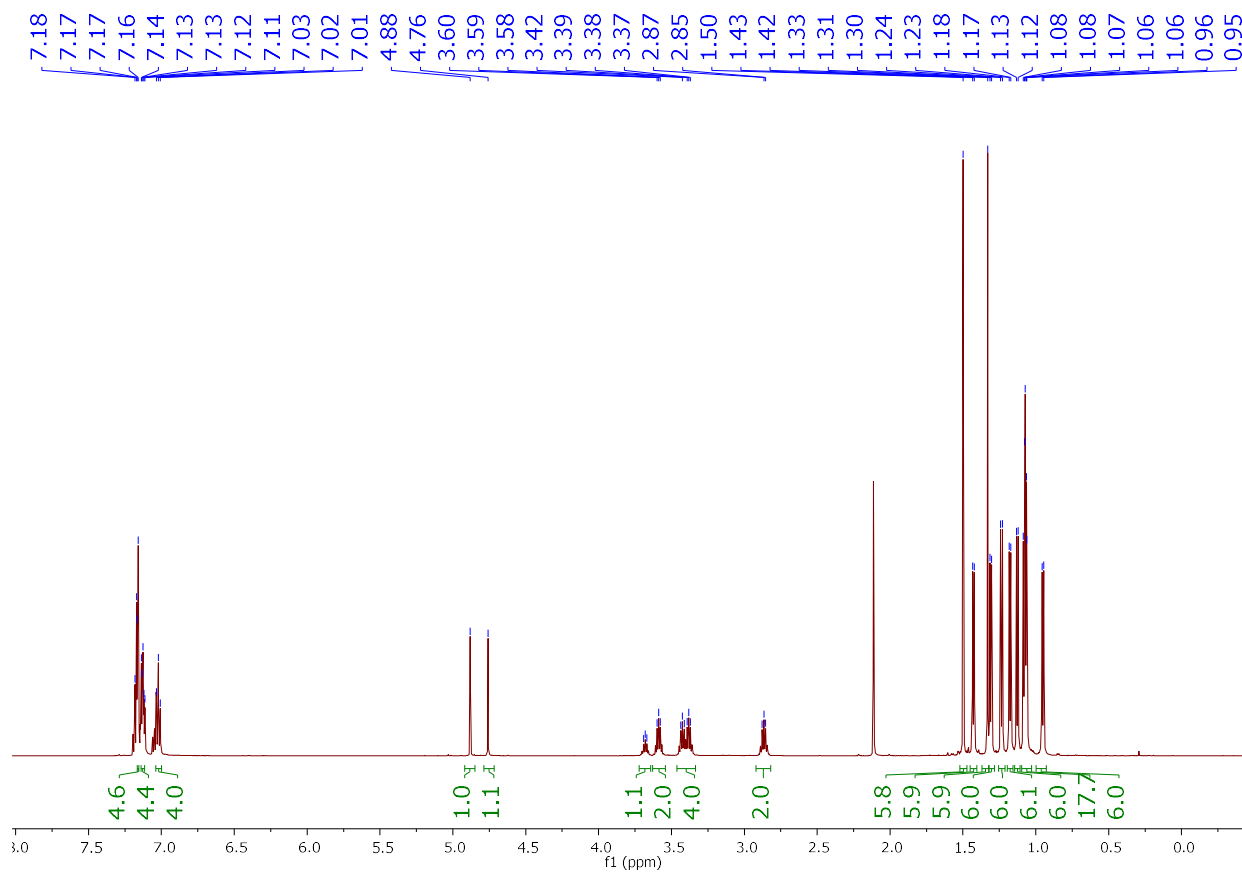


Figure S21. ^1H NMR (600 MHz, C_6D_6 , 298 K) spectrum of compound **5**.

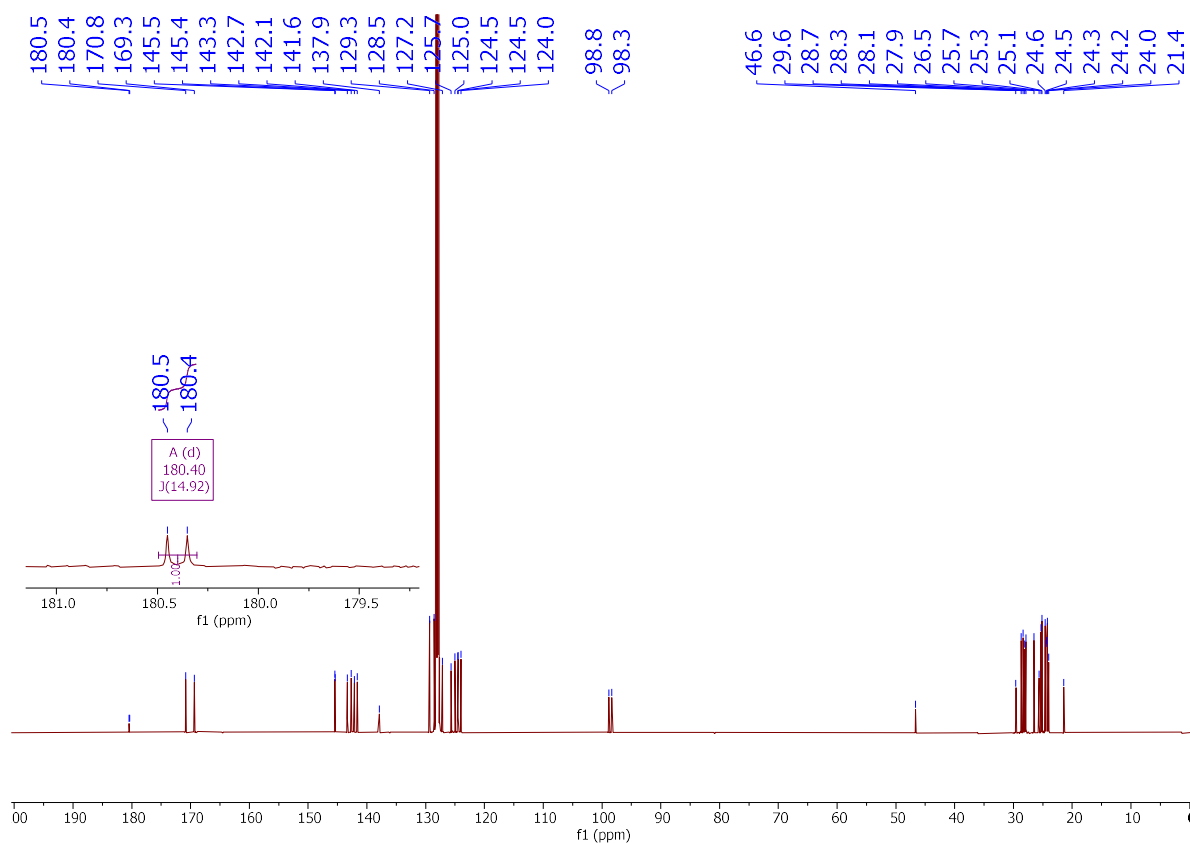


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, C_6D_6 , 298 K) spectrum of compound **5**.

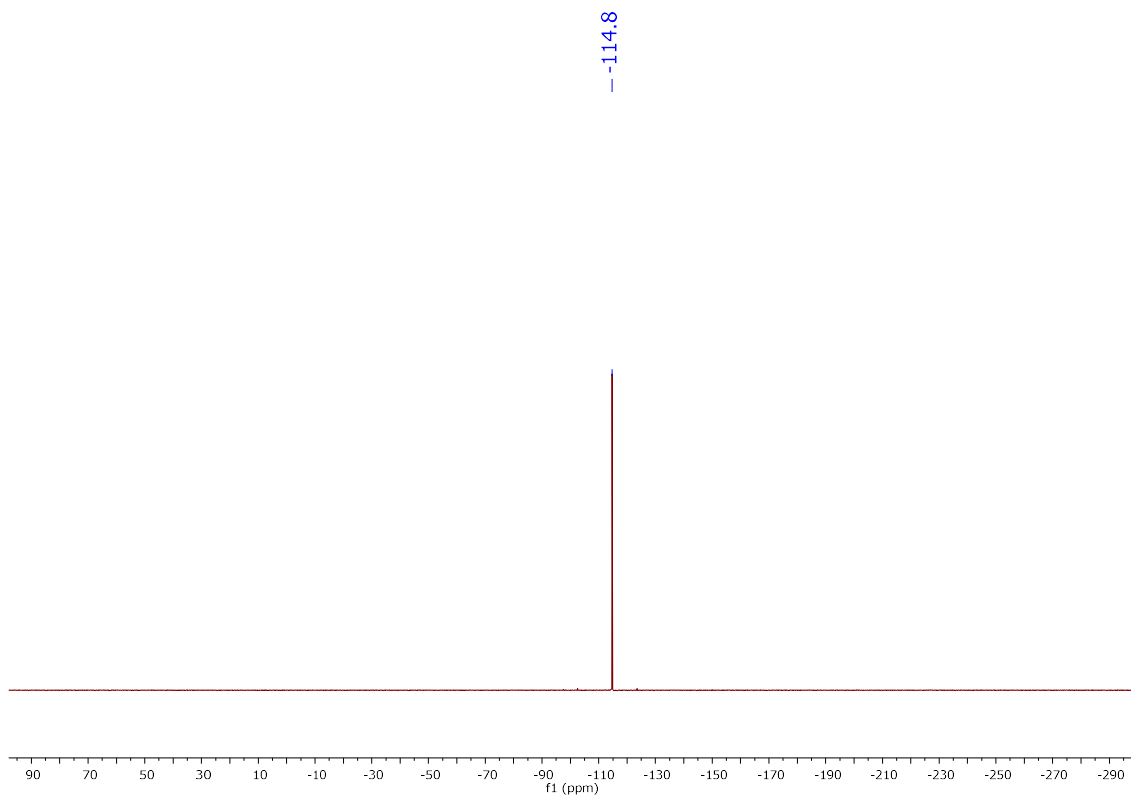


Figure S23. $^{31}\text{P}\{^1\text{H}\}$ NMR (243 MHz, C_6D_6 , 298 K) spectrum of compound **5**.

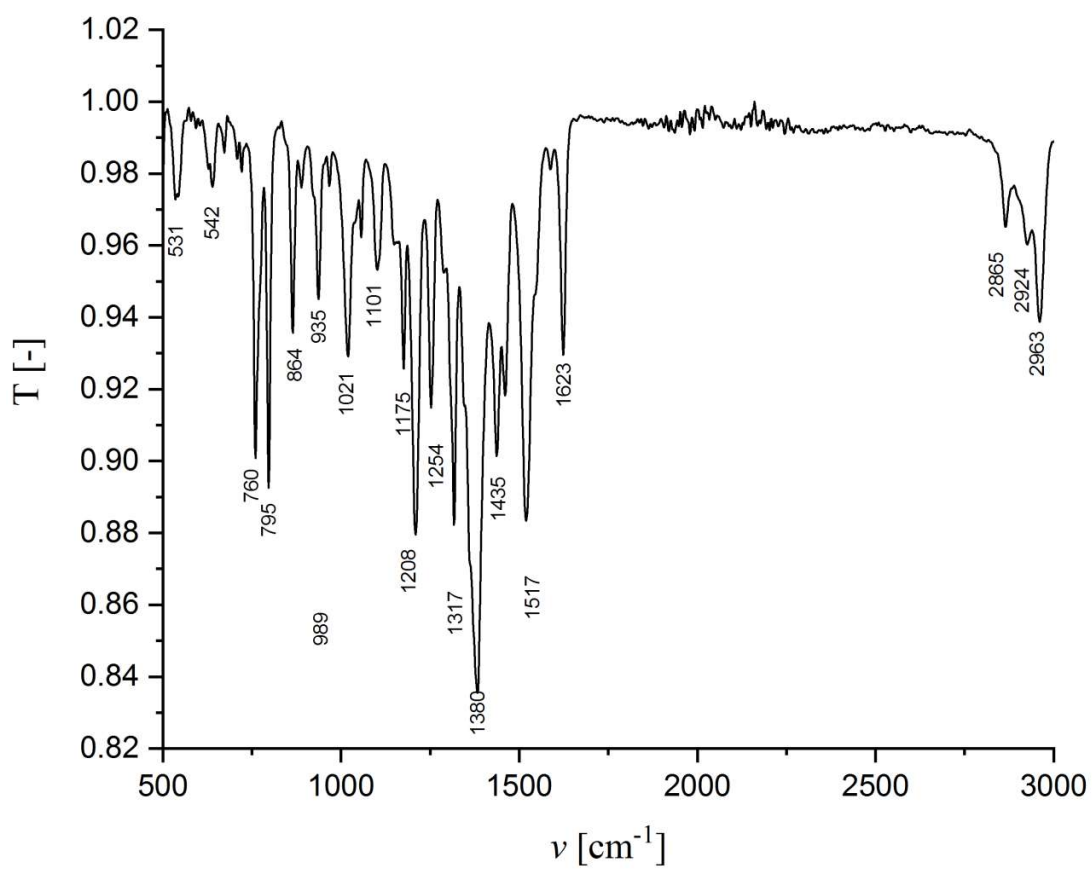


Figure S24. ATR-IR spectrum of **5**.

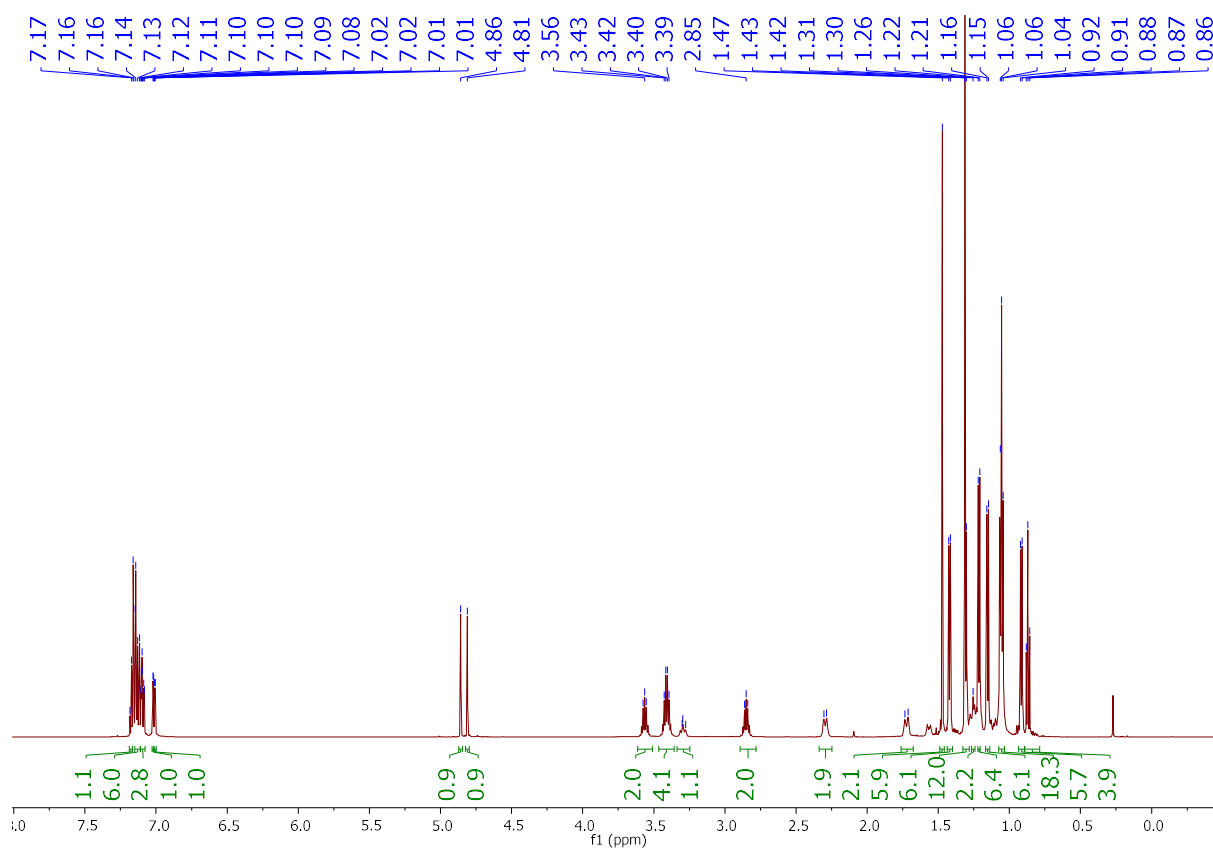


Figure S25. ^1H NMR (600 MHz, C_6D_6 , 298 K) spectrum of compound **6**.

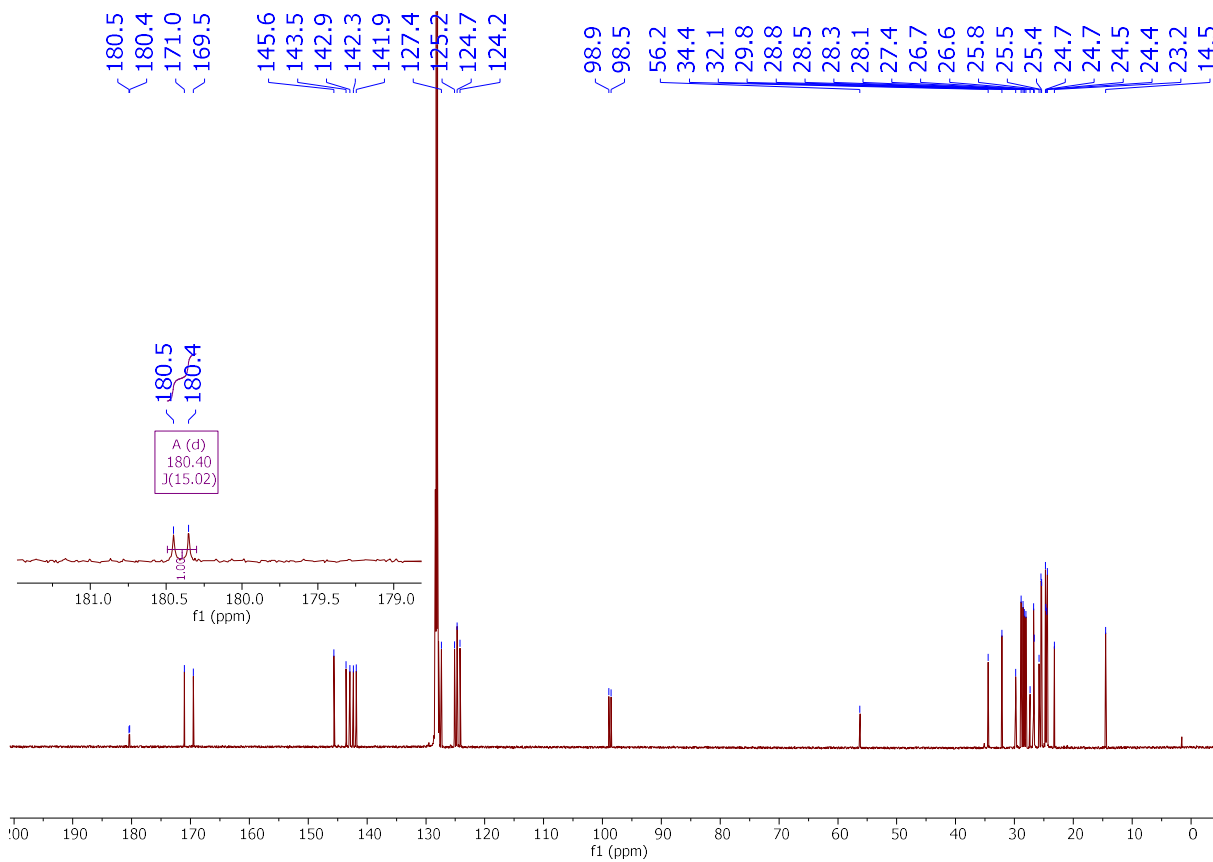


Figure S26. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, C_6D_6 , 298 K) spectrum of compound **6**.

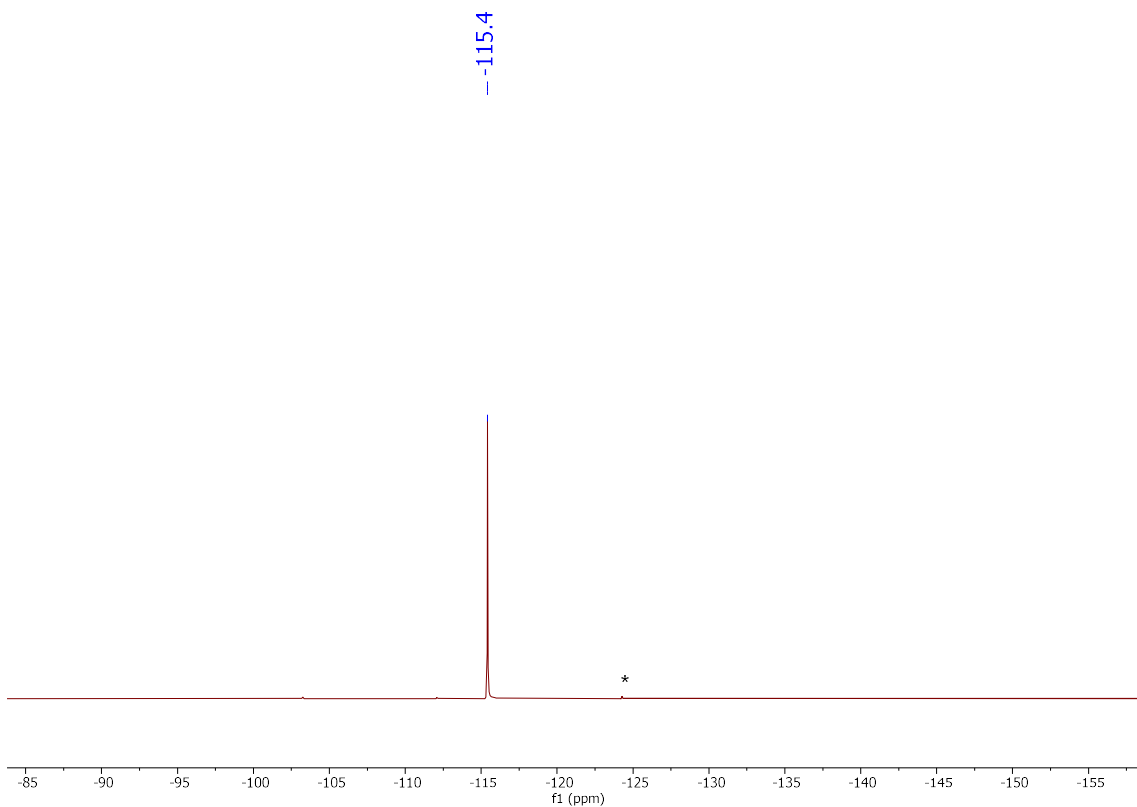


Figure S27. $^{31}\text{P}\{^1\text{H}\}$ NMR (243 MHz, C_6D_6 , 298 K) spectrum of compound **6**. *trace impurity.

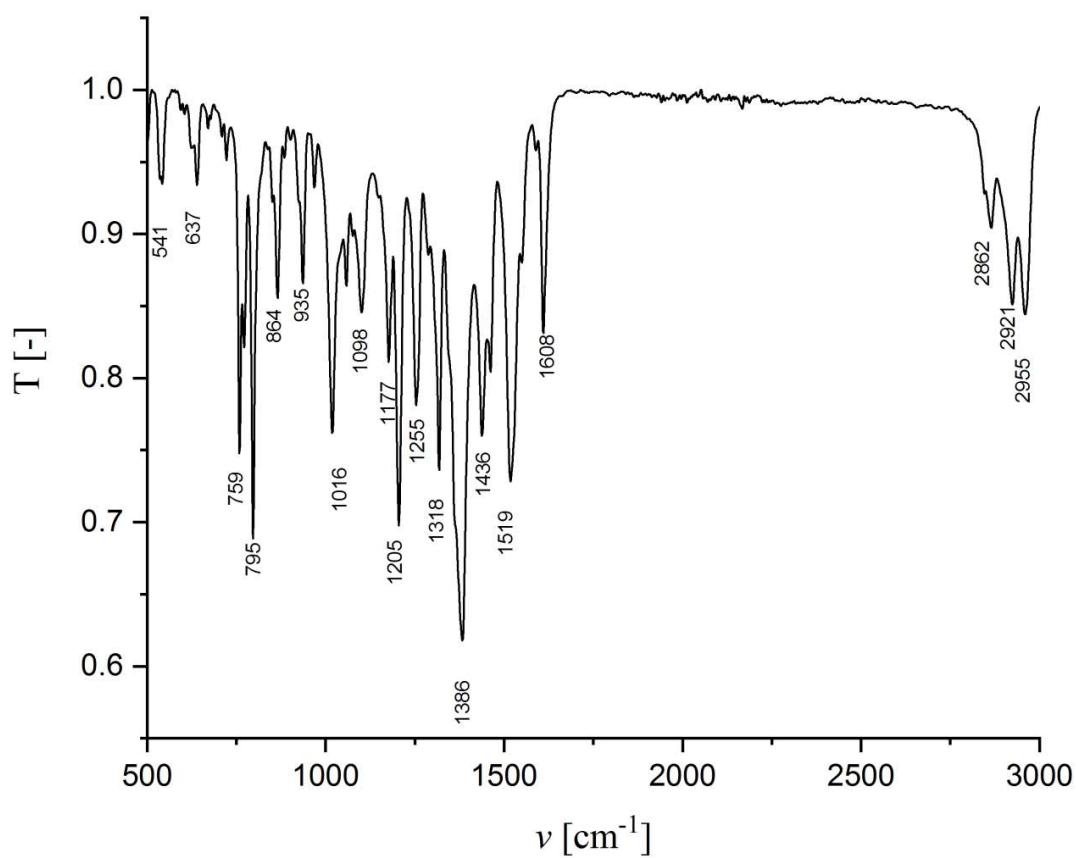


Figure S28. ATR-IR spectrum of **6**.

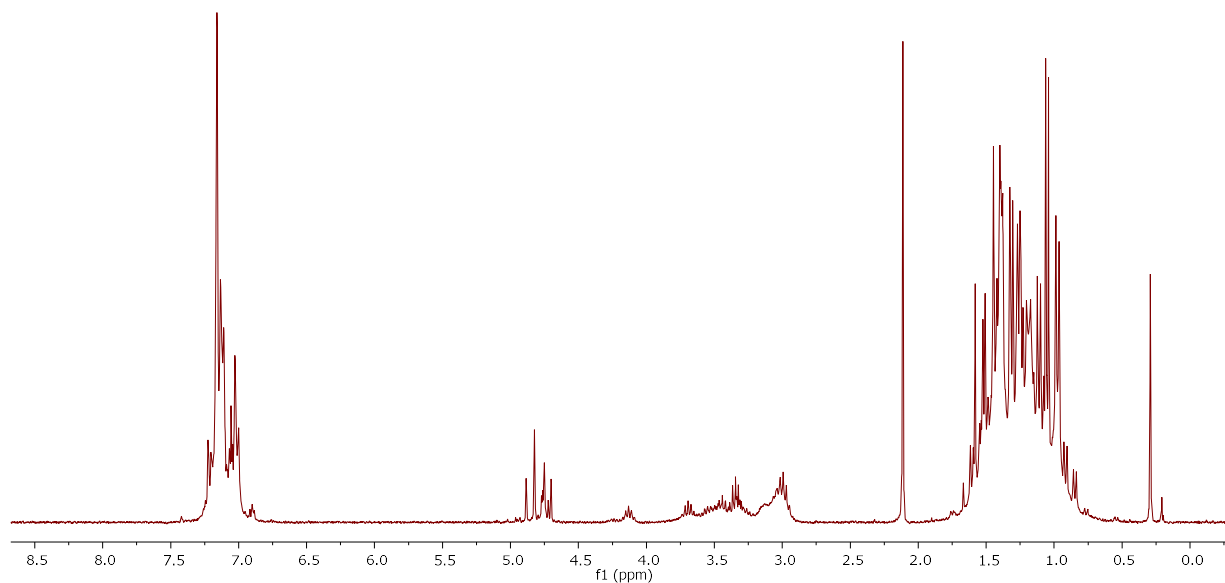


Figure S29. ^1H NMR (300 MHz, toluene- d_8 , 298 K) spectrum of reaction of **2** with CO_2 .

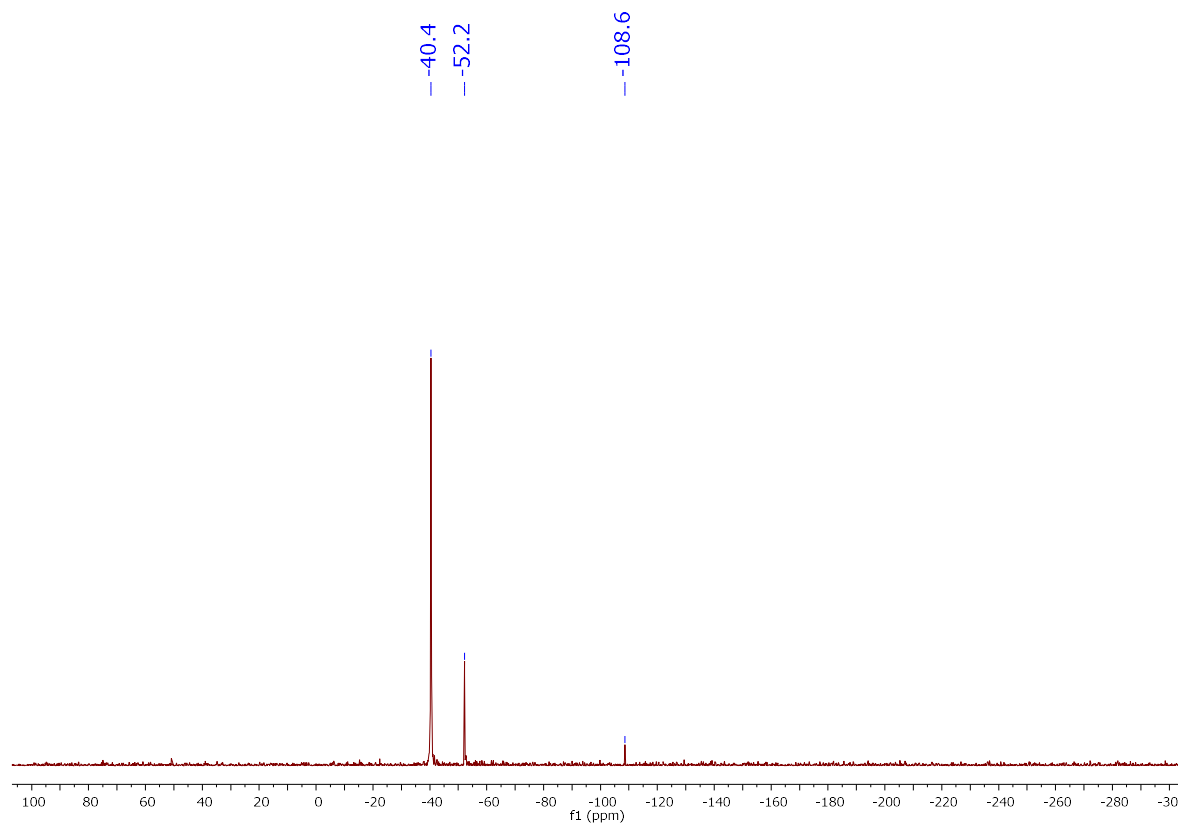


Figure S30. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8 , 298 K) spectrum of reaction of **2** with CO_2 .

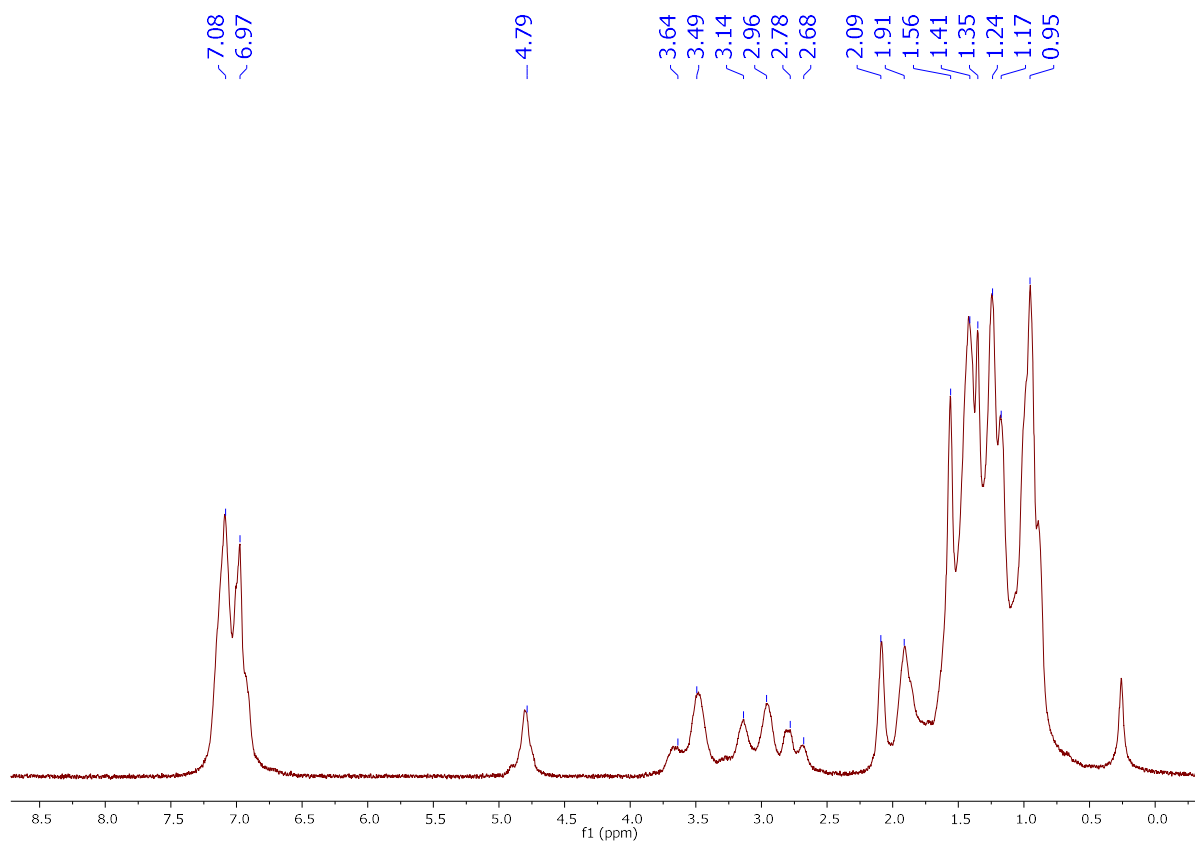


Figure S31. ^1H NMR (300 MHz, toluene- d_8 , 298 K) spectrum of reaction of **3** with CO_2 .

