Supporting Information

Multi-Talented Gallaphosphene for Ga–P–Ga Heteroallyl Cation Generation, CO₂ Storage, and C(sp³)–H Bond Activation

Mahendra K. Sharma, Christoph Wölper, Gebhard Haberhauer, and Stephan Schulz*

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1. Experimental Section

**General procedure.** All experiments and manipulations were carried out under a dry argon atmosphere using either standard Schlenk techniques or an MBraun LABmaster Pro glovebox. THF, toluene, benzene, and *n*-hexane were dried using Braun solvent drying system, degassed, and stored over 4Å molecular sieve. Deuterated solvents such as benzene-*d*$_6$ and toluene-*d*$_8$ were dried by refluxing over NaK, 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. LGaCl$_2$ (L = H[C(Me)N(Ar)]$_2$, Ar = 2,6-iPr$_2$C$_6$H$_3$),$^{[1]}$ LGa,$^{[2]}$ NaPCO(dioxane)$_{2.5}$,$^{[3]}$ and LiB(C$_6$F$_5$)$_4$,$^{[4]}$ were prepared according to literature procedures. NMR spectra ($^1$H, $^{13}$C, $^{31}$P, $^{19}$F) were recorded on Bruker Avance II 600 MHz, 400 MHz and 300 MHz spectrometers. Chemical shifts $\delta$ are given in ppm and referenced to the solvent residual peak(s).$^{[5]}$ 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 LGa(Cl)PCO (1):** LGaCl$_2$ (5.0 g, 8.95 mmol) and NaPCO(dioxane)$_{2.5}$ (2.7 g, 8.95 mmol) were dissolved in THF (50 mL) at 0 °C, warmed to ambient temperature and stirred overnight, yielding a clear pale yellow solution. All volatiles were removed in vacuo and the residue was extracted with toluene (50 mL) and dried. 1 was obtained as pale yellow crystalline powder. Yield: 95% (4.96 g). M.p. 121 °C (dec.). Single crystals suitable for X-ray diffraction were grown by cooling a hot toluene solution of 1 to ambient temperature. Anal. calcd. (%) for C$_{30}$H$_{41}$ClGaN$_2$OP (580.19): C, 61.93; H, 7.10; N, 4.81. Found: C, 62.20; H, 7.32; N, 4.89. $^1$H NMR (300 MHz, C$_6$D$_6$, 298 K) $\delta$ = 1.02 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(C$_6$H$_3$)$_2$), 1.20 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.36 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.50 (d, $^3$J$_{HH}$ = 6.7 Hz, 6H, CH(CH$_3$)$_2$), 1.55 (s, 6H, CCH$_3$), 3.11 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.75 (sept, $^3$J$_{HH}$ = 6.7 Hz, 2H, CH(CH$_3$)$_2$), 4.86 (s, 1H, CH), 7.05-7.16 (m, 6H, C$_6$H$_3$).$^{[13]}$C {$^1$H} NMR (75 MHz, C$_6$D$_6$, 298 K) $\delta$ = 24.1, 24.6, 24.7, 24.9 (CH(CH$_3$)$_2$), 27.2, 27.1, 28.6, 29.8, 29.9 (CH(CH$_3$)$_2$), 97.3 (CH), 124.6, 126.0, 139.6, 143.4, 146.4, 170.9 (C$_6$H$_3$), 181.6 (d, $\delta_{CP} = 100.6$ Hz, PCO). $^{31}$P {$^1$H} (121 MHz, C$_6$D$_6$, 298 K) $\delta$ = -371.4 ppm. ATR-IR: $v$ 2963, 2924, 2864, 1936, 1525, 1426, 1438, 1380, 1316, 1255, 1178, 1097, 1021, 933, 873, 797, 757, 637, 537 cm$^{-1}$.

**Synthesis of LGa(Cl)-P(GaL) (2):** LGaCl(PCO) (1) (1.5 g, 2.58 mmol) and LGa (1.26 g, 2.58 mmol) were dissolved in benzene (20 mL) at room temperature and stirred for 6 h to yield a red solution. All volatiles were removed in vacuo and the residue was washed with cold *n*-hexane (5 mL). 2 was obtained as red solid. Single crystals suitable for X-ray diffraction were grown upon storage of a saturated benzene solution of 2 at ambient temperature for 12 h. Yield: 83% (2.23 g).
M.p. 171 °C (dec.). Anal. calcd. (%) for C₈₅H₈₂ClGa₂Na₄P (1038.45): C, 66.91; H, 7.94; N, 5.26. Found: C, 66.89; H, 8.25; N, 5.32. ¹H NMR (300 MHz, C₆D₆, 298 K) δ = 1.07 (d, 3JHH = 6.8 Hz, 24H, CH(CH₃)₂), 1.17 (d, 3JHH = 6.8 Hz, 24H, CH(CH₃)₂), 1.43 (s, 12H, C₆H₃), 3.14 (sept, 3JHH = 6.8 Hz, 8H, CH(CH₃)₂), 4.82 (s, 2H, CH), 7.04-7.14 (m, 12H, C₆H₅). ¹³C {¹H} NMR (75 MHz, C₆D₆, 298 K) δ = 24.8, 26.4 (CH(CH₃)₂), 29.3 (CH(CH₃)₂), 98.3 (CH), 124.6, 142.3, 144.0, 169.1 (C₆H₅). ³¹P {¹H} (121 MHz, C₆D₆, 298 K) δ = -245.8. ATR-IR: ν 2956, 2923, 2835, 1535, 1436, 1380, 1317, 1254, 1176, 1100, 1019, 936, 880, 795, 758, 539, 531 cm⁻¹.

**Synthesis of LGa(OCP)-P(GaL) (3): Method A:** LGa(Cl)-P(GaL) (2) (100 mg, 0.10 mmol) and NaPCO(dioxane)₂ (29 mg, 0.10 mmol) were dissolved in THF (5 mL) at 0 °C, warmed to ambient temperature and stirred for 12 h. The solvent was removed in vacuo and the red residue extracted with toluene (10 mL). The filtrate was concentrated to 2 mL and stored at ambient temperature for 12 hours. Solid precipitates were filtered, the filtrate concentrated to 2 mL and stored at ambient temperature for 6 h. 3 was obtained as orange crystals. Yield: 67% (68 mg).

**Method B:** [LGa-P-GaL]⁺[B(C₆F₅)₄]⁻ (4) (150 mg, 0.09 mmol) and NaPCO·dioxane (27 mg, 0.09 mmol) were suspended in toluene (10 mL) at 0 °C, warmed to ambient temperature and stirred for 12 h. Solid precipitates were filtered, the filtrate concentrated to 2 mL and stored at ambient temperature for 6 h. 3 was obtained as orange crystals in 47% (45 mg) yield.

M.p. 127 °C (dec.). Anal. calcd. (%) for C₅₉H₈₂Ga₂Na₄O₂P (1062.45): C, 66.56; H, 7.76; N, 5.26. Found: C, 66.67; H, 7.83; N, 5.37. ¹H NMR (300 MHz, C₆D₆, 298 K) δ = 1.10 (d, 3JHH = 6.8 Hz, 48H, CH(CH₃)₂), 1.45 (s, 12H, C₆H₃), 3.31 (sept, 3JHH = 6.7 Hz, 8H, CH(CH₃)₂), 4.85 (s, 2H, CH), 7.03 (d, 3JHH = 7.5 Hz, 8H, C₆H₅), 7.13-7.18 (m, 4H, C₆H₅). ¹³C {¹H} NMR (150 MHz, THF-d₈, 298 K) δ = 24.7, 26.4 (CH(CH₃)₂), 29.1 (CH(CH₃)₂), 96.8, 100.3 (CH), 124.6, 124.8, 125.5, 125.9, 127.7, 128.0, 141.8, 142.4, 143.2, 143.8, 145.5, 146.1, 169.1, 169.3, 170.7 (C₆H₅), 183.3 (d, ¹JP-C = 40.1 Hz, OCP). ³¹P {¹H} (161 MHz, C₆D₆, 298 K) δ = -290.5, -320.8. ATR-IR: ν 2959, 2923, 2864, 1739, 1528, 1380, 1336, 1314, 1252, 1173, 1097, 1018, 935, 856, 795, 757, 626, 530 cm⁻¹.

**Synthesis of [LGa-P-GaL]⁺[B(C₆F₅)₄]⁻ (4):** LGa(Cl)-P(GaL) (2) (300 mg, 0.29 mmol) and LiB(C₆F₅)₄ (198 mg, 0.29 mmol) were dissolved in toluene (10 mL) at -60 °C, the resulting mixture warmed to ambient temperature and stirred for 2 h. The solid precipitate was filtered through a G4 frit, the resulting filtrate concentrated to 2 mL and stored at -30 °C for 12 h. Yellow crystals of 4 formed in 78% (378 mg) yield. M.p. 183 °C (dec.). Anal. calcd. (%) for C₇₀H₇₅BF₂₀Ga₂Na₄P (1639.40): C, 57.80; H, 4.60; N, 3.41. Found: C, 58.21; H, 4.78; N, 4.57. ¹H NMR (300 MHz, toluene-d₈, 298 K) δ = 0.83 (d, 3JHH = 6.8 Hz, 24H, CH(CH₃)₂), 1.00 (d, 3JHH = 6.8 Hz, 24H, CH(CH₃)₂), 1.41 (s, 12H, C₆H₃), 2.52 (sept, 3JHH = 6.8 Hz, 8H, CH(CH₃)₂), 5.15 (s, 2H, CH), 6.93 (d, 3JHH = 6.7 Hz, 8H, C₆H₅), 7.02 (m, 4H, C₆H₅). ¹³C {¹H} NMR (125 MHz, toluene-d₈, 298 K) δ =
23.5, 24.1, 25.3 (CH(CH$_3$)$_2$), 29.3 (CH(CH$_3$)$_2$), 101.9 (CH), 136.1, 138.2 (C$_6$F$_5$), 139.0, 143.1 (C$_6$H$_3$), 148.3, 150.3 (C$_6$F$_5$), 172.5 (C$_6$H$_3$). 31P$_1^1$H (121 MHz, toluene-$d_8$, 298 K) $\delta = -267.0$. 19F (282 MHz, toluene-$d_8$, 298 K) $\delta = -131.7$ (m, ortho-C$_6$F$_5$), -163.0 (t, $^3$J$_{CF} = 20.73$ Hz, para-C$_6$F$_5$), -166.73 (t, $^3$J$_{CF} = 18.22$ Hz, meta-C$_6$F$_5$). ATR-IR: $\nu$ 2963, 2927, 2867, 1643, 1514, 1458, 1364, 1317, 1254, 1084, 976, 870, 800, 755, 729, 660, 606, 503 cm$^{-1}$.

**Synthesis of LGa(Cl)-P(CO$_2$)$_2$GaL (5):** A toluene solution (5 mL) of LGa(Cl)-P(GaL) (2) (0.5 g, 0.48 mmol) in a J-Young Schlenk flask was degassed using the freeze-pump-thaw method. CO$_2$ (1 bar) gas was added and the solution immediately turned from red to colourless. All volatiles were then removed in vacuo, the resulting residue washed with $n$-hexane (5 mL) and dried in vacuo, to yield a colorless crystalline powder. Single crystals suitable for X-ray diffraction were grown by cooling a toluene solution of 5 at $-30$ °C for four days. Yield: 75% (0.4 g). M.p.: 100 °C (dec.).

Anal. calcd. (%) for C$_{60}$H$_{82}$ClGa$_2$Na$_4$OP (1126.43): C 63.82; H, 7.32; N, 4.96. Found: C, 63.21; H, 7.31; N, 5.17. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) $\delta = 0.97$ (d, $^3$J$_{HH} = 6.8$ Hz, 12H, CH(CH$_3$)$_2$), 1.11 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, CH(CH$_3$)$_2$), 1.25 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, CH(CH$_3$)$_2$), 1.81 (d, $^3$J$_{HH} = 6.7$ Hz, 18H, CH(CH$_3$)$_2$), 1.38 (d, $^3$J$_{HH} = 6.8$ Hz, 6H, CH(CH$_3$)$_2$), 1.45 (s, 6H, CCH$_3$), 1.57 (s, 6H, CCH$_3$), 2.99 (sept, $^3$J$_{HH} = 6.8$ Hz, 4H, CH(CH$_3$)$_2$), 3.33 (sept, $^3$J$_{HH} = 6.8$ Hz, 2H, CH(CH$_3$)$_2$), 3.69 (sept, $^3$J$_{HH} = 6.7$ Hz, 2H, CH(CH$_3$)$_2$), 4.71 (s, 1H, CH), 4.88 (s, 1H, CH), 7.04 (d, $^3$J$_{HH} = 6.7$ Hz, 4H, C$_6$H$_3$), 7.09-7.14 (m, 4H, C$_6$H$_3$), 7.19-7.23 (m, 4H, C$_6$H$_3$). $^{13}$C$_1^1$H NMR (150 MHz, C$_6$D$_6$, 298 K) $\delta = 23.2, 24.2, 24.3, 24.7, 24.9, 25.2, 26.1$ (CH(CH$_3$)$_2$), 28.3, 28.7, 29.5 (CH(CH$_3$)$_2$), 96.1, 98.1 (CH), 123.4, 124.9, 125.1, 127.3, 128.7, 137.0, 141.7, 142.6, 144.3, 145.9, 170.1, 172.7 (C$_6$H$_3$), 175.0 (d, $^1$J$_{CP} = 1.5$ Hz, PCO). 31P$_1^1$H (121 MHz, C$_6$D$_6$, 298 K) $\delta = -52.1$. ATR-IR: $\nu$ 2962, 2924, 2865, 1940, 1662, 1525, 1460, 1438, 1381, 1317, 1258, 1217, 1177, 1091, 1015, 935, 866, 795, 758, 665, 622, 528 cm$^{-1}$.