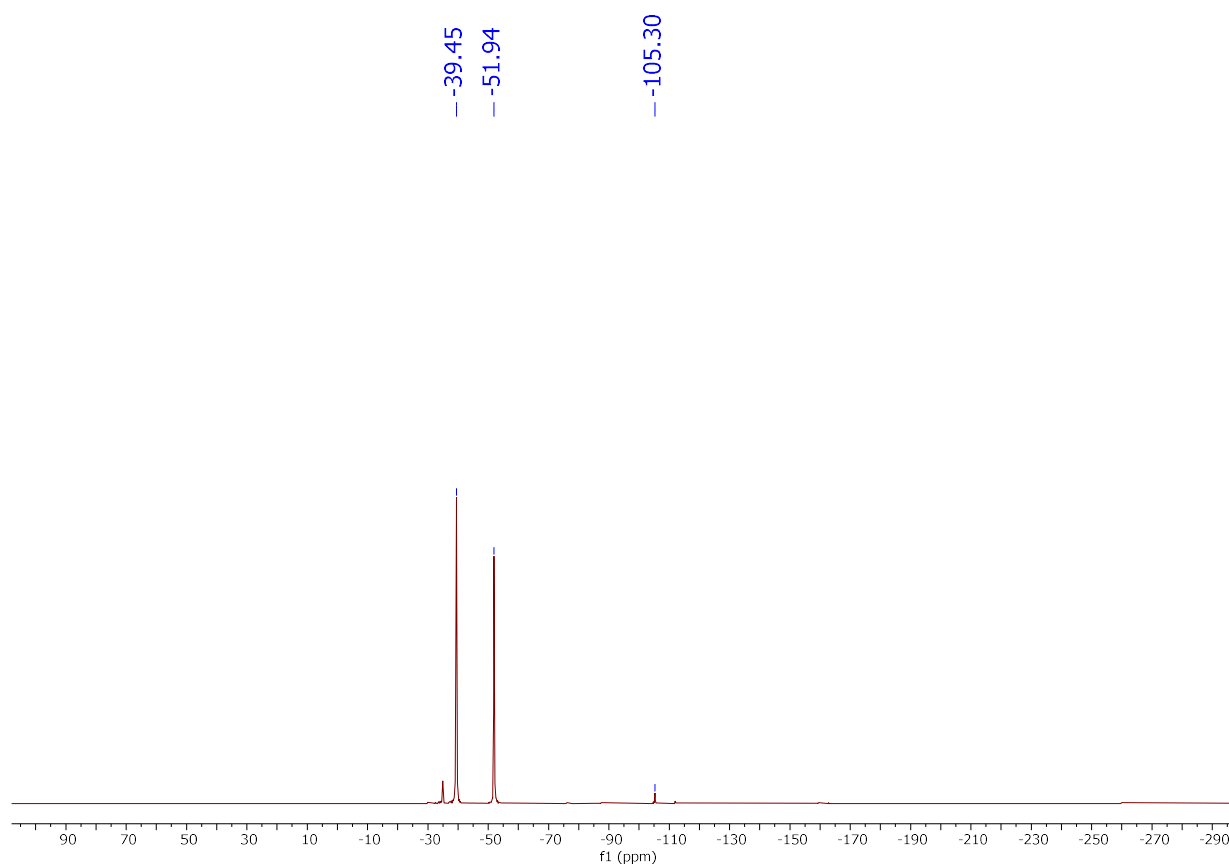


Figure S32. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8 , 298 K) spectrum of reaction of **3** with CO_2 .

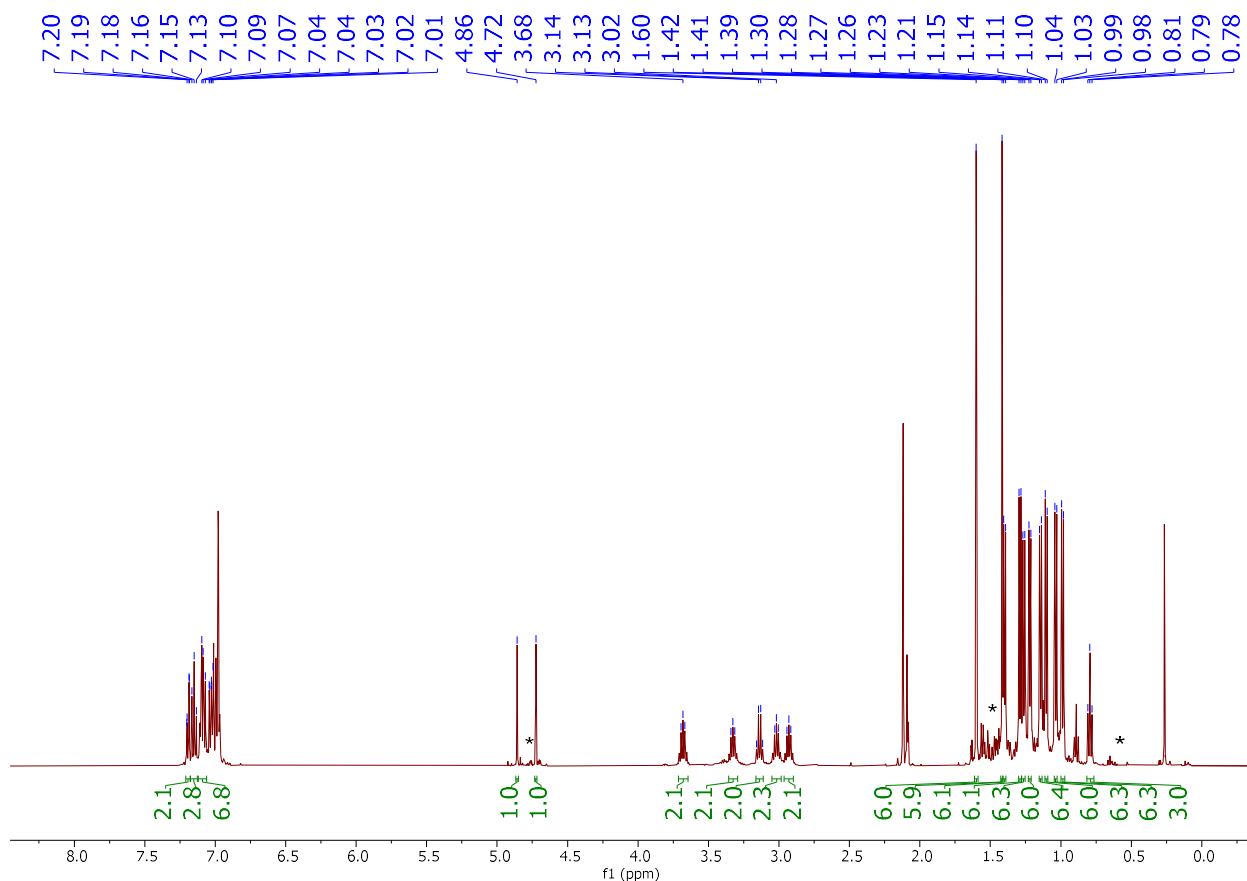


Figure S33. ^1H NMR (500 MHz, toluene- d_8 , 298 K) spectrum of compound 7. *trace impurities.

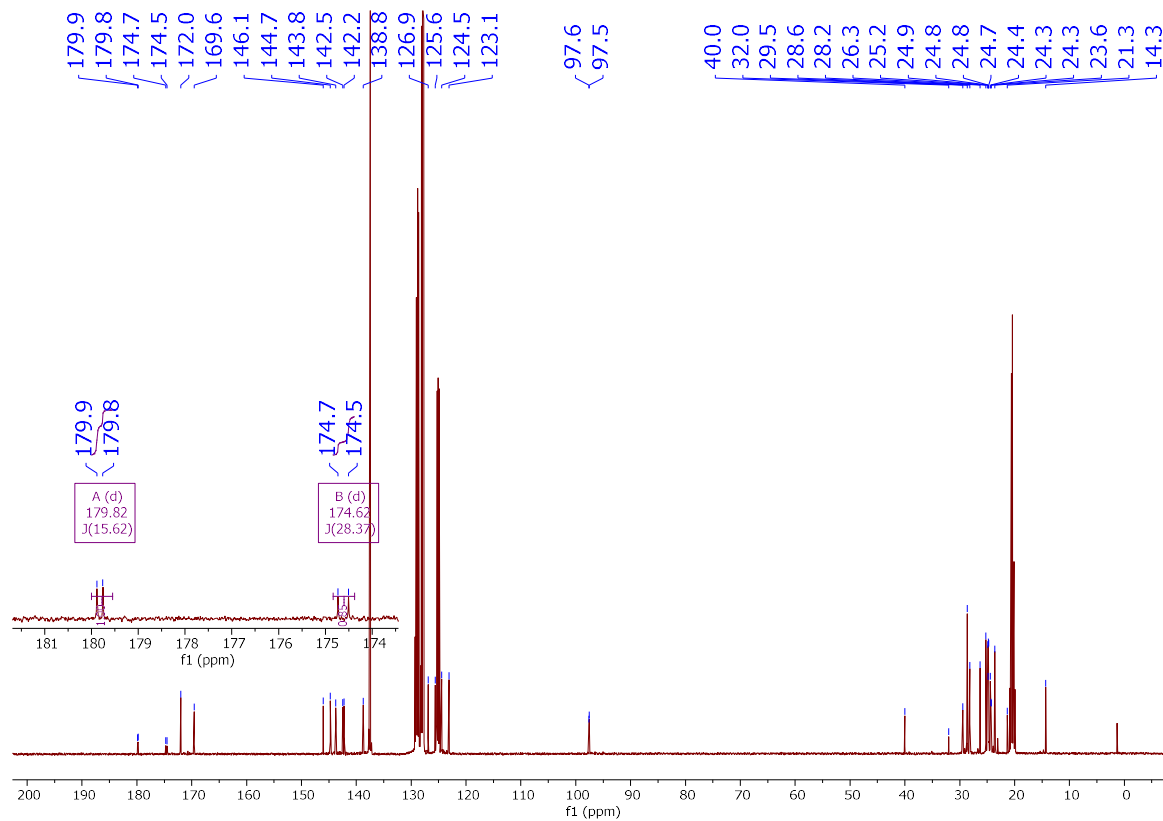


Figure S34. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, toluene- d_8 , 298 K) spectrum of compound 7.

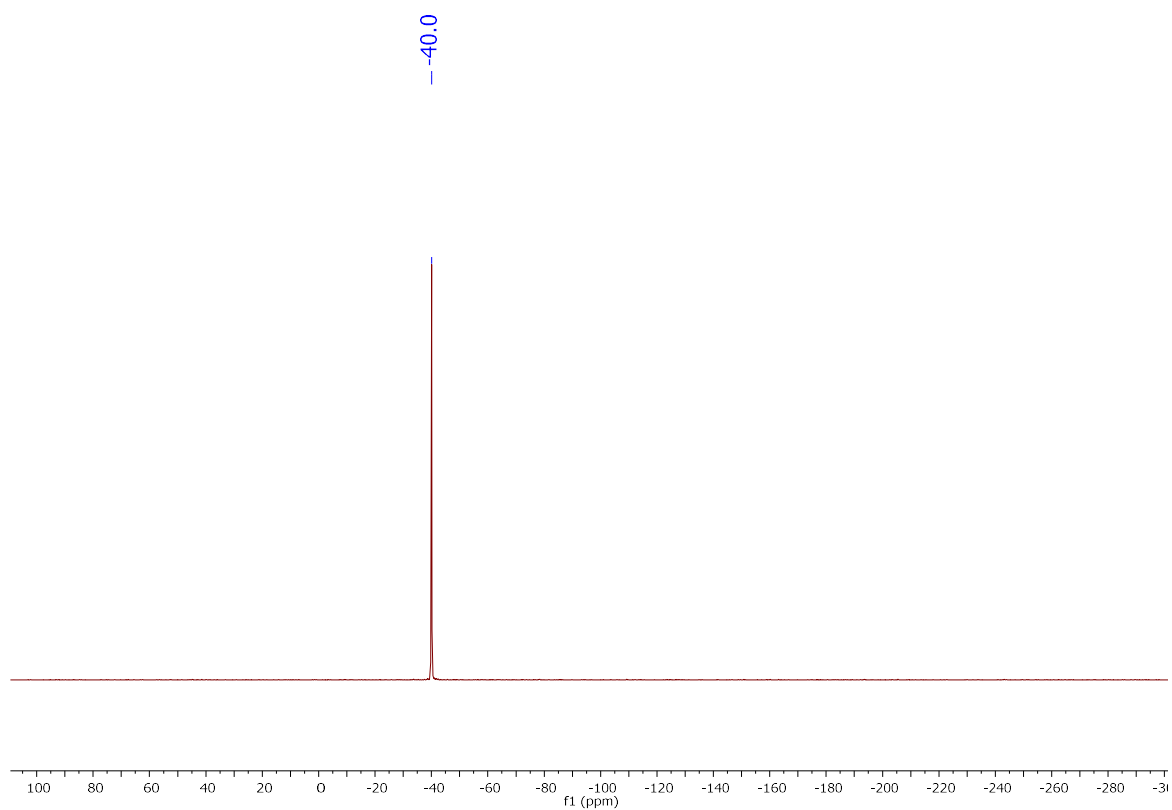


Figure S35. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, C_6D_6 , 298 K) spectrum of compound **7**.

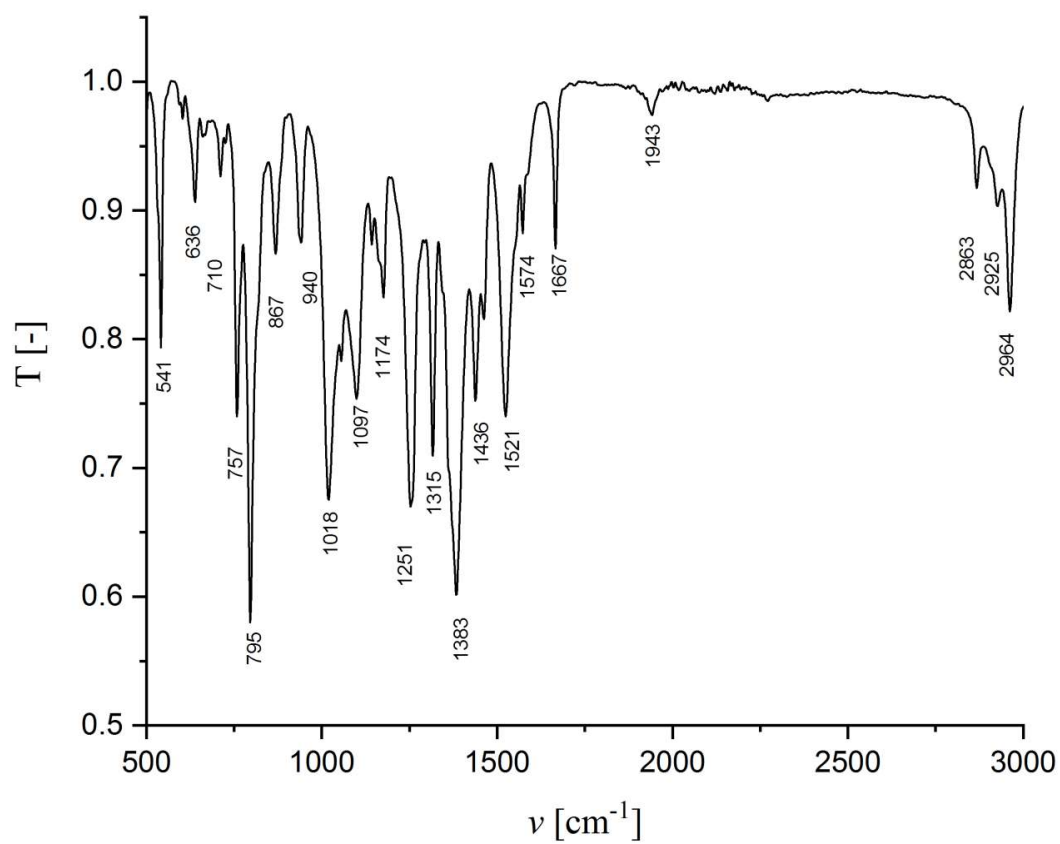


Figure S36. ATR-IR spectrum of **7**.

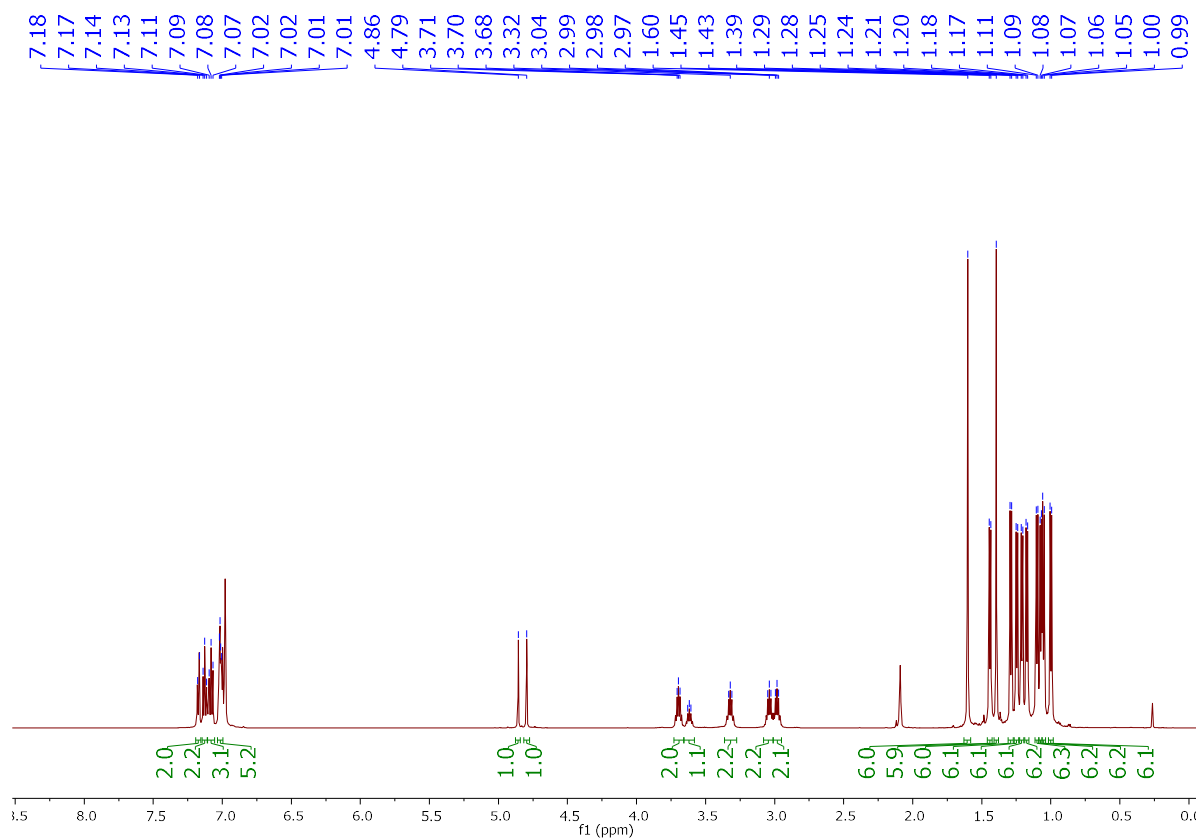


Figure S37. ^1H NMR (300 MHz, C_6D_6 , 298 K) spectrum of compound **8**.

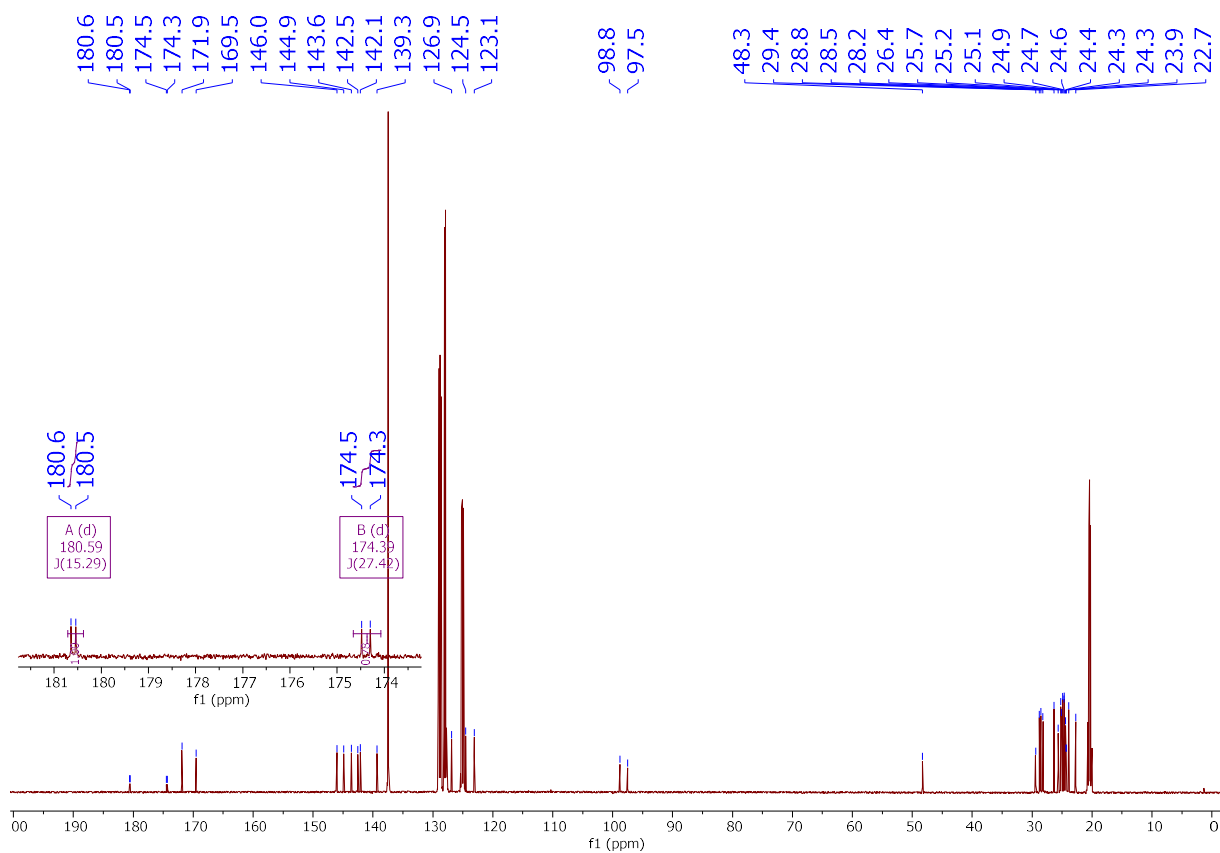


Figure S38. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, toluene- d_8 , 298 K) spectrum of compound **8**.

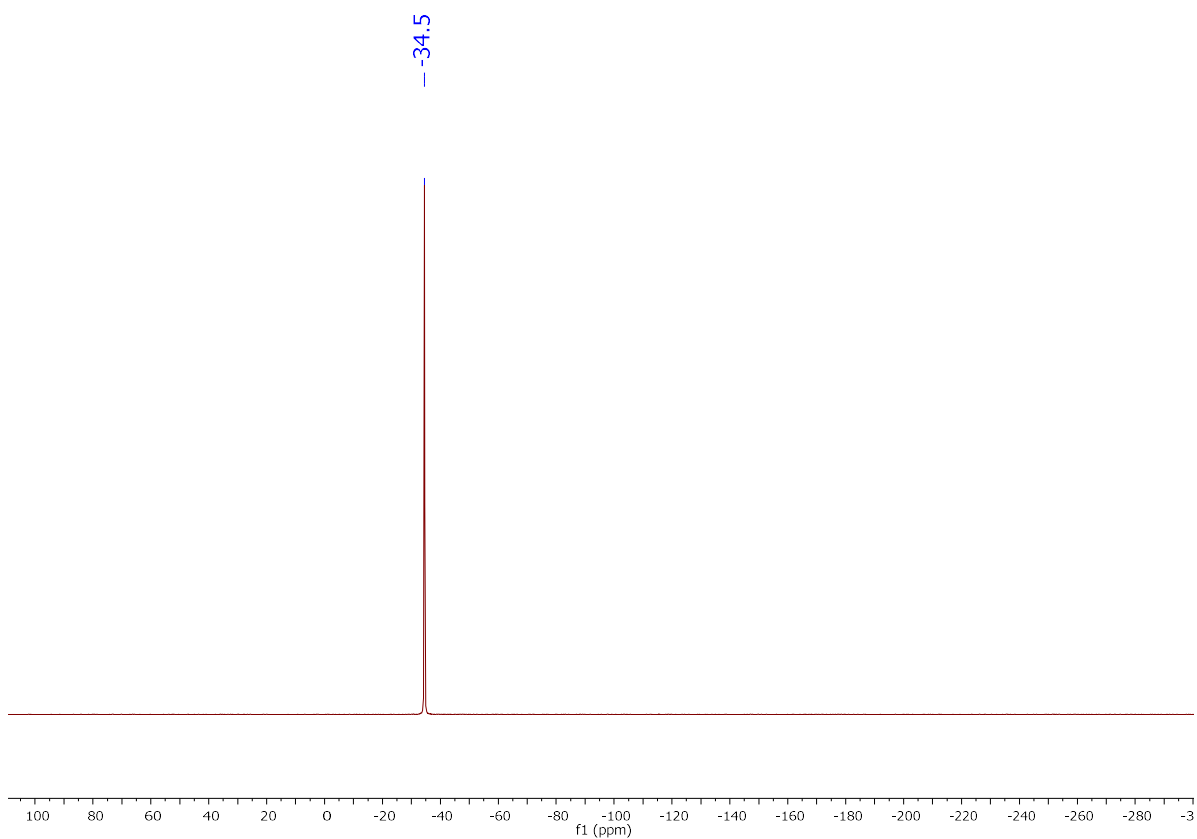


Figure S39. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8 , 298 K) spectrum of compound **8**.

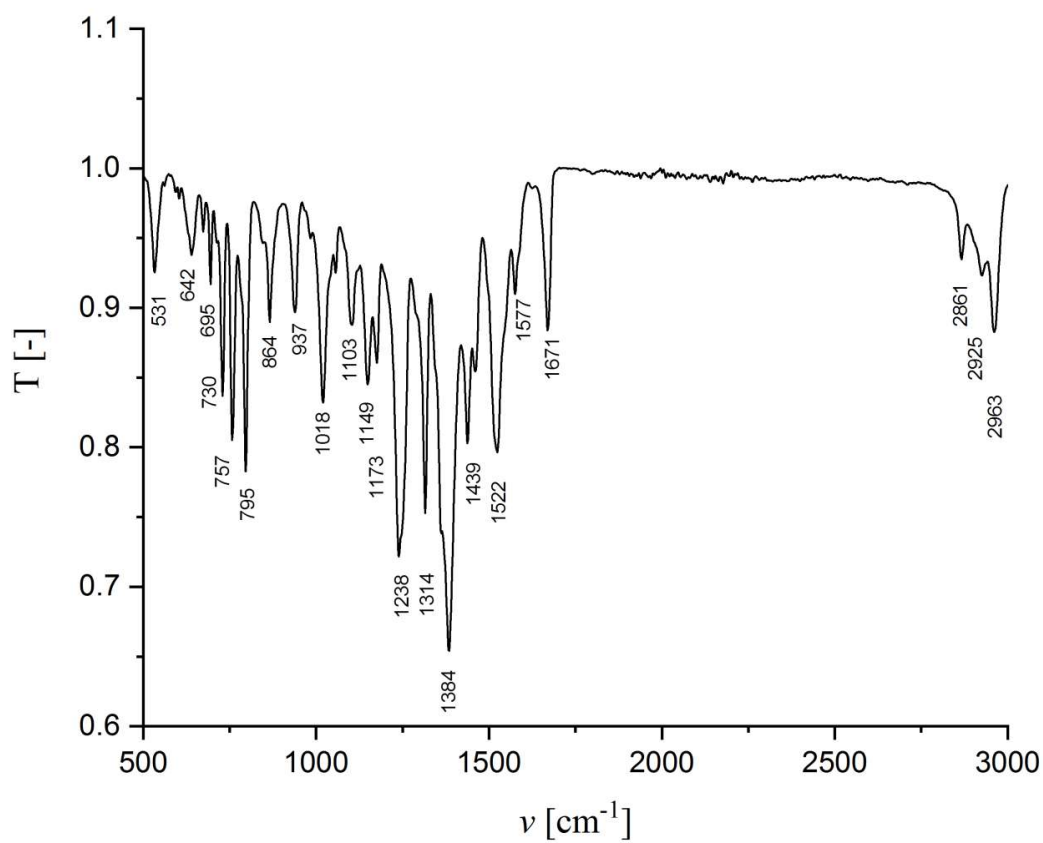


Figure S40. ATR-IR spectrum of **8**.

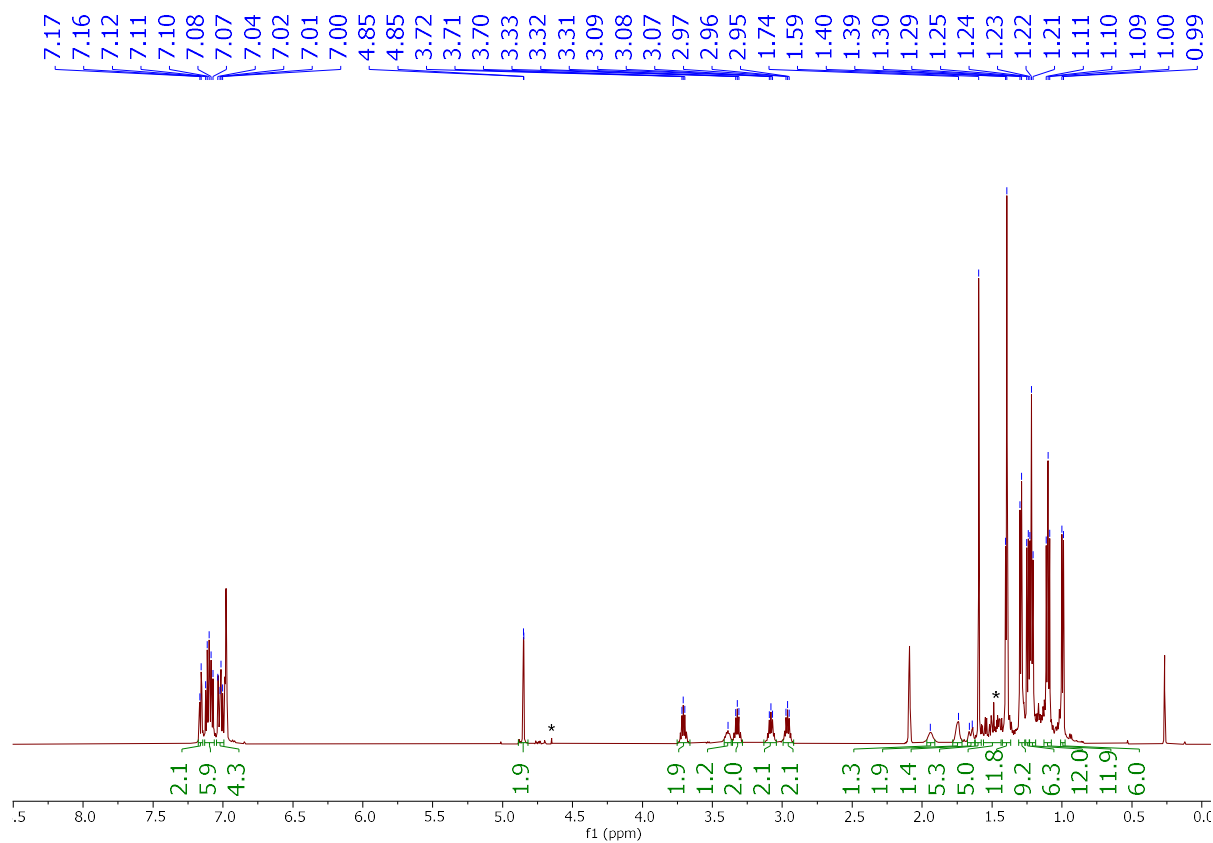


Figure S41. ^1H NMR (600 MHz, toluene- d_8 , 298 K) spectrum of compound **9**. *trace impurities.

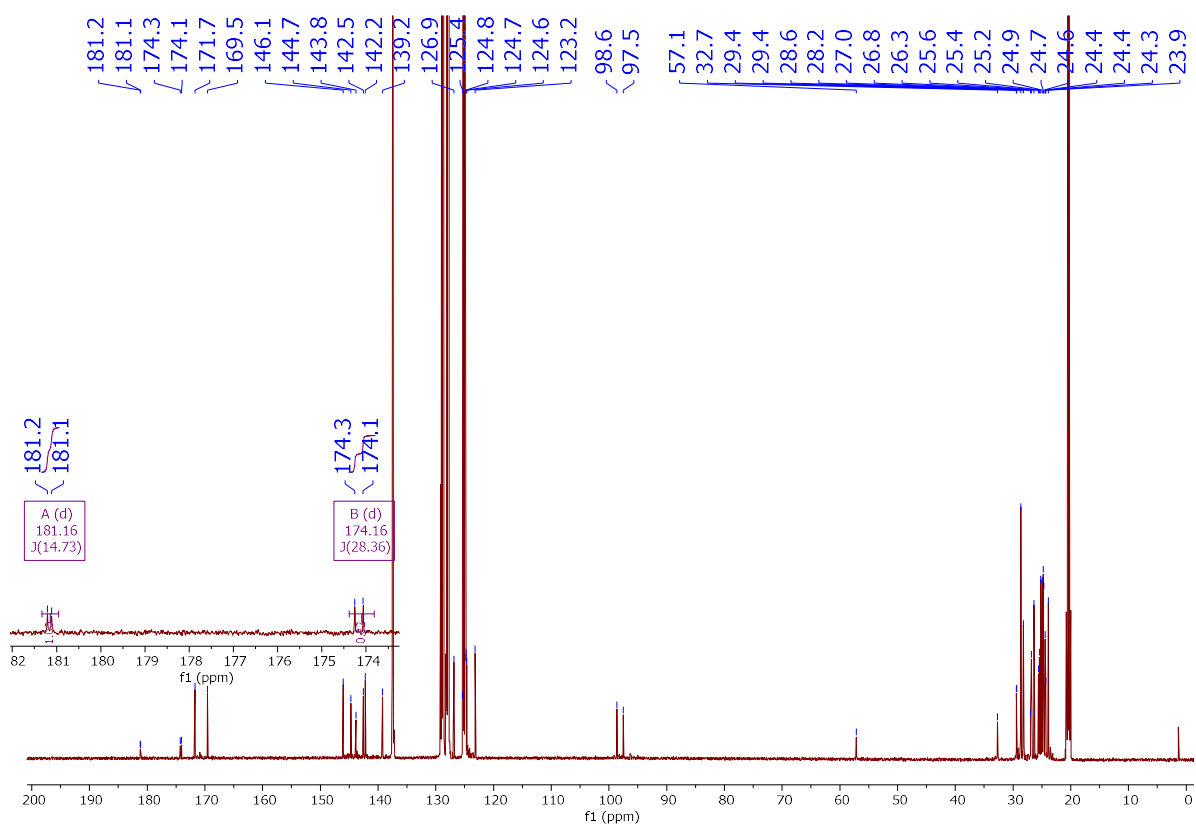


Figure S42. $^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, toluene- d_8 , 298 K) spectrum of compound **9**.

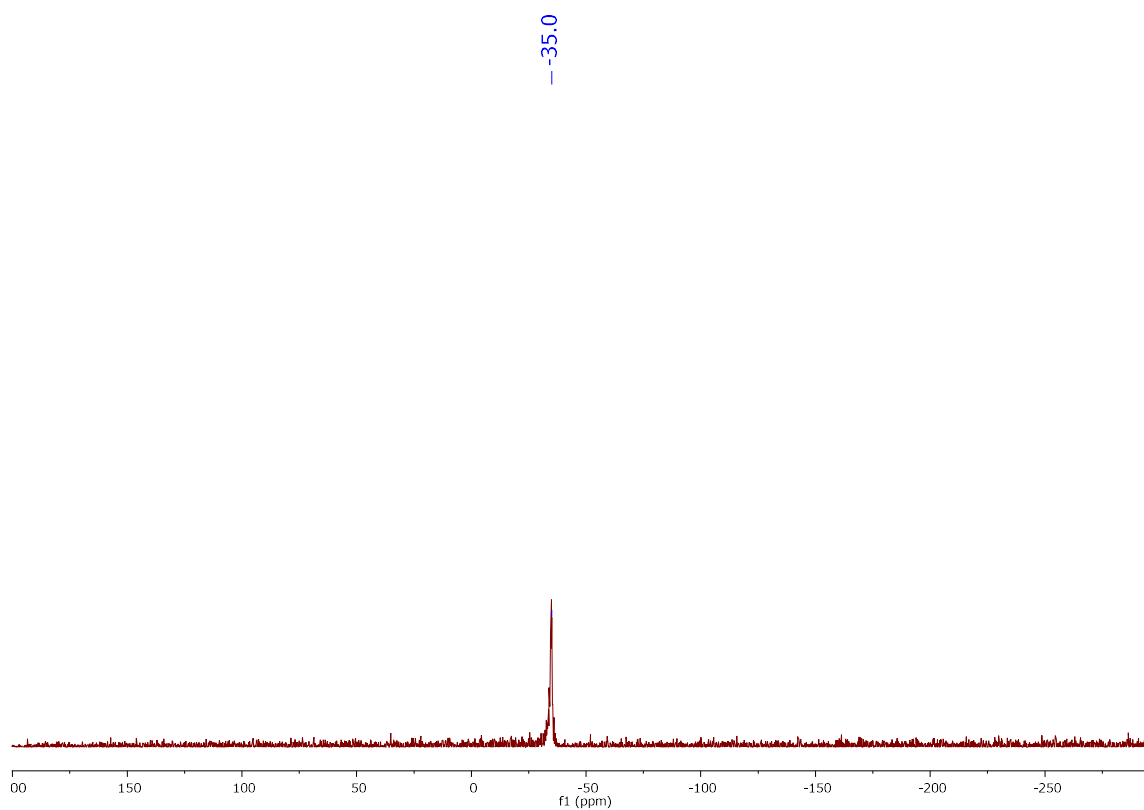


Figure S43. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8 , 298 K) spectrum of compound **9**.

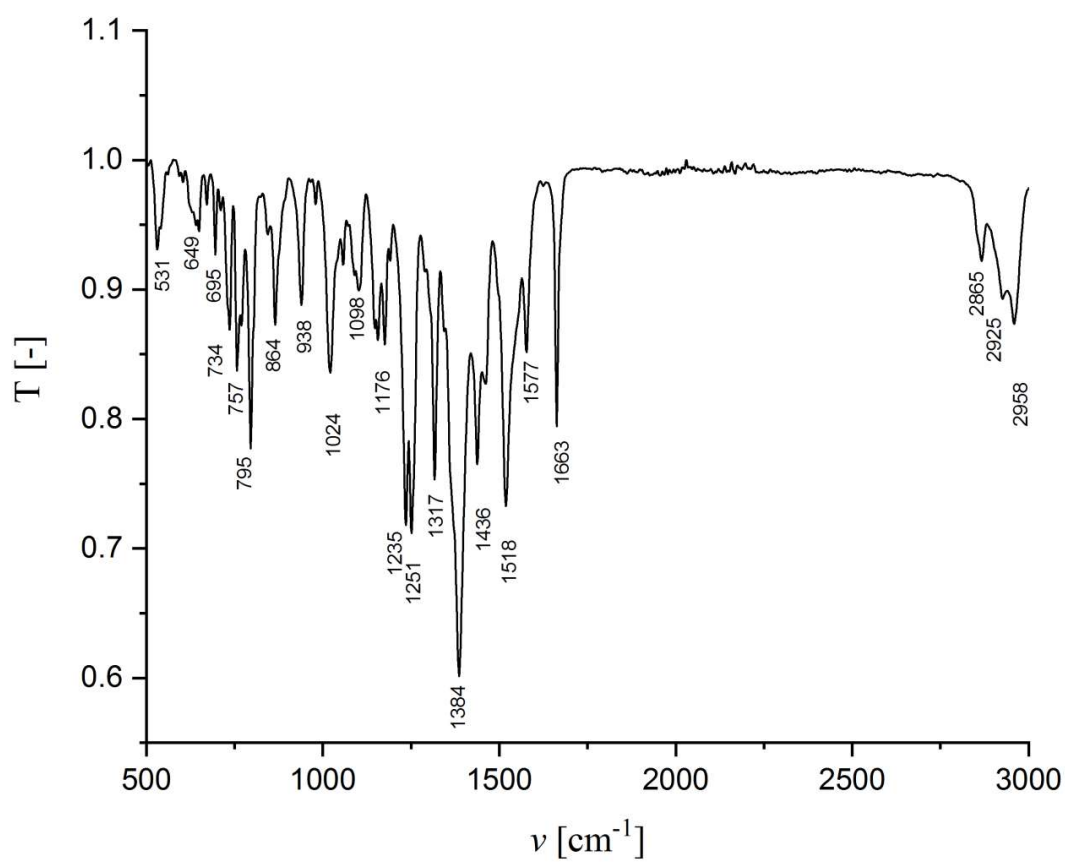


Figure S44. ATR-IR spectrum of **9**.

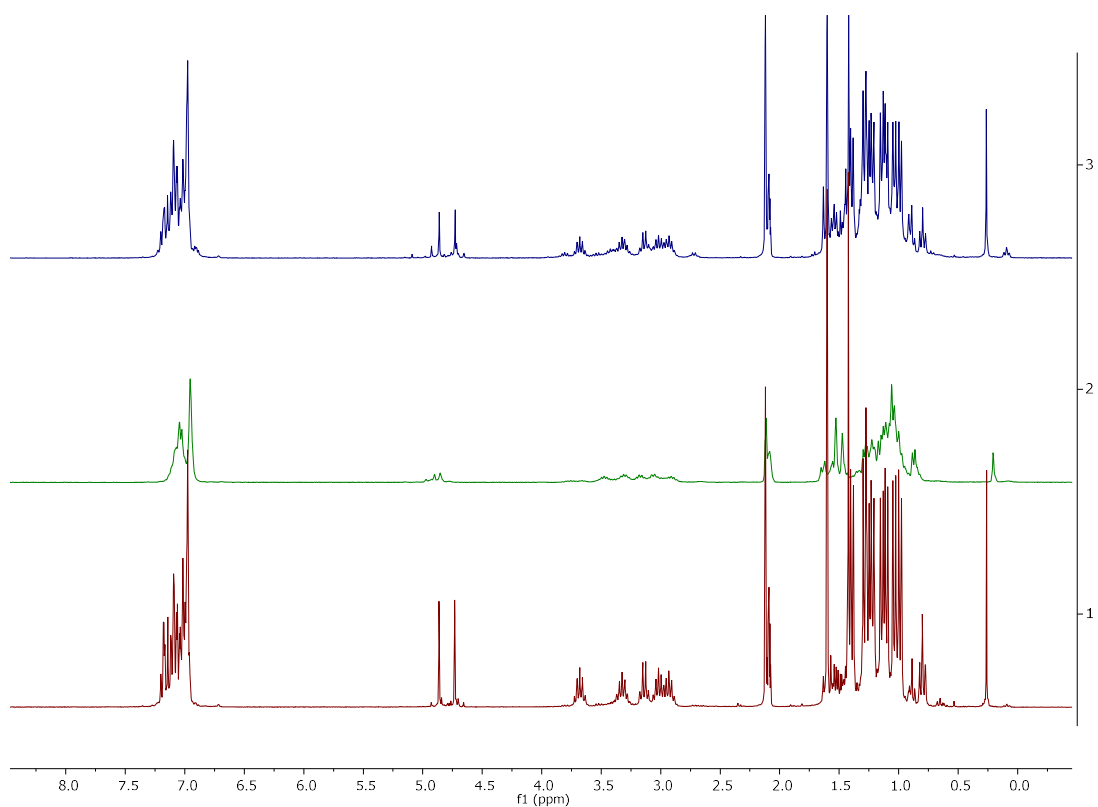


Figure S45. ^1H NMR (300 MHz, toluene- d_8) spectra of the temperature dependent reversible reaction of CO_2 and compound **4**; 1) compound **7**; 2) compound **7** after heating at $90\text{ }^\circ\text{C}$; 3) after cooling to ambient temperature.

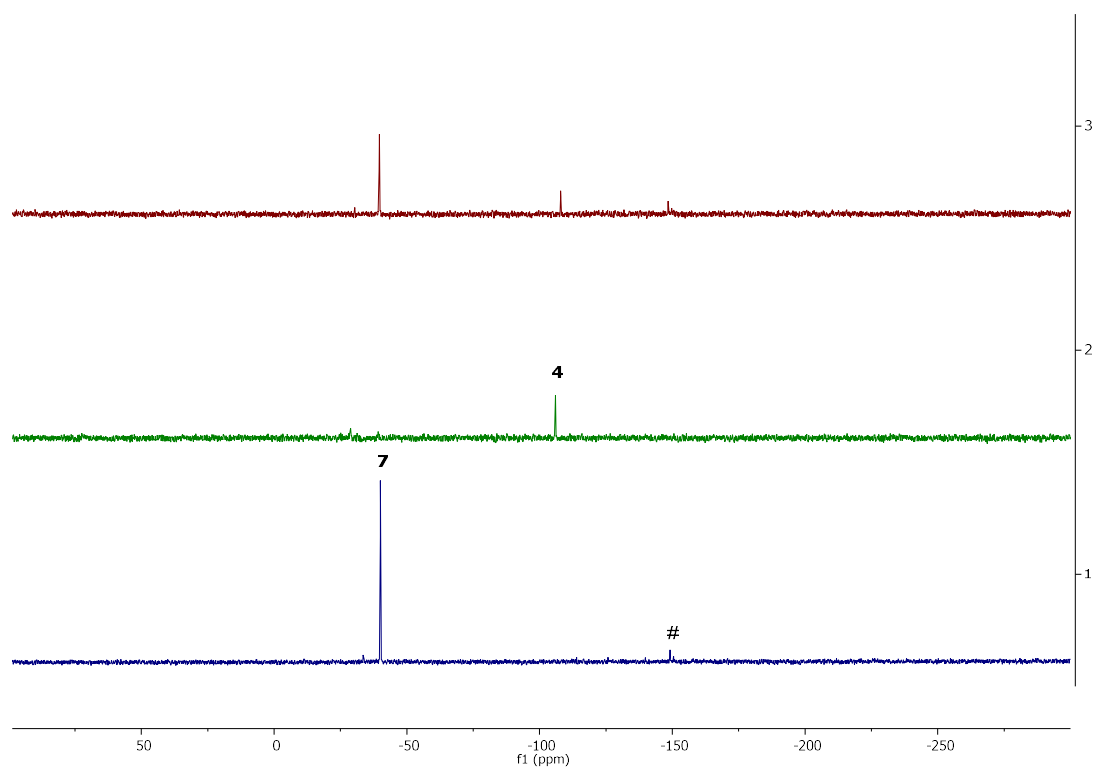


Figure S46. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8) spectra of the temperature dependent reversible reaction of CO_2 and compound **4**; 1) compound **7**; 2) compound **7** after heating at $90\text{ }^\circ\text{C}$; 3) after cooling to ambient temperature. #unidentified impurity.

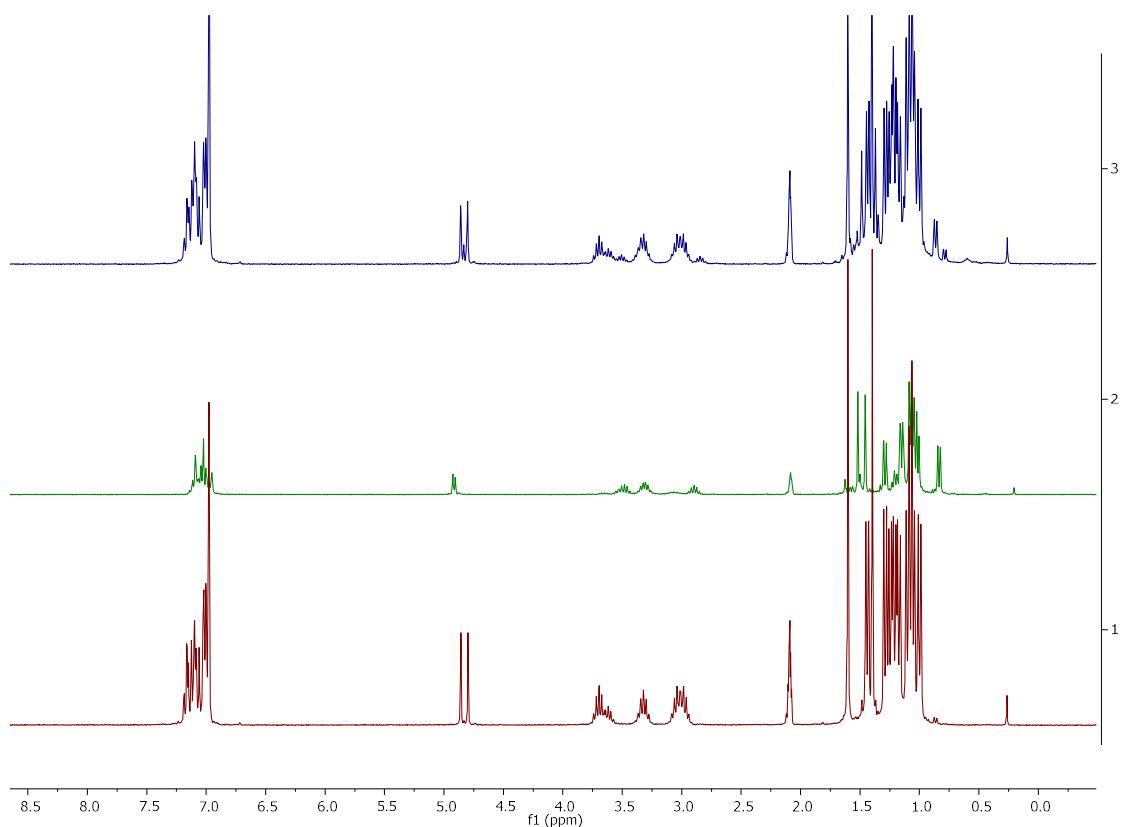


Figure S47. ^1H NMR (300 MHz, toluene- d_8) spectra of the temperature dependent reversible reaction of CO_2 and compound **5**; 1) compound **8**; 2) compound **8** after heating at 90 °C; 3) after cooling to ambient temperature.

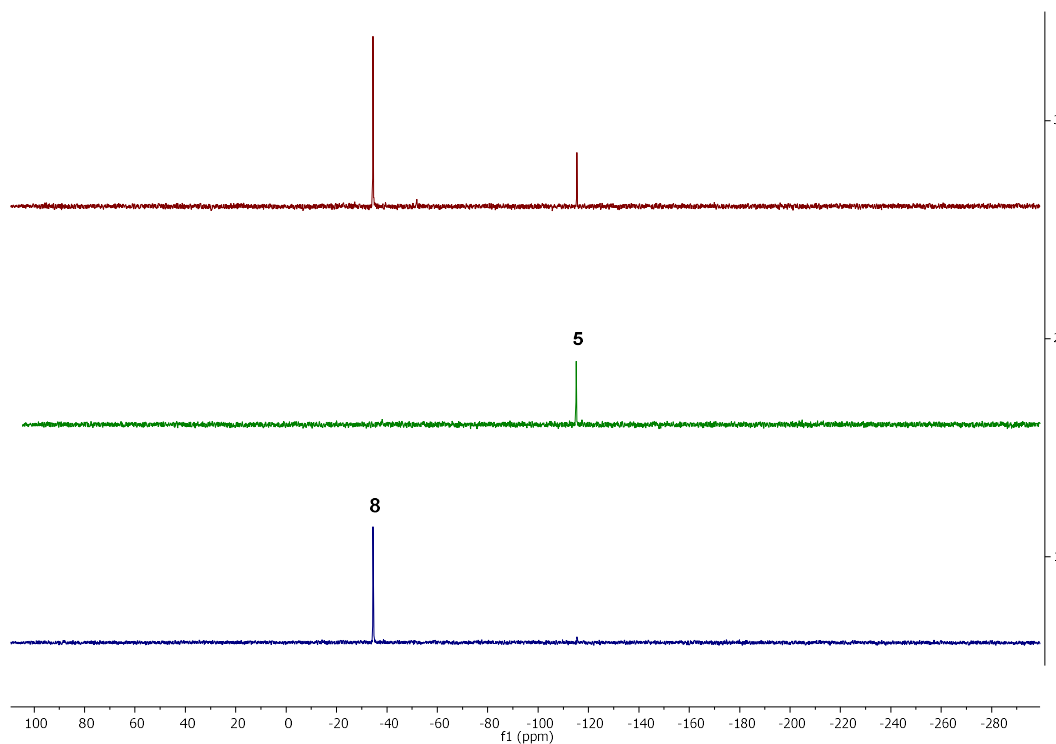


Figure S48. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8) spectra tracking the temperature dependent reversible reaction of CO_2 and compound **5**; 1) compound **8**; 2) compound **8** after heating at 90 °C; 3) after cooling to ambient temperature.

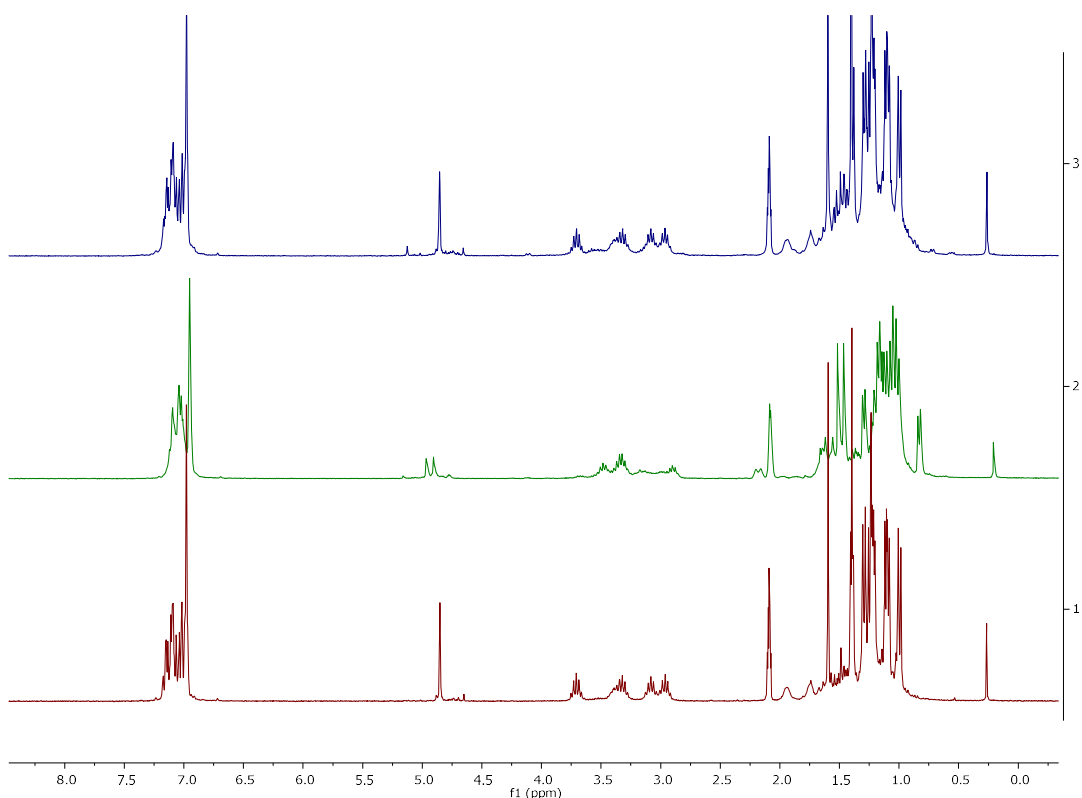


Figure S49. ^1H NMR (300 MHz, toluene- d_8) spectra of the temperature dependent reversible reaction of CO_2 and compound **6**; 1) compound **9**; 2) compound **9** after heating at 90 °C; 3) after cooling to ambient temperature.

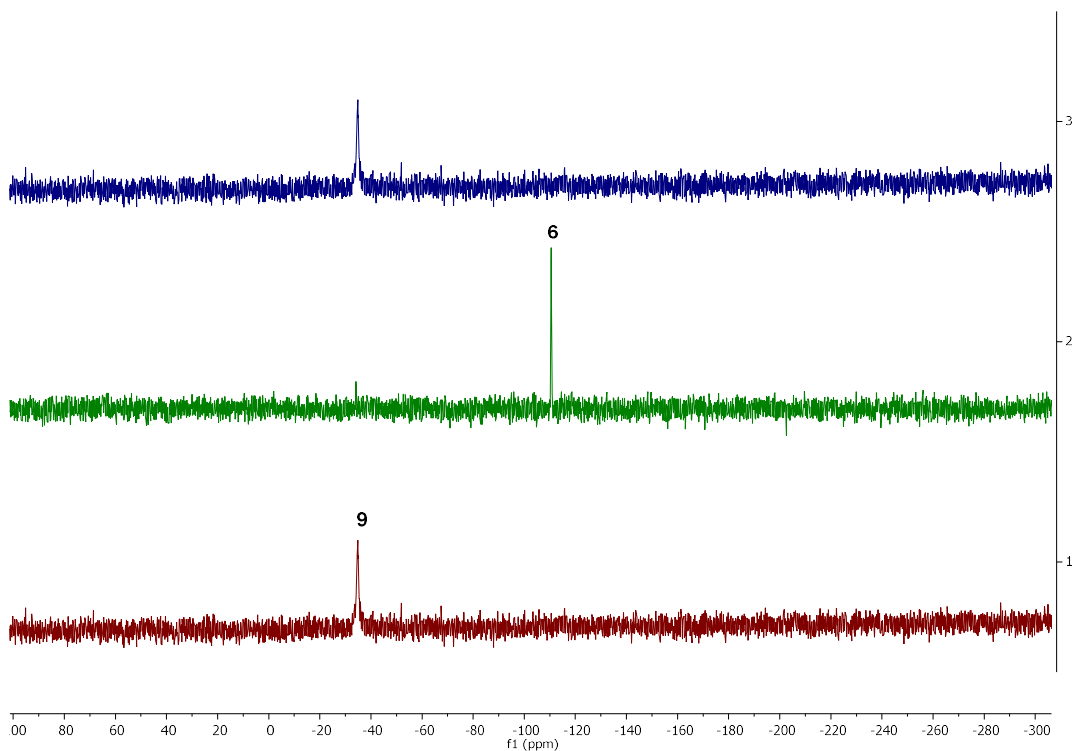


Figure S50. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene- d_8) spectra tracking the temperature dependent reversible reaction of CO_2 and compound **6**; 1) compound **9**; 2) compound **9** after heating at 90 °C; 3) after cooling to ambient temperature.

3. X-Ray Crystallographic Analysis

The crystals were mounted on nylon loops in inert oil. Data for **2** were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $\text{Mo}_{K\alpha}$ radiation, $\lambda = 0.71073 \text{ \AA}$) and for **6**, **8**, and **9** were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated $\text{Cu}_{K\alpha}$ radiation, $\lambda = 1.54178 \text{ \AA}$, micro-focus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)^[3] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2014).^[4-6] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. **2** was refined as a 2-component inversion twin. The toluene molecule is disordered over two alternate sites. The bond lengths and angles of its phenyl ring were constrained to be equal (SADI) and its anisotropic displacement parameters were restrained with RIGU. In **6** an *i*-Pr group in residue 2 is disordered over two positions. All its corresponding bond lengths and angles were restrained to be equal (SADI). In both residues the phosphorous atom is disordered over two positions. In addition, in the residual density near Cl1 of residue 1 the CNCO unit of an alternate orientation of the CyNCO ligand can be identified, however, finding and refining the whole moiety failed due to the low residual density. The small displacement ellipsoid of N5 suggests that in the elusive second orientation CyNCO and Cl swap places. N5 would then be over-layered with a Cl atom leading to more electron density in the place. A refinement of a partially occupied Cl here failed due to the low occupancy. Considering the unresolved disorder, quantitative results should be carefully assessed. The crystal of **8** was a non-merohedral twin of strongly overlapping components which was identified but not integrated separately. Consequently, only the connectivity should be taken for granted. Quantitative results should not be discussed since the obtained intensity data is strongly distorted by the ignored twin components as indicated by the high R_{int} . A more suitable specimen was not available. In addition, the structure contains a highly disordered toluene molecule. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run.^[7] The molecule was included in the sum formula for completeness. A toluene molecule in **9** is disordered over three alternate positions. The occupancies were constrained to the values of the free variables in the last refinement cycles to avoid correlations and ensure a convergence of the refinement. All bond lengths and angles of the solvents' phenyl rings were restrained to be equal (SADI) and RIGU restraints were applied to the anisotropic displacement parameters.

CCDC-2089048 (**2**), -2089049 (**6**), -2089050 (**8**), and -2089051 (**9**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement of **2** and **6**.

Compound	2	6
Emp. formula	C ₇₂ H ₁₀₄ ClGa ₂ N ₆ P	C ₆₈ H ₁₀₀ ClGa ₂ N ₅ OP
Formula weight	1259.47	1209.38
Temperature [K]	100(2)	100(2)
Crystal system	monoclinic	orthorhombic
Space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> [Å]	12.3792(15)	13.2671(8)
<i>b</i> [Å]	12.7475(15)	14.3515(9)
<i>c</i> [Å]	21.578(3)	68.902(4)
α [°]	90	90
β [°]	92.262(3)	90
γ [°]	90	90
<i>V</i> [Å ³]	3402.5(7)	13119.1(1)
<i>Z</i>	2	8
ρ [Mgm ⁻³]	1.229	1.225
μ [mm ⁻¹]	0.899	1.942
<i>F</i> (000)	1344	5160
Crystal size [mm]	0.411 × 0.215 × 0.130	0.162 × 0.096 × 0.057
θ max [°]	33.448	78.458
Index ranges	-19 ≤ <i>h</i> ≤ 19 -19 ≤ <i>k</i> ≤ 19 -33 ≤ <i>l</i> ≤ 33	-16 ≤ <i>h</i> ≤ 15 -18 ≤ <i>k</i> ≤ 18 -87 ≤ <i>l</i> ≤ 86
No. of reflect. collected	147001	482739
Unique reflect.	26323	27953
<i>R</i> _{int}	0.0306	0.1205
Data / restraints / params.	24791/223/830	25967/25/1497
Goodness-of-fit on F ²	1.013	1.069
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0214	0.0554
<i>wR</i> 2 [<i>I</i> > 2σ(<i>I</i>)]	0.0515	0.1288
<i>R</i> 1 [all data]	0.0242	0.0608
<i>wR</i> 2 [all data]	0.0522	0.1321
<i>x</i> (Flack)	0.115(3)	0.058(13)
Largest diff. peak and hole max./min. [e·Å ⁻³]	0.389/-0.253	1.630/-0.613

Table S2. Crystal data and structure refinement of **8** and **9**.

Compound	8	9
Emp. formula	C _{66.50} H ₉₃ ClGa ₂ N ₅ O ₃ P	C ₈₀ H ₁₀₉ ClGa ₂ N ₅ O ₃ P
Formula weight	1216.31	1394.58
Temperature [K]	100(2)	100(2)
Crystal system	triclinic	triclinic
Space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> [Å]	12.7138(13)	12.4401(7)
<i>b</i> [Å]	22.680(2)	12.7679(7)
<i>c</i> [Å]	23.894(2)	23.7801(12)
α [°]	82.361(5)	88.165(3)
β [°]	88.926(5)	83.535(3)
γ [°]	76.638(5)	85.239(3)
<i>V</i> [Å ³]	6643.2(11)	3739.1(4)
<i>Z</i>	4	2
ρ [Mgm ⁻³]	1.216	1.239
μ [mm ⁻¹]	1.946	1.794
<i>F</i> (000)	2580	1484
Crystal size [mm]	0.220 × 0.119 × 0.042	0.095 × 0.074 × 0.051
θ max [°]	75.564	81.135
Index ranges	-15 ≤ <i>h</i> ≤ 15 -28 ≤ <i>k</i> ≤ 28 -29 ≤ <i>l</i> ≤ 29	-15 ≤ <i>h</i> ≤ 14 -16 ≤ <i>k</i> ≤ 16 -30 ≤ <i>l</i> ≤ 30
No. of reflect. collected	247431	208100
Unique reflect.	27202	16280
<i>R</i> _{int}	0.2748	0.0714
Data / restraints / params.	17943/0/1396	13586/732/982
Goodness-of-fit on F ²	1.076	1.024
<i>R</i> 1 [<i>I</i> > 2σ(<i>I</i>)]	0.0806	0.0335
<i>wR</i> 2 [<i>I</i> > 2σ(<i>I</i>)]	0.2175	0.0810
<i>R</i> 1 [all data]	0.1266	0.0441
<i>wR</i> 2 [all data]	0.2516	0.0880
Largest diff. peak and hole max./min. [e·Å ⁻³]	1.360/-1.459	0.608/-0.414

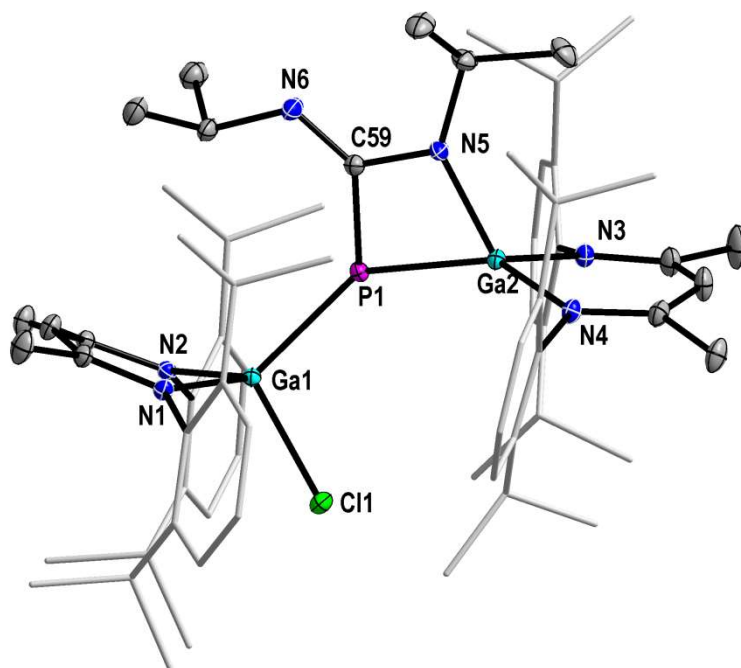


Figure S51. Molecular structure of **2** with thermal ellipsoids at 50% probability level. The hydrogen atoms and solvent molecules (toluene) are omitted for clarity. Selected bond length (Å) and angles (°): Ga1-N1 1.9511(11), Ga1-N2 1.9861(11), Ga1-Cl1 2.1967(4), Ga1-P1 2.3084(4), Ga2-N5 1.9279(11), Ga2-N4 1.9668(11), Ga2-N3 1.9704(12), Ga2-P1 2.3115(4), P1-C59 1.8860(13), N5-C59 1.3882(17), N6-C59 1.2834(17); N1-Ga1-N2 95.57(5), N1-Ga1-Cl1 108.52(3), N2-Ga1-Cl1 106.61(3), N1-Ga1-P1 128.82(4), N2-Ga1-P1 110.66(3), Cl1-Ga1-P1 104.915(14), N5-Ga2-N4 116.74(5), N5-Ga2-N3 116.42(5), N4-Ga2-N3 97.34(5), N5-Ga2-P1 75.96(4), N4-Ga2-P1 142.51(4), N3-Ga2-P1 108.21(4), C59-P1-Ga1 121.55(4), C59-P1-Ga2 75.66(4), Ga1-P1-Ga2 130.987(17), C59-N5-Ga2 101.82(8), N5-C59-P1 105.66(9).