**Synthesis of LGa(Cl)-PH(OC(Ph)=CH$_2$)GaL (6):** A benzene solution (1 mL) of acetonaphthone (12.3 µL, 0.10 mmol) was added dropwise to a solution of LGa(Cl)-P(GaL) (2) (0.11 g, 0.10 mmol) in benzene (1 mL) at ambient temperature. The red solution immediately turned colourless. All volatiles were removed in vacuo, the resulting residue washed with $n$-hexane (0.3 mL) and dried in vacuo, to yield a colorless crystalline powder. Single crystals suitable for X-ray diffraction were grown by diffusing $n$-hexane to a benzene solution of 6 at ambient temperature. Yield: 97% (0.12 g). M.p.: 197 °C (dec.). Anal. calcd. (%) for C$_{66}$H$_{90}$ClGa$_2$NaOP (1158.51): C, 68.26; H, 7.81; N, 4.82. Found: C, 68.39; H, 7.93; N, 4.81. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) $\delta = -0.64$ (d, $^1$J$_{PH} = 181.0$ Hz, 1H, PH), 0.89 (d, $^3$J$_{HH} = 2.4$ Hz, 6H, CH(CH$_3$)$_2$), 0.91 (d, $^3$J$_{HH} = 2.4$ Hz, 6H, CH(CH$_3$)$_2$), 0.98 (d, $^3$J$_{HH} = 6.7$ Hz, 6H, CH(CH$_3$)$_2$), 1.05 (d, $^3$J$_{HH} = 6.7$ Hz, 6H, CH(CH$_3$)$_2$), 1.15 (td, $^3$J$_{HH} = 7.1$ Hz, 6H, CH(CH$_3$)$_2$), 1.29 (d, $^3$J$_{HH} = 6.7$ Hz, 6H, CH(CH$_3$)$_2$), 1.45 (s, 6H, CCH$_3$), 1.57 (s, 6H, CCH$_3$), 2.98 (sept, $^3$J$_{HH} = 6.8$ Hz, 4H, CH(CH$_3$)$_2$), 3.33 (sept, $^3$J$_{HH} = 6.8$ Hz, 2H, CH(CH$_3$)$_2$), 3.69 (sept, $^3$J$_{HH} = 6.7$ Hz, 2H, CH(CH$_3$)$_2$), 4.71 (s, 1H, CH), 4.88 (s, 1H, CH), 7.04 (d, $^3$J$_{HH} = 6.7$ Hz, 4H, C$_6$H$_3$), 7.09-7.14 (m, 4H, C$_6$H$_3$), 7.19-7.23 (m, 4H, C$_6$H$_3$). $^{13}$C$_1^1$H NMR (150 MHz, C$_6$D$_6$, 298 K) $\delta = 23.2, 24.2, 24.3, 24.7, 24.9, 25.2, 26.1$ (CH(CH$_3$)$_2$), 28.3, 28.7, 29.5 (CH(CH$_3$)$_2$), 96.1, 98.1 (CH), 123.4, 124.9, 125.1, 127.3, 128.7, 137.0, 141.7, 142.6, 144.3, 145.9, 170.1, 172.7 (C$_6$H$_3$), 175.0 (d, $^1$J$_{CP} = 1.5$ Hz, PCO). 31P$_1^1$H (121 MHz, C$_6$D$_6$, 298 K) $\delta = -52.1$. ATR-IR: $\nu$ 2962, 2924, 2865, 1940, 1662, 1525, 1460, 1438, 1381, 1317, 1258, 1217, 1177, 1091, 1015, 935, 866, 795, 758, 665, 622, 528 cm$^{-1}$. 
18H, CH(CH$_3$)$_2$), 1.21 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.42 (s, 6H, CCH$_3$), 1.47 (s, 6H, CCH$_3$), 3.06 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.11 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.47 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.53 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 4.28 (bs, 1H, C=CH$_2$), 4.86 (s, 1H, CH), 5.00 (bs, 1H, C=CH$_2$), 5.01 (s, 1H, CH), 6.94 (t, $^3$J$_{HH}$ = 6.7 Hz, 6H, C$_6$H$_5$), 6.99 (d, $^3$J$_{HH}$ = 6.7 Hz, 2H, C$_6$H$_5$), 7.09-7.13 (m, 4H, C$_6$H$_5$), 7.19 (t, $^3$J$_{HH}$ = 7.2 Hz, 1H, C$_6$H$_5$), 7.37 (t, $^3$J$_{HH}$ = 7.5 Hz, 2H, C$_6$H$_5$), 8.32 (d, $^3$J$_{HH}$ = 7.9 Hz, 2H, C$_6$H$_5$). $^{13}$C {$^1$H} NMR (150 MHz, C$_6$D$_6$, 298 K) $\delta$ = 24.2, 24.3, 24.7, 25.0, 25.1, 25.2 (CH(CH$_3$)$_2$), 27.0, 27.9, 28.0, 28.8, 29.0, 29.1, 29.4, 29.9 (CH(CH$_3$)$_2$), 86.1 (C=CH$_2$), 98.1, 98.9 (CH), 124.1, 124.3, 125.4, 127.2, 127.4, 141.3, 141.4, 141.7, 142.3, 142.6, 145.7, 145.8 (C$_6$H$_5$), 162.4 (C(O)Ph), 168.9, 169.5 (C$_6$H$_5$). $^{31}$P {$^1$H} (242 MHz, C$_6$D$_6$, 298 K) $\delta$ = -313.3. $^{31}$P (242 MHz, C$_6$D$_6$, 298 K) $\delta$ = -313.3 (d, $^1$J$_{P-H}$ = 181.0 Hz). ATR-IR: $\nu$ 2956, 2923, 2864, 1731, 1616, 1527, 1438, 1386, 1317, 1258, 1100, 1021, 991, 940, 884, 797, 758, 699, 623, 567, 531 cm$^{-1}$.

**Synthesis of LGa(Cl)-PH(OC(CH$_3$)=CH$_2$)GaL (7):** Compound 7 was prepared using similar protocols used for compound 6 using acetone (14.3 μL, 0.19 mmol), LGa(Cl)-(GaL) (2) (0.2 g, 0.19 mmol) and toluene (2 mL). Yield: 98% (0.2 g, colorless crystalline powder). M.p.: 194 °C (dec.). Anal. calcd. (%) for C$_6$H$_8$SiClGa$_2$N$_2$OP (1096.49): C, 66.65; H, 8.07; N, 5.10. Found: C, 66.75; H, 8.18; N, 4.93. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) $\delta$ = -0.75 (d, $^1$J$_{HH}$ = 178.9 Hz, 1H, PPh), 0.99 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.04 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.16 (d, $^3$J$_{HH}$ = 6.7 Hz, 6H, CH(CH$_3$)$_2$), 1.18 (d, $^3$J$_{HH}$ = 6.8 Hz, 12H, CH(CH$_3$)$_2$), 1.22 (td, $^3$J$_{HH}$ = 7.4 Hz, 15H, CH(CH$_3$)$_2$; COCH$_3$), 1.26 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.41 (s, 6H, CCH$_3$), 1.49 (s, 6H, CCH$_3$), 3.06 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.15 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.49 (sept, $^3$J$_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.54 (sept, $^3$J$_{HH}$ = 6.7 Hz, 2H, CH(CH$_3$)$_2$), 3.84 (s, 1H, C=CH$_2$), 4.18 (s, 1H, C=CH$_2$), 4.84 (s, 1H, CH), 4.92 (s, 1H, CH), 6.97 (t, $^3$J$_{HH}$ = 6.7 Hz, 4H, C$_6$H$_5$), 7.15-7.17 (m, 8H, C$_6$H$_5$). $^{13}$C {$^1$H} NMR (150 MHz, C$_6$D$_6$, 298 K) $\delta$ = 24.0, 24.1, 24.8, 24.9, 25.0, 25.1, 25.2 (CH(CH$_3$)$_2$), 26.9, 27.9, 29.2, 29.5 (CH(CH$_3$)$_2$), 84.6 (C=CH$_2$), 97.8, 98.4 (CH), 123.9, 124.1, 125.9, 125.7, 127.2, 127.4, 128.6, 129.3, 137.9, 141.3, 141.4, 141.7, 142.5, 142.7, 145.7, 145.8 (C$_6$H$_5$), 162.7 (C(O)CH$_3$), 168.8, 169.2 (C$_6$H$_5$). $^{31}$P {$^1$H} (242 MHz, C$_6$D$_6$, 298 K) $\delta$ = -316.2. $^{31}$P (242 MHz, C$_6$D$_6$, 298 K) $\delta$ = -316.3 (d, $^1$J$_{P-H}$ = 178.9 Hz). ATR-IR: $\nu$ 2995, 2925, 2865, 1897, 1631, 1527, 1438, 1386, 1315, 1281, 1257, 1178, 1100, 1018, 989, 938, 884, 795, 757, 734, 639, 589, 531 cm$^{-1}$. 
2. Spectroscopic Characterization

**Figure S1.** $^1$H NMR (300 MHz, $\text{C}_6\text{D}_6$, 298 K) spectrum of compound 1.

**Figure S2.** $^{13}\text{C}$ {$^1$H} NMR (75 MHz, $\text{C}_6\text{D}_6$, 298 K) spectrum of compound 1.
Figure S3. $^{31}$P$^1$H NMR (121 MHz, C$_6$D$_6$, 298 K) spectrum of compound 1.

Figure S4. ATR-IR spectrum of 1.
Figure S5. $^1\text{H}$ NMR (300 MHz, C$_6$D$_6$, 298 K) spectrum of compound 2.

Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, C$_6$D$_6$, 298 K) spectrum of compound 2.
Figure S7. $^{31}$P\textsubscript{\textsuperscript{1}H} NMR (121 MHz, C\textsubscript{6}D\textsubscript{6}, 298 K) spectrum of compound 2.

Figure S8. ATR-IR spectrum of 2.
Figure S9. $^1$H NMR (300 MHz, C$_6$D$_6$, 298 K) spectrum of compound 3. (*THF which was used as solvent in the synthesis)

Figure S10. $^{13}$C{$^1$H} NMR (150 MHz, C$_6$D$_6$, 298 K) spectrum of compound 3.
**Figure S11.** $^{31}\text{P}^{1\text{H}}$ NMR (161 MHz, C$_6$D$_6$, 298 K) spectrum of compound 3. (*Impurity)

**Figure S12.** ATR-IR spectrum of 3.
Figure S13. $^1$H NMR (300 MHz, toluene-$d_8$, 298 K) spectrum of compound 4.

Figure S14. $^{13}$C{$^1$H} NMR (125 MHz, toluene-$d_8$, 298 K) spectrum of compound 4.
**Figure S15.** $^{31}$P{$^1$H} NMR (121 MHz, toluene-$d_8$, 298 K) spectrum of compound 4.

**Figure S16.** $^{19}$F{$^1$H} NMR (282 MHz, toluene-$d_8$, 298 K) spectrum of compound 4.
Figure S17. ATR-IR spectrum of 4.

Figure S18. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.
Figure S19. $^{13}\text{C\{^1\text{H}\}}$ NMR (150 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.

Figure S20. $^{31}\text{P\{^1\text{H}\}}$ NMR (121 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.
Figure S21. ATR-IR spectrum of 5.

Figure S22. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.
**Figure S23.** $^{13}$C{$^{1}$H} NMR (150 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.

**Figure S24.** $^{31}$P{$^{1}$H} NMR (242 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.
**Figure S25.** $^{31}$P NMR (242 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.

**Figure S26.** ATR-IR spectrum of 6.
Figure S27. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 7. *toluene

Figure S28. $^{13}$C-$^1$H NMR (150 MHz, C$_6$D$_6$, 298 K) spectrum of compound 7.
Figure S29. $^{31}$P{$^{1}$H} NMR (242 MHz, C$_{6}$D$_{6}$, 298 K) spectrum of compound 7.