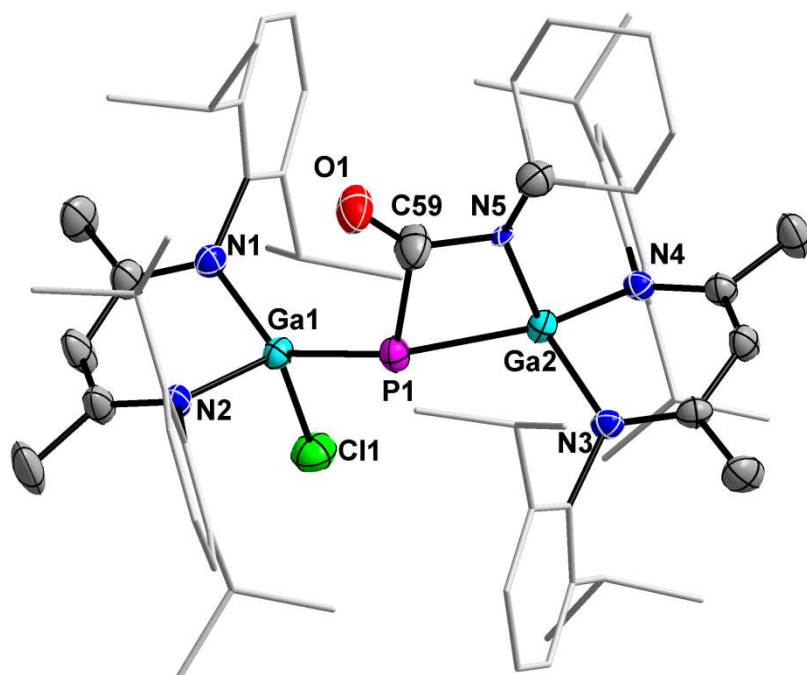


Figure S52. Molecular structure of **6** with thermal ellipsoids at 50% probability level. The hydrogen atoms, a solvent molecule (*n*-hexane) and the alternate positions of the disordered parts are omitted for clarity. Selected bond length (Å) and angles (°): Ga1-N2 1.949(5), Ga1-N1 1.949(5), Ga1-Cl1 2.2102(17), Ga1-P1 2.296(2), Ga2-N4 1.937(4), Ga2-N3 1.961(5), Ga2-N5 2.005(4), Ga2-P1 2.266(2), P1-C59 1.904(7), O1-C59 1.234(8), N5-C59 1.366(8); N2-Ga1-N1 95.9(2), N2-Ga1-Cl1 107.14(16), N1-Ga1-Cl1 105.83(15), N2-Ga1-P1 105.32(16), N1-Ga1-P1 135.06(16), Cl1-Ga1-P1 104.99(8), N4-Ga2-N3 95.92(19), N4-Ga2-N5 113.34(18), N3-Ga2-N5 112.03(18), N4-Ga2-P1 148.61(15), N3-Ga2-P1 107.98(15), N5-Ga2-P1 76.64(13), C59-P1-Ga2 75.9(2), C59-P1-Ga1 115.8(3), Ga2-P1-Ga1 132.96(11), O1-C59-N5 126.3(6), O1-C59-P1 124.1(5), N5-C59-P1 107.5(4).

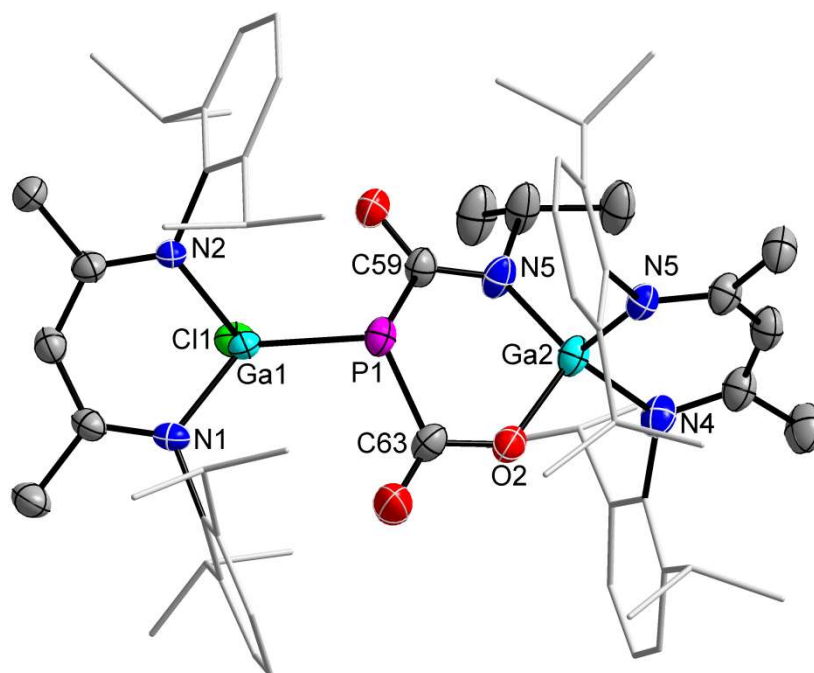


Figure S53. Molecular structure of **8** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. Selected bond length (Å) and angles (°): Ga1-N1 1.944(4), Ga1-N2 1.962(4), Ga1-Cl1 2.2015(14), Ga1-P1 2.3272(15), Ga2-O2 1.840(4), Ga2-N5 1.887(5), Ga2-N4 1.917(4), Ga2-N3 1.942(5), P1-C63 1.861(5), P1-C59 1.863(6), O1-C59 1.240(7), O2-C63 1.322(7), O3-C63 1.187(7); N1-Ga1-N2 95.93(16), N1-Ga1-Cl1 106.70(14), N2-Ga1-Cl1 104.62(14), N1-Ga1-P1 118.95(15), N2-Ga1-P1 113.13(13), Cl1-Ga1-P1 115.08(5), O2-Ga2-N5 107.17(19), O2-Ga2-N4 100.45(19), N5-Ga2-N4 124.8(2), O2-Ga2-N3 114.54(19), N5-Ga2-N3 110.2(2), N4-Ga2-N3 99.73(19), C63-P1-C59 109.2(2), C63-P1-Ga1 107.9(2), C59-P1-Ga1 95.26(18), C63-O2-Ga2 127.5(4).

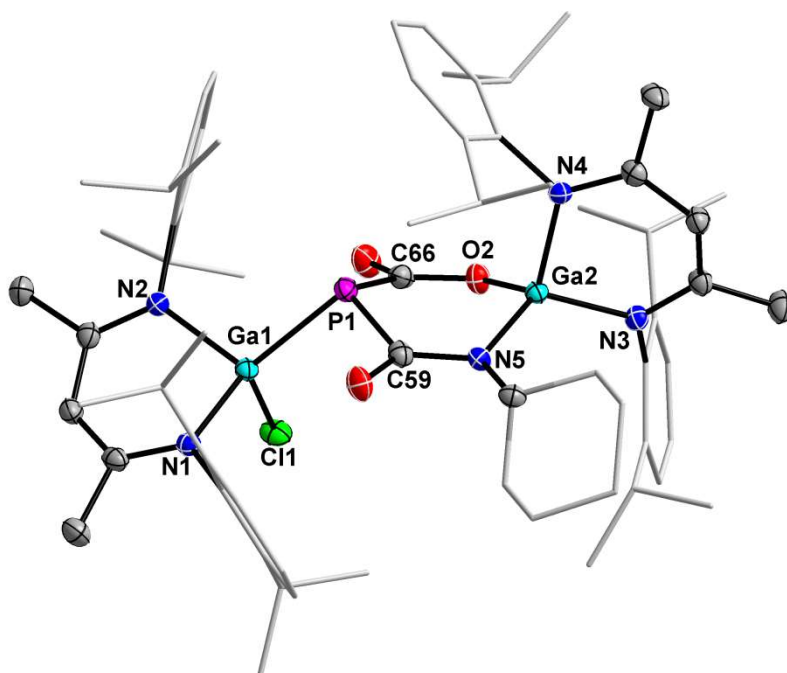


Figure S54. Molecular structure of **9** with thermal ellipsoids at 50% probability level. The hydrogen atoms and a solvent molecule (toluene) are omitted for clarity. Selected bond length (Å) and angles (°): Ga1-N1 1.9432(14), Ga1-N2 1.9604(14), Ga1-Cl1 2.1961(4), Ga1-P1 2.3215(5), Ga2-O2 1.8337(12), Ga2-N5 1.8963(14), Ga2-N3 1.9142(14), Ga2-N4 1.9407(13), P1-C66 1.8524(18), P1-C59 1.8563(18), O1-C59 1.228(2), O2-C66 1.323(2), O3-C66 1.214(2); N1-Ga1-N2 97.20(6), N1-Ga1-Cl1 104.46(4), N2-Ga1-Cl1 104.15(4), N1-Ga1-P1 125.76(4), N2-Ga1-P1 108.44(4), Cl1-Ga1-P1 113.815(18), O2-Ga2-N5 107.31(6), O2-Ga2-N3 102.60(6), N5-Ga2-N3 123.62(6), O2-Ga2-N4 110.11(6), N5-Ga2-N4 112.61(6), N3-Ga2-N4 99.79(6), C66-P1-C59 109.84(8), C66-P1-Ga1 99.52(5), C59-P1-Ga1 103.16(5), C66-O2-Ga2 125.50(11).

4. Computational Details

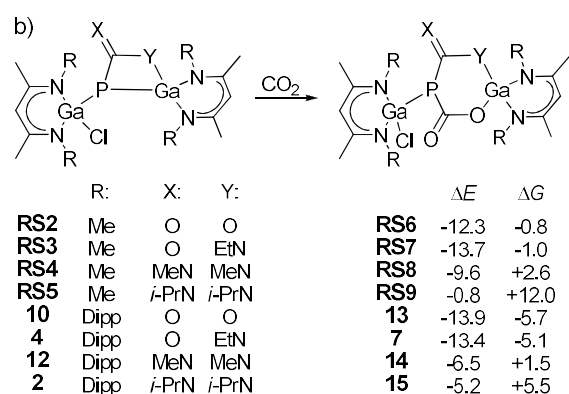
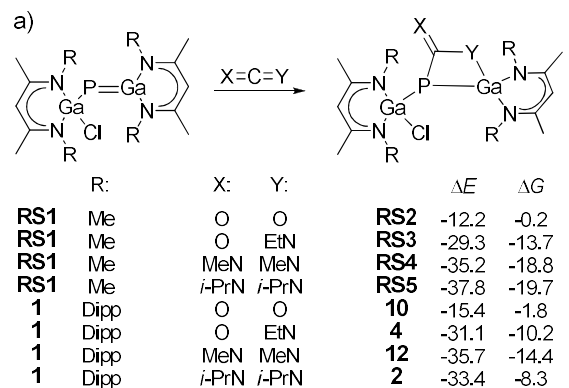
All calculations were performed by using the program package Gaussian 16^[8]. The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP^[9] together with the dispersion correction with Becke-Johnson damping^[10] (D3BJ). For the determination of the energetics of the reaction, the basis set def2-TZVP was applied. In order to calculate the reaction mechanism, the 6-31G* basis was used. For all structures C1 symmetry was applied. Frequency calculations were carried out at each of the stationary points to verify the nature of the stationary point. It turned out that all products have no imaginary frequency, whereas the two transition states have exactly one. Furthermore, single point calculations were performed on the B3LYP-D3BJ/6-31G*-optimized structures by means of B3LYP-D3BJ/def2-TZVP.

Influence of the Dipp groups on the reaction behavior

In order to determine the influence of the sterically demanding Dipp groups on the observed reaction behavior, the [2+2] cycloaddition of the reference system (RS) **RS1**, in which the Dipp groups in **1** are replaced by small methyl substituents, to the corresponding heterocycles **RS2–RS5** were studied (Scheme S2). In a second step, the energetic parameters of the cycloaddition reaction of the four-membered metallaheterocycles **2**, **4**, **10**, **12** and **RS2–RS5** with CO₂ to the six-membered metallaheterocycles **7**, **13–15** and **RS6–RS9** were calculated (Scheme S2). A comparison between the data for the gallaphosphenes **1** and **RS1** reveals, that only in the case of the carbodiimides a strong deviation from one another is found. For the addition of DMC to **1** and **RS1**, almost the same values are found, while this is not the case for the cycloaddition of the larger carbodiimide DIC. The reaction of DIC with **RS1** is energetically more favorable than that of DMC with **RS1**; in the case of **1**, the order is reversed. This demonstrates the influence of the Dipp groups of the β -diketiminato ligands: the large isopropyl groups lead to steric repulsive interactions making the formation of **2** (R = Dipp) approx. 4 kcal/mol less favorable than that of **RS5** (R = Me).

The calculated Gibbs free energies (ΔG) for the addition to the reference system **RS1** show the same trend as the calculated energies (ΔE): CO₂ addition is by far the most unfavorable, then EtNCO and DMC additions follow, and the addition of DIC exhibits the energetically most favored value. A different order is found for gallaphosphene **1**. Here, the addition of DIC is even less favorable than that of EtNCO. This means that starting from **1** the formation of **2** is less favorable than the formation of **4** due to entropic reasons. Presumably, the free

rotation of the large groups in **2** is severely restricted and the entropy loss during the cycloaddition is correspondingly high.



Dipp = 2,6-*i*-Pr₂C₆H₃

Scheme S2. a) Calculation of the [2+2] cycloaddition reactions of gallaphosphenes **1** and **RS1** with CO₂, isocyanate EtNCO and two carbodiimides DMC and DIC to the four-membered metallaheterocycles **2**, **4**, **10**, **12** and **RS2–RS5**. b) Calculation of the addition of CO₂ to the metallaheterocycles **2**, **4**, **10**, **12** and **RS2–RS5** yielding the six-membered metallaheterocycles **7**, **13–15** and **RS6–RS9**. The calculations were performed using B3LYP-D3BJ/def2-TZVP and the energy values are given in kcal/mol.

5. Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Table S3. Absolute energies [au] of **1**, **2**, **4**, **7**, **10-15** and **RS1-RS9** calculated by means B3LYP-D3BJ/def2-TZVP.

	<i>E</i>	<i>G</i>
CO ₂	-188.671581	-188.680564
EtN=C=O	-247.420958	-247.372101
MeN=C=NMe	-227.501536	-227.441922
<i>i</i> -PrN=C=Ni-Pr	-384.847226	-384.683500
RS1	-5420.153444	-5419.823496
1	-7131.516108	-7130.348273
RS2	-5608.844451	-5608.504329
10	-7320.212173	-7319.031643
RS6	-5797.535601	-5797.186198
13	-7508.905936	-7507.721369
RS3	-5667.621040	-5667.217459
4	-7378.986696	-7377.736580
RS7	-5856.314385	-5855.899541
7	-7567.679568	-7566.425322
RS4	-5647.711040	-5647.295424
12	-7359.074464	-7357.813111
RS8	-5836.397975	-5835.971878
14	-7547.756456	-7546.491359
RS5	-5805.060938	-5804.538370
2	-7516.416505	-7515.045034
RS9	-5993.733767	-5993.199743
15	-7705.096392	-7703.716865
11	-7378.975817	-7377.727521

Table S4. Absolute energies [au] of **1**, **4**, **10**, **TS₁₋₄** and **TS₁₋₁₀** calculated by means of different methods.

	<i>E^a</i>	<i>G^a</i>	<i>E^b</i>
CO ₂	-188.582581	-188.591707	-188.671227
EtN=C=O	-247.315618	-247.266333	-247.420578
1	-7126.709669	-7125.521419	-7131.508923
TS₁₋₁₀	-7315.300074	-7314.101426	-7320.177414
10	-7315.325668	-7314.129424	-7320.204522
TS₁₋₄	-7374.051336	-7372.786884	-7378.942449
4	-7374.090857	-7372.824263	-7378.980314

^a B3LYP-D3BJ/6-31G*. ^b B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G*.

Cartesian coordinates of the optimized geometry for CO₂ at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15970600
O	0.00000000	0.00000000	-1.15970600

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

C	-1.36084900	-0.06937300	-0.00004500
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O	-2.53286800	-0.04409200	0.00096600
N	-0.17352400	-0.22048700	-0.00222500
C	1.03821200	0.57224400	-0.00007500
H	1.04193100	1.21885800	-0.88123400
H	1.03978200	1.21786800	0.88182300
C	2.26674100	-0.32104500	0.00080900
H	3.17177700	0.28834300	0.00200200
H	2.27883000	-0.96031000	0.88402000
H	2.28066900	-0.95957200	-0.88291000

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

N	-1.15290000	0.40013900	-0.37850000
N	1.15255700	0.39858700	0.37923500
C	-0.00011700	0.32117800	0.00022100
C	2.28924100	-0.35503500	-0.11874500
H	3.04375600	0.34083500	-0.48810000
H	2.73411200	-0.92027800	0.70131800
H	2.02251700	-1.04604800	-0.92230200
C	-2.28896300	-0.35562000	0.11813600
H	-3.04348100	0.33878000	0.49023200
H	-2.73421800	-0.91854000	-0.70331300
H	-2.02124800	-1.04896300	0.91934100

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

N	-1.16163100	0.55712800	-0.35515100
N	1.16165000	0.55724600	0.35492800
C	-0.00000200	0.48622800	-0.00004300
C	-2.27882700	-0.22607800	0.18811700
H	-1.91232200	-0.88058300	0.98714400
C	-2.86745100	-1.08752800	-0.92349800
H	-3.21707600	-0.45700300	-1.74279000
H	-3.71083600	-1.66938000	-0.54711500
H	-2.12056400	-1.77707200	-1.31858100
C	-3.31097900	0.73194000	0.77217300
H	-2.87504600	1.33234800	1.57104200
H	-4.15758600	0.17561600	1.17890200
H	-3.67746000	1.40796200	-0.00226600
C	2.27885300	-0.22606300	-0.18815200
H	1.91240100	-0.88047400	-0.98727400
C	2.86718500	-1.08767100	0.92349800
H	3.71038100	-1.66981000	0.54712700
H	2.12006400	-1.77695900	1.31857800
H	3.21702100	-0.45726400	1.74279200
C	3.31121400	0.73188800	-0.77195900
H	4.15793000	0.17551900	-1.17840800
H	3.67746200	1.40791700	0.00257100
H	2.87553800	1.33226600	-1.57098700

Cartesian coordinates of the optimized geometry for **RS1** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Cl	0.00000300	0.00017800	-1.39219600
P	0.00000800	-0.00035100	2.33073900
Ga	1.47543700	-0.00010300	0.64121800
Ga	-1.47538100	-0.00010500	0.64116800
N	2.67788200	1.45120200	0.12498700
N	2.67792300	-1.45122800	0.12458700
N	-2.67786200	1.45120000	0.12501500
N	-2.67788800	-1.45123700	0.12459500
C	3.74612500	1.26225400	-0.63579700
C	4.22670400	0.00016500	-1.00936300

H	5.10120800	0.00026500	-1.64058200
C	3.74616500	-1.26203900	-0.63614000
C	4.50921300	2.46225100	-1.13296900
H	3.85483300	3.13101200	-1.69570000
H	5.33331800	2.16068800	-1.77397100
H	4.91420800	3.03807100	-0.29801300
C	4.50929500	-2.46187700	-1.13363000
H	5.33338200	-2.16011500	-1.77456200
H	3.85493800	-3.13052100	-1.69652600
H	4.91432300	-3.03789500	-0.29882600
C	-3.74619200	1.26224900	-0.63564500
C	-4.22681300	0.00016000	-1.00915600
H	-5.10139300	0.00025900	-1.64026900
C	-3.74622200	-1.26204500	-0.63600200
C	-4.50933800	2.46224400	-1.13273300
H	-3.85502400	3.13100500	-1.69554000
H	-4.91423900	3.03806600	-0.29773200
H	-5.33351600	2.16067800	-1.77364000
C	-4.50940300	-2.46188300	-1.13341700
H	-5.33356700	-2.16011800	-1.77424700
H	-4.91432600	-3.03791400	-0.29857200
H	-3.85510800	-3.13051500	-1.69640000
C	-2.24437500	-2.79791100	0.47642600
H	-1.88032300	-3.34613800	-0.39776900
H	-1.42746800	-2.71538900	1.19240200
H	-3.04586600	-3.37874700	0.93829400
C	-2.24430900	2.79776500	0.47721500
H	-3.04579000	3.37850800	0.93921700
H	-1.42742300	2.71502200	1.19318900
H	-1.88021400	3.34621000	-0.39682600
C	2.24437300	2.79776500	0.47724700
H	1.88021300	3.34623100	-0.39675300
H	1.42754400	2.71501900	1.19328600
H	3.04590000	3.37848900	0.93919400
C	2.24446600	-2.79790100	0.47649200
H	1.42762600	-2.71537600	1.19254400
H	1.88033700	-3.34615500	-0.39765400
H	3.04601300	-3.37871200	0.93829500

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

Cl	1.56549500	1.58878900	2.35197200
P	0.03116000	-0.71428500	-0.59498800
Ga	1.72048700	0.40792800	0.45053800
Ga	-1.94366600	-0.24406100	0.19322400
N	3.19467000	-0.89323000	0.84253000
N	2.89955900	1.59280200	-0.66475200
N	-3.26851000	-1.60217000	-0.37982100
N	-3.28001000	0.95289400	0.94558700
C	4.45837100	-0.48143900	0.89056500
C	4.90075000	0.73799000	0.37428100
H	5.95223400	0.94254500	0.49821700
C	4.20837600	1.63564200	-0.44706000
C	5.50887900	-1.37552400	1.50115400
H	5.32153700	-1.49570200	2.56857800
H	6.50031300	-0.95102400	1.36635500
H	5.48596800	-2.37304200	1.06537700
C	5.05298400	2.68814800	-1.12297900
H	6.09075000	2.36736700	-1.17049900
H	5.01117600	3.61691300	-0.55333900
H	4.69886900	2.90886600	-2.12685200
C	2.92768100	-2.27445400	1.13154900
C	2.72142900	-2.70136800	2.45245500
C	2.58053000	-4.06658200	2.69394100
H	2.42744500	-4.41198000	3.70789900
C	2.62954100	-4.98724500	1.66127500

H	2.52570900	-6.04461400	1.86992700
C	2.78579400	-4.54673500	0.35712500
H	2.79963600	-5.26691400	-0.45012600
C	2.92932500	-3.19259600	0.06656400
C	3.13149600	-2.74873100	-1.37049100
H	2.98810200	-1.67099800	-1.40066900
C	4.56437200	-3.03071100	-1.84154400
H	5.29726000	-2.50002600	-1.23348300
H	4.69651100	-2.71139400	-2.87701000
H	4.78873600	-4.09832100	-1.78548100
C	2.10661700	-3.37329000	-2.32025700
H	2.22396400	-4.45664100	-2.38893200
H	2.23544300	-2.96823900	-3.32560200
H	1.09100200	-3.15541700	-1.99394300
C	2.32002500	2.48910200	-1.62332600
C	2.07859500	3.83150800	-1.28740900
C	1.55595300	4.67348800	-2.26827900
H	1.36753800	5.71151600	-2.02724400
C	1.26765100	4.20651500	-3.53790000
H	0.85960600	4.87592700	-4.28467800
C	1.48943600	2.87325500	-3.84695100
H	1.25081000	2.51335200	-4.83752200
C	2.01686600	1.99365600	-2.90567900
C	2.33950900	4.38928400	0.09989600
H	2.86076800	3.63231500	0.68250400
C	3.20149500	5.65797400	0.07554000
H	3.46294100	5.95066700	1.09425400
H	2.66632300	6.49451300	-0.37807100
H	4.12558900	5.51868200	-0.48645700
C	1.01460000	4.66815400	0.81263600
H	0.39582100	3.77684700	0.85904700
H	0.45471400	5.44833100	0.29289500
H	1.19095100	4.99887400	1.83771900
C	2.30558900	0.54985100	-3.27460100
H	2.13122900	-0.04720000	-2.38123600
C	3.77059700	0.35593100	-3.68830600
H	4.45754400	0.58741100	-2.87623200
H	4.01826800	0.99548400	-4.53873500
H	3.94494800	-0.68043900	-3.98314600
C	1.37234200	0.00389100	-4.35340500
H	1.50750600	-1.07405600	-4.44601700
H	1.57543800	0.44466600	-5.33198700
H	0.33157300	0.18847600	-4.09795300
C	-4.56225400	-1.56757700	-0.11072300
C	-5.17237500	-0.50630500	0.57109600
H	-6.23707300	-0.59169300	0.71830600
C	-4.59105900	0.68167500	1.00228900
C	-5.45496000	-2.67699400	-0.59684800
H	-4.97613400	-3.64765700	-0.49214000
H	-5.66778700	-2.54106400	-1.65916900
H	-6.39901300	-2.67363500	-0.05697600
C	-5.52305700	1.73628000	1.54150800
H	-6.55150200	1.38750100	1.50554700
H	-5.43838100	2.65301900	0.95771100
H	-5.27356000	1.99872300	2.56907100
C	-2.72325600	-2.66533000	-1.17710800
C	-2.75997800	-2.55337800	-2.57477800
C	-2.13805700	-3.54758100	-3.32601300
H	-2.13868900	-3.47807100	-4.40577400
C	-1.50893400	-4.61924900	-2.71211100
H	-1.02194500	-5.37686100	-3.31251600
C	-1.49467900	-4.71555800	-1.32994600
H	-0.99376800	-5.55019100	-0.85808200
C	-2.09457200	-3.74189400	-0.53565600
C	-3.42121400	-1.37521700	-3.26998700
H	-3.99165600	-0.82042100	-2.52547200
C	-4.40548600	-1.81970000	-4.35755800
H	-3.89166400	-2.30917800	-5.18645600

H	-4.93435500	-0.95525900	-4.76374600
H	-5.14573100	-2.52081200	-3.96789000
C	-2.37213400	-0.41397400	-3.84054200
H	-1.68478500	-0.07998800	-3.06362600
H	-2.85332300	0.46136800	-4.28310800
H	-1.78233300	-0.90493600	-4.61685300
C	-2.06917200	-3.87183300	0.97596600
H	-2.45146600	-2.94180000	1.39718400
C	-2.99249300	-5.00218000	1.45168800
H	-2.66186400	-5.96500300	1.05670700
H	-4.02393500	-4.84762100	1.13130400
H	-2.98394900	-5.06562800	2.54181800
C	-0.65008700	-4.06554000	1.50880500
H	-0.65002400	-4.05185300	2.59989700
H	0.00775600	-3.27411400	1.15463100
H	-0.23046600	-5.02066200	1.19337400
C	-2.84456200	2.26637500	1.34227200
C	-2.70110500	3.25246700	0.35698400
C	-2.33244400	4.53241400	0.76570300
H	-2.21499900	5.31201800	0.02502900
C	-2.09730500	4.81587400	2.09929800
H	-1.79760500	5.81258500	2.39572100
C	-2.22791400	3.82017700	3.05614200
H	-2.03565100	4.05499400	4.09322600
C	-2.61290100	2.53092500	2.70184800
C	-2.78564200	1.44246600	3.74747500
H	-3.56361100	0.76508900	3.39188600
C	-1.50655300	0.61498800	3.89263200
H	-1.66166000	-0.21275200	4.58734700
H	-0.68313800	1.22833500	4.25705300
H	-1.18112500	0.20175200	2.93834600
C	-3.24272000	1.97174700	5.10838300
H	-3.47816300	1.13587600	5.76927100
H	-4.13238500	2.59845500	5.02116300
H	-2.46345200	2.55931100	5.59647300
C	-2.94336200	2.97148900	-1.11612000
H	-3.27897800	1.93893000	-1.21450900
C	-4.05639000	3.85719300	-1.68912100
H	-3.77833600	4.91222300	-1.66060000
H	-4.24990600	3.59291000	-2.73056700
H	-4.98788500	3.74308300	-1.13174800
C	-1.65157700	3.11636100	-1.92566000
H	-0.87424100	2.44581000	-1.56038200
H	-1.83012800	2.87901700	-2.97574000
H	-1.26636200	4.13431800	-1.87448100
C	2.60834900	-1.72126400	3.60300700
H	2.91195400	-0.73953100	3.24438900
C	1.14341400	-1.60594300	4.03748000
H	1.02885500	-0.83113700	4.79640900
H	0.51111100	-1.34558200	3.19113800
H	0.78559800	-2.55238500	4.45048500
C	3.49940600	-2.08310700	4.79545400
H	3.44775800	-1.29716400	5.55136400
H	3.18358500	-3.01504400	5.26844000
H	4.54358600	-2.20025900	4.50090300

Cartesian coordinates of the optimized geometry for **RS2** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Cl	0.87142800	-2.09710200	-1.63002300
P	0.17845100	1.42019900	-0.14733000
Ga	1.68133400	-0.31741400	-0.56119500
Ga	-1.87274400	0.45763300	0.29628600
N	3.22553800	0.30417100	-1.57586300
N	2.65379600	-0.86039600	1.02889300
N	-3.50493900	1.41651900	-0.11525100
N	-2.61667900	-1.32045200	0.29505100

C	4.31670300	0.70849600	-0.93842000
C	4.53925000	0.51346600	0.43064700
H	5.44096400	0.95301100	0.82588800
C	3.78538800	-0.24542700	1.34030600
C	5.39446700	1.41500000	-1.71780000
H	5.82776400	0.74957700	-2.46798500
H	6.19078000	1.75046300	-1.05908900
H	4.99068100	2.27911200	-2.24899900
C	4.31285400	-0.36384300	2.74350900
H	5.21252700	0.23216200	2.86991600
H	4.54942000	-1.40051700	2.99194800
H	3.55661300	-0.01772900	3.45082400
C	-4.59702400	0.79640700	-0.54374500
C	-4.71766100	-0.59633600	-0.63703800
H	-5.65161600	-0.95980200	-1.03491900
C	-3.81539100	-1.58087200	-0.20968300
C	-5.78853500	1.62175500	-0.94975800
H	-5.52844300	2.31133500	-1.75548300
H	-6.14241500	2.22718500	-0.11271600
H	-6.60401300	0.98738200	-1.28569400
C	-4.26319000	-3.01453800	-0.31198200
H	-5.20441900	-3.08671800	-0.85007200
H	-4.40380300	-3.44758300	0.68096300
H	-3.51486700	-3.62028500	-0.82542200
O	-1.18727100	0.83102900	2.07127000
C	0.04983300	1.21561000	1.76981600
O	0.93354100	1.41027200	2.56747700
C	-1.78183100	-2.39331200	0.82896700
H	-1.31346000	-2.97431900	0.03281200
H	-0.99272800	-1.94712400	1.42875700
H	-2.35179300	-3.05907000	1.47810800
C	-3.46788100	2.87118500	-0.00323300
H	-4.18691300	3.23635200	0.73415900
H	-2.47395300	3.17447500	0.31899000
H	-3.67276800	3.35974500	-0.95880200
C	3.07274900	0.51641000	-3.00833100
H	2.19900500	-0.03343400	-3.35275800
H	2.92800400	1.57430200	-3.24907000
H	3.93412600	0.15065900	-3.57080800
C	1.96695200	-1.69427400	2.00681100
H	1.47815500	-1.08841600	2.77361700
H	1.21265100	-2.28219600	1.48782500
H	2.64889600	-2.39527800	2.49035400

Cartesian coordinates of the optimized geometry for **10** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Cl	1.53505000	0.90862400	2.68492000
P	0.03398900	-0.48770200	-0.64690600
Ga	1.88376700	0.03220700	0.66521700
Ga	-2.09240300	0.39491300	-0.45416000
N	2.83554500	-1.66508000	1.08451100
N	3.46416500	0.95968500	-0.03482700
N	-3.49256800	-0.89556600	-0.91661000
N	-3.23462000	1.73889300	0.34337400
C	4.12598400	-1.62431500	1.38626500
C	4.92367700	-0.48183500	1.23553000
H	5.93285400	-0.57057200	1.60611700
C	4.64881800	0.67874600	0.51121000
C	4.82055300	-2.85118500	1.91969500
H	4.75377500	-2.86220400	3.00879400
H	5.87383000	-2.83747600	1.64900800
H	4.36549800	-3.76783100	1.55437000
C	5.78360600	1.65680500	0.34683700
H	6.73666200	1.18417200	0.57028800
H	5.63852800	2.48575700	1.04235600
H	5.81578200	2.08040300	-0.65344300

C	2.10519300	-2.89818400	1.15589900
C	1.65207800	-3.38838600	2.39175600
C	0.95925700	-4.59890600	2.40347300
H	0.60866400	-4.99659500	3.34688000
C	0.70092100	-5.29178100	1.23424700
H	0.15473000	-6.22621900	1.26558500
C	1.13333300	-4.78099400	0.02011100
H	0.91257400	-5.31789600	-0.89085500
C	1.84461800	-3.58723600	-0.04463500
C	2.37008100	-3.07501800	-1.37259500
H	2.40172800	-1.98910900	-1.30688700
C	3.80543900	-3.55524600	-1.62491700
H	4.49120600	-3.20489200	-0.85448900
H	4.16529700	-3.18125800	-2.58510200
H	3.84810700	-4.64650000	-1.64746100
C	1.46638700	-3.41748000	-2.55572300
H	1.49223900	-4.48288800	-2.79508600
H	1.79962600	-2.87530900	-3.44157600
H	0.43552400	-3.13459500	-2.35299600
C	3.36655900	2.01889300	-1.00590000
C	3.10319100	3.33165700	-0.59326900
C	2.99694600	4.31930700	-1.57194100
H	2.77851700	5.33705200	-1.27612200
C	3.17237600	4.01969400	-2.91096900
H	3.08445200	4.79877400	-3.65754800
C	3.45210900	2.71812000	-3.29811100
H	3.56804900	2.49251700	-4.34823400
C	3.54370000	1.69313700	-2.36343400
C	2.94766800	3.70788700	0.86814400
H	3.18751400	2.83565000	1.47262800
C	3.90333100	4.83635900	1.27637700
H	3.84579100	5.00504300	2.35364400
H	3.64731300	5.77482800	0.78093400
H	4.93824200	4.60328100	1.02179100
C	1.50377000	4.09378600	1.18981300
H	0.80848800	3.29565100	0.93811600
H	1.20735200	4.98440100	0.63420400
H	1.38887800	4.30045200	2.25437200
C	3.83521300	0.26726400	-2.80344400
H	3.32749000	-0.38973900	-2.09765000
C	5.33535900	-0.05775000	-2.73598100
H	5.72687700	-0.00652700	-1.72269600
H	5.90432000	0.63778900	-3.35725500
H	5.51807800	-1.06807700	-3.10748300
C	3.30327800	-0.06677900	-4.19873300
H	3.40745400	-1.13878800	-4.37899900
H	3.87255400	0.44344800	-4.97904100
H	2.25473100	0.20398000	-4.29154400
C	-4.78092000	-0.59063600	-0.85159700
C	-5.26408100	0.64109700	-0.39104800
H	-6.33422900	0.76493000	-0.43440300
C	-4.56240200	1.69001200	0.20593700
C	-5.80391700	-1.62525300	-1.23580300
H	-5.92596000	-2.34058600	-0.41966100
H	-5.49272100	-2.19218300	-2.10966800
H	-6.76738800	-1.15853200	-1.42582300
C	-5.38453500	2.82041400	0.76625000
H	-6.41575500	2.74253800	0.43246200
H	-4.98017200	3.78682000	0.47242600
H	-5.36943000	2.79286900	1.85699100
C	-3.07998100	-2.22612800	-1.27572600
C	-2.69290300	-2.50209400	-2.59616400
C	-2.27001100	-3.79630700	-2.89462900
H	-1.96908300	-4.03290400	-3.90625800
C	-2.20923200	-4.77692500	-1.91874700
H	-1.86268300	-5.77121300	-2.17016700
C	-2.57937100	-4.47909400	-0.61762400
H	-2.51002400	-5.24297200	0.14477700