Figure S30. $^{31}$P NMR (242 MHz, C$_{6}$D$_{6}$, 298 K) spectrum of compound 7.
Figure S31. ATR-IR spectrum of 7.
Figure S32. Stacked $^1$H NMR (300 MHz, C$_6$D$_6$) spectra of the temperature dependent binding/release of CO$_2$ on gallaphosphene 2; 1) compound 5; 2) compound 5 after heating at 95 °C; 3) after cooling to ambient temperature; 4) after heating 2$^{nd}$ time to 95 °C; 5) compound 2 for comparison.
Figure S33. Stacked $^{31}\text{P}\{^1\text{H}\}$ NMR (300 MHz, C$_6$D$_6$) spectra tracking the temperature dependent binding/release of CO$_2$ on gallaphosphene 2: 1) compound 5; 2) compound 5 after heating at 95 °C; 3) after cooling to ambient temperature; 4) after heating 2$^{nd}$ time to 95 °C; 5) compound 2 for comparison. *protonated species
Figure S34. Stacked variable temperature (VT) $^1$H NMR (300 MHz, toluene-$d_8$) spectra of compound 2.
Figure S35. $^1$H NMR (400 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with two drops of THF. (#coordinated THF molecule protons)

Figure S36. $^{13}$C{^1}H NMR (121 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with two drops of THF.
Figure S37. $^1$H, $^{13}$C, $^{31}$P and $^{19}$F NMR spectra of the reaction of a solution of compound 4 in toluene-$d_8$ with two drops of THF.

Figure S38. $^{19}$F{$^1$H} NMR (282 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with two drops of THF.
Figure S39. $^1$H NMR (400 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with DMAP.

Figure S40. $^{13}$C-$^1$H) NMR (100 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with DMAP.
**Figure S41.** $^{31}$P$\{^1$H$\}$ NMR (121 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with DMAP.

**Figure S42.** $^{19}$F$\{^1$H$\}$ NMR (282 MHz, toluene-$d_8$, 298 K) spectrum of the reaction of a solution of compound 4 in toluene-$d_8$ with DMAP.
3. X-Ray Crystallographic Analysis

The crystals were mounted on nylon loops in inert oil. Data for 1 - 6 were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (mono-chromated Cu$_{K\alpha}$ radiation, $\lambda = 1.54178$ Å, micro-focus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-97)\cite{[6]} and refined anisotropically by full-matrix least-squares on $F^2$ (SHELXL-2014).\cite{[7]-[9]}

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. In 1, the Dipp group is disordered over two positions. All corresponding bond length and angle of the alternate positions were restrained to be equal (SADI). RIGU restraints were applied to the anisotropic displacement parameters of the Dipp residue’s atoms. The PCO moiety is disordered over two positions and the mirror plane. Bond length and angle of the components were restrained to be equal (SADI). RIGU and SIMU restraints were used to refine the anisotropic displacement parameters. For C16 and C16’ additional ISOR restraints were necessary. Due to the disorder and the high number of restraints applied quantitative results should be carefully accessed since they are biased and might be unreliable. In 2, the ClGaPGa moiety is disordered over two positions. In addition, two isopropyl groups are disordered over two positions each. The corresponding bond lengths were restrained to be equal (SADI) and the anisotropic displacement parameters of the disordered atoms were refined with RIGU restraints. C13’ and C14’ (occupancy approx. 6%) could only be refined isotropically. 3 was refined as a 2-component inversion twin. The corresponding centro-symmetric space group $P2_1/n$ yielded significantly higher $R$-values ($R_I = 0.961$, $wR_2 = 0.248$) thus the model was discarded. The bridging P and PCO moieties are also disordered over two positions, and bond lengths and angles of both orientations of the PCO were restrained to be equal (SADI). RIGU restraints were applied to the anisotropic displacement parameters of all disordered atoms. C59, C59’, P1 and P1’ were refined with common displacement parameters (EADP) due to their proximity. In 6, the PH hydrogen atom was refined freely and is disordered over two position. The P–H bond lengths of both orientations were restrained to be equal (SADI). Since the electron density maxima were very small the existence of this hydrogen atom was confirmed by $^1$H and $^{31}$P NMR spectroscopic studies (vide supra). The displacement parameters of the benzene molecule and the residual electron density in its vicinity suggest disorder. However, no second orientation of the molecule could be identified and refined. RIGU restraints were applied to the anisotropic displacement parameters of the benzene molecule atoms.

CCDC-2038994 (1), -2038996 (2), -2038997 (3), -2038998 (4), -2038999 (5), and -2040133 (6) contain the supplementary crystallographic data for this paper. These data can be obtained free of
Table S1. Crystal data and structure refinement of 1–3.

| Compound | 1                  | 2                  | 3                  |
|----------|--------------------|--------------------|--------------------|
| Emp. formula | C₃₀H₄₁ClGaN₃P     | C₅₉H₈₂ClGa₂N₄P     | C₅₉H₈₂Ga₂N₄OP₂     |
| Formula weight | 581.79          | 1041.13           | 1064.66            |
| Temperature [K] | 100(2)          | 100(2)            | 100(2)             |
| Crystal system | orthorhombic     | monoclinic         | monoclinic         |
| Space group | Pnma             | P2₁/n              | Pn                |
| a [Å]  | 14.3388(7)        | 20.1951(14)        | 14.0653(6)         |
| b [Å]  | 21.4252(10)       | 13.7533(9)         | 13.8476(6)         |
| c [Å]  | 9.9470(5)         | 20.9985(14)        | 15.1248(6)         |
| α [°]  | 90                | 90                | 90                 |
| β [°]  | 90                | 105.0285(15)       | 106.0732(16)       |
| γ [°]  | 90                | 90                | 90                 |
| V [Å³] | 3055.8(3)         | 5632.8(7)          | 2830.7(2)          |
| Z      | 4                 | 4                 | 2                  |
| ρ [Mgm⁻³] | 1.265            | 1.228             | 1.249              |
| μ [mm⁻¹] | 2.707            | 2.163             | 2.013              |
| F (000) | 1224             | 2208              | 1128               |
| Crystal size [mm] | 0.194 × 0.143 × 0.079 | 0.409 × 0.329 × 0.229 | 0.116 × 0.067 × 0.046 |
| θ max [°] | 80.934          | 79.628            | 80.726             |
| Index ranges | -14 ≤ h ≤ 18     | -25 ≤ h ≤ 25      | -17 ≤ h ≤ 18      |
|          | -27 ≤ k ≤ 27     | -16 ≤ k ≤ 17      | -16 ≤ k ≤ 17      |
|          | -12 ≤ l ≤ 12     | -26 ≤ l ≤ 26      | -19 ≤ l ≤ 19      |
| No. of reflect. collected | 62988           | 285456            | 118666             |
| Unique reflect. | 3454            | 12213             | 12296              |
| Rint | 0.0423           | 0.0368            | 0.0486             |
| Data / restraints / params. | 3454 / 440 / 339 | 12213 / 28 / 684 | 12296 / 22 / 653 |
| Goodness-of-fit on F² | 1.059           | 1.106             | 1.049              |
| R1 [I>2σ(I)] | 0.0274          | 0.0317            | 0.0355             |
| wR2 [I>2σ(I)] | 0.0781          | 0.0774            | 0.0862             |
| R1 [all data] | 0.0301          | 0.0317            | 0.0389             |
| wR2 [all data] | 0.0805          | 0.0774            | 0.0885             |
| Flack parameter | -              | -                 | 0.46(3)            |
| Largest diff. peak and hole max./min. [e·Å⁻³] | 0.615/-0.323 | 0.377/-0.298 | 0.469/-0.655 |
Table S2. Crystal data and structure refinement of 4–6.

| Compound | 4 | 5 | 6 |
|----------|---|---|---|
| Emp. formula | C₈₈H₈₈BF₂₀Ga₄N₄P | C₆₂H₉₀ClGa₂N₄O₄P | C₇₂H₉₀ClGa₂N₄OP |
| Formula weight | 1762.84 | 1221.28 | 1239.38 |
| Temperature [K] | 100(2) | 100(2) | 100(2) |
| Crystal system | triclinic | orthorhombic | orthorhombic |
| Space group | P-1 | Pbca | Pbca |
| a [Å] | 12.4094(5) | 13.3069(6) | 22.0196(9) |
| b [Å] | 16.3929(6) | 21.1072(9) | 21.2959(9) |
| c [Å] | 20.9728(8) | 46.161(2) | 28.6737(13) |
| α [°] | 90.7416(10) | 90 | 90 |
| β [°] | 105.8792(10) | 90 | 90 |
| γ [°] | 94.3128(11) | 90 | 90 |
| V [Å³] | 4089.5(3) | 12965.2(10) | 13445.9(10) |
| Z | 2 | 8 | 8 |
| ρ [Mgm⁻³] | 1.432 | 1.251 | 1.224 |
| μ [mm⁻¹] | 1.806 | 2.005 | 1.906 |
| F (000) | 1812 | 5168 | 5264 |
| Crystal size [mm] | 0.281 × 0.223 × 0.095 | 0.158 × 0.050 × 0.033 | 0.300 × 0.200 × 0.111 |
| θ max [°] | 81.034 | 79.870 | 81.017 |
| Index ranges | -15 ≤ h ≤ 15 | -14 ≤ h ≤ 16 | -27 ≤ h ≤ 28 |
| | -20 ≤ k ≤ 20 | -26 ≤ k ≤ 26 | -27 ≤ k ≤ 26 |
| | -26 ≤ l ≤ 26 | -58 ≤ l ≤ 58 | -36 ≤ l ≤ 36 |
| No. of reflect. collected | 365331 | 439052 | 655773 |
| Unique reflect. | 17813 | 13753 | 14792 |
| R(int) | 0.0273 | 0.1563 | 0.0359 |
| Data / restraints / params. | 17813 / 0 / 1065 | 13753 / 0 / 733 | 14792 / 37 / 759 |
| Goodness-of-fit on F² | 1.027 | 1.126 | 1.056 |
| R1 [I>2σ(I)] | 0.0266 | 0.0653 | 0.0321 |
| wR2 [I>2σ(I)] | 0.0680 | 0.1738 | 0.0902 |
| R1 [all data] | 0.0269 | 0.0829 | 0.0329 |
| wR2 [all data] | 0.0692 | 0.1853 | 0.0908 |
| Largest diff. peak and hole max./min. [e·Å⁻³] | 0.486/-0.627 | 1.813/-0.802 | 0.855/-0.506 |
Figure S43. Molecular structure of 1 with thermal ellipsoids at 50% probability level. The hydrogen atoms and alternate positions of the disordered parts are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)-N(1)#1 1.9294(10), Ga(1)-N(1) 1.9294(10), Ga(1)-Cl(1) 2.2147(6), Ga(1)-P(1) 2.340(10), P(1)-C(16) 1.642(13), O(1)-C(16) 1.165(12); N(1)#1-Ga(1)-N(1) 97.67(6), N(1)-Ga(1)-Cl(1) 102.52(4), N(1)-Ga(1)-P(1) 122.0(3), Cl(1)-Ga(1)-P(1) 116.6(4). Coordinates used to generate equivalent atoms: 1 x,-y+1/2,z.

Figure S44. Molecular structure of 2 with thermal ellipsoids at 50% probability level. The hydrogen atoms and alternate positions of the disordered parts are omitted for clarity. Selected bond length (Å) and angels (°): Cl(1)-Ga(1) 2.2360(5), P(1)-Ga(2) 2.1613(6), P(1)-Ga(1) 2.2688(5), Ga(1)-N(1) 1.9900(13), Ga(1)-N(2) 1.9937(13), Ga(2)-N(4) 1.9159(14), Ga(2)-N(3) 1.9555(13); Ga(2)-P(1)-Ga(1) 113.87(2), N(1)-Ga(1)-N(2) 94.68(5), N(1)-Ga(1)-Cl(1) 105.04(4), N(2)-Ga(1)-Cl(1) 99.77(4), N(1)-Ga(1)-P(1) 105.74(4), N(2)-Ga(1)-P(1) 118.57(4), Cl(1)-Ga(1)-P(1) 127.65(2), N(4)-Ga(2)-N(3) 95.39(6), N(4)-Ga(2)-P(1) 149.10(5), N(3)-Ga(2)-P(1) 112.81(5).
**Figure S45.** Molecular structure of 3 with thermal ellipsoids at 50% probability level. The hydrogen atoms and alternate positions of the disordered parts are omitted for clarity. Selected bond length (Å) and angles (°): Ga(1)-O(1) 1.977(4), Ga(1)-P(1) 2.2943(16), Ga(1)-N(1) 1.981(4), Ga(1)-N(2) 1.983(4), O(1)-C(59) 1.223(7), C(59)-P(2) 1.592(6), Ga(2)-P(2) 2.4798(16), Ga(2)-P(1) 2.297(2), Ga(2)-N(3) 1.988(4), Ga(2)-N(4) 1.977(4); Ga(1)-P(1)-Ga(2) 99.86(7), O(1)-C(59)-P(2) 176.9(7), O(1)-Ga(1)-P(1) 110.48(13), P(1)-Ga(1)-N(1) 126.68(12), P(1)-Ga(1)-N(2) 112.46(12), N(2)-Ga(1)-N(1) 93.62(16), O(1)-Ga(1)-N(1) 99.39(17), O(1)-Ga(1)-N(2) 99.84(18), N(4)-Ga(2)-N(3) 93.90(16), N(4)-Ga(2)-P(1) 120.92(13), N(3)-Ga(2)-P(1) 119.04(12), P(1)-Ga(2)-P(2) 127.22(6).

**Figure S46.** Molecular structure of 4 with thermal ellipsoids at 50% probability level. The hydrogen atoms, a solvent molecule (benzene) and anion (B(C₆F₅)₄) are omitted for clarity. Selected bond length (Å) and angels (°): Ga1-N2 1.9117(10), Ga1-N1 1.9183(10), Ga1-P1 2.2026(4), Ga2-N3 1.9018(10), Ga2-N4 1.9304(10), Ga2-P1 2.1860(4); N2-Ga1-N1 98.19(4), N2-Ga1-P1 117.319(17).
**Figure S47.** Molecular structure of 5 with thermal ellipsoids at 50% probability level. The hydrogen atoms and a solvent molecule (toluene) are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)-N(1) 1.946(3), Ga(1)-N(2) 1.949(3), Ga(1)-Cl(1) 2.1902(11), Ga(1)-P(1) 2.3319(12), Ga(2)-O(4) 1.826(3), Ga(2)-O(2) 1.832(3), Ga(2)-N(3) 1.887(3), Ga(2)-N(4) 1.900(3), P(1)-C(59) 1.865(4), P(1)-C(60) 1.871(4), O(1)-C(59) 1.217(6), O(2)-C(59) 1.298(5); N(1)-Ga(1)-N(2) 96.62(13), N(1)-Ga(1)-Cl(1) 105.42(10), N(2)-Ga(1)-Cl(1) 104.41(10), N(1)-Ga(1)-P(1) 116.83(11), N(2)-Ga(1)-P(1) 114.25(10), Cl(1)-Ga(1)-P(1) 116.79(4), O(4)-Ga(2)-O(2) 104.43(13), O(4)-Ga(2)-N(3) 112.57(14), O(2)-Ga(2)-N(3) 110.02(14), O(4)-Ga(2)-N(4) 114.94(14), O(2)-Ga(2)-N(4) 113.50(14), N(3)-Ga(2)-N(4) 101.59(15), C(59)-P(1)-C(60) 103.36(19), C(59)-P(1)-Ga(1) 101.51(15), C(60)-P(1)-Ga(1) 102.09(14).
**Figure S48.** Molecular structure of 6 with thermal ellipsoids at 50% probability level. The hydrogen atoms, a solvent molecule (benzene) and the alternate position of the disordered P bond hydrogen are omitted for clarity. Selected bond length (Å) and angles (°): Ga(1)-P(1) 2.3068(4), Ga(2)-P(1) 2.3220(4), Ga(1)-N(1) 1.9598(12), Ga(1)-N(2) 1.9658(13), Ga(1)-Cl(1) 2.2156(4), Ga(2)-O(1) 1.8523(10), Ga(2)-N(4) 1.9606(12), Ga(2)-N(3) 1.9705(12); Ga(1)-P(1)-Ga(2) 116.793(17), N(1)-Ga(1)-N(2) 95.19(5), N(1)-Ga(1)-Cl(1) 102.45(4), N(2)-Ga(1)-Cl(1) 103.72(4), N(1)-Ga(1)-P(1) 117.03(4), N(2)-Ga(1)-P(1) 111.01(4), Cl(1)-Ga(1)-P(1) 123.208(17), O(1)-Ga(2)-N(4) 109.88(5), O(1)-Ga(2)-N(3) 110.61(5), N(4)-Ga(2)-N(3) 94.64(5), O(1)-Ga(2)-P(1) 115.78(3), N(4)-Ga(2)-P(1) 115.03(4), N(3)-Ga(2)-P(1) 108.86(4).
4. Computational Details

All calculations were performed by using the program package Gaussian 16.[10] The geometrical parameters of all stationary points were optimized by means of the density functional B3LYP[11-13] with the dispersion correction D3BJ.[14] 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 stationary states have none imaginary frequency. As basis set def2-TZVP was employed. In order to analyze the electronic structures of the compounds, NBO analyses[15] were performed and the Mayer bond orders[16] were calculated at the B3LYP/def2-TZVP level of theory.

As compound 2 exhibits a remarkably small HOMO-LUMO gap (2.94 eV), we performed CASSCF(2/2)/def2-TZVP and CASSCF(4/4)/def2-TZVP calculations on the B3LYP-D3BJ/def2-TZVP-optimized structure of 2 to check for an open-shell singlet diradical character of 2. The occupation numbers of the orbitals in the active space amount to 2.00 and 0.00 for the CASSCF(2/2) calculation (Figure S51). In the case of the CASSCF(4/4) approximation the occupation numbers of the orbitals in the active space are computed to be 2.00, 1.96, 0.00 and 0.04 (Figure S52). Thus, the analysis of the CASSCF wave functions shows that compound 2 has almost no open-shell singlet diradical character.

![Figure S49. Structures of the isomers of 1 (a) and 3 (b) as well as the chloride exchange reaction of 2 (c). The relative energies, ΔE, are calculated at the B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory.](image)

To figure out why the phosphaethynolate ion binds via the phosphorus atom in compound 1, whereas in compound 3, binding via the oxygen is observed, the compounds 1, 3, S1, S2 and S3 were calculated at the B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory.
A comparison of the relative energies shows following (Figure S49): If the phosphaethynolate ion acts as a monodentate ligand (1, S1, S2 and S3), binding via the phosphorus atom is energetically preferred (1 and S3). However, if the phosphaethynolate ion binds via two sites (as found in compound 3), a binding via the oxygen atom combined with a donating phosphorus atom is the energetically preferred way. This is properly due to the higher donor character of phosphorus compared to oxygen.

Table S3. NBO charges [e] of 2 and the cationic part of 4 calculated by means of B3LYP-D3BJ/def2-TZVP.

| Compound                  | Ga(1) | P(1)  | Ga(2) |
|---------------------------|-------|-------|-------|
| 2                         | +1.404| -1.122| +1.353|
| Cationic part of 4        | +1.479| -1.090| +1.468|

Figure S50. Selected molecular orbitals of 2 calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.04). Hydrogen atoms are omitted for clarity.
**Figure S51.** Orbitals in the active space of 2 calculated at CASSCF(2/2)/def2-TZVP//B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.04). Hydrogen atoms are omitted for clarity.

**Figure S52.** Orbitals in the active space of 2 calculated at CASSCF(4/4)/def2-TZVP//B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.04). Hydrogen atoms are omitted for clarity.
Figure S53. Selected molecular orbitals of 4 calculated at B3LYP-D3BJ/def2-TZVP level of theory (isovalue 0.04). Hydrogen atoms are omitted for clarity.
5. Cartesian Coordinates and Absolute Energies for All Calculated Compounds

Absolute energy of 1 at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -4079.978522 au.

Absolute energy of 1 at B3LYP-D3BJ/6-31G* level of theory: -4077.487184 au. Cartesian coordinates of the optimized geometry for 1 at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Cl   | 0.22435100 | -2.87039900 | 0.24826700 |
| P    | -0.28971000 | 0.23198700 | 2.46402400 |
| Ga   | -0.03543100 | -0.67498700 | 0.34266200 |
| N    | -1.55127700 | -0.23053200 | -0.77087400 |
| N    | 1.33422500  | 0.03454400  | -0.83780100 |
| C    | -1.40127600 | -0.21557500 | -2.10197900 |
| C    | -0.15480900 | -0.14814600 | -2.73530600 |
| H    | -0.17161600 | -0.16445700 | -3.81744300 |
| C    | 1.10858700  | 0.07406000  | -2.15052600 |
| C    | -2.63958300 | -0.22602800 | -2.96405100 |
| H    | -3.23969000 | -1.11503700 | -2.74197600 |
| H    | -2.38021300 | -0.22784100 | -4.02406800 |
| H    | -3.27378200 | 0.63976800  | -2.75707400 |
| C    | 2.24781300  | 0.38992900  | -3.08957800 |
| H    | 1.87224100  | 0.81130000  | -4.02418100 |
| H    | 2.79462100  | -0.52907400 | -3.32700600 |
| H    | 2.95953500  | 1.08401100  | -2.63981100 |
| C    | -2.81731100 | 0.08913700  | -0.17047600 |
| C    | -3.66107900 | -0.93808500 | 0.29369700  |
| C    | -4.86453400 | -0.57979800 | 0.91084900  |
| H    | -5.52482400 | -1.36134500 | 1.27473800  |
| C    | -5.22697300 | 0.75365000  | 1.06481700  |
| H    | -6.16804300 | 1.01215100  | 1.54205100  |
| C    | -4.37583200 | 1.75644700  | 0.61097400  |
| H    | -4.65726700 | 2.79727300  | 0.74129800  |
| C    | -3.15536000 | 1.44908400  | 0.00150400  |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -2.242963 | 2.581200  | -0.45209  |
| H       | -1.315408 | 2.147430  | -0.83693  |
| C       | -2.871471 | 3.406861  | -1.58795  |
| H       | -3.106033 | 2.787141  | -2.45928  |
| H       | -2.181683 | 4.194765  | -1.91178  |
| H       | -3.800417 | 3.887603  | -1.26092  |
| C       | -1.871836 | 3.489886  | 0.72999   |
| H       | -2.757395 | 3.970222  | 1.16008   |
| H       | -1.193957 | 4.283560  | 0.39874   |
| H       | -1.377251 | 2.921087  | 1.52250   |
| C       | 2.614330  | 0.381868  | -0.27379  |
| C       | 3.656488  | -0.565728 | -0.22625  |
| C       | 4.866212  | -0.186010 | 0.36727   |
| H       | 5.679545  | -0.903784 | 0.41049   |
| C       | 5.036498  | 1.077207  | 0.91619   |
| H       | 5.982313  | 1.350773  | 1.37516   |
| C       | 3.985517  | 1.988942  | 0.88875   |
| H       | 4.122840  | 2.967002  | 1.33498   |
| C       | 2.756519  | 1.661461  | 0.31012   |
| C       | 3.517669  | -1.986114 | -0.75173  |
| H       | 2.521019  | -2.104711 | -1.18230  |
| C       | 4.553696  | -2.300737 | -1.84573  |
| H       | 4.378755  | -3.302265 | -2.25448  |
| H       | 5.573718  | -2.280700 | -1.44548  |
| H       | 4.513407  | -1.582878 | -2.67165  |
| C       | 3.643441  | -2.999467 | 0.40064   |
| H       | 2.945397  | -2.771086 | 1.20831   |
| H       | 4.658770  | -2.997110 | 0.81438   |
| H       | 3.424631  | -4.010302 | 0.04017   |
| C       | 1.625194  | 2.681352  | 0.27778   |
| H       | 0.684895  | 2.127501  | 0.34414   |
| C       | 1.605365  | 3.457478  | -1.05056  |
| H       | 1.438556  | 2.792496  | -1.90263  |
Absolute energy of S1 at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -4079.949666 au.