C	-3.02741800	-3.20699100	-0.27322700
C	-2.73340700	-1.45398800	-3.69340600
H	-2.89619700	-0.48375600	-3.23028300
C	-3.89325600	-1.70893600	-4.66560900
H	-3.78881100	-2.68032000	-5.15406100
H	-3.91053300	-0.94140400	-5.44188800
H	-4.85879500	-1.69277400	-4.15821500
C	-1.40451400	-1.36840400	-4.45214500
H	-0.56375000	-1.25418500	-3.77150500
H	-1.41036200	-0.50497300	-5.11810900
H	-1.23037500	-2.26004000	-5.05829600
C	-3.39175900	-2.90115200	1.16786100
H	-3.88454200	-1.92979200	1.19700600
C	-4.36953100	-3.92266100	1.75827800
H	-3.91410800	-4.91053000	1.84391100
H	-5.26571500	-4.02314200	1.14355200
H	-4.67591100	-3.61477200	2.75986500
C	-2.12616600	-2.80228100	2.02323700
H	-2.37219100	-2.52583600	3.04897100
H	-1.43485800	-2.06003600	1.62536900
H	-1.59559000	-3.75304400	2.04233600
C	-2.65217300	2.82790000	1.08645700
C	-2.18903000	3.96462400	0.40594600
C	-1.67366300	5.01194900	1.16765900
H	-1.31804400	5.90187400	0.66616500
C	-1.59232900	4.92806000	2.54624500
H	-1.17280200	5.74760100	3.11534800
C	-2.03884700	3.78883700	3.19730700
H	-1.96509000	3.72848000	4.27448300
C	-2.58964600	2.72684000	2.48652700
C	-3.09323100	1.49652400	3.22135400
H	-3.74688800	0.94462900	2.54597000
C	-1.92789200	0.57175600	3.58233300
H	-2.29076800	-0.32965900	4.07891200
H	-1.22363000	1.07187600	4.24799200
H	-1.36568500	0.27618600	2.69805100
C	-3.92088500	1.84216700	4.46326000
H	-4.35906400	0.93501100	4.88355400
H	-4.73143800	2.53409500	4.22723000
H	-3.30936300	2.29918900	5.24264700
C	-2.24793800	4.10167000	-1.10533100
H	-2.63221900	3.17321300	-1.51956100
C	-3.19678900	5.22974000	-1.53142600
H	-2.85369400	6.19828700	-1.16185700
H	-3.24659100	5.28609600	-2.62048000
H	-4.20971300	5.07140100	-1.15741500
C	-0.85372400	4.31282600	-1.70650500
H	-0.16177200	3.52973500	-1.40715100
H	-0.90863600	4.29593400	-2.79527300
H	-0.43031200	5.27223300	-1.40170600
C	1.87831600	-2.65634000	3.70311100
H	2.50964600	-1.79143800	3.50782600
C	0.55744900	-2.12322000	4.26851700
H	0.73918200	-1.55529500	5.18278900
H	0.07036500	-1.46010100	3.55984300
H	-0.12550500	-2.94206800	4.50424000
C	2.57847900	-3.53852400	4.74531000
H	2.83318900	-2.94724700	5.62695500
H	1.93147600	-4.35447000	5.07291500
H	3.49434600	-3.98378600	4.35618400
O	-1.42384000	1.14139100	-2.10908500
C	-0.15068200	0.77242000	-2.06836100
O	0.69372900	1.10776200	-2.85807200

Cartesian coordinates of the optimized geometry for **RS6** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	2.30377600	-0.00130400	-0.30422600
Ga	-2.50061300	0.00080200	0.25717100
Cl	1.32495500	-0.00861200	-2.30341100
P	0.72448000	0.00449400	1.43736500
O	0.44518400	-2.56393000	0.87476700
O	-1.46989800	-1.49849800	0.54598200
O	0.44530300	2.56934700	0.85924500
O	-1.46938600	1.50186900	0.53496400
N	3.57274700	-1.46140800	-0.21143300
N	3.57190900	1.46020100	-0.22191700
N	-3.31853000	-0.00486400	-1.46667900
N	-4.04863400	0.00481400	1.37811800
C	4.76945900	-1.26162900	0.32208700
C	5.28824400	0.00293300	0.63987500
H	6.26167900	0.00489500	1.10375100
C	4.76867100	1.26490200	0.31312900
C	5.65439700	-2.45170500	0.58300100
H	5.95176300	-2.92368200	-0.35611600
H	5.12886300	-3.20708800	1.16948700
H	6.55421200	-2.15451200	1.11484800
C	5.65283000	2.45734200	0.56582500
H	5.94958600	2.92334400	-0.37645700
H	6.55299900	2.16438600	1.09940900
H	5.12683400	3.21619000	1.14742500
C	-4.63978100	-0.00530200	-1.59592800
C	-5.53840900	-0.00167700	-0.51771400
H	-6.58247600	-0.00260500	-0.78661900
C	-5.27190800	0.00300500	0.85734200
C	-5.22563000	-0.00994200	-2.98110400
H	-4.89552400	0.86593300	-3.54313500
H	-6.31120000	-0.01009900	-2.94415700
H	-4.89504400	-0.88926900	-3.53743000
C	-6.45100600	0.00617100	1.79123900
H	-6.43131900	0.88656000	2.43687700
H	-6.43121200	-0.86970800	2.44297800
H	-7.38532600	0.00418800	1.23731700
C	-0.18728900	-1.53008200	0.86491400
C	-0.18712500	1.53542100	0.85506100
C	3.15147400	-2.79818300	-0.62368000
H	2.22850300	-2.71687100	-1.19016400
H	3.90256300	-3.27252400	-1.25846200
H	2.94753300	-3.43748400	0.23660700
C	3.14994800	2.79375800	-0.64372800
H	3.90086400	3.26397300	-1.28177100
H	2.22714600	2.70785900	-1.20982800
H	2.94549000	3.43905600	0.21194000
C	-2.44458800	-0.00865700	-2.64050200
H	-1.40545700	-0.00696800	-2.32020900
H	-2.60330200	-0.89840500	-3.25333800
H	-2.60424300	0.87643300	-3.25978300
C	-3.84619600	0.00971600	2.82455500
H	-2.77828100	0.01011300	3.03406000
H	-4.27712400	0.89876400	3.29017300
H	-4.27764100	-0.87586200	3.29626100

Cartesian coordinates of the optimized geometry for **13** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-2.47997200	0.56501200	0.58553500
Ga	2.66423700	-0.47388800	0.20177000
Cl	-2.05878900	1.55797600	2.51866200
P	-0.58765500	-0.41342400	-0.40237500
O	-0.63103200	-1.86182700	1.84441800
O	1.43671600	-1.41986200	1.19489000
O	-0.01073500	2.10189500	-1.10026800
O	1.79471700	0.99523700	-0.47057700
N	-3.94153400	-0.71793900	0.89925800

N	-3.51535400	1.82040800	-0.51901200
N	4.21958700	0.03685500	1.17154300
N	3.45590400	-1.59767200	-1.14086700
C	-5.20140300	-0.30229500	0.85101300
C	-5.59458800	0.94209100	0.34545400
H	-6.65114900	1.14974400	0.40398300
C	-4.83907200	1.87277200	-0.37383100
C	-6.30528900	-1.19418900	1.35710700
H	-6.44667300	-1.01110700	2.42409900
H	-6.06754600	-2.24734200	1.23749500
H	-7.24138500	-0.97134500	0.85033800
C	-5.60469300	2.98653000	-1.04042500
H	-5.35772100	3.94195500	-0.57853200
H	-6.67508700	2.82086000	-0.95246100
H	-5.33898800	3.07143500	-2.09290300
C	-3.63255300	-2.08761700	1.21270000
C	-3.42533500	-2.97340500	0.14029000
C	-3.07652800	-4.28904500	0.43053400
H	-2.90906800	-4.98791900	-0.37719400
C	-2.94049600	-4.71892800	1.74098500
H	-2.66214200	-5.74434600	1.94876800
C	-3.15662200	-3.83332800	2.78176900
H	-3.03883900	-4.17290100	3.80232700
C	-3.50017200	-2.50454200	2.54430500
C	-3.63849300	-2.53700300	-1.29942600
H	-3.53044600	-1.45457800	-1.33365900
C	-5.06678300	-2.85863200	-1.76117100
H	-5.81127000	-2.37226400	-1.13189800
H	-5.24904800	-3.93506600	-1.72561000
H	-5.22259200	-2.51970000	-2.78754600
C	-2.61357600	-3.12102300	-2.27141700
H	-1.59898400	-2.85976200	-1.97807700
H	-2.78519200	-2.72309200	-3.27280200
H	-2.68683800	-4.20800700	-2.33859800
C	-3.69706800	-1.56962900	3.72353400
H	-3.96975300	-0.58851600	3.33739200
C	-4.82640700	-2.05223500	4.64476500
H	-5.01472800	-1.31518900	5.42810400
H	-4.56002800	-2.99206000	5.13250000
H	-5.75688600	-2.21858300	4.10100400
C	-2.40138800	-1.39442900	4.52560900
H	-1.59156000	-1.05163100	3.88915700
H	-2.09757400	-2.33829200	4.98410300
H	-2.55279100	-0.66316700	5.32213300
C	-2.89026800	2.73257700	-1.44341500
C	-2.63349900	2.28299500	-2.74805500
C	-2.09674700	3.18188100	-3.66386400
H	-1.89708200	2.85749300	-4.67594700
C	-1.79445100	4.48276900	-3.29427800
H	-1.37453500	5.16947800	-4.01833800
C	-2.00163600	4.89024500	-1.98837400
H	-1.72531500	5.89420400	-1.69424600
C	-2.54335200	4.02795900	-1.03729200
C	-2.90426200	0.84716600	-3.15853500
H	-2.92682700	0.25119200	-2.24824600
C	-4.27334300	0.68746700	-3.83000100
H	-5.08290800	0.98230600	-3.16215500
H	-4.44040800	-0.35310500	-4.11699000
H	-4.33626100	1.30242100	-4.73059100
C	-1.78947600	0.27042700	-4.03396200
H	-1.76424300	0.73588000	-5.02110600
H	-1.94194100	-0.79925400	-4.17838100
H	-0.81548700	0.40755900	-3.56698000
C	-2.66401600	4.49446800	0.40106400
H	-3.17961900	3.72262700	0.96990600
C	-3.46151500	5.79634400	0.54239500
H	-3.58025400	6.04964400	1.59768900
H	-4.45630800	5.71906600	0.10060000

H	-2.95156800	6.63156600	0.05858400
C	-1.26698900	4.65591000	1.01739600
H	-0.72356700	5.46916100	0.53079000
H	-0.68144700	3.74655000	0.90453500
H	-1.34700500	4.88291500	2.08192500
C	5.36862300	-0.61870900	0.99265900
C	5.56956900	-1.59202600	0.01021800
H	6.55043900	-2.04239000	-0.00333500
C	4.71658300	-1.99224400	-1.03296200
C	6.53433800	-0.26686700	1.87388500
H	6.95809100	0.69323900	1.57784600
H	7.31167700	-1.02314700	1.80042800
H	6.21842400	-0.16661000	2.91127500
C	5.31129900	-2.91115100	-2.06633000
H	6.22542700	-2.47304300	-2.46704900
H	4.62430900	-3.11062500	-2.88242200
H	5.58340000	-3.85757300	-1.59680300
C	4.14598900	1.20786600	2.00770400
C	4.59744000	2.43497600	1.48925600
C	4.48525300	3.56479100	2.29471900
H	4.82004700	4.52131200	1.91579200
C	3.93436100	3.48955400	3.56440500
H	3.85178300	4.38095800	4.17280200
C	3.47129400	2.27656300	4.04453700
H	3.02291700	2.22742300	5.02776900
C	3.55913300	1.11497000	3.27863100
C	5.14757200	2.57812800	0.07958200
H	5.24078500	1.58323500	-0.35503200
C	4.17795700	3.37328900	-0.80654100
H	4.07197200	4.39685600	-0.44174700
H	3.19069400	2.91557800	-0.82426600
H	4.55732200	3.42125500	-1.82993600
C	6.54221400	3.21600100	0.06213800
H	6.51052900	4.24869900	0.41316100
H	6.93928400	3.22587600	-0.95471100
H	7.24662800	2.67451900	0.69562800
C	3.01362800	-0.18713200	3.83468500
H	3.09046300	-0.94904600	3.06191800
C	1.52901700	-0.06159700	4.19897300
H	1.38601100	0.58681400	5.06568800
H	1.11391400	-1.04154900	4.43514400
H	0.94685500	0.35209800	3.37707800
C	3.83659300	-0.67211400	5.03490800
H	4.88572500	-0.81757800	4.77000200
H	3.44543300	-1.62298800	5.40170800
H	3.79736700	0.04623400	5.85620200
C	2.59333600	-1.95548400	-2.23657800
C	2.45076200	-1.04492200	-3.29864900
C	1.55933000	-1.36874300	-4.31801900
H	1.42776000	-0.68558700	-5.14526900
C	0.82744800	-2.54477000	-4.28324900
H	0.13435000	-2.77392700	-5.08223100
C	0.96630700	-3.41548400	-3.21627900
H	0.37477600	-4.32015200	-3.18710200
C	1.83746000	-3.13719900	-2.16479000
C	3.26003700	0.23898300	-3.37335200
H	3.63293300	0.46049400	-2.37440500
C	2.43039000	1.44712600	-3.81568000
H	1.56250700	1.59831500	-3.17668200
H	2.08825600	1.34710000	-4.84729400
H	3.04017100	2.35016800	-3.76121200
C	4.48131100	0.05328900	-4.28509000
H	5.08510400	0.96289600	-4.30335100
H	4.16862900	-0.16637700	-5.30815200
H	5.11459500	-0.76783100	-3.94820900
C	1.94238800	-4.10889500	-1.00187600
H	2.51624100	-3.62754500	-0.21086800
C	0.57130500	-4.46388400	-0.41593400

H	0.69414500	-5.05270300	0.49400500
H	-0.01942100	-5.05673100	-1.11644200
H	-0.00639500	-3.58134600	-0.15728900
C	2.68381900	-5.38850900	-1.41522500
H	3.67567100	-5.17669000	-1.81275500
H	2.12602200	-5.92357000	-2.18667400
H	2.79509400	-6.05584400	-0.55831200
C	0.12286700	-1.30772300	1.08156600
C	0.48833100	1.09274500	-0.66223800

Cartesian coordinates of the optimized geometry for **RS3** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Cl	1.14727600	-1.66660000	1.92489400
P	0.13175600	-0.28555400	-1.52790400
Ga	1.78716800	-0.55956600	0.07287900
Ga	-1.87112400	0.06038800	-0.39106400
N	3.30357100	-1.58987000	-0.59475200
N	2.77693100	1.02347900	0.61660200
N	-3.52458300	-0.56923700	-1.20308900
N	-2.44853900	-0.08000600	1.45301300
C	4.55361300	-1.16741000	-0.49163900
C	4.91892800	0.08176800	0.02828000
H	5.97623900	0.29343100	0.03283600
C	4.09558800	1.10509900	0.51815400
C	5.66683200	-2.06383600	-0.96823900
H	5.63083100	-3.03086400	-0.46269300
H	6.63640200	-1.61017000	-0.78197100
H	5.57701600	-2.25743100	-2.03938400
C	4.77367100	2.37779900	0.95286200
H	5.84961500	2.30945700	0.81829500
H	4.56729300	2.59137600	2.00362400
H	4.40340200	3.22591000	0.37341200
C	-4.48554900	-1.15441200	-0.50313700
C	-4.47142900	-1.26917600	0.89362900
H	-5.30720800	-1.79296300	1.32934600
C	-3.54285900	-0.74364500	1.80302800
C	-5.67217100	-1.72743000	-1.23149800
H	-5.35609700	-2.47375900	-1.96317100
H	-6.20337100	-0.94705900	-1.78063500
H	-6.36627000	-2.19338500	-0.53755200
C	-3.83234600	-0.93827600	3.26761900
H	-4.71738700	-1.55243200	3.40887600
H	-3.99725300	0.02143600	3.76226600
H	-2.98809900	-1.41607900	3.76782000
C	-0.09783400	1.62704200	-1.45342400
O	0.69718300	2.46797800	-1.83414300
N	-1.34631100	1.84694900	-0.93899500
C	-1.86904200	3.20374300	-0.87180200
H	-1.48132100	3.77255200	-1.72043500
H	-2.95629500	3.15263800	-0.97432000
C	-1.50755400	3.91965900	0.42710200
H	-1.93253700	4.92603100	0.44876700
H	-1.88849400	3.37231300	1.29193000
H	-0.42491900	4.00522600	0.52235600
C	2.00810300	2.15506500	1.11996200
H	2.30325900	2.42704900	2.13643000
H	2.09993300	3.02541200	0.46871700
H	0.95626300	1.88469000	1.13914600
C	3.00408000	-2.90292500	-1.14957100
H	1.92714600	-2.99292000	-1.28122200
H	3.47009000	-3.05260300	-2.12570600
H	3.32617400	-3.70686600	-0.48175800
C	-1.58505800	0.50140600	2.47642500
H	-2.14563100	1.15547700	3.14790600
H	-1.07136700	-0.26381900	3.05865600
H	-0.82288700	1.10232800	1.98896200

C	-3.61700400	-0.46434600	-2.65488800
H	-2.74092200	0.06405800	-3.02514100
H	-3.64183600	-1.44637900	-3.13434900
H	-4.50391800	0.09358000	-2.96541900

Cartesian coordinates of the optimized geometry for **4** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Cl	-1.51423300	0.95822400	-2.83290200
P	-0.14305800	-0.71048700	0.39277200
Ga	-1.88089300	0.34251500	-0.71037600
Ga	2.06216700	0.00749300	0.36483700
N	-3.32016800	-1.02009200	-0.93597300
N	-3.08238700	1.71751900	0.01682300
N	3.15978800	-1.58544300	0.86885900
N	3.46905000	0.93404700	-0.59730000
C	-4.55504200	-0.62367700	-1.18836600
C	-4.96334800	0.71878200	-1.11815400
H	-5.96643400	0.91708100	-1.46288800
C	-4.31573500	1.78449400	-0.49803000
C	-5.61637800	-1.62255000	-1.57104200
H	-5.68769400	-1.67763700	-2.65889700
H	-6.58580200	-1.30897400	-1.18921200
H	-5.38719200	-2.61880000	-1.20299800
C	-5.07392800	3.08481400	-0.41696800
H	-6.13523900	2.92654400	-0.59119200
H	-4.69498600	3.75903500	-1.18786300
H	-4.93656300	3.58120200	0.53982200
C	-2.95951200	-2.40750500	-0.92404100
C	-2.72907100	-3.09477900	-2.12593900
C	-2.33474800	-4.43138900	-2.05211000
H	-2.15327100	-4.97907600	-2.96776700
C	-2.16486300	-5.06405300	-0.83417000
H	-1.85389400	-6.10073500	-0.79903000
C	-2.38300900	-4.36479300	0.34372400
H	-2.22694400	-4.85898600	1.29130600
C	-2.77882700	-3.03238700	0.32538400
C	-3.03030600	-2.27952400	1.61873600
H	-2.74039200	-1.24273500	1.45153300
C	-4.52075300	-2.27893400	1.98368000
H	-5.12814900	-1.80969000	1.21060400
H	-4.68116800	-1.72896100	2.91268100
H	-4.88175600	-3.30005800	2.12608300
C	-2.18535900	-2.77683000	2.78979800
H	-2.51605200	-3.75583900	3.14515800
H	-2.26365200	-2.07357100	3.61844800
H	-1.13616400	-2.84603900	2.50891000
C	-2.62956500	2.75131200	0.90881300
C	-1.96051100	3.87270200	0.39766400
C	-1.50649200	4.83985000	1.29418000
H	-0.97599300	5.70466300	0.91766400
C	-1.73763100	4.71608100	2.65200600
H	-1.37887900	5.47441700	3.33649600
C	-2.42754700	3.61521600	3.13828400
H	-2.59671100	3.52826500	4.20148900
C	-2.88214800	2.61071300	2.28939400
C	-1.74804300	4.07429900	-1.09017200
H	-2.29102300	3.29535100	-1.61941200
C	-2.29251300	5.42550200	-1.57064000
H	-2.22493800	5.48956900	-2.65852900
H	-1.72201100	6.25823400	-1.15472800
H	-3.33576600	5.56620300	-1.28423700
C	-0.27526400	3.93238100	-1.47109200
H	0.13903300	2.98414600	-1.13147500
H	0.31705800	4.73513400	-1.03276000
H	-0.15391100	3.97142400	-2.55276900
C	-3.64840600	1.42024900	2.84835100

H	-3.35443600	0.55395600	2.25815600
C	-5.17012700	1.59110000	2.71241500
H	-5.50097200	1.60580800	1.67775600
H	-5.49763700	2.51681500	3.19166600
H	-5.68021700	0.76044500	3.20439500
C	-3.31756100	1.11113000	4.31025900
H	-3.76407400	0.15345400	4.58503500
H	-3.73534100	1.86328000	4.98404900
H	-2.24521500	1.04093200	4.46626800
C	4.47492100	-1.58242000	0.78588900
C	5.21505000	-0.49604700	0.28560100
H	6.28677100	-0.61267800	0.32771800
C	4.75920500	0.60326200	-0.43399700
C	5.27813200	-2.80302000	1.15610600
H	5.65731600	-3.27201900	0.24611900
H	4.69439600	-3.53857100	1.69823800
H	6.14123600	-2.50904200	1.75336600
C	5.81305500	1.44094200	-1.11182600
H	6.78672500	0.96672800	-1.02518800
H	5.86699000	2.43112900	-0.66269300
H	5.57896700	1.58488700	-2.16555400
C	2.44713400	-2.79199400	1.19589500
C	2.08565400	-3.05829900	2.52567000
C	1.36355600	-4.22146100	2.78678600
H	1.07630000	-4.44813500	3.80431000
C	0.99428900	-5.08375400	1.76837500
H	0.42062400	-5.97383300	1.99254800
C	1.34810400	-4.79593900	0.46136300
H	1.03983400	-5.46106400	-0.33381100
C	2.07947500	-3.65373800	0.15053800
C	2.48356900	-2.14855300	3.67352500
H	2.82285700	-1.20825700	3.24257100
C	3.65211800	-2.74140000	4.47447100
H	3.36933200	-3.69817300	4.91888900
H	3.93703900	-2.06590800	5.28385000
H	4.53041600	-2.90983400	3.85229300
C	1.30888100	-1.83828200	4.60711000
H	0.46414900	-1.41207300	4.07079400
H	1.61876100	-1.12026300	5.36897000
H	0.96873400	-2.73459300	5.12899500
C	2.44347500	-3.37459300	-1.29570100
H	2.96112200	-2.41775600	-1.33686400
C	3.40519400	-4.43417200	-1.84790600
H	2.93135000	-5.41733900	-1.87338000
H	4.30444000	-4.51598100	-1.23617800
H	3.70700500	-4.18133300	-2.86641100
C	1.19613800	-3.26048100	-2.17381300
H	1.47204100	-2.99583500	-3.19524700
H	0.51523700	-2.50217800	-1.79146600
H	0.64351100	-4.19939000	-2.20984100
C	3.14088100	1.97784600	-1.53314900
C	3.27592300	3.32267400	-1.15553800
C	3.03494500	4.30267700	-2.11586900
H	3.13511800	5.34579700	-1.84757900
C	2.65306900	3.96396900	-3.40110800
H	2.46482200	4.73879700	-4.13312600
C	2.48061400	2.63190300	-3.74425600
H	2.14987400	2.38469300	-4.74165900
C	2.71799200	1.61244800	-2.82599100
C	2.54110900	0.15325400	-3.22520000
H	2.05500000	-0.35352400	-2.38677600
C	1.63436700	-0.03707300	-4.44131000
H	1.43409200	-1.09914800	-4.58294000
H	2.10998000	0.32593500	-5.35509100
H	0.67995000	0.46859700	-4.31344800
C	3.88313700	-0.54930700	-3.48130100
H	3.70870500	-1.57624100	-3.80771300
H	4.51379500	-0.59000600	-2.59664300

H	4.43447500	-0.03654400	-4.27266000
C	3.63145100	3.73732200	0.26155100
H	3.97410100	2.85201700	0.79666000
C	4.75147600	4.78263200	0.32005100
H	4.42541000	5.73886100	-0.09209000
H	5.04534100	4.95778500	1.35656900
H	5.63689000	4.47094000	-0.23561000
C	2.38761600	4.25698000	0.99041800
H	1.58507600	3.52288800	0.97846800
H	2.62269100	4.49009400	2.02990800
H	2.01620900	5.16725000	0.51692300
C	-2.88604000	-2.44680300	-3.49080900
H	-3.25460700	-1.43269100	-3.34776500
C	-1.53861600	-2.32905300	-4.21106100
H	-1.66767400	-1.83047000	-5.17366300
H	-0.83641200	-1.74128200	-3.62695300
H	-1.10254200	-3.31362300	-4.39262100
C	-3.89076700	-3.20445200	-4.36941700
H	-4.07224000	-2.65401200	-5.29475000
H	-3.51179500	-4.19129400	-4.64216600
H	-4.84587700	-3.34895400	-3.86411000
C	0.08427500	0.30186400	1.99637000
O	-0.73651900	0.35087800	2.89819500
N	1.34703900	0.81635200	1.98799000
C	1.91489600	1.46470700	3.16996700
H	2.12892000	0.71950800	3.94288700
H	2.87809800	1.87632200	2.86022400
C	1.05692200	2.56996700	3.78060500
H	0.70997900	3.26768200	3.02205800
H	0.17990500	2.15410200	4.26739400
H	1.64407400	3.12387500	4.51756100

Cartesian coordinates of the optimized geometry for **RS7** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-2.40950400	-0.00109100	-0.23309000
Ga	2.32426700	-0.11207400	0.25593400
Cl	-1.46907600	-0.25743500	-2.24420700
P	-0.82498900	0.62571700	1.38745300
O	-0.49857700	2.73739100	-0.13940200
O	-0.68087100	-1.91786500	2.09430500
N	-3.90468400	1.22579800	-0.36317900
N	-3.40923400	-1.61960200	0.13183900
N	3.07034800	-0.98896900	-1.28138200
N	3.94568300	0.20053100	1.24520600
C	-5.10701000	0.88361900	0.07796700
C	-5.44177100	-0.39330300	0.55116800
H	-6.45088500	-0.50616800	0.91402800
C	-4.67232900	-1.56612200	0.52677300
C	-6.20225900	1.91737600	0.06598800
H	-6.37935100	2.28160000	-0.94795600
H	-5.92609400	2.78251500	0.67213400
H	-7.12972500	1.50350100	0.45198300
C	-5.35165300	-2.84062000	0.95324500
H	-5.44788800	-3.52847700	0.11021800
H	-6.34547900	-2.63698700	1.34269400
H	-4.76829200	-3.35194300	1.72072400
C	4.36554800	-1.26220200	-1.37081300
C	5.31385200	-0.90865600	-0.39892000
H	6.32935300	-1.20021200	-0.61407000
C	5.12453200	-0.23133500	0.81301800
C	4.86600700	-1.99277900	-2.58719600
H	4.35516700	-2.95089500	-2.70022000
H	5.93499600	-2.17370600	-2.51978300
H	4.66754100	-1.41689300	-3.49351600
C	6.34086900	0.01644600	1.66350000
H	6.21756200	-0.42500300	2.65443800

H	6.50123700	1.08707400	1.80757000
H	7.22952600	-0.40621400	1.20348200
C	0.12174200	1.73335600	0.20805800
C	-0.01209800	-1.05549300	1.56568200
N	1.38826600	1.46204400	-0.17799300
C	2.03535600	2.43825600	-1.06530100
H	1.28886300	2.82192900	-1.76071900
H	2.79371400	1.91055800	-1.64951400
C	2.67589700	3.58849400	-0.29737400
H	1.92015000	4.12236100	0.27793700
H	3.44002000	3.21897800	0.39005000
H	3.14903600	4.29403200	-0.98403200
O	1.24334300	-1.26562400	1.20931000
C	2.14065700	-1.38996800	-2.33706900
H	2.06671600	-2.47750400	-2.41306400
H	1.14943100	-1.00115800	-2.11364000
H	2.44014400	-0.99394500	-3.30953100
C	3.82170300	0.88831600	2.52685100
H	4.46707100	1.76750300	2.58260000
H	2.79387500	1.22485000	2.65011900
H	4.05991400	0.22828000	3.36447300
C	-3.66214800	2.55910100	-0.91083700
H	-2.60375000	2.66853500	-1.12716400
H	-4.22979200	2.71756600	-1.83180400
H	-3.93002900	3.34139700	-0.19749800
C	-2.71921300	-2.90197400	0.01851400
H	-1.77255100	-2.74623000	-0.49234700
H	-2.49775900	-3.32622700	0.99801900
H	-3.30113900	-3.61527900	-0.56873700

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

Ga	2.56739700	0.64157700	-0.57765700
Ga	-2.52540600	-0.54517100	-0.33280500
Cl	2.30772400	1.52032800	-2.59543500
P	0.65223500	-0.31846900	0.38322400
O	0.96561200	-1.68637800	-1.86924600
O	-0.06507100	2.15664200	1.12382400
N	4.08471100	-0.61602100	-0.71875200
N	3.50742800	1.99089700	0.50733800
N	-4.13530000	-0.03446800	-1.24427300
N	-3.30418000	-1.64002200	1.08024600
C	5.32572100	-0.15373200	-0.63739400
C	5.65224800	1.13743400	-0.20653500
H	6.70298100	1.37922600	-0.23361200
C	4.83326000	2.08555600	0.41341100
C	6.48624200	-1.03684500	-1.01821500
H	6.72829800	-0.86703700	-2.06927800
H	6.25534200	-2.09150400	-0.90114300
H	7.36587900	-0.78859100	-0.42830600
C	5.52819300	3.27085600	1.03294500
H	5.24738400	4.18665400	0.51352500
H	6.60717200	3.15286000	0.97929300
H	5.23217000	3.39980000	2.07302200
C	3.82674900	-2.01155400	-0.94745400
C	3.57727500	-2.82242400	0.17431800
C	3.24600100	-4.15751200	-0.03804300
H	3.04689200	-4.79958400	0.80867300
C	3.17079000	-4.67909100	-1.32008200
H	2.90499300	-5.71835200	-1.46761700
C	3.44242400	-3.86966900	-2.40956000
H	3.38392400	-4.28354500	-3.40771000
C	3.77290800	-2.52593200	-2.25068400
C	3.74390500	-2.28717700	1.58695400
H	3.64388800	-1.20449100	1.54205300
C	5.15618700	-2.58536300	2.11092000

H	5.92236500	-2.15727300	1.46566000
H	5.32687700	-3.66303300	2.16383800
H	5.28864500	-2.16900700	3.11169900
C	2.68909700	-2.79546700	2.56895900
H	1.68586000	-2.52851000	2.24363400
H	2.85349000	-2.34753400	3.55016000
H	2.73799800	-3.87836000	2.69707900
C	4.06098600	-1.68353000	-3.48035500
H	4.29193400	-0.67157300	-3.15096600
C	5.27201900	-2.22598400	-4.25378800
H	5.53015400	-1.55082900	-5.07232300
H	5.05234900	-3.20349300	-4.68805800
H	6.14854800	-2.34124100	-3.61589500
C	2.84613400	-1.58537500	-4.41105700
H	1.98637000	-1.18496000	-3.88323100
H	2.57936400	-2.56757700	-4.80870000
H	3.07827700	-0.93159000	-5.25432400
C	2.81455700	2.93468100	1.34791100
C	2.53019200	2.56177500	2.67088800
C	1.94320200	3.50133600	3.51142600
H	1.72243900	3.23657500	4.53632000
C	1.61145900	4.76480300	3.04897200
H	1.15085400	5.48339400	3.71506000
C	1.83831000	5.09109900	1.72378900
H	1.53644400	6.06282300	1.35574200
C	2.43544600	4.18707100	0.84734200
C	2.81422400	1.15871000	3.17428300
H	2.85993200	0.50988400	2.30159500
C	4.17235900	1.05885900	3.87829400
H	4.99057700	1.32140200	3.20747000
H	4.34644600	0.04066700	4.23339000
H	4.21143000	1.72968000	4.73955900
C	1.68941500	0.62051300	4.06165800
H	1.64032400	1.14230300	5.01934700
H	1.85053000	-0.43683200	4.27149300
H	0.72391300	0.72045800	3.56825500
C	2.58070400	4.55812000	-0.61590200
H	3.15685900	3.77934200	-1.11204800
C	3.31058900	5.88918600	-0.82842200
H	3.45272200	6.07156400	-1.89543700
H	4.29226100	5.89791100	-0.35162300
H	2.74109000	6.72813100	-0.42399300
C	1.19779400	4.59310300	-1.28221100
H	0.59076500	5.40105300	-0.86744700
H	0.66327000	3.65886900	-1.12433300
H	1.29856600	4.75167500	-2.35726400
C	-5.17917400	-0.87294800	-1.18121500
C	-5.28440700	-1.91813200	-0.26349600
H	-6.17700000	-2.51991200	-0.34514200
C	-4.49087500	-2.18375800	0.87503500
C	-6.32452900	-0.66001600	-2.13369800
H	-6.91121200	0.21330500	-1.85115800
H	-6.98029600	-1.52726400	-2.14236900
H	-5.95017700	-0.47448600	-3.14078000
C	-5.08182600	-3.13282800	1.88270300
H	-6.10513500	-2.83830100	2.11341200
H	-4.50269000	-3.16890600	2.79986100
H	-5.12001000	-4.13638600	1.45550500
C	-4.29732700	1.26093600	-1.85884300
C	-5.05542200	2.23341700	-1.18061000
C	-5.25198500	3.46731300	-1.79515700
H	-5.83681800	4.22332500	-1.28806500
C	-4.68858500	3.75626200	-3.02680500
H	-4.84899000	4.72337800	-3.48557200
C	-3.89413900	2.81128200	-3.65179100
H	-3.42402700	3.04919600	-4.59649900
C	-3.68228500	1.55601000	-3.08553700
C	-5.58382600	2.03201200	0.22904100