Absolute energy of S1 at B3LYP-D3BJ/6-31G* level of theory: -4077.459277 au. Cartesian coordinates of the optimized geometry for S1 at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Cl      | 0.02243000 | -2.66238600 | 1.01348600 |
| Ga      | -0.08481800 | -0.61222100 | 0.32663200 |
| N       | -1.61899500 | -0.22005900 | -0.74836800 |
| N       | 1.28785000  | -0.15279200 | -0.92898800 |
| C       | -1.51029000 | -0.21255600 | -2.08324100 |
| C       | -0.28624400 | -0.28148200 | -2.76410500 |
| H       | -0.35169900 | -0.31569700 | -3.84327600 |
| C       | 1.01195200  | -0.16050900 | -2.23801900 |
| C       | -2.76403000 | -0.06398800 | -2.90753000 |
|   |   |   |   |   |
|---|---|---|---|---|
| H | 4.40826500 | 2.87388000 | 0.55266700 |
| C | 2.87524900 | 1.52056700 | -0.10895600 |
| C | 3.30650900 | -2.29375200 | -0.60001700 |
| H | 2.27054600 | -2.39509600 | -0.93466300 |
| C | 4.21182900 | -2.91214600 | -1.67917400 |
| H | 3.93649400 | -3.95920300 | -1.84777800 |
| H | 5.26455400 | -2.89162700 | -1.37604700 |
| H | 4.13611700 | -2.38449800 | -2.63630400 |
| C | 3.44679500 | -3.07129200 | 0.72188100 |
| H | 2.84599400 | -2.61673300 | 1.51267700 |
| H | 4.49150100 | -3.08803900 | 1.05354500 |
| H | 3.11404900 | -4.10690300 | 0.59171700 |
| C | 1.77449200 | 2.57683900 | -0.11520800 |
| H | 0.84300300 | 2.07196900 | 0.14996200 |
| C | 1.57039300 | 3.20640100 | -1.50444400 |
| H | 1.23432600 | 2.47173000 | -2.24137400 |
| H | 2.49931700 | 3.66027500 | -1.86941500 |
| H | 0.80810200 | 3.99304500 | -1.45403000 |
| C | 2.00210200 | 3.66491500 | 0.94283500 |
| H | 1.11796800 | 4.30495100 | 1.01304800 |
| H | 2.84896000 | 4.31262400 | 0.68860800 |
| H | 2.18282800 | 3.22160700 | 1.92626800 |
| C | -3.43877400 | -2.37694600 | 0.09280700 |
| H | -2.44642700 | -2.46056700 | -0.35462100 |
| C | -3.39920200 | -3.11088700 | 1.44388100 |
| H | -3.07009300 | -4.14576500 | 1.30143600 |
| H | -2.70328600 | -2.63010200 | 2.13568200 |
| H | -4.39023000 | -3.13242800 | 1.91206900 |
| C | -4.44029900 | -3.05601400 | -0.85751500 |
| H | -4.17164500 | -4.10850900 | -1.00146200 |
| H | -5.45818200 | -3.02287400 | -0.45262700 |
| H | -4.46018400 | -2.57625100 | -1.84227500 |
| C | 0.89200400 | 0.46255300 | 2.61912300 |
Absolute energy of $3$ at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -7126.003294 au.

Absolute energy of $3$ at B3LYP-D3BJ/6-31G* level of theory: -7121.168822 au. Cartesian coordinates of the optimized geometry for $3$ at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | -0.08664100 | 0.55670800 | 1.80364600 |
| P    | 2.10841000  | 0.35541500  | 3.60183500  |
| Ga   | 1.62117200  | 0.15833100  | 0.56872300  |
| Ga   | -1.61889800 | -0.15852100 | -0.41429100 |
| P    | -0.39981400 | -0.10389000 | 1.43562000  |
| P    | -0.70698800 | -0.09404500 | -2.97412300 |
| O    | 1.65825800  | 0.19426600  | -1.45879400 |
| C    | 0.63930700  | 0.06874900  | -2.12878300 |
| N    | 3.08600100  | -1.13299900 | 0.92733700  |
| N    | 2.76213500  | 1.73276300  | 0.96986800  |
| N    | -2.75712900 | -1.74778500 | -0.78966400 |
| N    | -3.06985500 | 1.12607900  | -0.86066100 |
| C    | 4.12725400  | -0.83771700 | 1.71352100  |
| C    | 4.42661200  | 0.45156300  | 2.16632800  |
| H    | 5.27649000  | 0.53746900  | 2.82941200  |
| C    | 3.84100300  | 1.65388900  | 1.75745900  |
| C    | 5.08414300  | -1.93308600 | 2.12823700  |
| H    | 5.92148200  | -1.51722100 | 2.69106400  |
| H    | 5.47337600  | -2.47110600 | 1.26065800  |
| H    | 4.57782700  | -2.67407800 | 2.75148900  |
| C    | 4.52140800  | 2.92318000  | 2.21915100  |
| H    | 5.41043900  | 2.68942700  | 2.80721300  |
| H    | 3.84485700  | 3.52504800  | 2.83041600  |
| H    | 4.81290100  | 3.54901800  | 1.37225600  |
| C    | 3.03255900  | -2.46885700 | 0.39317100  |
| C    | 2.45066400  | -3.51171000 | 1.14067500  |
| C    | 2.53975600  | -4.81358400 | 0.63333800  |
|    |  X            |  Y            |  Z            |
|----|---------------|---------------|---------------|
| H  | 2.09538500   | -5.63018400  | 1.19427900    |
| C  | 3.19445200   | -5.07988200  | -0.56468600   |
| H  | 3.26740300   | -6.10033000  | -0.93116800   |
| C  | 3.73855900   | -4.03253800  | -1.30282000   |
| H  | 4.23464100   | -4.24105400  | -2.24629300   |
| C  | 3.65931900   | -2.71304300  | -0.84799500   |
| C  | 1.74063400   | -3.27463500  | 2.46596600    |
| H  | 1.85343600   | -2.22111300  | 2.73712800    |
| C  | 2.32610900   | -4.12389400  | 3.60882300    |
| H  | 3.40193300   | -3.96846700  | 3.74360100    |
| H  | 2.16856600   | -5.19383600  | 3.43125500    |
| H  | 1.82909000   | -3.87095800  | 4.55208200    |
| C  | 0.24105600   | -4.56240900  | 2.32199500    |
| H  | -0.27594500  | -3.34880400  | 3.26502400    |
| H  | 0.06621000   | -4.61230000  | 2.07016800    |
| H  | -0.20844400  | -2.93647000  | 1.55333600    |
| C  | 4.28599900   | -1.59181200  | -1.66749900   |
| H  | 3.99972900   | -0.64457500  | -1.20972300   |
| C  | 5.82269600   | -1.66256800  | -1.65019300   |
| H  | 6.24795500   | -0.84352600  | -2.24247200   |
| H  | 6.18164800   | -2.60737100  | -2.07499200   |
| H  | 6.21832400   | -1.57913900  | -0.63296600   |
| C  | 3.75889000   | -1.57791200  | -3.10963600   |
| H  | 4.15107100   | -0.70605900  | -3.64496500   |
| H  | 2.66899300   | -1.52431100  | -3.12671000   |
| H  | 4.06696200   | -2.47235100  | -3.66316000   |
| C  | 2.41961800   | 3.03695200   | 0.46633100    |
| C  | 1.59106700   | 3.89502500   | 1.21604600    |
| C  | 1.38598000   | 5.19489300   | 0.73744100    |
| H  | 0.74799900   | 5.86964800   | 1.30015900    |
| C  | 1.99404300   | 5.63964900   | -0.43175100   |
| H  | 1.83610800   | 6.65853700   | -0.77515200   |
| C  | 2.79153400   | 4.76980600   | -1.17049000   |

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H     3.25266600  5.11487200  -2.09148600
C     3.00974900  3.45593700  -0.74621800
C     0.93108400  3.46741600   2.51943400
H     1.26793400  2.45608000   2.76385800
C     1.30396200  4.38888200   3.69522800
H     2.38589600  4.46002600   3.85019000
H     0.85620500  4.00998700   4.62080500
H     0.92671200  5.40606400   3.53942900
C    -0.59336700  3.42601600   2.35712200
H    -1.06292400  3.06919200   3.28061200
H    -0.88203800  2.74369300   1.55758600
H    -0.99124500  4.42042300   2.13645900
C     3.90499700  2.53708500  -1.56914700
H     3.87242400  1.54410600  -1.11816700
C     5.37206600  3.00026300  -1.54954200
H     5.47816800  4.00345700  -1.97858600
H     5.99437200  2.31541200  -2.13773600
H     5.77418800  3.02612700  -0.53181800
C     3.40095700  2.39997300  -3.01335400
H     3.44873900  3.35394700  -3.55089700
H     2.36925700  2.04669700  -3.03261500
H     4.01886400  1.67935000  -3.56098400
C    -3.74632500  -1.68790800  -1.68515800
C    -4.24214200  -0.48861300  -2.21995200
H    -5.02153400  -0.59140800  -2.96287900
C    -4.02333500   0.81048800  -1.74088000
C    -4.44805800  -2.95667500  -2.11573200
H    -4.80602300  -3.51156700  -1.24374100
H    -3.76968300  -3.62192700  -2.65606500
H    -5.29794700  -2.72529400  -2.76000900
C    -4.98272800   1.88012600  -2.21034400
H    -5.53858000   2.29234900  -1.36202800
H    -5.69434600   1.47159200  -2.92981200
| Element | X-Center | Y-Center | Z-Center |
|---------|----------|----------|----------|
| H       | -4.45158700 | 2.71657400 | -2.67211200 |
| C       | -2.46570400 | -3.03230200 | -0.20285500 |
| C       | -2.98480100 | -3.33269000 | 1.07513300  |
| C       | -2.83800300 | -4.63820300 | -0.20285500 |
| C       | -2.83800300 | -4.63820300 | 1.07513300  |
| H       | -3.24285500 | -4.90012900 | 2.52433000  |
| C       | -2.16159000 | -5.60705500 | 0.81785600  |
| H       | -2.06002500 | -6.61519300 | 1.21060900  |
| C       | -1.58551400 | -5.26966900 | -0.40022800 |
| H       | -1.01919700 | -6.01321500 | -0.95192800 |
| C       | -1.72702300 | -3.98370500 | -0.93213300 |
| C       | -3.68820000 | -2.27026300 | 1.91083200  |
| H       | -3.11952600 | -1.34207000 | 1.78964300  |
| C       | -5.12610200 | -2.01948400 | 1.42323100  |
| H       | -5.63600800 | -1.31324500 | 2.08736900  |
| H       | -5.70252000 | -2.95246900 | 1.42058100  |
| H       | -5.14213000 | -1.59731400 | 0.41636900  |
| C       | -3.68209000 | -2.58690300 | 3.41141500  |
| H       | -2.66967500 | -2.80120400 | 3.76741600  |
| H       | -4.32409800 | -3.44177800 | 3.65434800  |
| H       | -4.06265500 | -1.72782500 | 3.97222300  |
| C       | -1.04429800 | -3.62590900 | -2.23986900 |
| H       | -1.50392600 | -2.71474900 | -2.62898700 |
| C       | -1.17224200 | -4.70618700 | -3.32363300 |
| H       | -0.75749700 | -4.33458800 | -4.26720500 |
| H       | -2.21589600 | -4.99109000 | -3.50013200 |
| H       | -0.61949000 | -5.61520200 | -3.06127900 |
| C       | 0.43113400  | -3.31364600 | -1.96223100 |
| H       | 0.53539400  | -2.54246200 | -1.19569500 |
| H       | 0.92971900  | -2.96607500 | -2.87205700 |
| H       | 0.94990000  | -4.20467500 | -1.60315900 |
| C       | -3.08979400 | 2.44996600  | -0.29198900 |
| C       | -3.77216700 | 2.65169600  | 0.92283800  |
| C       | -3.84715300 | 3.94973800  | 1.43790600  |
Absolute energy of $S_2$ at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -7125.989013 au.

Absolute energy of $S_2$ at B3LYP-D3BJ/6-31G* level of theory: -7121.138823 au. Cartesian coordinates of the optimized geometry for $S_2$ at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

Ga                   -1.55188900    0.81492200   -0.68015800
Ga  1.42385100  -0.68931000  0.28860000
P  0.19250100  -0.20196800  -1.50986100
C  1.14783500  -0.12961400  3.09675300
N  -3.43220100  0.30961000  -1.00716900
N  -1.94012900  2.74008700  -0.74361400
N   1.65704300  -2.57854300  0.78516200
N   3.33960600  -0.28636100  0.44220200
C  -4.32657500  1.12460600  -1.58225200
C  -4.11479500  2.49105300  -1.77646000
H  -4.91710700  3.03554600  -2.25632900
C  -3.04937200  3.25742800  -1.29222900
C  -5.68255200  0.58540500  -1.97457800
H  -6.14113400  1.23225000  -2.72587600
H  -6.34767000  0.55412400  -1.10492700
H  -5.61658100  -0.43143000  -2.36279300
C  -3.21131600  4.75857000  -1.36377400
H  -4.10189400  5.02000000  -1.93784900
H  -2.34012000  5.24130500  -1.81051800
H  -3.31243600  5.17366500  -0.35527700
C  -3.88605100  -0.98455600  -0.56823600
C  -3.58295500  -2.12742300  -1.32845200
C  -3.99485300  -3.37135700  -0.83656000
H  -3.74976600  -4.26831600  -1.39539900
C  -4.71652300  -3.47285100  0.34741600
H  -5.02872100  -4.44744700  0.71231300
C  -5.05051400  -2.32316600  1.05957400
H  -5.62524200  -2.41007700  1.97645400
C  -4.64337700  -1.06027500  0.62080600
C  -2.90453400  -2.03461900  -2.68532500
H  -2.55390000  -1.00888000  -2.82307400
C  -3.89550600  -2.35068300  -3.82091800
H  -4.75132600  -1.66733300  -3.82830900
H  -4.28487800  -3.37113600  -3.72759400
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | 2.39689600| 3.79625100| -2.54107200|
| C     | -2.10647500| 3.52900900| 2.05005700 |
| H     | -2.80857800| 2.91930200| 1.47260000 |
| C     | -2.94182800| 4.56911000| 2.81185500 |
| H     | -2.32577600| 5.16830400| 3.49109300 |
| H     | -3.70200400| 4.06610300| 3.42018200 |
| H     | -3.45293400| 5.25686700| 2.12828300 |
| C     | -1.36386900| 2.59832000| 3.02664800 |
| H     | -0.61371100| 3.15687300| 3.59622700 |
| H     | -0.84131600| 1.78986000| 2.50725800 |
| H     | -2.06280200| 2.15145400| 3.74088500 |
| C     | 2.66137800  | -2.97765000| 1.57618400 |
| C     | 3.80021500  | -2.20675600| 1.83095300 |
| H     | 4.53154800  | -2.64022300| 2.49899600 |
| C     | 4.16154800  | -1.00417500| 1.21578000 |
| C     | 2.63174100  | -4.36736500| 2.16718800 |
| H     | 2.52532300  | -5.12217800| 1.38281900 |
| H     | 1.77712100  | -4.48264500| 2.83990000 |
| H     | 3.54634200  | -4.56555500| 2.72826500 |
| C     | 5.58354000  | -0.53458900| 1.41012500 |
| H     | 6.07919900  | -0.39455100| 0.44474500 |
| H     | 6.15071000  | -1.25833500| 1.99744100 |
| H     | 5.61169000  | 0.43103500 | 1.92213300 |
| C     | 0.69758200  | -3.56693600| 0.37200100 |
| C     | 0.90183100  | -4.24267300| -0.85166700|
| C     | 0.04305400  | -5.30338800| -1.15684300|
| H     | 0.18171600  | -5.85542600| -2.07942400|
| C     | -1.01682200 | -5.64082000| -0.31786500|
| H     | -1.67613600 | -6.46332800| -0.58284700|
| C     | -1.24450800 | -4.91069700| 0.84308200 |
| H     | -2.09030100 | -5.15542800| 1.47742200 |
| C     | -0.38442700 | -3.87270400| 1.21592700 |
| C     | 1.98853500  | -3.79723300| -1.82954400|
H  1.93962100  -2.70162500  -1.86403300
C  3.40955200  -4.19610300  -1.39069900
H  4.13143100  -3.91622900  -2.16687900
H  3.47963500  -5.28108700  -1.24658600
H  3.71505700  -3.70195200  -0.46827800
C  1.75103600  -4.28746500  -3.26434500
H  0.74532900  -4.04545000  -3.61698600
H  1.89704200  -5.37074800  -3.35318700
H  2.47050700  -3.80818700  -3.93677500
C  -0.61511600  -3.08064100  2.49051100
H  0.31545300  -2.57471400  2.75157800
C  -1.00550500  -3.94978900  3.69367100
H  -1.03098400  -3.33289700  4.59830800
H  -0.28856200  -4.76241900  3.85799800
H  -1.99766500  -4.39960100  3.56972200
C  -1.66636400  -1.98901100  2.25644700
H  -1.43316600  -1.40864600  1.35977800
H  -1.69073300  -1.30802200  3.11234200
H  -2.65821600  -2.42698300  2.12055300
C  3.86638900  0.86223000  -0.24302400
C  4.30212800  0.72310100  -1.57423600
C  4.83015800  1.84774600  -2.21684100
H  5.17595500  1.76014800  -3.24296800
C  4.91982800  3.07233600  -1.56172000
H  5.33322700  3.93531300  -2.07694100
C  4.47398400  3.19160300  -0.24808800
H  4.53936200  4.15031500  0.25772800
C  3.94663300  2.09279400  0.43676600
C  4.23927200  -0.61201200  -2.30054400
H  3.82700400  -1.34875600  -1.60712300
C  5.63956700  -1.10362000  -2.70230800
H  5.57615900  -2.08937600  -3.17768000
H  6.29807300  -1.19010000  -1.83086700
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | 6.11545600 | -0.41961300| -3.41427800|
| C       | 3.30268200 | -0.54561900| -3.51592800|
| H       | 2.29772700 | -0.23958900| -3.21271100|
| H       | 3.23304800 | -1.52791200| -3.99778000|
| H       | 3.66760900 | 0.16916000 | -4.26300700|
| C       | 3.45699800 | 2.22902400 | 1.86801100 |
| H       | 3.28834400 | 1.23026900 | 2.27352000 |
| C       | 4.46662400 | 2.93016000 | 2.78909000 |
| H       | 4.60947400 | 3.98081600 | 2.51033100 |
| H       | 5.44926900 | 2.44528200 | 2.76799600 |
| H       | 4.10007600 | 2.90681100 | 3.82106000 |
| C       | 2.11267200 | 2.96277000 | 1.89548700 |
| H       | 2.24628300 | 4.01429400 | 1.63322900 |
| H       | 1.67280300 | 2.90571500 | 2.89573000 |
| H       | 1.40453900 | 2.53152600 | 1.18433000 |
| O       | 0.70616200 | 0.08132100 | 1.94139800 |
| P       | 1.65740700 | -0.36121700| 4.57167500 |

Absolute energy of **S3** at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -7125.976788 au.

Absolute energy of **S3** at B3LYP-D3BJ/6-31G* level of theory: -7121.144376 au. Cartesian coordinates of the optimized geometry for **S3** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Element | X       | Y      | Z       |
|---------|---------|--------|---------|
| Ga      | -1.60724100 | 0.70626000 | -0.65800500 |
| Ga      | 1.39841400 | -0.56717600 | 0.50560400 |
| P       | 0.21637500 | -0.23542000 | -1.38336600 |
| P       | 0.32444100 | 0.24368800 | 2.53035800 |
| O       | 1.81814200 | -1.39973900 | 4.28613000 |
| C       | 1.22539500 | -0.71851500 | 3.53153700 |
| N       | -3.43952300 | 0.06348200 | -0.98662100 |
| N       | -2.11839800 | 2.59914200 | -0.79548300 |
| N       | 1.91169900 | -2.48698200 | 0.73966100 |
| N       | 3.30607300 | 0.03860600 | 0.58588500 |
| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| C     | -4.37177100 | 0.79394300 | -1.61225600 |
| C     | -4.22622500 | 2.15433200 | -1.89726700 |
| H     | -5.04016400 | 2.61893000 | -2.43718700 |
| C     | -3.22135400 | 3.01290800 | -1.43646200 |
| C     | -5.69307200 | 0.15727200 | -1.97351600 |
| H     | -6.24783300 | 0.79582300 | -2.66373800 |
| H     | -6.30274000 | 0.01014500 | -1.07569600 |
| H     | -5.55426700 | -0.82754000 | -2.42334400 |
| C     | -3.44081200 | 4.49203400 | -1.66099700 |
| H     | -4.41029200 | 4.66685300 | -2.13045100 |
| H     | -2.65978000 | 4.91139000 | -2.29941700 |
| H     | -3.39988800 | 5.04142000 | -0.71674000 |
| C     | -3.82928100 | -1.23833300 | -0.50707900 |
| C     | -3.56317500 | -2.38312200 | -1.27716000 |
| C     | -4.01110400 | -3.61852700 | -0.79374700 |
| H     | -3.80871300 | -4.51597700 | -1.36995500 |
| C     | -4.71377500 | -3.71189900 | 0.40234100 |
| H     | -5.06107500 | -4.67884700 | 0.75585100 |
| C     | -4.95954000 | -2.56592500 | 1.15500800 |
| H     | -5.49210200 | -2.64779400 | 2.09771500 |
| C     | -4.51930800 | -1.31291000 | 0.72169800 |
| C     | -2.83650500 | -2.31553300 | -2.61102500 |
| H     | -2.54942900 | -1.27713800 | -2.79674300 |
| C     | -3.73673700 | -2.76500700 | -3.77546900 |
| H     | -4.64246400 | -2.15373300 | -3.85848900 |
| H     | -4.04968400 | -3.80854000 | -3.65538600 |
| H     | -3.19158500 | -2.68778800 | -4.72304600 |
| C     | -1.55272300 | -3.15057000 | -2.56308400 |
| H     | -0.98125100 | -3.01400700 | -3.48827700 |
| H     | -1.77279800 | -4.21724600 | -2.45707700 |
| H     | -0.92058800 | -2.83816700 | -1.73179700 |
| C     | -4.77317600 | -0.07666400 | 1.57598000 |
| H     | -4.54848300 | 0.80833000 | 0.97522000 |
|   | X      | Y      | Z      |
|---|--------|--------|--------|
| C | -6.23851100 | 0.04316700 | 2.02355300 |
| H | -6.39587000 | 0.99422200 | 2.54479600 |
| H | -6.51983900 | -0.75988700 | 2.71354800 |
| H | -6.92605100 | 0.00563300 | 1.17127200 |
| C | -3.83007600 | -0.05500900 | 2.79007700 |
| H | -4.00872200 | 0.83801200 | 3.39900000 |
| H | -2.77961300 | -0.05604400 | 2.48497600 |
| H | -3.98915200 | -0.93437900 | 3.42383800 |
| C | -1.26576200 | 3.62689100 | -0.25405400 |
| C | -0.32240600 | 4.26174800 | -1.08092300 |
| C | 0.32407000  | 5.39779000 | -0.57878700 |
| H | 1.05337200  | 5.90997100 | -1.19879300 |
| C | 0.04195500  | 5.88067200 | 0.69357000  |
| H | 0.53531900  | 6.77809200 | 1.05669600 |
| C | -0.83167000 | 5.18412300 | 1.52647400 |
| H | -0.99315200 | 5.53344100 | 2.54031900 |
| C | -1.48010900 | 4.02949500 | 1.08185100 |
| C | 0.02872000  | 3.73737300 | -2.46551400 |
| H | -0.65886500 | 2.92433100 | -2.71586100 |
| C | -0.09121400 | 4.80736600 | -3.56381700 |
| H | -1.09493400 | 5.24360300 | -3.61747500 |
| H | 0.13413100  | 4.36455800 | -4.54033000 |
| H | 0.61811200  | 5.62718300 | -3.40415400 |
| C | 1.45037200  | 3.15620800 | -2.44365200 |
| H | 1.68972000  | 2.70047600 | -3.41092700 |
| H | 1.54843000  | 2.38367000 | -1.67932900 |
| H | 2.18914000  | 3.93808400 | -2.24461700 |
| C | -2.39373100 | 3.22971500 | 2.00550700 |
| H | -2.31593800 | 2.17794700 | 1.70405400 |
| C | -3.87195900 | 3.63623500 | 1.86566900 |
| H | -3.99926400 | 4.70403800 | 2.08018700 |
| H | -4.48841800 | 3.07518600 | 2.57712300 |
| H | -4.26110900 | 3.43817000 | 0.86417700 |
C  -1.96110600  3.29503600  3.47572400
H  -2.12355700  4.29030000  3.90517800
H  -0.90664600  3.03138700  3.59074800
H  -2.55036500  2.58544000  4.06517100
C  2.95293100  -2.80519300  1.51640800
C  3.95602700  -1.89615900  1.87931700
H  4.72083800  -2.27584400  2.54284000
C  4.19090100  -0.62766400  1.33318300
C  3.13078100  -4.23220500  1.98301000
H  3.15305000  -4.92163700  1.13443000
H  2.29494700  -4.53573000  2.61955800
H  4.05747300  -4.33902400  2.54926000
C  5.56297000  -0.03642000  1.56721700
H  6.08744800  0.09776000  0.61566700
H  6.15965200  -0.69020000  2.20537000
H  5.50029500  0.95113000  2.03018700
C  1.14213200  -3.57405500  -0.78390700
C  1.48716300  -4.07520000  -1.08766500
C  0.84353100  -5.23140300  -1.53888000
H  1.10398000  -5.64455000  -2.50650300
C  -0.14917400  -5.85019600  -0.78390700
H  -0.63926800  -6.74502300  -1.15850900
C  -0.52850100  -5.30107800  0.43369000
H  -1.32702200  -5.76066400  1.00785100
C  0.11417900  -4.16745900  0.94313300
C  2.52687500  -3.37837900  -1.95698400
H  2.38182200  -2.30293800  -1.81311500
C  3.96763600  -3.72658900  -1.54020100
H  4.68281900  -3.28746500  -2.24457400
H  4.11852200  -4.81284200  -1.54321400
H  4.20898200  -3.34405600  -0.54676600
C  2.33810400  -3.65777700  -3.45387000
H  1.31537800  -3.44091100  -3.77597100
|   |         |         |         |
|---|---------|---------|---------|
| H | 2.56783200 | -4.69902400 | -3.70845400 |
| H | 3.01907600 | -3.02938700 | -4.03566600 |
| C | -0.33328900 | -3.57329800 | 2.26351100  |
| H | 0.44121000 | -2.88734200 | 2.60385600  |
| C | -0.54209000 | -4.61171000 | 3.37469800  |
| H | -0.75773300 | -4.10258500 | 4.32053400  |
| H | 0.34656600 | -5.23575500 | 3.52219800  |
| H | -1.38554000 | -5.27792800 | 3.15993400  |
| C | -1.61024900 | -2.75899300 | 2.02958000  |
| H | -1.46792500 | -2.04815500 | 1.21114000  |
| H | -1.88294300 | -2.20174000 | 2.92980500  |
| H | -2.44043600 | -3.41576200 | 1.75846000  |
| C | 3.74884600 | 1.25353600 | -0.04622600 |
| C | 4.26404000 | 1.20125800 | -1.35683400 |
| C | 4.75193800 | 2.37866100 | -1.93285600 |
| H | 5.15264300 | 2.34789100 | -2.94195700 |
| C | 4.73424300 | 3.58215500 | -1.23691900 |
| H | 5.12018600 | 4.48692000 | -1.69898100 |
| C | 4.21247900 | 3.62112700 | 0.05154200  |
| H | 4.18958800 | 4.56198700 | 0.59328500  |
| C | 3.71912100 | 2.46748300 | 0.66940800  |
| C | 4.32427700 | -0.09369900 | -2.14884100 |
| H | 3.95499000 | -0.89412400 | -1.50488500 |
| C | 5.76640700 | -0.45146900 | -2.54436300 |
| H | 5.78973900 | -1.40763300 | -3.07924000 |
| H | 6.41236800 | -0.54138000 | -1.66383200 |
| H | 6.20348900 | 0.30735700 | -3.20321600 |
| C | 3.41039300 | -0.01824500 | -3.38124400 |
| H | 2.37255700 | 0.14620100 | -3.07843500 |
| H | 3.46011300 | -0.94873000 | -3.95592600 |
| H | 3.70839100 | 0.80097400 | -4.04603300 |
| C | 3.14616300 | 2.55886700 | 2.07239100  |
| H | 2.95690100 | 1.54795700 | 2.43958600  |
Absolute energy of **2** at B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G* level of theory: -7131.508923 au.