H	-5.36366900	1.01253500	0.54128500
C	-4.84554200	2.97578700	1.18718900
H	-5.04844000	4.01870000	0.93811600
H	-3.76840300	2.82079500	1.13476500
H	-5.17488300	2.80867800	2.21357900
C	-7.10022400	2.22678000	0.33703200
H	-7.38991600	3.24735900	0.08131100
H	-7.43179000	2.03542400	1.35945600
H	-7.64583900	1.55174200	-0.32350400
C	-2.75618800	0.58000500	-3.77498200
H	-2.85221300	-0.36952300	-3.26069700
C	-1.29964400	1.04679400	-3.64576300
H	-1.13920100	1.97610600	-4.19514200
H	-0.60905200	0.30097400	-4.04022000
H	-1.02672800	1.23365600	-2.60825100
C	-3.13213100	0.32798900	-5.23802300
H	-4.16667800	-0.00834800	-5.33095800
H	-2.48392100	-0.44050600	-5.66352200
H	-3.01678400	1.22694900	-5.84566200
C	-2.51553200	-1.86562000	2.26626100
C	-2.49076800	-0.86412200	3.25533500
C	-1.67868600	-1.06008600	4.36870800
H	-1.64101200	-0.30247400	5.13737700
C	-0.90890000	-2.20289700	4.50650600
H	-0.27915600	-2.33140700	5.37720000
C	-0.93619100	-3.16956500	3.51952700
H	-0.32162400	-4.05305700	3.62387400
C	-1.72409600	-3.02125000	2.37899000
C	-3.35635700	0.37929900	3.16347500
H	-3.55379100	0.57256100	2.11164700
C	-2.66950900	1.62743300	3.72222700
H	-1.71455400	1.80978800	3.23053300
H	-2.50106700	1.55278000	4.79778000
H	-3.29817900	2.50123900	3.55643700
C	-4.70822600	0.13660500	3.84932100
H	-5.34642400	1.01790100	3.76280900
H	-4.56914200	-0.07826000	4.91103800
H	-5.23750200	-0.70717600	3.40513200
C	-1.68183800	-4.11302900	1.32606500
H	-2.27295900	-3.78267300	0.47305600
C	-0.25087800	-4.36158100	0.83782200
H	-0.23962800	-5.12190700	0.05736600
H	0.38241500	-4.71629600	1.65083600
H	0.20226000	-3.46009900	0.43346100
C	-2.28813000	-5.42371800	1.84799600
H	-3.29927100	-5.28594000	2.22852900
H	-1.68359300	-5.83201100	2.66011300
H	-2.32073900	-6.16928500	1.05086600
C	0.08199200	-1.24969000	-1.14210300
C	-0.49002400	1.14193600	0.62552000
N	-1.23532400	-1.51197300	-1.32111500
C	-1.58571600	-2.33924300	-2.48843100
H	-1.09902700	-1.92087100	-3.37127300
H	-2.66361200	-2.25740600	-2.63621100
C	-1.21277900	-3.81068100	-2.37028400
H	-0.14648200	-3.92498000	-2.19101600
H	-1.76431800	-4.29587500	-1.56617500
H	-1.46276600	-4.31976300	-3.30397300
O	-1.77444900	0.98930400	0.34607500

Cartesian coordinates of the optimized geometry for **RS4** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	1.58620300	0.61321500	-0.23742200
Ga	-1.94403900	-0.42110900	-0.09481900
Cl	0.86537600	2.61222100	0.50401100
P	0.01309600	-0.67082900	-1.35379000

N	2.57079600	-0.25008300	1.20711400
N	3.12569800	1.03715100	-1.36340300
N	-3.63799800	-0.53886100	-1.05530400
N	-2.56142900	0.82096800	1.26103100
N	-1.21324600	-2.07294700	0.55521000
N	0.82703900	-3.08973200	0.03072100
C	3.89400400	-0.31262800	1.22779300
C	4.72777800	0.19362800	0.22142000
H	5.78609300	0.07585800	0.39121900
C	4.37338600	0.81454400	-0.98460800
C	4.56803200	-0.98020300	2.39815100
H	5.64914400	-0.91840800	2.30947300
H	4.28514300	-2.03360400	2.45429000
H	4.26711700	-0.51698300	3.33965200
C	5.49789900	1.23704000	-1.89412300
H	6.46285400	1.03603700	-1.43689000
H	5.43434300	2.30285900	-2.12191800
H	5.44906000	0.70184300	-2.84498700
C	-4.58686800	0.37629200	-0.92565900
C	-4.55315700	1.39865600	0.03327100
H	-5.37251100	2.09909300	0.00307100
C	-3.63550300	1.57826800	1.07774200
C	-5.78103800	0.32556900	-1.84138200
H	-5.47133300	0.35441800	-2.88794400
H	-6.45100800	1.15996900	-1.65274600
H	-6.33819800	-0.60296000	-1.69847200
C	-3.91726800	2.68834100	2.05548900
H	-3.04362400	3.33196400	2.17085300
H	-4.15623700	2.28669800	3.04280900
H	-4.75764600	3.29117500	1.72202800
C	-0.02447100	-2.15892200	-0.13911700
C	-3.74851000	-1.59444300	-2.05483800
H	-3.72585300	-1.19628700	-3.07298500
H	-2.90386400	-2.27137600	-1.94269300
H	-4.66512800	-2.17628900	-1.93211700
C	-1.71970300	1.00435300	2.43943600
H	-1.07539200	0.13421800	2.53911000
H	-1.08013200	1.88359900	2.34540600
H	-2.31427400	1.08208700	3.35081900
C	1.79316800	-0.82127000	2.30056500
H	2.04705700	-1.86640400	2.47931400
H	1.92653300	-0.25499300	3.22694300
H	0.74132400	-0.79711400	2.03286400
C	2.83751700	1.68870100	-2.63407000
H	3.12147900	2.74471800	-2.61981300
H	3.34530100	1.20274700	-3.46979300
H	1.76680400	1.63396000	-2.82277500
C	-1.56297400	-3.12062300	1.49226000
H	-1.61053400	-4.09970800	1.00501800
H	-0.82644900	-3.20544900	2.29876600
H	-2.53710300	-2.89613100	1.92891500
C	2.04995000	-3.10860500	-0.73079300
H	2.10508000	-2.31771800	-1.49254600
H	2.91403700	-2.99380200	-0.06740200
H	2.16354800	-4.07229800	-1.23609500

Cartesian coordinates of the optimized geometry for **12** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-1.87698600	-0.18671800	0.21768900
Ga	2.28363500	0.21095300	0.04361200
Cl	-1.89589700	-0.35774500	-2.00075400
P	0.14064800	0.77372400	0.73965600
N	-2.78050900	-1.75996400	0.96562800
N	-3.31179800	1.11922700	0.73894300
N	3.13209200	1.79056500	-0.78123500
N	3.35270700	-1.13783200	-0.90691200

N	2.33601700	0.12791400	1.97177500
N	0.58184900	0.06609700	3.51429300
C	-3.70422000	-1.64138000	1.92203300
C	-4.30271400	-0.43944300	2.28588200
H	-5.03047800	-0.50256600	3.08039500
C	-4.20090200	0.81880900	1.67016700
C	-4.13653800	-2.86879400	2.68178500
H	-5.08625800	-2.69771400	3.18219500
H	-3.38624700	-3.09904400	3.44047500
H	-4.21912200	-3.74135700	2.03910100
C	-5.20938600	1.83663200	2.14273700
H	-6.21228800	1.41519100	2.08069900
H	-5.17505500	2.75837000	1.57277000
H	-5.02020600	2.06454200	3.19258000
C	-2.42981200	-3.06347400	0.47304200
C	-3.15661000	-3.58096900	-0.61626300
C	-2.82300800	-4.84918100	-1.08371200
H	-3.36961200	-5.26963700	-1.91662800
C	-1.79109800	-5.57737500	-0.51001600
H	-1.53934200	-6.55681700	-0.89680600
C	-1.07893900	-5.04586800	0.55091700
H	-0.26711800	-5.61189800	0.98740100
C	-1.38918600	-3.78930300	1.06994700
C	-4.30514500	-2.81230100	-1.24772600
H	-4.17246300	-1.76312200	-0.99446400
C	-5.65733900	-3.25710900	-0.67315100
H	-6.46942800	-2.69443600	-1.13877300
H	-5.71350600	-3.09358600	0.40236200
H	-5.82939800	-4.31922400	-0.86209800
C	-4.31537100	-2.90660600	-2.77495600
H	-4.55996000	-3.91318000	-3.11985200
H	-3.35022700	-2.62105000	-3.18910700
H	-5.07056200	-2.23103400	-3.18070100
C	-0.60659200	-3.25725000	2.25372300
H	-1.03421200	-2.29831400	2.53934200
C	-0.68658300	-4.18884400	3.46945200
H	-1.71670700	-4.41957900	3.74340500
H	-0.19956800	-3.72090400	4.32687800
H	-0.17850900	-5.13529200	3.27420100
C	0.85169200	-3.01387600	1.87367000
H	1.34504500	-3.94331800	1.59193200
H	1.38722400	-2.56436600	2.70822900
H	0.91749500	-2.33247800	1.03013700
C	-3.32142800	2.40192500	0.08390700
C	-4.00599100	2.52297000	-1.14096400
C	-3.96552800	3.74814600	-1.80137200
H	-4.48225500	3.85948600	-2.74439300
C	-3.26898000	4.82441900	-1.27620400
H	-3.23899800	5.76502800	-1.81158700
C	-2.61445700	4.69318400	-0.06435900
H	-2.07700100	5.53726800	0.34560200
C	-2.63121200	3.49306600	0.64544300
C	-4.83230200	1.38532600	-1.71705500
H	-4.45749500	0.45738600	-1.29232600
C	-6.30731300	1.51928800	-1.31174300
H	-6.88743100	0.68549000	-1.71343100
H	-6.73246000	2.44673500	-1.70200200
H	-6.43231900	1.52502900	-0.23044400
C	-4.71494300	1.26627300	-3.23830600
H	-5.19469900	0.34513600	-3.57353400
H	-3.67304000	1.23559200	-3.55011000
H	-5.20943400	2.09502300	-3.74894100
C	-1.97026400	3.44625200	2.01263400
H	-1.93069900	2.40669300	2.32913600
C	-2.78859500	4.23306100	3.04929200
H	-3.82086400	3.89649400	3.11138400
H	-2.80265100	5.29562400	2.79740400
H	-2.33654100	4.13043100	4.03811500

C	-0.53708500	3.98261500	2.00018000
H	-0.51516900	5.05957000	1.82754300
H	0.05949600	3.49814200	1.23390700
H	-0.06453500	3.79382600	2.96565500
C	4.22477300	1.71393900	-1.52896800
C	4.81491200	0.50642400	-1.91884100
H	5.68342200	0.59945900	-2.55057100
C	4.37850600	-0.79983300	-1.69507600
C	4.88463900	2.97761700	-2.01692300
H	4.15739100	3.67389400	-2.42916300
H	5.63551100	2.75205800	-2.76968100
H	5.36998000	3.48630400	-1.18369800
C	5.09903600	-1.86582200	-2.48702200
H	5.20105000	-2.80277800	-1.95181100
H	6.08220700	-1.51097200	-2.78664800
H	4.52506500	-2.07690500	-3.39092100
C	2.51895500	3.07899800	-0.59116700
C	1.49539300	3.46759900	-1.47611700
C	0.99092600	4.76001800	-1.36189800
H	0.20224500	5.08308600	-2.02494000
C	1.46812000	5.63553100	-0.39818600
H	1.06740500	6.63917500	-0.33290800
C	2.42038400	5.20814200	0.50845000
H	2.74890000	5.87723300	1.29280700
C	2.95101900	3.92006600	0.44274900
C	0.94014200	2.51501100	-2.52372400
H	0.98823700	1.50870600	-2.10368200
C	1.76839000	2.51261700	-3.81596200
H	1.31306200	1.84272800	-4.54788500
H	2.79000800	2.17405200	-3.65304700
H	1.80531800	3.51407800	-4.25120100
C	-0.52971500	2.78715300	-2.84324700
H	-0.92615400	1.98055300	-3.45761200
H	-0.65912100	3.72031800	-3.39510200
H	-1.13128100	2.83940000	-1.93849900
C	3.92327100	3.46483000	1.51524300
H	4.25105900	2.45536000	1.26787600
C	5.16766900	4.35568600	1.60875000
H	4.90582100	5.37057700	1.91344400
H	5.69540300	4.42414100	0.65682100
H	5.86184500	3.95705100	2.35114200
C	3.20974200	3.40165800	2.87233600
H	2.34779500	2.73903400	2.83018700
H	2.86352400	4.39214800	3.17367900
H	3.88903100	3.03418900	3.64324300
C	3.06067300	-2.54161400	-0.76920500
C	2.06613400	-3.12669800	-1.57429100
C	1.91361800	-4.51059200	-1.50216400
H	1.15638500	-4.99459500	-2.09798200
C	2.70459600	-5.28468800	-0.66774800
H	2.57311900	-6.35910800	-0.64377600
C	3.63097500	-4.67959400	0.16196300
H	4.21122600	-5.28513200	0.84455900
C	3.81235600	-3.29810800	0.14575500
C	1.13822700	-2.29416400	-2.45367100
H	0.76373300	-1.47540200	-1.83141400
C	1.81397100	-1.65707200	-3.67682600
H	2.27504500	-2.42114600	-4.30739700
H	2.56885000	-0.92228500	-3.41096900
H	1.05927300	-1.14282500	-4.27392900
C	-0.08450500	-3.08033300	-2.92475600
H	-0.63128000	-3.52150500	-2.09459000
H	0.19683000	-3.87676600	-3.61820800
H	-0.76321900	-2.41015200	-3.44638500
C	4.78867400	-2.65893300	1.12100200
H	4.52799700	-1.60523400	1.19134500
C	6.25126500	-2.74345300	0.66090400
H	6.90971200	-2.35483200	1.44046400

H	6.43515500	-2.16601300	-0.24234000
H	6.53760600	-3.77960200	0.46615300
C	4.66155900	-3.25931200	2.52615800
H	3.62533600	-3.28232600	2.85837200
H	5.23572500	-2.66362800	3.23709400
H	5.05314900	-4.27750400	2.56410200
C	1.00664200	0.22688700	2.32359900
C	3.31379900	-0.04312100	3.02517300
H	3.24543800	-1.02862000	3.49355600
H	4.31637300	0.07858000	2.61362700
H	3.16704400	0.69243900	3.81859100
C	-0.81142800	0.23476500	3.82227900
H	-1.45231000	0.34734900	2.93691400
H	-1.18071400	-0.62545500	4.38880800
H	-0.96691600	1.11843000	4.45083000

Cartesian coordinates of the optimized geometry for **RS8** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-2.20042100	-0.47646900	0.02499400
Ga	2.36625400	-0.01785700	-0.20617000
Cl	-1.29910800	-2.06139700	1.30428900
P	-0.74707400	0.40262200	-1.59004000
N	-2.96697700	0.81025300	1.25713400
N	-3.84419300	-1.13340100	-0.76389700
N	3.99044000	0.59717300	-1.05040400
N	3.14463200	-0.91265100	1.30570700
N	1.19125100	1.37557900	0.23343700
N	-0.49559800	2.83374000	-0.31760800
C	-4.26248100	1.09270300	1.25123700
C	-5.20309000	0.46773200	0.42124100
H	-6.21806400	0.81682800	0.52483200
C	-5.01716700	-0.58836100	-0.48642600
C	-4.77474000	2.14268500	2.20124000
H	-5.83554500	2.32065200	2.04781900
H	-4.23684400	3.08295300	2.06585200
H	-4.62304100	1.83342900	3.23765900
C	-6.24467400	-1.12247700	-1.17638200
H	-7.13813600	-0.60807100	-0.83348300
H	-6.36145000	-2.19103700	-0.98581900
H	-6.16524400	-0.99782400	-2.25837200
C	5.19136100	0.29943800	-0.57334400
C	5.40400800	-0.44823100	0.59306100
H	6.43603400	-0.61556700	0.85670200
C	4.45929000	-1.00913800	1.46437500
C	6.40742500	0.78780000	-1.31330700
H	6.40906300	0.41934700	-2.34111300
H	7.31929300	0.45646100	-0.82458500
H	6.41819200	1.87865500	-1.36430700
C	4.98696300	-1.76460600	2.65419800
H	4.63134700	-1.32001300	3.58587700
H	6.07322100	-1.76573200	2.66310800
H	4.63688900	-2.79864500	2.64084800
C	0.04723000	1.68110600	-0.46453200
O	1.54561500	-1.21266500	-1.35504300
C	0.28170400	-1.16457600	-1.71521300
O	-0.28813800	-2.10111800	-2.23296300
C	-3.72848900	-2.24672800	-1.70395000
H	-4.18616400	-3.15489500	-1.30251300
H	-4.19865900	-2.01511900	-2.66186300
H	-2.67557800	-2.44883800	-1.89068200
C	-2.07062300	1.43886300	2.22325300
H	-1.96444700	2.50947800	2.04125000
H	-2.41184800	1.27875700	3.24854600
H	-1.08362300	0.99308500	2.12753500
C	3.84145100	1.38394300	-2.27031800
H	4.23748800	0.85829600	-3.14267100

H	2.78297300	1.56815700	-2.44538300
H	4.33873000	2.35350000	-2.19356700
C	2.22962800	-1.52564000	2.26784600
H	1.20383700	-1.33643700	1.96265100
H	2.36030000	-2.60886600	2.31361500
H	2.36879700	-1.11572500	3.27117800
C	1.71510200	2.42966200	1.09820300
H	1.96026600	3.33508900	0.53566900
H	0.97990300	2.71683400	1.85264700
H	2.61319900	2.06678700	1.60150700
C	-1.69897100	3.20616300	-1.02857400
H	-1.72776400	2.84684900	-2.06423200
H	-2.60056200	2.82864900	-0.53153800
H	-1.77273000	4.29487700	-1.04518500

Cartesian coordinates of the optimized geometry for **14** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	2.51899400	-0.20800400	-0.00612500
Ga	-2.85473700	0.52118400	-0.20092500
Cl	2.98703100	0.30375700	2.09413700
P	0.38040800	0.76373200	-0.30944800
N	2.89367900	-2.07771200	-0.54526000
N	4.06221500	0.57277700	-0.95716800
N	-3.44988300	2.20207800	0.57838100
N	-4.55387500	-0.42396000	-0.15844400
N	-1.91740500	0.70625300	-1.81373500
N	-0.04442300	0.43515800	-3.10405800
C	3.68132600	-2.34001000	-1.58151000
C	4.34305700	-1.36567300	-2.34740000
H	4.83937500	-1.73263600	-3.23166900
C	4.59215700	-0.03610100	-2.01869900
C	3.96804500	-3.76923600	-1.97258900
H	4.18260500	-3.82851400	-3.03773600
H	3.15901800	-4.44782400	-1.72511600
H	4.85685900	-4.10842400	-1.43729600
C	5.51573300	0.73846000	-2.92346100
H	5.99598500	0.08235800	-3.64486500
H	6.27722900	1.27755900	-2.36543600
H	4.93252900	1.48610900	-3.46558900
C	2.29015600	-3.18259700	0.15715100
C	2.94393600	-3.75235000	1.25524800
C	2.36991100	-4.87944600	1.84419000
H	2.86094700	-5.34221100	2.69011100
C	1.18177400	-5.40856400	1.37225800
H	0.75392300	-6.28541800	1.84162900
C	0.52178200	-4.79283400	0.31847300
H	-0.43071700	-5.18208800	-0.01366800
C	1.05264100	-3.66605200	-0.29969100
C	4.22567600	-3.17920800	1.83136600
H	4.42897700	-2.23897700	1.32306000
C	5.42741900	-4.10346200	1.60159000
H	6.33634200	-3.65165400	2.00451600
H	5.59111300	-4.29966100	0.54182700
H	5.28308300	-5.06510600	2.09853600
C	4.06726400	-2.86091100	3.32250300
H	3.93806200	-3.77171600	3.91075400
H	3.20806300	-2.21419800	3.48883900
H	4.95557100	-2.34675400	3.69280300
C	0.28825800	-2.96182200	-1.40558900
H	0.58324900	-1.91566200	-1.37646700
C	0.61720200	-3.47516800	-2.81331300
H	1.65538800	-3.30062500	-3.08713200
H	-0.00534300	-2.95705400	-3.54533900
H	0.41873600	-4.54678300	-2.89186500
C	-1.22320700	-3.00716100	-1.18679000
H	-1.64454200	-3.97815600	-1.44921900

H	-1.69857800	-2.26446500	-1.82402500
H	-1.49192600	-2.79096300	-0.15623900
C	4.74425200	1.71652600	-0.41583100
C	5.89107300	1.49032200	0.37022400
C	6.59111400	2.59481000	0.84529000
H	7.48007300	2.44291800	1.44298700
C	6.16317400	3.88681000	0.57814400
H	6.72292500	4.73321600	0.95540400
C	5.00592100	4.08804100	-0.15361300
H	4.65976400	5.09654000	-0.33929900
C	4.27443400	3.01236300	-0.65585000
C	6.37502100	0.09013700	0.71179000
H	5.57996400	-0.60473800	0.45032400
C	7.61720300	-0.30354500	-0.09868800
H	7.93835100	-1.31249100	0.16890500
H	8.44589800	0.37858700	0.10414500
H	7.42519100	-0.28858200	-1.17088700
C	6.64084500	-0.07611800	2.21124800
H	6.88257300	-1.11785700	2.43093900
H	5.76299700	0.20201400	2.79143900
H	7.48515700	0.53156700	2.54197500
C	2.99207600	3.27328600	-1.41613900
H	2.55755900	2.30764600	-1.66814800
C	3.23230700	4.02220400	-2.73144200
H	3.93165700	3.48832600	-3.37631000
H	3.64478100	5.01654800	-2.54840700
H	2.29321700	4.14359200	-3.27546400
C	1.98305400	4.01797000	-0.53997900
H	2.33197100	5.02627800	-0.30564400
H	1.80798500	3.49225100	0.39683200
H	1.02689400	4.10166500	-1.05149400
C	-4.73913600	2.48216500	0.71459300
C	-5.77094000	1.58224800	0.41142900
H	-6.76973700	1.96562500	0.55268900
C	-5.69331300	0.22739600	0.08538700
C	-5.16445800	3.83611300	1.21874400
H	-4.40530700	4.29620300	1.84427700
H	-6.09645800	3.75713600	1.77414100
H	-5.33804500	4.49846100	0.36867800
C	-7.00459300	-0.51122900	0.00847200
H	-6.89403000	-1.57026100	0.22065100
H	-7.40568700	-0.41547900	-1.00264100
H	-7.72778400	-0.07821000	0.69557300
C	-2.43853600	3.13925100	0.99539600
C	-1.84383800	2.96417000	2.25713700
C	-0.86968500	3.87705100	2.65293700
H	-0.39258200	3.75917300	3.61547700
C	-0.49657200	4.92879700	1.83234000
H	0.26441100	5.62612800	2.15762500
C	-1.07919900	5.07007200	0.58518900
H	-0.76406800	5.87907500	-0.06015300
C	-2.04611000	4.17493000	0.13372100
C	-2.26241600	1.84536400	3.19498700
H	-2.70508100	1.05537400	2.59462300
C	-3.33852100	2.32543100	4.17846300
H	-3.63858600	1.50917800	4.83905300
H	-4.22957100	2.68132000	3.66016200
H	-2.96164600	3.14204400	4.79825400
C	-1.08084600	1.22025100	3.94109100
H	-1.40928600	0.31985700	4.46134700
H	-0.66916400	1.89938600	4.69018600
H	-0.27778100	0.93549600	3.26319600
C	-2.61166200	4.34321300	-1.26546300
H	-3.34948500	3.55818000	-1.42986800
C	-3.31230700	5.69654400	-1.44533500
H	-2.59822100	6.51867000	-1.37080100
H	-4.08099000	5.86230300	-0.69075100
H	-3.78105000	5.75367200	-2.42980800

C	-1.51594800	4.17549600	-2.32539300
H	-0.99904000	3.22481500	-2.21381300
H	-0.77783700	4.97588300	-2.25041600
H	-1.94724300	4.21784100	-3.32723300
C	-4.52736600	-1.86787400	-0.17195500
C	-4.29115700	-2.53276600	1.04741400
C	-4.23828800	-3.92387000	1.03636600
H	-4.05389300	-4.45299400	1.96088700
C	-4.41826300	-4.64153000	-0.13496700
H	-4.37246400	-5.72300700	-0.12156700
C	-4.65410300	-3.97101600	-1.32171300
H	-4.79436100	-4.53638400	-2.23341400
C	-4.70978400	-2.57876400	-1.36800400
C	-4.15970100	-1.79297200	2.36851100
H	-3.95149200	-0.74870700	2.15127200
C	-5.48330400	-1.83943000	3.14625100
H	-5.75397000	-2.86880700	3.39103800
H	-6.30465700	-1.40534700	2.57577000
H	-5.39150100	-1.28250300	4.08096900
C	-3.00506400	-2.30831100	3.23112100
H	-2.06206600	-2.27624100	2.68944100
H	-3.18193300	-3.32836000	3.57744400
H	-2.90431500	-1.68006100	4.11821900
C	-4.99924500	-1.90221500	-2.69573900
H	-4.93915000	-0.82537900	-2.54239900
C	-6.41482300	-2.23133500	-3.19302900
H	-6.64049800	-1.66600900	-4.09957000
H	-7.17376600	-1.99942300	-2.44724900
H	-6.50341200	-3.29282400	-3.43193000
C	-3.97665000	-2.28394800	-3.77249600
H	-2.95905200	-2.06390400	-3.45918900
H	-4.17587400	-1.73420600	-4.69413900
H	-4.03059500	-3.34908400	-4.00395300
C	-0.55132800	0.53352800	-1.93667800
O	-1.75355600	-0.42393400	0.94652100
C	-0.44280800	-0.47553400	0.82794200
O	0.22756600	-1.24012400	1.48903600
C	-2.65137800	0.92275600	-3.05535600
H	-2.25205900	1.78210000	-3.59612600
H	-2.58502800	0.06884400	-3.72874300
H	-3.70134800	1.10993500	-2.82255500
C	1.36207400	0.26531000	-3.33592100
H	1.88422500	1.22585000	-3.39530200
H	1.86017800	-0.33878500	-2.57340700
H	1.51054800	-0.23909000	-4.29218200

Cartesian coordinates of the optimized geometry for **RS5** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-1.60001300	-0.97281800	-0.21811400
Ga	1.95136500	0.04929800	-0.25017500
Cl	-0.83569700	-2.98200600	0.45399400
P	-0.06390200	0.28032900	-1.41180300
N	-2.51812800	-0.16533200	1.29930100
N	-3.19695700	-1.38369100	-1.26834600
N	3.59051300	0.08047100	-1.30385400
N	2.59846700	-1.14020900	1.13701100
N	1.29902000	1.76922800	0.32175500
N	-0.75588300	2.79803800	-0.15872500
C	-3.83213900	-0.24587300	1.45538800
C	-4.70810900	-0.79008200	0.50774300
H	-5.75056000	-0.79025300	0.78336700
C	-4.41819700	-1.29686200	-0.76726800
C	-4.44712200	0.29425400	2.72017500
H	-5.51386200	0.08980300	2.74828000
H	-4.30361100	1.37493800	2.78773300
H	-3.98142400	-0.14885500	3.60220200

C	-5.58499500	-1.75464500	-1.60334300
H	-6.51489000	-1.67670000	-1.04672000
H	-5.45310300	-2.79056400	-1.92152900
H	-5.67416000	-1.14922800	-2.50805300
C	4.57780400	-0.78158000	-1.11464300
C	4.60353200	-1.71774100	-0.07160900
H	5.45290000	-2.38194700	-0.05830800
C	3.70010600	-1.86474900	0.98993900
C	5.75138700	-0.76526400	-2.05776100
H	5.42515200	-0.92071000	-3.08810800
H	6.46858400	-1.53951300	-1.79949200
H	6.25924100	0.20111700	-2.02574700
C	4.02991000	-2.90163200	2.03103400
H	3.18794200	-3.57952900	2.18087000
H	4.24229800	-2.43250600	2.99433400
H	4.90004000	-3.48157100	1.73574400
C	0.06829600	1.83693300	-0.29623300
C	1.79181700	2.88636900	1.11980000
H	1.52343800	3.81153400	0.59853400
C	3.30978400	2.79233200	1.22473100
H	3.60682400	1.86019600	1.71407800
H	3.71080100	3.62054800	1.81141300
H	3.77271200	2.81608900	0.23684000
C	1.13922800	2.92954400	2.50248000
H	0.05861500	3.00939000	2.39960800
H	1.49599500	3.78890400	3.07560100
H	1.37843800	2.02314700	3.06575300
C	-1.99229500	2.81800200	-0.91552200
H	-2.21788300	1.81562300	-1.31181800
C	-1.85599200	3.76612600	-2.10737600
H	-2.78828000	3.82179100	-2.67493000
H	-1.06478500	3.42187100	-2.77496900
H	-1.59852400	4.76912100	-1.76035000
C	-3.14266400	3.23666400	-0.00386500
H	-4.08721500	3.26367000	-0.55161500
H	-2.95056800	4.22777200	0.41232100
H	-3.24785400	2.53503000	0.82285300
C	3.64216100	1.04667000	-2.39396900
H	3.66532400	0.55904500	-3.37201000
H	2.75040200	1.66880600	-2.35305100
H	4.51355900	1.70174700	-2.31489200
C	1.76086500	-1.30294300	2.32113200
H	1.17810400	-2.22464500	2.27914200
H	2.35172500	-1.28638100	3.23842200
H	1.06180500	-0.47239600	2.36496400
C	-1.68775600	0.44260000	2.33056300
H	-2.08271300	1.40157600	2.66558300
H	-1.57833500	-0.21548500	3.19824900
H	-0.70300600	0.63695300	1.91773800
C	-2.97719700	-1.91913500	-2.60544000
H	-3.15493800	-2.99777300	-2.64136900
H	-3.61260200	-1.43683000	-3.35081200
H	-1.94187300	-1.73900200	-2.88949600

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

Ga	-1.89288500	-0.22742500	0.15200800
Ga	2.25067300	0.26232000	-0.04565500
Cl	-1.96539100	-0.41672300	-2.05495600
P	0.10857900	0.78580400	0.66493700
N	-2.72653800	-1.83976600	0.90643200
N	-3.38338300	1.01356600	0.65072900
N	2.99540300	1.86401100	-0.96079000
N	3.29860000	-1.09313800	-1.04409300
N	2.34207200	0.20604300	1.90142700
N	0.59682800	0.30369800	3.46768600

C	-3.60332700	-1.73746800	1.90518900
C	-4.20395200	-0.54154000	2.29739200
H	-4.87178500	-0.61435100	3.14227000
C	-4.19073200	0.70602500	1.65332600
C	-3.97876800	-2.96708600	2.69078200
H	-4.97283500	-2.86317500	3.11920200
H	-3.26897900	-3.08881800	3.51169600
H	-3.93704000	-3.86896200	2.08652000
C	-5.17864800	1.71463500	2.18189400
H	-6.13866000	1.23893400	2.37495900
H	-5.32044100	2.54946400	1.50346900
H	-4.80825700	2.10353400	3.13227200
C	-2.34299300	-3.12361400	0.38330600
C	-3.06462100	-3.65129400	-0.70474100
C	-2.65798400	-4.87393400	-1.23270000
H	-3.19746500	-5.29729000	-2.06820100
C	-1.56611600	-5.55452100	-0.71562000
H	-1.25820300	-6.49677200	-1.15096100
C	-0.87007600	-5.02260000	0.35425000
H	-0.01291200	-5.54985500	0.75047900
C	-1.24769700	-3.80916100	0.92711500
C	-4.28365500	-2.94615100	-1.27052800
H	-4.18479000	-1.89058200	-1.03104600
C	-5.57379700	-3.44969500	-0.60847100
H	-6.43929200	-2.92390400	-1.01763200
H	-5.56491400	-3.28847800	0.46865900
H	-5.71011900	-4.51866800	-0.78777900
C	-4.38466200	-3.05698700	-2.79243300
H	-4.57699800	-4.08179500	-3.11521300
H	-3.47122600	-2.70621300	-3.27035200
H	-5.21243000	-2.44578900	-3.15311900
C	-0.46998500	-3.27607100	2.11012500
H	-0.91572800	-2.32936600	2.40436800
C	-0.52637800	-4.22587700	3.31273400
H	-1.55095600	-4.47116300	3.59339000
H	-0.03471000	-3.76906600	4.17350000
H	-0.01145200	-5.16335900	3.09365500
C	0.97791300	-2.99584500	1.72625400
H	1.48659300	-3.91144400	1.42873200
H	1.51463600	-2.54773900	2.55881600
H	1.02181800	-2.30551100	0.88835300
C	-3.53945900	2.22643400	-0.11171500
C	-4.30273900	2.17110700	-1.29643400
C	-4.37653700	3.31091000	-2.09143500
H	-4.95075300	3.28380100	-3.00641600
C	-3.72219400	4.47931100	-1.73583100
H	-3.78097300	5.35152200	-2.37459600
C	-3.00398100	4.52750600	-0.55605600
H	-2.50829800	5.44546300	-0.27203100
C	-2.90321300	3.41689000	0.28254100
C	-5.09167800	0.93296700	-1.68457900
H	-4.59444000	0.07608000	-1.23852700
C	-6.51618000	0.98849400	-1.11408200
H	-7.06745300	0.08519000	-1.38472700
H	-7.05854300	1.84918200	-1.51199100
H	-6.51579000	1.06676800	-0.02846700
C	-5.13909300	0.69550000	-3.19458900
H	-5.60744500	-0.26701900	-3.40159900
H	-4.13744300	0.68346500	-3.62074800
H	-5.72961600	1.45680600	-3.70765800
C	-2.17431400	3.57826600	1.60379500
H	-2.06523100	2.59235300	2.05054700
C	-2.97962900	4.46359700	2.56851700
H	-3.99503500	4.10227300	2.71772300
H	-3.04693900	5.48312900	2.18326200
H	-2.48523600	4.50538300	3.54069600
C	-0.77766500	4.17310100	1.42607000
H	-0.82721900	5.19719200	1.05656300