Absolute energy of **2** at B3LYP-D3BJ/6-31G* level of theory: -7126.709669 au. Cartesian coordinates of the optimized geometry for **2** at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| Cl   | -1.048179 | -1.768832 | 2.357834 |
| P    | -0.161373 | 0.657761 | -0.720227 |
| Ga   | -1.527939 | -0.677086 | 0.456037 |
| Ga   | 1.783649 | 0.609674 | 0.221385 |
| N    | -3.221046 | 0.253635 | 0.940212 |
| N    | -2.479788 | -2.092514 | -0.579940 |
| N    | 2.810441 | 2.192638 | -0.356753 |
| N    | 3.344996 | -0.253911 | 0.987581 |
| C    | -4.367491 | -0.422826 | 1.068011 |
| C    | -4.572795 | -1.711677 | 0.564870 |
| H    | -5.547896 | -2.143218 | 0.748121 |
| C    | -3.739088 | -2.431766 | -0.304036 |
| C    | -5.554181 | 0.245419 | 1.727677 |
| H    | -5.310128 | 0.539912 | 2.752675 |
| H    | -6.412881 | -0.428029 | 1.750342 |
| H    | -5.838066 | 1.159724 | 1.199197 |
| C    | -4.362866 | -3.631532 | -0.984154 |
| H    | -5.449896 | -3.600974 | -0.888977 |
| H    | -4.006129 | -4.561052 | -0.531611 |
| Element | x       | y       | z       |
|---------|---------|---------|---------|
| 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       | -1.23932300  | -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  | -3.05485800 | -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   4.04586900  3.78643700   -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
|  | X          | Y          | Z          |
|---|------------|------------|------------|
| 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 |

Absolute energy of 2-TS at B3LYP-D3BJ/def-TZVP//B3LYP-D3BJ/6-31G* level of theory: -7131.495731 au.
Absolute energy of 2-TS at B3LYP-D3BJ/6-31G* level of theory: -7126.692628 au.
Cartesian coordinates of the optimized geometry for 2-TS at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 1):

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Cl   | 0.000000 | 0.000000 | 1.940195 |
| P    | 0.000000 | 0.000000 | -1.651767 |
| Ga   | 0.299486 | -1.544135 | -0.084325 |
| Ga   | -0.299486 | 1.544135 | -0.084326 |
| N    | -0.794285 | -3.079314 | 0.560641 |
| N    | 1.902564 | -2.712473 | -0.356945 |
| N    | -1.902564 | 2.712473 | -0.356946 |
| N    | 0.794285 | 3.079314 | 0.560640 |
| C    | -0.404555 | -4.363565 | 0.557670 |
| C    | 0.896971 | -4.797601 | 0.301095 |
| H    | 1.074008 | -5.860235 | 0.395643 |
| C    | 1.978118 | -4.026867 | -0.126099 |
| C    | -1.422373 | -5.464359 | 0.784174 |
| H    | -2.103305 | -5.262964 | 1.609351 |
| H    | -0.916687 | -6.415508 | 0.960672 |
| H    | -2.041207 | -5.569300 | -0.113408 |
| C    | 3.290126 | -4.755217 | -0.321716 |
| H    | 3.135259 | -5.835684 | -0.296833 |
| H    | 3.983464 | -4.490021 | 0.483453 |
| H    | 3.778010 | -4.484002 | -1.258862 |
| C    | -2.168093 | -2.863966 | 0.936379 |
| C    | -2.496520 | -2.823472 | 2.310373 |
| C    | -3.849590 | -2.856094 | 2.658694 |
| H    | -4.128813 | -2.856442 | 3.707984 |
| C    | -4.845018 | -2.880167 | 1.684282 |
| H    | -5.891230 | -2.904874 | 1.977457 |
| C    | -4.499069 | -2.847389 | 0.338253 |
| H    | -5.278859 | -2.840440 | -0.417356 |
| C    | -3.157499 | -2.855134 | -0.063770 |
| C    | -2.822089 | -2.890064 | -1.549543 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -1.73834400| -2.97676800| -1.67172900|
| C    | -3.45683800| -4.09466800| -2.26577000|
| H    | -3.15884400| -4.10155300| -3.32039100|
| H    | -4.55123700| -4.04969600| -2.23229200|
| C    | -3.25672800| -1.57837100| -2.21277400|
| H    | -4.34590700| -1.47190200| -2.19702700|
| H    | -2.92868100| -1.55081700| -3.25835700|
| H    | -2.81196800| -0.72260200| -1.70486100|
| C    | 3.05393300 | -2.10236800| -0.96439000|
| C    | 4.10602000 | -1.66183500| -0.14300600|
| C    | 5.25487200 | -1.15116900| -0.75533200|
| H    | 6.07671100 | -0.79814700| -0.13969900|
| C    | 5.36237300 | -1.10674500| -2.14183100|
| H    | 6.26692900 | -0.72201600| -2.60518100|
| C    | 4.30661600 | -1.54427000| -2.93777800|
| H    | 4.39806800 | -1.49622200| -4.01831100|
| C    | 3.12736000 | -2.03865500| -2.37102200|
| C    | 3.99994600 | -1.74424900| 1.37171500 |
| H    | 3.14581800 | -2.38104100| 1.61814800 |
| C    | 5.24664200 | -2.36004300| 2.02587400 |
| H    | 5.08326400 | -2.48488600| 3.10231000 |
| H    | 6.12465400 | -1.71625600| 1.90153300 |
| H    | 5.49289600 | -3.34018200| 1.60221900 |
| C    | 3.71697900 | -0.35774700| 1.95538900 |
| H    | 2.85477200 | 0.11320600 | 1.47988100 |
| H    | 4.57443400 | 0.30175700 | 1.80648700 |
| H    | 3.52137800 | -0.42256500| 3.03124300 |
| C    | 2.00491200 | -2.55127700| -3.26829900|
| H    | 1.09473400 | -2.64303700| -2.66880700|
| C    | 2.32470400 | -3.95389100| -3.81836100|
| H    | 2.41969000 | -4.69335100| -3.01744600|
| H    | 3.26245100 | -3.94751400| -4.38663100|
H  1.52547900  -4.28974100  -4.48945300
C  1.69159300  -1.58240300  -4.41780700
H  0.80031900  -1.92287400  -4.95721100
H  2.51291600  -1.53046500  -5.14231300
H  1.49250100  -0.57978600  -4.03273200
C  -1.97811800  4.02686700  -0.12610000
C  -0.89697100  4.79760100   0.30109300
H  -1.07400800  5.86023600   0.39564100
C  0.40455500  4.36356500   0.55766900
C  -3.29012600  4.75521800  -0.32171700
H  -3.98346300  4.49002300   0.48345200
H  -3.77801100  4.48400200  -1.25886300
H  -3.13525800  5.83568500  -0.29683600
C  1.42237400  5.46435900   0.78417300
H  0.91668800  6.41550900   0.96066900
H  2.04120900  5.56929900  -0.11340700
H  2.10330400  5.26296500   1.60935200
C  -3.05393300  2.10236800  -0.96439000
C  -3.12737700  2.03865400  -2.37102200
C  -4.30661700  1.54426900  -2.93777700
H  -4.39806900  1.49622100  -4.01831000
C  -5.36237400  1.10674400  -2.14183000
H  -6.26693000  0.72201400  -2.60517900
C  -5.25487200  1.15116900  -0.75533100
H  -6.07671100  0.79814700  -0.13969700
C  -4.10601900  1.66183500  -0.14300500
C  -2.00491300  2.55127600  -3.26830000
H  -1.09473500  2.64303700  -2.66880800
C  -2.32470600  3.95389000  -3.81836300
H  -3.26245400  3.94751100  -4.38663200
H  -1.52548100  4.28973900  -4.48945500
H  -2.41969300  4.69335000  -3.01744900
C  -1.69159400  1.58240100  -4.41780700
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| H    | -1.49250200  | 0.57978500   | -4.03273100  |
| H    | -0.80032100  | 1.92287300   | -4.95721200  |
| H    | -2.51291800  | 1.53046200   | -5.14231200  |
| C    | -3.99994500  | 1.74425000   | 1.37171600   |
| H    | -3.14581700  | 2.38104200   | 1.61814800   |
| C    | -5.24641000  | 2.36004500   | 2.02587400   |
| H    | -6.12465300  | 1.71625800   | 1.90153400   |
| H    | -5.49289400  | 3.34018400   | 1.60221900   |
| H    | -5.03262000  | 2.48488800   | 3.10231000   |
| C    | -3.71697800  | 0.35774800   | 1.95539000   |
| H    | -3.52137700  | 0.42256700   | 3.03124400   |
| H    | -2.85477200  | -0.11320500  | 1.47988200   |
| H    | -4.57443300  | -0.30175600  | 1.80648900   |
| C    | 2.16809300   | 2.86396600   | 0.93637900   |
| C    | 3.15750000   | 2.85513400   | -0.06377000  |
| C    | 4.49906900   | 2.84739000   | 0.33825300   |
| H    | 5.27886000   | 2.84044200   | -0.41735600  |
| C    | 4.84501800   | 2.88016800   | 1.68428200   |
| H    | 5.89123000   | 2.90487600   | 1.97745800   |
| C    | 3.84958900   | 2.85609500   | 2.65869400   |
| H    | 4.12881200   | 2.85644300   | 3.70798400   |
| C    | 2.49652000   | 2.82347200   | 2.31037300   |
| C    | 1.43289200   | 2.81284000   | 3.40603000   |
| H    | 0.47028800   | 2.59088700   | 2.93970500   |
| C    | 1.69767900   | 1.71486800   | 4.44935800   |
| H    | 0.86342900   | 1.66893300   | 5.15855800   |
| H    | 2.60932600   | 1.91342200   | 5.02508500   |
| H    | 1.79046800   | 0.73734700   | 3.97385100   |
| C    | 1.30433300   | 4.17828200   | 4.10763400   |
| H    | 0.58493200   | 4.11041500   | 4.93189300   |
| H    | 0.95441200   | 4.95975300   | 3.42792400   |
| H    | 2.26572700   | 4.49843200   | 4.52694400   |
| C    | 2.82209000   | 2.89006400   | -1.54954300  |

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H  1.73834500  2.97676800  -1.67172900
C  3.45683900  4.09466700  -2.26577100
H  4.55123800  4.04969600  -2.23229200
H  3.15884500  4.10155200  -3.32039100
H  3.15090300  5.04896200  -1.82314400
C  3.25672900  1.57837100  -2.21277300
H  2.81196900  0.72260200  -1.70486100
H  2.92868200  1.55081600  -3.25835700
H  4.34590800  1.47190100  -2.19702600
C  -1.43289300 -2.81284000  3.40603000
H  -0.47028900 -2.59088800  2.93970600
C  -1.69767900 -1.71486800  4.44935800
H  -0.86343000 -1.66893400  5.15855900
H  -1.79046700 -0.73734700  3.97385100
H  -2.60932700 -1.91342200  5.02508500
C  -1.30433500 -4.17828200  4.10763500
H  -0.58493400 -4.11041500  4.93189400
H  -2.26572900 -4.49843100  4.52694400
H  -0.95441400 -4.95975300  3.42792500

Absolute energy of 2 at CASSCF(2/2)/def2-TZVP//B3LYP-D3BJ/def2-TZVP level of theory: -7109.6329748 au.