H	-0.18422600	3.58435900	0.73400400
H	-0.25446700	4.19872100	2.38226800
C	4.13866400	1.79672600	-1.63359900
C	4.79320100	0.59835500	-1.93761900
H	5.70228300	0.70590700	-2.50670200
C	4.34963800	-0.71782700	-1.78118200
C	4.77818800	3.06013800	-2.14966100
H	4.05977100	3.67637100	-2.68700200
H	5.61263600	2.82762100	-2.80581800
H	5.14633700	3.65888300	-1.31633900
C	5.10384400	-1.74003200	-2.60143200
H	5.17093500	-2.71103100	-2.12607900
H	6.10467200	-1.37558200	-2.82042500
H	4.58169600	-1.88183900	-3.54876000
C	2.29148400	3.12655900	-0.94495400
C	1.28764400	3.34895000	-1.90690400
C	0.69368700	4.60807300	-1.96047100
H	-0.08176300	4.79719900	-2.68729400
C	1.07106200	5.62208000	-1.09637600
H	0.60084700	6.59498400	-1.16269300
C	2.02398900	5.37336400	-0.12710200
H	2.28965400	6.15350300	0.57348400
C	2.63929600	4.12750900	-0.02458100
C	0.86974300	2.28173500	-2.90418500
H	0.95490100	1.31234200	-2.40952100
C	1.79695400	2.27201100	-4.12897300
H	1.43932500	1.55380300	-4.86777300
H	2.81907500	1.99917800	-3.87264200
H	1.81377900	3.25838100	-4.59810300
C	-0.58345000	2.43044100	-3.35904200
H	-0.88134500	1.54905700	-3.92467600
H	-0.71322700	3.29865300	-4.00849400
H	-1.26518200	2.52572900	-2.51588200
C	3.62622500	3.88797800	1.09743200
H	4.13964100	2.95423700	0.88416900
C	4.69148300	4.98282400	1.21693100
H	4.25880600	5.93083400	1.54053600
H	5.20278100	5.16019200	0.26949900
H	5.43966500	4.69598400	1.95834700
C	2.87738900	3.71872800	2.42521600
H	2.14541200	2.91605700	2.36486700
H	2.34956900	4.63872000	2.68385500
H	3.57425100	3.48982400	3.23336200
C	2.96630600	-2.50174100	-1.06528700
C	2.00524900	-2.97562800	-1.97707000
C	1.82491500	-4.35592900	-2.07174800
H	1.08726800	-4.75023800	-2.75169900
C	2.56559300	-5.23779300	-1.30649100
H	2.41665600	-6.30487600	-1.41263300
C	3.46611600	-4.75006700	-0.37701200
H	4.00427100	-5.44467100	0.25076800
C	3.66696500	-3.38136400	-0.21682900
C	1.15085800	-2.04719500	-2.83269300
H	0.78305900	-1.25065600	-2.17975300
C	1.92064600	-1.38496400	-3.98399800
H	2.39715900	-2.14030900	-4.61338900
H	2.67944400	-0.68762500	-3.64094600
H	1.22432900	-0.82396100	-4.60820600
C	-0.07875600	-2.74865300	-3.41312100
H	-0.67578600	-3.23461300	-2.64322100
H	0.20604900	-3.49442800	-4.15919400
H	-0.71154700	-2.01462500	-3.90625600
C	4.58155600	-2.88423400	0.89360000
H	4.13041600	-1.96294300	1.25730000
C	6.01566500	-2.55857100	0.44934400
H	6.62729400	-2.33405900	1.32501200
H	6.06739600	-1.69602500	-0.20947900
H	6.46708800	-3.41120100	-0.06280400

C	4.65264500	-3.85632600	2.07634700
H	3.66323200	-4.15788500	2.41772400
H	5.16809000	-3.37903500	2.90994900
H	5.21752100	-4.75569900	1.82393200
C	1.01205300	0.33852900	2.26278700
C	3.35907400	0.28517100	2.95650200
H	3.09805600	1.14094600	3.58748700
C	4.73518200	0.53657500	2.35167600
H	5.04707700	-0.28079200	1.70295200
H	5.48158200	0.63362500	3.14178600
H	4.75220200	1.44999300	1.76209500
C	3.37807500	-0.93805900	3.87575700
H	2.40725400	-1.05875100	4.34896800
H	4.13337300	-0.80550600	4.65503400
H	3.61760200	-1.84385900	3.32510500
C	-0.78245400	0.57359000	3.79933900
H	-1.39946300	0.62976900	2.88791600
C	-0.88075700	1.91742100	4.52233900
H	-1.91835100	2.15914700	4.76483000
H	-0.47150500	2.71530000	3.90606800
H	-0.30636600	1.87920700	5.44988100
C	-1.34103000	-0.53952100	4.68415800
H	-2.38267200	-0.34152500	4.94441400
H	-0.75628000	-0.61095500	5.60336100
H	-1.29172700	-1.50300900	4.18121000

Cartesian coordinates of the optimized geometry for **RS9** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-2.66138800	-1.07744700	0.20803100
Ga	2.68406900	-0.17580700	0.19463200
Cl	-2.94576000	-3.25083100	0.50093200
P	-0.40140400	-0.71426000	-0.32972300
N	-3.60416500	-0.05657000	1.56339700
N	-3.81731500	-0.64781500	-1.30900200
N	3.63998400	-1.31814600	-1.03125500
N	4.17491300	0.42687600	1.25797400
N	1.58776800	1.12779300	-0.61828000
N	-0.48060600	2.12866400	-0.73739100
C	-4.67239700	0.67247300	1.27378500
C	-5.25043000	0.77193600	-0.00039800
H	-6.12051800	1.40540500	-0.06572900
C	-4.87145100	0.14210000	-1.19425700
C	-5.32479900	1.46230100	2.37746100
H	-6.17626600	2.02279300	2.00177500
H	-4.61441300	2.16270800	2.82100300
H	-5.66733500	0.80343800	3.17763700
C	-5.72388900	0.39876800	-2.40837000
H	-6.54021300	1.07645700	-2.17416600
H	-6.14560600	-0.53420300	-2.78814400
H	-5.12956400	0.83430500	-3.21396400
C	4.96509700	-1.34564400	-1.06212700
C	5.79081200	-0.63988400	-0.17325700
H	6.85070400	-0.75958900	-0.33074100
C	5.42911700	0.14403800	0.93007200
C	5.64638500	-2.18430200	-2.10973500
H	5.35352500	-3.23201300	-2.01819700
H	6.72681000	-2.11744500	-2.01913900
H	5.36001500	-1.85911800	-3.11206500
C	6.54122500	0.68326400	1.78839900
H	6.49500100	1.77274300	1.84516000
H	7.51141600	0.39637400	1.39278700
H	6.45862300	0.30575000	2.80970000
C	0.20796000	1.07783900	-0.52808400
C	2.17634000	2.37157300	-1.14470700
H	1.45361300	2.76339900	-1.86205800
C	3.48034100	2.07731900	-1.88146100

H	4.26159000	1.70802400	-1.21220900
H	3.86043500	2.99027400	-2.34343000
H	3.32509500	1.33583500	-2.66642200
C	2.36732600	3.43316000	-0.06211000
H	1.42667600	3.60621500	0.45746300
H	2.69805000	4.37759200	-0.50148700
H	3.12168600	3.11964800	0.66225800
C	-1.91674000	2.20297000	-0.71075200
H	-2.36033500	1.24777800	-0.42779000
C	-2.44419900	2.56301300	-2.09856000
H	-3.53098400	2.66302700	-2.08378400
H	-2.17376400	1.79162700	-2.82171900
H	-2.00984300	3.50688500	-2.43337600
C	-2.34555900	3.23218400	0.33378300
H	-3.43245000	3.32916000	0.35470700
H	-1.90683100	4.20588800	0.10734500
H	-2.00386400	2.92886700	1.32489600
O	1.64508300	-1.07453400	1.45084500
C	0.33925900	-1.20769300	1.33184800
O	-0.34681600	-1.69245900	2.20452000
C	-3.49567700	-1.27908200	-2.58214800
H	-4.29854800	-1.93625900	-2.92487800
H	-3.29592900	-0.53912700	-3.36180700
H	-2.60312900	-1.88856800	-2.45929600
C	-3.09190100	-0.10987600	2.93187900
H	-2.76431000	0.87626100	3.27257200
H	-3.84852600	-0.48079500	3.62696000
H	-2.23824500	-0.78048400	2.96428500
C	2.85586800	-2.10039800	-1.98505900
H	3.03272000	-3.17191600	-1.86628000
H	1.79764300	-1.91255300	-1.81240600
H	3.08442200	-1.82373600	-3.01713900
C	3.87277900	1.15375200	2.48780500
H	2.79616900	1.28316800	2.56642600
H	4.20319500	0.59987600	3.36939400
H	4.33616900	2.14268400	2.50426000

Cartesian coordinates of the optimized geometry for **15** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	-2.47667800	-0.29132400	-0.12354900
Ga	2.80654300	0.51727400	0.16679600
Cl	-2.87244500	0.03773200	-2.27996500
P	-0.38951300	0.78937100	0.23759800
N	-2.77115500	-2.11101800	0.61924200
N	-4.11904200	0.51423400	0.63953400
N	3.23507100	2.20759000	-0.72641300
N	4.50625100	-0.41313700	-0.14002900
N	1.90365200	0.69138100	1.82446800
N	-0.03620000	0.82353400	3.04318000
C	-3.59201100	-2.27358300	1.65032300
C	-4.33087100	-1.24442700	2.26018900
H	-4.83435700	-1.52362500	3.17212800
C	-4.64857000	0.01246500	1.75616400
C	-3.84692400	-3.65101700	2.21372200
H	-4.01624700	-3.58699900	3.28723100
H	-3.04588900	-4.35234100	2.01132600
H	-4.75807000	-4.04885000	1.76241800
C	-5.64905100	0.83672300	2.52391000
H	-6.10502100	0.25693100	3.32236600
H	-6.42850400	1.23379000	1.87763400
H	-5.13572800	1.69517000	2.96326300
C	-2.12146800	-3.27531200	0.06314000
C	-2.72111600	-3.95609500	-1.00381800
C	-2.12366700	-5.13229600	-1.45586900
H	-2.57943900	-5.67605200	-2.27254100
C	-0.95927300	-5.61132200	-0.88393400

H	-0.51152200	-6.52833500	-1.24546700
C	-0.35168800	-4.89428600	0.13457400
H	0.58122300	-5.24957900	0.54972700
C	-0.90668800	-3.71363300	0.61818900
C	-3.98176600	-3.46187500	-1.68696300
H	-4.19857200	-2.46607900	-1.30917200
C	-5.18680100	-4.35520100	-1.36847800
H	-6.08586400	-3.97487700	-1.85704500
H	-5.38054600	-4.40103100	-0.29648500
H	-5.02076800	-5.37570300	-1.71986800
C	-3.77914900	-3.33272000	-3.20058900
H	-3.62185300	-4.30721400	-3.66691700
H	-2.92086300	-2.69983000	-3.41927100
H	-4.65875900	-2.88145000	-3.66060300
C	-0.17785500	-2.93887000	1.70154000
H	-0.53702100	-1.91131400	1.67246700
C	-0.45090300	-3.48489300	3.10956900
H	-1.49995000	-3.41269900	3.38849300
H	0.12817000	-2.92370100	3.84538800
H	-0.15758500	-4.53529400	3.17491400
C	1.33487800	-2.91006100	1.46077900
H	1.79391000	-3.86940600	1.70367600
H	1.78988400	-2.15487100	2.09962900
H	1.57948100	-2.67937400	0.42751100
C	-4.85212700	1.52071900	-0.08343600
C	-5.90734500	1.09834600	-0.91668800
C	-6.62735900	2.06290800	-1.61406500
H	-7.44416900	1.75634300	-2.25320600
C	-6.30690700	3.40829200	-1.52040600
H	-6.87317800	4.14281400	-2.07884700
C	-5.25505800	3.80412100	-0.71482400
H	-5.00136800	4.85388000	-0.64668800
C	-4.51759200	2.87597200	0.01984900
C	-6.28085300	-0.36584200	-1.07153600
H	-5.45040200	-0.95701800	-0.69290300
C	-7.52006700	-0.73044500	-0.24267300
H	-7.76393900	-1.78710200	-0.37235100
H	-8.38477800	-0.14273500	-0.55910800
H	-7.36444900	-0.55285200	0.82069100
C	-6.48606800	-0.75761700	-2.53735200
H	-6.64903400	-1.83339800	-2.61482900
H	-5.61229100	-0.49738500	-3.13218300
H	-7.35998700	-0.26667400	-2.96885900
C	-3.39185300	3.36750600	0.90313000
H	-2.99436400	2.50754000	1.43798400
C	-3.89169700	4.37857500	1.94223500
H	-4.68426900	3.95763700	2.56289000
H	-4.29071400	5.27241000	1.45985200
H	-3.07710100	4.69050800	2.59667600
C	-2.25517500	3.96441600	0.07112800
H	-2.58157900	4.87055900	-0.44406600
H	-1.89517000	3.26217800	-0.67775600
H	-1.41000300	4.22604900	0.70771900
C	4.50830700	2.53014600	-0.94244800
C	5.58912400	1.67159700	-0.70845200
H	6.56164500	2.09442900	-0.90870200
C	5.58488600	0.29111000	-0.48232200
C	4.84377700	3.89123100	-1.49335800
H	4.15924300	4.17666800	-2.28908400
H	5.86311800	3.91097500	-1.86939300
H	4.75145300	4.64320400	-0.70938900
C	6.91101600	-0.39422700	-0.71119600
H	6.90066400	-1.44236900	-0.43617700
H	7.68318300	0.12009100	-0.13799100
H	7.18661300	-0.31501200	-1.76227300
C	2.19149300	3.10809900	-1.16452000
C	1.55028700	2.84896800	-2.38984000
C	0.58393100	3.74952600	-2.83086400

H	0.07637900	3.56484900	-3.76616700
C	0.25245000	4.87078200	-2.09029900
H	-0.50445100	5.55520100	-2.45047900
C	0.87232000	5.09516800	-0.87529200
H	0.59062200	5.95715100	-0.28570600
C	1.84117100	4.22279200	-0.38508400
C	1.89989700	1.64764500	-3.25013900
H	2.26310200	0.86376700	-2.59295800
C	3.02985300	1.97906700	-4.23433300
H	3.25999100	1.10937800	-4.85299000
H	3.94495800	2.27028800	-3.71778900
H	2.73972100	2.79769300	-4.89674500
C	0.68550100	1.07466200	-3.98605400
H	0.94627300	0.12083700	-4.44235300
H	0.34551800	1.73539600	-4.78588400
H	-0.15162100	0.89919300	-3.31137200
C	2.43925300	4.50077300	0.98022600
H	3.25982300	3.80389600	1.13352900
C	3.00567900	5.92035700	1.10769900
H	2.21239700	6.66853300	1.07088500
H	3.71249200	6.15433100	0.31088200
H	3.51983200	6.03503200	2.06396400
C	1.40007200	4.24746300	2.07912700
H	0.97729500	3.24947800	2.00311700
H	0.58149800	4.96602700	2.00365400
H	1.84948600	4.35659000	3.06808700
C	4.53204200	-1.85386000	-0.29086300
C	4.32304000	-2.40414200	-1.56767800
C	4.38309500	-3.79034700	-1.70568800
H	4.22197800	-4.22944200	-2.68060300
C	4.63963700	-4.61167800	-0.62456500
H	4.68357900	-5.68549800	-0.75398800
C	4.82638700	-4.05445500	0.62984800
H	5.00932900	-4.70453000	1.47245600
C	4.76947000	-2.67729000	0.82554700
C	4.05216000	-1.57147800	-2.80894900
H	3.90976000	-0.53744000	-2.50329700
C	5.24167400	-1.61059000	-3.77928500
H	5.39928200	-2.62191300	-4.15939900
H	6.16831900	-1.28844000	-3.30665600
H	5.05202900	-0.95797900	-4.63357000
C	2.77673000	-2.02318500	-3.52929300
H	1.91260800	-1.98541200	-2.87052300
H	2.87854600	-3.03993900	-3.91238600
H	2.58912500	-1.37443600	-4.38593100
C	4.96222200	-2.10158900	2.21659900
H	4.28076800	-1.25749600	2.29240800
C	6.38034900	-1.56488000	2.45468800
H	6.48194400	-1.22681900	3.48770600
H	6.61682200	-0.72301600	1.81007500
H	7.12263500	-2.34672200	2.28025200
C	4.60315100	-3.07875000	3.33818000
H	3.61602400	-3.51611900	3.19662000
H	4.60808400	-2.55539600	4.29489700
H	5.33049100	-3.88922800	3.41253000
C	0.51399400	0.68851100	1.90264300
C	2.60606200	1.04504600	3.07986600
H	2.05560500	1.88342800	3.51137300
C	4.03207900	1.50712200	2.79858400
H	4.65877400	0.71100200	2.39807600
H	4.49751400	1.84476200	3.72536100
H	4.05673500	2.34040300	2.09780400
C	2.58424400	-0.07185300	4.12547700
H	1.55956100	-0.29906200	4.40228100
H	3.12615800	0.24759900	5.01938100
H	3.05300300	-0.97885100	3.75525900
C	-1.44636000	0.94058900	3.29569700
H	-2.04001700	0.80133400	2.38364300

C	-1.72875700	2.33812300	3.84755900
H	-2.79180900	2.47186700	4.05517100
H	-1.41405900	3.10394800	3.14039500
H	-1.17123500	2.48534200	4.77423600
C	-1.86179200	-0.12554900	4.30763300
H	-2.91574300	-0.02500200	4.56938600
H	-1.26187800	-0.02281700	5.21405900
H	-1.70504000	-1.12375100	3.90457500
O	1.71832100	-0.57045000	-0.86950500
C	0.41373300	-0.57884500	-0.74601800
O	-0.27856000	-1.40208000	-1.31487200

Cartesian coordinates of the optimized geometry for **11** at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga	1.84270400	0.21633200	0.12488000
Ga	-2.26851500	-0.21537700	-0.09823500
Cl	1.76498100	0.40040600	-2.09130200
P	-0.16619400	-0.76172200	0.66584800
N	2.73360300	1.79357900	0.87581900
N	3.28477700	-1.08192600	0.62683800
N	-3.15715800	-1.80073400	-0.83625700
N	-3.42853900	1.11869400	-0.91112800
N	-0.73765200	0.01498700	3.38390600
C	3.66614800	1.67304300	1.82450300
C	4.26620800	0.47088800	2.18494900
H	4.99925400	0.53467900	2.97442900
C	4.17203500	-0.78309900	1.56111800
C	4.11528200	2.89994900	2.57516100
H	5.06907800	2.72232100	3.06524100
H	3.37640500	3.14075800	3.34126800
H	4.19878700	3.76876800	1.92752300
C	5.19170200	-1.79532300	2.02147900
H	6.18973300	-1.36233500	1.96045100
H	5.16627600	-2.71205200	1.44325100
H	5.00819800	-2.03493700	3.06964400
C	2.37913500	3.10292600	0.39723800
C	3.07891900	3.61768100	-0.71071500
C	2.74923200	4.89368700	-1.15927100
H	3.27509400	5.31195400	-2.00637400
C	1.74856100	5.63347000	-0.54673600
H	1.49981800	6.61953100	-0.91832900
C	1.06474600	5.10607300	0.53462900
H	0.27904100	5.68224700	1.00418200
C	1.37178500	3.84123000	1.03510600
C	4.20027100	2.84005000	-1.37864800
H	4.05738000	1.78968100	-1.13707800
C	5.57123700	3.25466000	-0.82649300
H	6.36405000	2.68481300	-1.31600100
H	5.64622100	3.07539200	0.24546500
H	5.75721400	4.31623300	-1.00468200
C	4.17856600	2.95449500	-2.90412000
H	4.42915300	3.96205900	-3.24150800
H	3.20069500	2.68704900	-3.30053700
H	4.91543100	2.27447300	-3.33510800
C	0.62694300	3.31703200	2.24615900
H	1.07040100	2.36376400	2.52554200
C	0.74043800	4.26047800	3.45052600
H	1.77628800	4.50859600	3.68515500
H	0.29026100	3.79495300	4.32907400
H	0.21170300	5.19766100	3.26669600
C	-0.84281000	3.06332000	1.92027200
H	-1.34873000	3.98934400	1.65345800
H	-1.34918100	2.61754100	2.77357000
H	-0.93759300	2.37874900	1.08120800
C	3.30775300	-2.36069000	-0.03496100
C	3.97733500	-2.45976500	-1.26982900

C	3.96679000	-3.68530300	-1.93014600
H	4.47371000	-3.78061000	-2.88017200
C	3.31482700	-4.78366200	-1.39353300
H	3.31007500	-5.72598500	-1.92660900
C	2.67044300	-4.67185200	-0.17455800
H	2.16607200	-5.53292100	0.24198400
C	2.65500300	-3.47051700	0.53382400
C	4.75894300	-1.29537200	-1.85407500
H	4.35648700	-0.38044400	-1.42687300
C	6.24016000	-1.37658400	-1.45832400
H	6.78809600	-0.52351300	-1.86458800
H	6.69553700	-2.28934100	-1.84900400
H	6.37077400	-1.37527700	-0.37745200
C	4.62248200	-1.18065700	-3.37367000
H	5.07351700	-0.24722800	-3.71439300
H	3.57638400	-1.17755300	-3.67347900
H	5.13287700	-1.99602000	-3.89001700
C	1.99420400	-3.44313100	1.90234500
H	1.94076800	-2.40638700	2.22872600
C	2.81826500	-4.22993200	2.93407100
H	3.84701200	-3.88362600	3.00081400
H	2.84339200	-5.29005000	2.67334200
H	2.36372300	-4.13924200	3.92239400
C	0.56930000	-4.00046600	1.87503200
H	0.56625300	-5.07129200	1.66945800
H	-0.03615500	-3.50452500	1.12347400
H	0.09072800	-3.85262500	2.84418500
C	-4.26614000	-1.73383700	-1.56192000
C	-4.87350100	-0.53129700	-1.93827800
H	-5.75855600	-0.62917100	-2.54594700
C	-4.48759800	0.77773100	-1.65188900
C	-4.94060600	-3.00348800	-2.01090200
H	-4.22273900	-3.73318800	-2.37821100
H	-5.67390800	-2.79349800	-2.78542000
H	-5.45398300	-3.46307600	-1.16522800
C	-5.36141000	1.86360800	-2.22586000
H	-6.03059200	2.25107300	-1.45802700
H	-5.96728600	1.46690400	-3.03659300
H	-4.77402900	2.70257000	-2.59048000
C	-2.56702200	-3.08990400	-0.59215200
C	-1.55796600	-3.53715200	-1.46382500
C	-1.08068200	-4.83405000	-1.29610900
H	-0.30618600	-5.20455800	-1.95179800
C	-1.56776800	-5.65172100	-0.28736900
H	-1.18857500	-6.65992800	-0.17830800
C	-2.50079800	-5.16169500	0.60904200
H	-2.83439200	-5.78622200	1.42720800
C	-3.00872400	-3.86874400	0.48592500
C	-0.99583700	-2.64160500	-2.55620000
H	-1.07806700	-1.61094500	-2.20668000
C	-1.79529300	-2.74430600	-3.86204100
H	-1.34483700	-2.10915200	-4.62732800
H	-2.82973400	-2.42754000	-3.73712300
H	-1.79629700	-3.77207200	-4.23256100
C	0.48844200	-2.89655200	-2.81812300
H	0.88469900	-2.12110400	-3.47224400
H	0.65685400	-3.85968100	-3.30334600
H	1.06321600	-2.87622100	-1.89495200
C	-3.97206300	-3.33840400	1.53247900
H	-4.30647300	-2.35070500	1.21687800
C	-5.21249700	-4.22475500	1.69582200
H	-4.94826400	-5.21119300	2.08143200
H	-5.73829700	-4.37099800	0.75110700
H	-5.90851400	-3.77024300	2.40328200
C	-3.25388600	-3.16584000	2.87798100
H	-2.39708800	-2.50311500	2.78729900
H	-2.90896600	-4.12984300	3.25859900
H	-3.93065100	-2.73041600	3.61518500

C	-3.20080300	2.51779200	-0.65711300
C	-2.22808800	3.19341700	-1.41733100
C	-2.07713000	4.56199100	-1.20886900
H	-1.33489100	5.10782700	-1.77014100
C	-2.85255100	5.23743900	-0.27867300
H	-2.71980300	6.30263100	-0.13674000
C	-3.77397000	4.54553100	0.48616100
H	-4.35187600	5.07410300	1.23238700
C	-3.96472100	3.17420800	0.32114600
C	-1.36362200	2.46370600	-2.43652000
H	-1.04552800	1.52062700	-1.98158500
C	-2.12356000	2.11823100	-3.72568500
H	-2.51335400	3.02444400	-4.19539400
H	-2.95362900	1.43689700	-3.55540400
H	-1.44486300	1.63814000	-4.43292400
C	-0.08909500	3.22652200	-2.79038900
H	0.48040600	3.49468800	-1.90428500
H	-0.30918400	4.13934600	-3.34864900
H	0.54584800	2.60092100	-3.41425100
C	-4.96732900	2.45689500	1.21075700
H	-5.09698600	1.44341600	0.83245000
C	-6.34286800	3.13800000	1.20601100
H	-7.06459100	2.52347200	1.74694400
H	-6.72356800	3.29924000	0.19640400
H	-6.30632300	4.10991400	1.70111100
C	-4.44123400	2.34009100	2.64820200
H	-3.53288600	1.74388600	2.68635800
H	-5.18841200	1.85484500	3.28024600
H	-4.23799800	3.32875300	3.06561100
C	-1.11446800	-0.18267800	2.19382400
C	0.64874200	-0.15129800	3.73954300
H	1.27727100	-0.37467100	2.86300100
H	1.02002900	0.79231200	4.15425100
C	0.83309900	-1.25127800	4.77865600
H	1.88460000	-1.34664600	5.05971600
H	0.24971200	-1.02914400	5.67292400
H	0.49141700	-2.20880500	4.38487400
O	-2.39894400	-0.07955600	1.81705100

Cartesian coordinates of the optimized geometry for CO₂ at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16912200
O	0.00000000	0.00000000	-1.16912200

Cartesian coordinates of the optimized geometry for EtN=C=O at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

C	-1.36399500	-0.06272500	-0.00035500
O	-2.54517700	-0.04673000	0.00145300
N	-0.16889400	-0.22509600	-0.00297500
C	1.04037000	0.57462300	-0.00009300
H	1.04659400	1.22483400	-0.88382000
H	1.04370800	1.22342300	0.88468500
C	2.27380700	-0.32220000	0.00112400
H	3.18190300	0.28967400	0.00299100
H	2.28383000	-0.96399100	0.88736000
H	2.28654900	-0.96261300	-0.88607300

Cartesian coordinates of the optimized geometry for **1** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

Cl	-1.04817900	-1.76883200	2.35783400
P	-0.16137300	0.65776100	-0.72022700
Ga	-1.52793900	-0.67708600	0.45603700

Ga	1.78364900	0.60967400	0.22138500
N	-3.22104600	0.25363500	0.94021200
N	-2.47978800	-2.09251400	-0.57994000
N	2.81044100	2.19263800	-0.35675300
N	3.34499600	-0.25391100	0.98758100
C	-4.36749100	-0.42282600	1.06801100
C	-4.57279500	-1.71167700	0.56487000
H	-5.54789600	-2.14321800	0.74812100
C	-3.73908800	-2.43176600	-0.30403600
C	-5.55418100	0.24541900	1.72767700
H	-5.31012800	0.53991200	2.75267500
H	-6.41288100	-0.42802900	1.75034200
H	-5.83806600	1.15972400	1.19919700
C	-4.36286600	-3.63153200	-0.98415400
H	-5.44989600	-3.60097400	-0.88897700
H	-4.00612900	-4.56105200	-0.53161100
H	-4.09952300	-3.66937800	-2.04329000
C	-3.26707700	1.66998100	1.18320800
C	-3.06479600	2.17621500	2.48170500
C	-3.24639900	3.54574500	2.69927400
H	-3.10078100	3.94866700	3.69712600
C	-3.61047400	4.39768800	1.66168100
H	-3.75712100	5.45764800	1.85159600
C	-3.76624600	3.88890800	0.37636500
H	-4.03503100	4.55724300	-0.43678100
C	-3.59357000	2.52645700	0.11175100
C	-3.80668500	2.00679200	-1.30224600
H	-3.55695200	0.94362400	-1.31266900
C	-5.27990800	2.12637100	-1.72934800
H	-5.93782000	1.56295200	-1.05915300
H	-5.41758500	1.73292900	-2.74309600
H	-5.61150000	3.17133200	-1.72600800
C	-2.88131100	2.71863700	-2.30053100
H	-3.10264100	3.79096800	-2.35899300
H	-3.01630700	2.30120500	-3.30466100
H	-1.83303600	2.60082500	-2.01497000
C	-1.76356500	-2.84497500	-1.57105700
C	-1.23933200	-4.11341600	-1.24979700
C	-0.59925500	-4.84005100	-2.26011200
H	-0.19401100	-5.82137900	-2.03123200
C	-0.46220400	-4.32309000	-3.54271600
H	0.03958700	-4.90127800	-4.31400800
C	-0.95732400	-3.05458500	-3.83365900
H	-0.83472200	-2.65394900	-4.83380700
C	-1.61509000	-2.29335100	-2.86287000
C	-1.30529700	-4.68753800	0.15813700
H	-1.97205300	-4.06517800	0.75866900
C	-1.83065700	-6.13259300	0.19385900
H	-1.95804400	-6.45820800	1.23236900
H	-1.12943400	-6.82762700	-0.28233300
H	-2.79379800	-6.23948100	-0.31677800
C	0.08190100	-4.61563000	0.80922600
H	0.47175000	-3.59770400	0.80278300
H	0.79072600	-5.25931600	0.27639500
H	0.03861700	-4.94418900	1.85332900
C	-2.20715000	-0.93295400	-3.20881600
H	-2.09911400	-0.30189300	-2.32431700
C	-3.71020800	-1.03240100	-3.52386700
H	-4.28509300	-1.35043500	-2.65046900
H	-3.89351200	-1.74361100	-4.33827800
H	-4.09699300	-0.05524100	-3.83528300
C	-1.46382400	-0.22514600	-4.34640100
H	-1.81771900	0.80625100	-4.43503700
H	-1.63037200	-0.71348200	-5.31409300
H	-0.38988000	-0.19414200	-4.15046400
C	4.07118300	2.47355200	-0.04849800
C	4.89623900	1.58115100	0.65121500
H	5.91569000	1.90070600	0.82058100

C	4.57711700	0.28302700	1.05093300
C	4.67452800	3.77170700	-0.52403500
H	4.04586900	4.61881000	-0.23669800
H	4.73980600	3.78643700	-1.61668100
H	5.67561100	3.91198400	-0.11173600
C	5.72644400	-0.58054200	1.52365600
H	6.64801400	0.00246700	1.56228800
H	5.87127300	-1.41753400	0.83243700
H	5.54280000	-1.01878600	2.50677200
C	2.08601700	3.03697800	-1.26877500
C	2.15950500	2.74753300	-2.64504000
C	1.33717000	3.47266200	-3.51177700
H	1.36576400	3.25983200	-4.57659900
C	0.47009700	4.44898800	-3.02763900
H	-0.17267600	4.99273700	-3.71426300
C	0.42611700	4.72833300	-1.66474600
H	-0.25635100	5.48662000	-1.29256000
C	1.22774900	4.02603400	-0.76002000
C	3.09706800	1.67755400	-3.19200500
H	3.68777200	1.28094000	-2.36060900
C	4.08302300	2.25962500	-4.21880400
H	3.55962200	2.63155900	-5.10668000
H	4.79043200	1.48978900	-4.54807400
H	4.65777000	3.09371100	-3.80070600
C	2.31859100	0.49511600	-3.78973100
H	1.63011300	0.07265800	-3.05338100
H	3.01070400	-0.29022400	-4.11717300
H	1.73173900	0.80992500	-4.66016700
C	1.15482500	4.32935300	0.72776400
H	1.86777000	3.67881600	1.24468800
C	1.55652200	5.78370200	1.02933700
H	0.85938300	6.49002500	0.56440800
H	2.56099900	6.01818200	0.65831500
H	1.54233800	5.96578000	2.11013300
C	-0.23928100	4.02426700	1.28828500
H	-0.24326800	4.12468300	2.37896100
H	-0.55965000	3.01369800	1.02565900
H	-0.98443900	4.71924700	0.89080500
C	3.20995700	-1.64116500	1.34887800
C	3.27411900	-2.60485500	0.32912500
C	3.25860800	-3.95308100	0.70388200
H	3.31475900	-4.71859500	-0.06388300
C	3.15281800	-4.32256100	2.03857900
H	3.13190400	-5.37393300	2.31047300
C	3.05459400	-3.34814400	3.03113000
H	2.96275100	-3.65467000	4.06657000
C	3.09015200	-1.98943500	2.71136800
C	3.05126700	-0.90121500	3.78014900
H	3.86819500	-0.20074000	3.56435200
C	1.74757300	-0.09706900	3.70852100
H	1.79001700	0.77508400	4.36967900
H	0.89011300	-0.71442400	3.97908200
H	1.57308600	0.25372200	2.68893200
C	3.27524500	-1.41964800	5.20473900
H	3.32416900	-0.57546300	5.90070400
H	4.20858500	-1.98688200	5.29322300
H	2.45104700	-2.06393600	5.53079200
C	3.36140100	-2.22466400	-1.14286300
H	3.43099100	-1.13565000	-1.22432800
C	4.62507500	-2.79457800	-1.80823300
H	4.61728400	-3.89027100	-1.80992000
H	4.68575400	-2.46166900	-2.85066600
H	5.53585000	-2.46750300	-1.29347100
C	2.09883200	-2.66788100	-1.89554300
H	1.19237100	-2.21997500	-1.48006400
H	2.16110000	-2.37189900	-2.94730300
H	1.98305200	-3.75484200	-1.86351400
C	-2.63310100	1.27539300	3.62576200

H	-2.75354500	0.23655600	3.31115500
C	-1.14032500	1.48887000	3.91727200
H	-0.80191000	0.78936800	4.68746800
H	-0.53461500	1.32690900	3.02263900
H	-0.95472400	2.51018800	4.27284700
C	-3.46670500	1.47585200	4.90085300
H	-3.17381200	0.74001400	5.65816700
H	-3.31807600	2.47110800	5.33555500
H	-4.53884900	1.35523200	4.70859700

Cartesian coordinates of the optimized geometry for **TS₁₋₁₀** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 1):

Cl	-1.58512700	-0.53035600	2.36424100
P	0.15006000	0.47891300	-0.98808900
Ga	-1.61963000	0.55640200	0.41211200
Ga	1.66647700	-0.90653900	-0.23290800
N	-2.04788500	2.44586500	0.92724500
N	-3.42732700	0.19797100	-0.31631900
N	3.47368900	-0.36855200	-0.77947700
N	2.16794400	-2.58079000	0.57426400
C	-3.30262800	2.86926000	1.08499800
C	-4.43597100	2.10565000	0.77511700
H	-5.38724800	2.57353200	0.99035000
C	-4.49644700	0.91417100	0.04586700
C	-3.57758600	4.26818400	1.59558300
H	-3.53017700	4.28785100	2.68843600
H	-4.57706600	4.59033300	1.29697800
H	-2.84580400	4.98810800	1.22715100
C	-5.87171100	0.50062400	-0.42898400
H	-6.59354400	1.29844100	-0.24668700
H	-6.21313000	-0.39688800	0.09065600
H	-5.86239800	0.26802600	-1.49628900
C	-0.98184700	3.38251100	1.16532400
C	-0.59203000	3.69519200	2.48584700
C	0.39426000	4.67057300	2.66967800
H	0.70014700	4.92953700	3.67896800
C	0.99581200	5.30423200	1.58769100
H	1.76182700	6.05741200	1.75343200
C	0.61536200	4.96790400	0.29259500
H	1.08552200	5.46388000	-0.55005900
C	-0.38345300	4.01803900	0.05556200
C	-0.88093000	3.78787900	-1.36470300
H	-1.40342900	2.83041600	-1.38704300
C	-1.90189000	4.87086000	-1.75831300
H	-2.78579900	4.84563200	-1.11335000
H	-2.23748800	4.72238400	-2.79087100
H	-1.45692000	5.87037600	-1.68578400
C	0.25882500	3.71485600	-2.38890000
H	0.71453900	4.69684400	-2.56459700
H	-0.12839800	3.35797500	-3.35043000
H	1.03644200	3.02501700	-2.05819800
C	-3.62735600	-0.89733700	-1.22783600
C	-4.13423800	-2.11981700	-0.73772900
C	-4.36483800	-3.15459500	-1.65065300
H	-4.74956600	-4.10448200	-1.29111000
C	-4.10960100	-2.98403200	-3.00450800
H	-4.29406500	-3.79651700	-3.70215400
C	-3.61444000	-1.76911000	-3.47035700
H	-3.41646000	-1.65815100	-4.52867000
C	-3.36009400	-0.69925200	-2.60573500
C	-4.43663500	-2.35447500	0.73912800
H	-4.35498100	-1.40103100	1.26612200
C	-5.85164900	-2.91684800	0.96864600
H	-6.07324500	-2.94509500	2.04148900
H	-5.93876000	-3.94180100	0.59042700
H	-6.62819200	-2.32260800	0.47594700

C	-3.40373400	-3.29655400	1.36992800
H	-2.39297800	-2.91285000	1.24745400
H	-3.45878500	-4.29374000	0.91707600
H	-3.58694400	-3.40129700	2.44530800
C	-2.81292500	0.62447300	-3.15495600
H	-1.86476300	0.81355000	-2.63622700
C	-3.73281500	1.83830300	-2.90908200
H	-3.76570900	2.14316100	-1.86502500
H	-4.75518500	1.63267200	-3.24845200
H	-3.36435800	2.69459800	-3.48440700
C	-2.48306700	0.58219800	-4.65458500
H	-1.99765100	1.52266800	-4.93778000
H	-3.39174300	0.48714200	-5.26262400
H	-1.80337100	-0.23175900	-4.90722900
C	4.51890100	-1.18827800	-0.74317500
C	4.44072300	-2.51385400	-0.28379900
H	5.34894400	-3.09564300	-0.36556400
C	3.37216100	-3.14133300	0.35797500
C	5.87471000	-0.67598800	-1.16255100
H	6.16264500	0.17692000	-0.53898200
H	5.85973700	-0.31613100	-2.19378000
H	6.63347100	-1.45473300	-1.06912600
C	3.62308700	-4.52711400	0.90372100
H	4.60361800	-4.89053700	0.59209000
H	2.85752800	-5.22821900	0.56166600
H	3.58043900	-4.52650900	1.99752900
C	3.65725300	1.00873100	-1.16282100
C	3.63494600	1.38571200	-2.52014700
C	3.80036200	2.74042000	-2.82785800
H	3.78421100	3.05115100	-3.86826500
C	3.95696700	3.69636700	-1.82932400
H	4.07018700	4.74457600	-2.09157800
C	3.95076400	3.30661200	-0.49465500
H	4.05004700	4.05471200	0.28566600
C	3.80800700	1.96187000	-0.13952700
C	3.39492200	0.39111000	-3.64650800
H	3.30744700	-0.60705300	-3.21166900
C	4.54691800	0.36564300	-4.66559400
H	4.65781200	1.33417800	-5.16607700
H	4.35060600	-0.38637100	-5.43823500
H	5.50814200	0.12455600	-4.19884000
C	2.06608300	0.70522700	-4.35797300
H	1.24971700	0.80600000	-3.63956500
H	1.81108900	-0.08999200	-5.06755100
H	2.13377700	1.64582200	-4.91711900
C	3.79486600	1.57094300	1.32930300
H	3.72914900	0.48100600	1.40496400
C	5.09047700	1.98222400	2.04776800
H	5.21972100	3.07028500	2.04880200
H	5.97292700	1.54164600	1.56944300
H	5.06727300	1.64928100	3.09189700
C	2.56639400	2.17563500	2.01679000
H	2.50372800	1.84903700	3.05758700
H	1.63979900	1.89919600	1.50517300
H	2.61966900	3.26596300	2.01340000
C	1.24054100	-3.27341700	1.43633600
C	0.31033400	-4.17140100	0.88410000
C	-0.55819600	-4.83225300	1.75831900
H	-1.28561300	-5.52942500	1.35561200
C	-0.51804500	-4.59702800	3.12833500
H	-1.21563800	-5.10594400	3.78727500
C	0.41934600	-3.71332100	3.65454000
H	0.45126900	-3.53975500	4.72563700
C	1.32679800	-3.05171300	2.82343500
C	2.37631300	-2.12097200	3.41236800
H	3.12137900	-1.91207400	2.63866300
C	1.73901300	-0.78274200	3.80125900
H	2.49641600	-0.08630000	4.17733200

H	0.97913700	-0.92002800	4.57777300
H	1.23474600	-0.32825400	2.94599100
C	3.12304800	-2.74732000	4.59991300
H	3.92895600	-2.08223600	4.93038100
H	3.56633300	-3.71363800	4.33356600
H	2.46017800	-2.90959000	5.45675100
C	0.24617900	-4.43982700	-0.61081000
H	1.09781600	-3.94810700	-1.08288500
C	0.34973400	-5.93907900	-0.93737800
H	-0.50604400	-6.49881500	-0.54365000
H	0.36824000	-6.08557800	-2.02320200
H	1.25918800	-6.38627200	-0.51998300
C	-1.03376400	-3.85200400	-1.22340500
H	-1.18774300	-2.80272900	-0.95610000
H	-1.00851800	-3.92181700	-2.31535600
H	-1.91539000	-4.40027200	-0.88081500
C	-1.20781800	3.02492700	3.70825400
H	-2.05791700	2.42142000	3.37977000
C	-0.20584400	2.05977200	4.35663000
H	-0.66367600	1.54897400	5.21161900
H	0.09921600	1.30200000	3.63899300
H	0.68436400	2.59352200	4.71024500
C	-1.70507300	4.04238500	4.75057400
H	-2.25743500	3.52660400	5.54409600
H	-0.86881800	4.56888600	5.22453000
H	-2.36211400	4.80139300	4.31400600
O	1.48835500	-1.99248400	-2.33889200
C	0.44288400	-1.54317300	-2.74972800
O	-0.43954100	-1.49966400	-3.52672600

Cartesian coordinates of the optimized geometry for **10** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

Cl	1.61952000	1.16711300	2.94759000
P	0.23072100	-0.67231400	-0.23568600
Ga	1.79883700	0.65229800	0.78237500
Ga	-2.05642500	-0.42554000	-0.20340400
N	3.46046600	-0.40778600	0.83546100
N	2.63801700	2.20541600	-0.04941000
N	-2.84831000	-2.15741700	-0.66647600
N	-3.69003700	0.38819500	0.40939300
C	4.61493800	0.21566900	1.03442200
C	4.74430100	1.61880900	0.99190700
H	5.69783700	2.01554500	1.31652900
C	3.84980600	2.53718500	0.43802600
C	5.86985200	-0.57983800	1.30504900
H	5.96565700	-0.77654200	2.37868100
H	6.75286100	-0.02352000	0.98355300
H	5.84717000	-1.54541100	0.79678100
C	4.29342600	3.98025100	0.35927400
H	5.32642100	4.08872400	0.69505500
H	3.64938200	4.59359300	1.00040400
H	4.20573000	4.38139100	-0.65178000
C	3.36744700	-1.83822300	0.77815000
C	3.33254300	-2.59961500	1.96178600
C	3.18679900	-3.98828800	1.84434100
H	3.16393700	-4.59519700	2.74494500
C	3.06545600	-4.59757300	0.60133800
H	2.95627400	-5.67675100	0.53183600
C	3.07997500	-3.82299400	-0.55668800
H	2.96089400	-4.30201400	-1.52159400
C	3.21470900	-2.43566200	-0.49293900
C	3.23322800	-1.58755900	-1.75627100
H	2.76883000	-0.62886100	-1.51133500
C	4.67395300	-1.29012100	-2.20680400
H	5.21994600	-0.71171100	-1.45597300
H	4.66962800	-0.70926500	-3.13551500

H	5.22320100	-2.22134000	-2.38981200
C	2.40983000	-2.17825300	-2.90398800
H	2.88740900	-3.06487900	-3.33939200
H	2.30076000	-1.43145000	-3.69522500
H	1.41063800	-2.45758000	-2.56290800
C	1.97682300	3.13543000	-0.92761100
C	1.07298400	4.06850200	-0.38857400
C	0.47274700	4.99064900	-1.25112300
H	-0.23304100	5.71315100	-0.85415100
C	0.77078300	4.99232200	-2.60939100
H	0.29830700	5.71460800	-3.26966100
C	1.66905200	4.06227700	-3.12517500
H	1.88231500	4.06409700	-4.18845000
C	2.28678100	3.11333500	-2.30467300
C	0.72255100	4.03012500	1.08693400
H	1.55090800	3.56574500	1.62508600
C	0.50648300	5.41576100	1.70886500
H	0.37542700	5.31810400	2.79221200
H	-0.39146400	5.90680200	1.31642900
H	1.36055000	6.07791100	1.52541400
C	-0.51918600	3.15633100	1.29409200
H	-0.39962900	2.16949600	0.83791600
H	-1.38766100	3.62522300	0.83262000
H	-0.71925300	3.00556000	2.35655800
C	3.26442600	2.10249200	-2.89472000
H	3.19972300	1.20563300	-2.27678700
C	4.72387400	2.59572000	-2.84873100
H	5.10193400	2.68299200	-1.82800900
H	4.82228700	3.57185400	-3.33932400
H	5.37351200	1.88783300	-3.37685900
C	2.91015600	1.69888900	-4.33391200
H	3.52082600	0.83873600	-4.63270600
H	3.12585300	2.50487400	-5.04617200
H	1.85868100	1.42113600	-4.41307700
C	-4.14063600	-2.44288400	-0.57028800
C	-5.10254800	-1.51210900	-0.14455300
H	-6.12720500	-1.85870700	-0.13821400
C	-4.89004700	-0.21848600	0.32829100
C	-4.62334400	-3.84298500	-0.86072800
H	-4.47328000	-4.46928100	0.02670400
H	-4.06906400	-4.30726400	-1.67595000
H	-5.68948500	-3.84230300	-1.09709900
C	-6.10595700	0.53470700	0.81638400
H	-7.01062000	-0.05231500	0.65129600
H	-6.20685400	1.49544400	0.30460100
H	-6.02127300	0.75874300	1.88460200
C	-1.91074800	-3.17474800	-1.05775100
C	-1.57078900	-3.31400300	-2.41752500
C	-0.62532400	-4.29071700	-2.75195500
H	-0.34905200	-4.42490700	-3.79321900
C	-0.02363700	-5.07776600	-1.77501100
H	0.71862600	-5.81931600	-2.05676800
C	-0.36708100	-4.91175600	-0.43671900
H	0.12064000	-5.51522800	0.32200900
C	-1.31938000	-3.96487900	-0.05321100
C	-2.22568800	-2.48382200	-3.51658600
H	-2.80737000	-1.68377200	-3.05214400
C	-3.19110100	-3.34482000	-4.35379300
H	-2.65769600	-4.16787700	-4.84379100
H	-3.65992200	-2.73644200	-5.13571400
H	-3.98987300	-3.78137600	-3.74559600
C	-1.19550600	-1.80996000	-4.43638600
H	-0.48611400	-1.19645100	-3.88224800
H	-1.71297300	-1.15618200	-5.14728200
H	-0.63238400	-2.54900000	-5.01892100
C	-1.68352500	-3.80330500	1.41723600
H	-2.48443500	-3.06155100	1.49854900
C	-2.21785800	-5.11673800	2.01482600

H	-1.44326300	-5.89167200	2.02255900
H	-3.06802000	-5.50603200	1.44401400
H	-2.54240500	-4.96138000	3.05008000
C	-0.49792600	-3.28526100	2.24430100
H	-0.80781900	-3.09876100	3.27873800
H	-0.09284100	-2.35888900	1.83327800
H	0.32281800	-4.00916300	2.25967800
C	-3.64789300	1.68990300	1.02182700
C	-3.82107700	2.83223500	0.22009300
C	-3.88848300	4.07296300	0.86566800
H	-4.02748600	4.97279400	0.27388700
C	-3.76164700	4.17126900	2.24823700
H	-3.81171800	5.14392400	2.72953700
C	-3.55120300	3.02762800	3.01611600
H	-3.43454200	3.11929900	4.09127500
C	-3.49708300	1.76390800	2.42101200
C	-3.27593500	0.50447900	3.25208600
H	-3.61943800	-0.35191100	2.66331900
C	-1.78079100	0.28465700	3.54254500
H	-1.63200400	-0.65464300	4.08795800
H	-1.37287300	1.09848200	4.15076600
H	-1.17883300	0.24181700	2.63203600
C	-4.08720100	0.50333700	4.55644200
H	-3.98623100	-0.46479200	5.05923900
H	-5.15223900	0.68191500	4.36944700
H	-3.73584600	1.27026500	5.25538200
C	-3.89704900	2.74770100	-1.29870600
H	-3.94023100	1.69548400	-1.59045900
C	-5.15763700	3.42909300	-1.85648000
H	-5.16219700	4.50507300	-1.64831500
H	-5.20155100	3.30385400	-2.94400800
H	-6.07371900	3.00386100	-1.43014400
C	-2.62799900	3.34234000	-1.93396600
H	-1.72478000	2.86603000	-1.55272800
H	-2.64241900	3.19159300	-3.01844200
H	-2.55817400	4.41880700	-1.73814500
C	3.44703200	-1.97360300	3.34537100
H	3.65153400	-0.90716400	3.22664600
C	2.12065700	-2.08061800	4.11481800
H	2.21042600	-1.59385400	5.09249300
H	1.31868100	-1.58259700	3.56853900
H	1.83913700	-3.12760400	4.27694200
C	4.59311700	-2.59530700	4.16238000
H	4.72204100	-2.05367500	5.10635000
H	4.38625200	-3.64275500	4.41001600
H	5.54337000	-2.56893100	3.61869600
O	-1.54501500	0.35700300	-1.91636200
C	-0.21908100	0.27498300	-1.82938200
O	0.56704700	0.64911700	-2.67594000

Cartesian coordinates of the optimized geometry for **TS₁₋₄** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 1):

Cl	-1.72649900	-1.04684500	2.44577800
P	-0.15367100	0.44844600	-0.91534700
Ga	-1.84580900	-0.33821600	0.31810600
Ga	1.80392800	0.05037800	-0.04720200
N	-3.34602000	0.99635700	0.41382000
N	-3.00505300	-1.72145900	-0.50941600
N	3.04206700	1.57773000	-0.33979700
N	2.92381900	-0.85824000	1.25542300
C	-4.62833000	0.63494700	0.39060800
C	-5.07632400	-0.66871900	0.12780600
H	-6.14519800	-0.82379100	0.19826200
C	-4.33095600	-1.74374400	-0.36471800
C	-5.71255700	1.66645800	0.62460700
H	-5.44516900	2.63845900	0.20768900

H	-5.87598400	1.80637800	1.69773700
H	-6.65401100	1.33473000	0.18182900
C	-5.10660200	-2.97433600	-0.77986700
H	-6.16872300	-2.74626000	-0.88847200
H	-4.99980800	-3.75262900	-0.01649300
H	-4.73287200	-3.39303900	-1.71579700
C	-3.01581100	2.38587800	0.56884700
C	-3.07032100	2.99620200	1.83883900
C	-2.76464500	4.35948700	1.93113100
H	-2.80696500	4.84628400	2.90122400
C	-2.39524900	5.09357400	0.81057500
H	-2.15732800	6.15020700	0.90373100
C	-2.33000300	4.47059400	-0.43298800
H	-2.03321400	5.04709500	-1.30167600
C	-2.64392500	3.11710000	-0.58204200
C	-2.66063600	2.47258400	-1.96250100
H	-2.37761100	1.42697800	-1.83362000
C	-4.06977500	2.48975700	-2.57901700
H	-4.77980200	1.91416300	-1.97900400
H	-4.04763300	2.04572200	-3.58166700
H	-4.44781100	3.51525500	-2.67047400
C	-1.63418300	3.08589000	-2.91923900
H	-1.90555300	4.10575100	-3.21876100
H	-1.57277800	2.48348100	-3.83105600
H	-0.64498500	3.10671300	-2.45850800
C	-2.36288400	-2.73519700	-1.29216300
C	-1.94419300	-3.93703000	-0.69175300
C	-1.29989900	-4.88573800	-1.49369500
H	-0.97179900	-5.82105100	-1.04888600
C	-1.07866500	-4.65251000	-2.84738600
H	-0.57376800	-5.39978100	-3.45386200
C	-1.52111500	-3.46658600	-3.42751900
H	-1.35973600	-3.29617200	-4.48752100
C	-2.16719300	-2.48826400	-2.66766900
C	-2.20792900	-4.22726100	0.77782700
H	-2.81540000	-3.41347200	1.17926400
C	-2.97930100	-5.54415500	0.97250600
H	-3.24174500	-5.67547200	2.02864600
H	-2.37525800	-6.40898400	0.67353300
H	-3.90264800	-5.57104600	0.38416500
C	-0.90952200	-4.25369700	1.58981100
H	-0.32821800	-3.34187000	1.45247100
H	-0.28522700	-5.10801900	1.30421600
H	-1.12939100	-4.33988600	2.65862200
C	-2.73782200	-1.24507700	-3.34045400
H	-3.04966000	-0.54935900	-2.55772100
C	-3.99582400	-1.60134800	-4.15450200
H	-4.76621000	-2.06278600	-3.52885500
H	-3.75475100	-2.30324300	-4.96178700
H	-4.42513200	-0.69930900	-4.60663700
C	-1.71818000	-0.51282500	-4.22061800
H	-2.18308300	0.37579600	-4.66330600
H	-1.35790500	-1.14101500	-5.04319400
H	-0.86153100	-0.19496900	-3.62500000
C	4.31882000	1.54421700	0.01451200
C	4.89357500	0.46369500	0.71224000
H	5.95909800	0.53084100	0.88749200
C	4.24038900	-0.60138700	1.34417100
C	5.20390900	2.73105100	-0.28329100
H	5.14283900	3.01296000	-1.33791400
H	6.24362400	2.52023800	-0.02578300
H	4.87098400	3.60154200	0.29123600
C	5.09192800	-1.47192900	2.24067600
H	6.11715000	-1.10003600	2.27613300
H	5.10427000	-2.50777800	1.89098200
H	4.68621000	-1.49013400	3.25592700
C	2.46519200	2.80575200	-0.82471800
C	2.41887000	3.08359400	-2.20266100

C	1.83181600	4.28320200	-2.61770200
H	1.78719000	4.51215100	-3.67854700
C	1.27874800	5.16988100	-1.69912800
H	0.81263400	6.08934000	-2.04217200
C	1.30754900	4.86461000	-0.34239500
H	0.85021400	5.54145300	0.37244900
C	1.90184800	3.68651400	0.11745500
C	2.94543000	2.10372200	-3.23700400
H	3.40698600	1.27884200	-2.69350700
C	4.01452900	2.72236800	-4.15072200
H	3.60319100	3.54110800	-4.75129600
H	4.40650100	1.96962000	-4.84540100
H	4.85710400	3.12443300	-3.57666900
C	1.78473800	1.51796400	-4.05732000
H	1.02042600	1.10237100	-3.39662700
H	2.13869000	0.72640600	-4.72914000
H	1.30932500	2.28946500	-4.67352400
C	1.91617700	3.37417800	1.60325100
H	2.45283900	2.43499600	1.74957200
C	2.66153600	4.44768500	2.41257100
H	2.16380700	5.42113500	2.33776100
H	3.69388800	4.57350100	2.06603700
H	2.69245300	4.17054900	3.47265200
C	0.49097400	3.17773000	2.13041700
H	0.51843800	2.81131900	3.16139200
H	-0.06694100	2.46671300	1.51525400
H	-0.06748500	4.11779700	2.12615600
C	2.38164000	-1.89103600	2.10636900
C	2.52152600	-3.23687100	1.71420600
C	2.14845800	-4.23517400	2.61689700
H	2.25937100	-5.27817300	2.33793500
C	1.61359400	-3.90583700	3.85604700
H	1.32325500	-4.68966800	4.54987800
C	1.41149600	-2.57095200	4.19451000
H	0.94892700	-2.33616700	5.14471000
C	1.78372500	-1.53217400	3.33391100
C	1.53378800	-0.07186800	3.71291500
H	1.01330600	0.39025800	2.86345300
C	0.61180400	0.08319900	4.92900700
H	0.38231900	1.14257500	5.07792400
H	1.09469700	-0.27760600	5.84554400
H	-0.33225700	-0.44722900	4.79005800
C	2.82791400	0.71963400	3.98219100
H	2.57649000	1.73137700	4.31955000
H	3.45864800	0.81875200	3.09981800
H	3.41306500	0.24266800	4.77803100
C	3.02094500	-3.59776300	0.32472600
H	3.52355100	-2.71757400	-0.07428800
C	4.03103700	-4.75389300	0.31150000
H	3.56918500	-5.69954500	0.61522100
H	4.42548500	-4.89792400	-0.70131000
H	4.87708200	-4.56677900	0.98245400
C	1.83668600	-3.90728100	-0.60630900
H	1.06902000	-3.12900400	-0.57734400
H	2.17461300	-4.02172200	-1.64299100
H	1.35151000	-4.84288300	-0.31521500
C	-3.43782100	2.23190500	3.10411800
H	-3.77422400	1.23225500	2.81833100
C	-2.20379300	2.04113200	3.99752500
H	-2.46124000	1.45313900	4.88583400
H	-1.42896000	1.50347700	3.45382100
H	-1.80210700	3.00683000	4.32738500
C	-4.56440600	2.91704200	3.89744100
H	-4.88257300	2.27698700	4.72824600
H	-4.22921100	3.86786700	4.32747400
H	-5.43952800	3.13097300	3.27519100
C	1.84255200	-1.40138100	-2.54741900
O	1.11588200	-1.86930400	-3.33067300

N	2.76542800	-0.98430000	-1.82634600
C	4.18688900	-1.19491800	-2.21851000
H	4.71183900	-0.28247000	-1.93441500
H	4.58318300	-1.99728500	-1.58901700
C	4.39370500	-1.50971600	-3.69392700
H	3.88441100	-2.43394500	-3.98621200
H	4.02227300	-0.69746500	-4.32648400
H	5.46290600	-1.63621300	-3.89345900

Cartesian coordinates of the optimized geometry for **4** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

Cl	-1.44763700	1.13148900	-2.94253400
P	-0.25205700	-0.71364200	0.31797400
Ga	-1.76611300	0.57093200	-0.80067700
Ga	2.00144500	-0.26862000	0.31764800
N	-3.39468100	-0.53756700	-0.98426400
N	-2.73169600	2.09231200	-0.03678800
N	2.83824700	-1.95564500	0.94276900
N	3.57146400	0.42748900	-0.57919100
C	-4.55340700	0.04460000	-1.26345100
C	-4.73543100	1.44198000	-1.22922400
H	-5.67709600	1.80656500	-1.61968500
C	-3.91515300	2.38642100	-0.61042200
C	-5.76071700	-0.79145400	-1.61800500
H	-5.78683600	-0.97641200	-2.69759100
H	-6.68021100	-0.27002300	-1.34337700
H	-5.73460400	-1.76222000	-1.12016700
C	-4.41502100	3.81265900	-0.55822900
H	-5.42307500	3.88632500	-0.97065000
H	-3.74800100	4.45426400	-1.14574600
H	-4.41923400	4.20891900	0.45864800
C	-3.25855800	-1.96506600	-0.93482400
C	-3.13280500	-2.71070800	-2.12282800
C	-2.94511500	-4.09480000	-2.01311600
H	-2.85007000	-4.68863000	-2.91767700
C	-2.86826500	-4.71523700	-0.77226400
H	-2.72133300	-5.79033200	-0.70859000
C	-2.97685500	-3.95682300	0.39143700
H	-2.89487200	-4.44434300	1.35596800
C	-3.16278000	-2.57471200	0.33634500
C	-3.29935400	-1.74836700	1.60700700
H	-2.83708900	-0.77655800	1.41668800
C	-4.77784400	-1.49145000	1.94671400
H	-5.27520400	-0.90816600	1.16658900
H	-4.86006600	-0.93067600	2.88415600
H	-5.31921400	-2.43740500	2.06728300
C	-2.55606900	-2.34044500	2.80738800
H	-3.04502600	-3.24553000	3.18942600
H	-2.52873200	-1.60418600	3.61528300
H	-1.52579900	-2.58795900	2.54267600
C	-2.17627400	3.04162500	0.89119900
C	-1.28220200	4.02181000	0.42332300
C	-0.79841900	4.97148300	1.32882500
H	-0.10333100	5.73194800	0.98651500
C	-1.21005000	4.96020600	2.65755000
H	-0.83382800	5.70782400	3.35077700
C	-2.09571600	3.98251600	3.10341900
H	-2.39745400	3.97548600	4.14525200
C	-2.58963700	2.99901000	2.24056700
C	-0.83543200	4.01567000	-1.02632700
H	-1.58292800	3.47693400	-1.60991800
C	-0.71306100	5.41535400	-1.64198400
H	-0.48397400	5.33060700	-2.71007500
H	0.09266100	5.99920700	-1.18182500
H	-1.64323300	5.98552600	-1.53534800
C	0.48811300	3.25485200	-1.15884900

H	0.45033000	2.29244800	-0.63957900
H	1.29853800	3.83498500	-0.71825100
H	0.72615000	3.05865700	-2.20504200
C	-3.56092300	1.93927900	2.74957300
H	-3.40974800	1.05269700	2.13196100
C	-5.03284200	2.37015900	2.59689800
H	-5.33376900	2.45936300	1.55112200
H	-5.21169900	3.33242000	3.09226000
H	-5.68942400	1.62571600	3.06235300
C	-3.29904300	1.53660600	4.20816900
H	-3.90633900	0.65886700	4.45858800
H	-3.58491100	2.33168800	4.90781800
H	-2.24971300	1.28227800	4.35887200
C	4.14308500	-2.17345100	0.90333200
C	5.06200900	-1.25362900	0.36002400
H	6.10185700	-1.54911000	0.41408200
C	4.79147200	-0.11999400	-0.40564700
C	4.71991600	-3.49604300	1.35215300
H	4.91362300	-4.12271300	0.47370300
H	4.04727500	-4.04433800	2.00862100
H	5.67625100	-3.33604100	1.85807700
C	5.96815200	0.48199800	-1.14172400
H	6.85219200	-0.14560800	-1.02010800
H	6.20309400	1.48476800	-0.77907300
H	5.74510300	0.57490600	-2.20823700
C	1.93438400	-3.02154200	1.29235900
C	1.52323900	-3.19938200	2.62686900
C	0.63713600	-4.24706700	2.90568100
H	0.31749200	-4.40982100	3.93014000
C	0.14912100	-5.07063900	1.89745600
H	-0.54799500	-5.86896200	2.13606300
C	0.54967600	-4.86313400	0.58183000
H	0.15032600	-5.49161000	-0.20772900
C	1.44681100	-3.84404100	0.25661100
C	2.04070100	-2.33438700	3.76748200
H	2.58427500	-1.49258400	3.33034300
C	3.02394500	-3.11485200	4.66005100
H	2.53152300	-3.98070400	5.11791900
H	3.39397200	-2.47355900	5.46843600
H	3.88914700	-3.48137300	4.09939500
C	0.89529700	-1.76693400	4.62182300
H	0.18535800	-1.19340100	4.02425700
H	1.29935900	-1.10478500	5.39649000
H	0.34698900	-2.56582900	5.13389800
C	1.85931300	-3.64162000	-1.19281900
H	2.51954200	-2.77319800	-1.24321500
C	2.65408500	-4.84436400	-1.72843700
H	2.03796300	-5.75069300	-1.73816300
H	3.53690600	-5.05012200	-1.11367400
H	2.98929100	-4.65590500	-2.75499700
C	0.64755400	-3.35069200	-2.08775400
H	0.97814400	-3.08554200	-3.09755700
H	0.04483500	-2.53101900	-1.69219900
H	-0.01216700	-4.22027500	-2.16944400
C	3.44208600	1.51188200	-1.51891200
C	3.87626700	2.80112700	-1.15022300
C	3.81703000	3.81617800	-2.11061100
H	4.14445900	4.81745200	-1.84886700
C	3.33649900	3.56415900	-3.38976700
H	3.29932900	4.36320900	-4.12477200
C	2.88047700	2.29168700	-3.72471600
H	2.48284600	2.11835300	-4.71708900
C	2.91500400	1.24090200	-2.80192700
C	2.40516300	-0.15041400	-3.17936300
H	1.73875000	-0.49254900	-2.37512600
C	1.56529000	-0.16254300	-4.46223100
H	1.12284400	-1.15426900	-4.59680300
H	2.18035300	0.04391700	-5.34652400

H	0.74766400	0.55895700	-4.41764700
C	3.55057500	-1.17100200	-3.32482300
H	3.15146700	-2.13202600	-3.66740700
H	4.08400200	-1.35190600	-2.39108800
H	4.27280100	-0.82635500	-4.07463900
C	4.35794600	3.12035800	0.26095900
H	4.58964900	2.17789200	0.76526300
C	5.62600000	3.98873800	0.28568700
H	5.42823500	5.00109000	-0.08324200
H	5.99416400	4.08369100	1.31315000
H	6.43029300	3.56631400	-0.32670700
C	3.23510800	3.78986900	1.06867800
H	2.34422500	3.16117300	1.08593600
H	3.55428100	3.96436200	2.10219600
H	2.96128400	4.75694800	0.63085100
C	-3.18317500	-2.07144600	-3.50428800
H	-3.43211600	-1.01417600	-3.38818400
C	-1.80619400	-2.12245200	-4.18472400
H	-1.84514800	-1.62476500	-5.16030700
H	-1.06336700	-1.60486800	-3.57756800
H	-1.47705000	-3.15689300	-4.33818800
C	-4.25031700	-2.72251600	-4.40113800
H	-4.33648000	-2.17394600	-5.34602000
H	-3.99003600	-3.75876700	-4.64539700
H	-5.23450600	-2.73656800	-3.92118700
C	0.05211900	0.33424100	1.89170800
O	-0.79799600	0.53506500	2.75566800
N	1.37688600	0.67286800	1.91417800
C	1.97622000	1.28033100	3.10556200
H	2.01635000	0.54669800	3.92049300
H	3.01594800	1.51243400	2.84663800
C	1.26105000	2.53572600	3.60979300
H	1.09769400	3.25581200	2.80586800
H	0.28331400	2.27892400	4.01570800
H	1.86027600	3.01668600	4.39298000

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