Absolute energy of 2 at CASSCF(4/4)/def2-TZVP//B3LYP-D3BJ/def2-TZVP level of theory: -7109.6458729 au.

Absolute energy of 2 at B3LYP-D3BJ/def2-TZVP level of theory: -7131.516108 au.

Cartesian coordinates of the optimized geometry for 2 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
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| N    | -3.26851  | -1.60217  | -0.37982  |
| N    | -3.28010  | 0.95289   | 0.94558   |
| C    | 4.45837   | -0.48144  | 0.89056   |
| C    | 4.90075   | 0.73799   | 0.37428   |
| H    | 5.95223   | 0.94254   | 0.49821   |
| C    | 4.20837   | 1.63564   | -0.44706  |
| C    | 5.50888   | -1.37552  | 1.50115   |
| H    | 5.32154   | -1.49570  | 2.56857   |
| H    | 6.50031   | -0.95102  | 1.36636   |
| H    | 5.48597   | -2.37304  | 1.06547   |
| C    | 5.05298   | 2.68814   | -1.12297  |
| H    | 6.09075   | 2.36737   | -1.17049  |
| H    | 5.01118   | 3.61691   | -0.55339  |
| H    | 4.69887   | 2.90887   | -2.12685  |
| C    | 2.92768   | -2.27445  | 1.13154   |
| C    | 2.72143   | -2.70136  | 2.45245   |
| C    | 2.58053   | -4.06658  | 2.69394   |
| H    | 2.42745   | -4.41198  | 3.70789   |
| C    | 2.62954   | -4.98724  | 1.66127   |
| H    | 2.52571   | -6.04461  | 1.86992   |
| C    | 2.78579   | -4.54673  | 0.35712   |
| H    | 2.79963   | -5.26691  | -0.45012  |
| C    | 2.92933   | -3.19259  | 0.06656   |
| C    | 3.13149   | -2.74873  | -1.37049  |
| H    | 2.98810   | -1.67099  | -1.40067  |
| C    | 4.56437   | -3.03071  | -1.84154  |
| H    | 5.29726   | -2.50026  | -1.23348  |
| H    | 4.69651   | -2.71139  | -2.87701  |
| H    | 4.78873   | -4.09832  | -1.78548  |
| C    | 2.10661   | -3.37329  | -2.32026  |
| H    | 2.22396   | -4.45664  | -2.38893  |
| H    | 2.23544   | -2.96823  | -3.32560  |
| H    | 1.09100   | -3.15541  | -1.99394  |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| 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
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -0.650087 | -4.06554  | 1.508805  |
| H | -0.650024 | -4.05185  | 2.599897  |
| H | 0.007756  | -3.27411  | 1.154631  |
| H | -0.230466 | -5.02066  | 1.193374  |
| C | -2.844562 | 2.266375  | 1.342272  |
| C | -2.701105 | 3.252467  | 0.356984  |
| C | -2.332444 | 4.532414  | 0.765703  |
| H | -2.214999 | 5.312018  | 0.025029  |
| C | -2.097305 | 4.815874  | 2.099298  |
| H | -1.797605 | 5.812585  | 2.395721  |
| C | -2.227914 | 3.820177  | 3.056142  |
| H | -2.035651 | 4.054994  | 4.093226  |
| C | -2.612901 | 2.530925  | 2.701848  |
| C | -2.785642 | 1.442466  | 3.747475  |
| H | -3.563611 | 0.765089  | 3.391866  |
| C | -1.506553 | 0.614988  | 3.892632  |
| H | -1.661660 | -0.212752 | 4.587347  |
| H | -0.683138 | 1.228335  | 4.257053  |
| H | -1.181125 | 0.201752  | 2.938346  |
| C | -3.242720 | 1.971747  | 5.108383  |
| H | -3.478163 | 1.135876  | 5.769271  |
| H | -4.132385 | 2.598455  | 5.021163  |
| H | -2.463452 | 2.559311  | 5.596473  |
| C | -2.943362 | 2.971489  | -1.116120 |
| H | -3.278978 | 1.938930  | -1.214509 |
| C | -4.056390 | 3.857193  | -1.689121 |
| H | -3.778336 | 4.912223  | -1.660600 |
| H | -4.249906 | 3.592910  | -2.730567 |
| H | -4.987885 | 3.743083  | -1.131748 |
| C | -1.651577 | 3.116361  | -1.925660 |
| H | -0.874241 | 2.445810  | -1.560382 |
| H | -1.830128 | 2.879017  | -2.975740 |
| H | -1.266362 | 4.134318  | -1.874481 |
Absolute energy of the cationic part of 4 at B3LYP-D3BJ/def2-TZVP level of theory: -6671.034025 au. Cartesian coordinates of the optimized geometry for the cationic part of 4 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

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

Ga  1.62215100   -0.88822500    0.04191500
Ga -1.63011500    0.86720200    0.43087700
P  0.06126100   -0.15307300    1.42019600
N  3.47994100   -0.89987300    0.61413900
N  1.75643300   -2.27667300   -1.28106200
N -1.90367000    2.59474300   -0.37032700
N -3.43301900    0.62981400    1.10608300
C  4.34969500   -1.82440900    0.20438500
C  4.03341900   -2.83349400   -0.70925300
H  4.82792200   -3.53096200   -0.92160900
C  2.84969300   -3.03962000   -1.41341500
C  5.76858000   -1.79420600    0.70248300
H  6.38024400   -1.20099300    0.02019900
H  6.17927800   -2.80135800    0.72166100
H  5.85164000   -1.34654800    1.68796900
C  2.81474600   -4.21379300   -2.35279800
H  2.25594500   -5.02979600   -1.89236300
H  3.82175400   -4.56510600   -2.56021100
H  2.31578800   -3.97553900   -3.28799700
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 3.92255900| 0.16359200| 1.48250600|
| C       | 4.63610100| 1.24159100| 0.93588500|
| C       | 5.03355800| 2.26473700| 1.79381300|
| H       | 5.58238100| 3.10783100| 1.39654400|
| C       | 4.73388600| 2.22293900| 3.14409600|
| H       | 5.05017700| 3.02766500| 3.79469800|
| C       | 4.02761900| 1.14942200| 3.66343400|
| H       | 3.80220600| 1.12739700| 4.71966100|
| C       | 3.60845900| 0.09922100| 2.85043800|
| C       | 4.96169200| 1.34687700| -0.54439900|
| H       | 4.71474500| 0.39849600| -1.02094500|
| C       | 4.10025600| 2.42598200| -1.20696300|
| H       | 3.03893300| 2.24159900| -1.05591000|
| H       | 4.28897600| 2.46643100| -2.28123700|
| H       | 4.32508900| 3.40813000| -0.78821500|
| C       | 6.44968100| 1.61443000| -0.80001900|
| H       | 6.66186800| 1.57050000| -1.86950600|
| H       | 7.08558300| 0.88636700| -0.29566900|
| H       | 6.74267500| 2.60450300| -0.44856300|
| C       | 2.89180400| -1.09681400| 3.45293600|
| H       | 2.25202100| -1.53071700| 2.68265800|
| C       | 1.98149600| -0.72270900| 4.62243200|
| H       | 1.30356900| 0.08492300| 4.34878000|
| H       | 2.55279200| -0.41562200| 5.49974800|
| H       | 1.38180900| -1.58520900| 4.91329400|
| C       | 3.88895800| -2.18526900| 3.87591400|
| H       | 4.59225400| -1.79576200| 4.61451900|
| H       | 4.46376900| -2.56267600| 3.03123000|
| H       | 3.36077700| -3.02903600| 4.32343700|
| C       | 0.61299700| -2.55398700| -2.11203700|
| C       | 0.48231400| -1.86907000| -3.33161100|
| C       | -0.57931400| -2.22559700| -4.16195600|
| H       | -0.69228800| -1.71909500| -5.11195600|
C  -1.48124700  -3.21269000  -3.79995000
H  -2.29143100  -3.47780600  -4.46638100
C  -1.35169400  -3.84596600  -2.57647700
H  -2.06907200  -4.60266700  -2.28969400
C  -0.31323300  -3.52774300  -1.70409400
C   1.43934900  -0.79888700  -3.84597600
H   0.90472200  -0.33931700  -4.67987000
C   1.76663700   0.33987100  -2.87340200
H   2.10385600  1.21831500  -3.42304600
H   2.58315600   0.07019000  -2.20252500
H   0.90184600   0.65172700  -2.28697100
C   2.73309700  -1.37779000  -4.43540000
H   2.52337800  -2.17274400  -5.15150800
H   3.38527200  -1.77628700  -3.65843400
H   3.28711200  -0.59386100  -4.95530400
C  -0.22826100  -4.23406500  -0.36145500
H   0.70279900  -3.93705200   0.12196900
H  -1.38263400  -3.80501300   0.55346100
H  -1.38488900  -2.72884700   0.71797000
H  -1.29640900  -4.29188900  1.52624900
H  -2.34487000  -4.08821600  0.12609200
C  -0.20700300  -5.76127400  -0.50694600
H  -1.15506300  -6.13557800  -0.89598600
H  -0.04514000  -6.22765500  0.46590800
H   0.58066500  -6.10071200  -1.18026200
C  -3.02033600  3.31296100  -0.18549600
C  -4.12889400  2.85854300  0.52390800
H  -4.94891500  3.55427800  0.60367600
C  -4.35409800  1.59436800  1.07578900
C  -3.11775300  4.68135900  -0.80227000
H  -3.91310400  5.25258300  -0.33083900
H  -3.34664300  4.59518700  -1.86623600
H  -2.18169400  5.22819700  -0.72358100
| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| C       | -5.73357400  | 1.32477000   | 1.61095400   |
| H       | -6.21015500  | 2.25573100   | 1.90913200   |
| H       | -5.72087300  | 0.63451100   | 2.44934300   |
| H       | -6.34638000  | 0.87105900   | 0.82919700   |
| C       | -0.8465600   | 3.1354400    | -1.18059500  |
| C       | 0.24693300   | 3.75619400   | -0.55072900  |
| C       | 1.24279900   | 4.2919200    | -1.36561000  |
| H       | 2.08640500   | 4.79067900   | -0.91007800  |
| C       | 1.16885100   | 4.20258400   | -2.74555800  |
| H       | 1.95511800   | 4.62565500   | -3.35708800  |
| C       | 0.08459900   | 3.57962600   | -3.34454800  |
| H       | 0.03451000   | 3.52189900   | -4.42313700  |
| C       | -0.9466400   | 3.04362500   | -2.57811800  |
| C       | 0.33633600   | 3.91657600   | 0.95794200   |
| H       | -0.41853800  | 3.27465600   | 1.41188500   |
| C       | 0.02021600   | 5.36026900   | 1.37489600   |
| H       | -0.97661400  | 5.66743300   | 1.05800300   |
| H       | 0.73861800   | 6.05701900   | 0.93891300   |
| H       | 0.07173800   | 5.45950500   | 2.46037400   |
| C       | 1.69016100   | 3.47655200   | 1.51674900   |
| H       | 2.50417900   | 4.10305300   | 1.15135500   |
| H       | 1.90583800   | 2.44243800   | 1.25771100   |
| H       | 1.68623200   | 3.54880300   | 2.60483300   |
| C       | -2.13260900  | 2.36887900   | -3.24790400  |
| H       | -2.95101900  | 2.33028200   | -2.53003000  |
| C       | -2.64280000  | 3.13423300   | -4.47242300  |
| H       | -3.56680100  | 2.68279000   | -4.83665800  |
| H       | -1.92496900  | 3.11140000   | -5.29342800  |
| H       | -2.84472600  | 4.18015900   | -4.23734000  |
| C       | -1.79334100  | 0.92246300   | -3.61676800  |
| H       | -2.65530300  | 0.41952200   | -4.05687200  |
| H       | -1.47991500  | 0.34211300   | -2.74851000  |
| H       | -0.97925400  | 0.89479300   | -4.34131600  |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -3.80495100 | -0.68885400 | 1.55547000 |
| C    | -3.43985100 | -1.10673100 | 2.84359100 |
| C    | -3.81283200 | -2.39066000 | 3.23733400 |
| H    | -3.55103200 | -2.74115300 | 4.22525800 |
| C    | -4.51704100 | -3.22678600 | 2.38651100 |
| H    | -4.79821400 | -4.21884200 | 2.71471500 |
| C    | -4.85687000 | -2.79597400 | 1.11438400 |
| H    | -5.39848200 | -3.46050300 | 0.45546700 |
| C    | -4.50731900 | -1.52328400 | 0.67190700 |
| C    | -2.70939900 | -0.18995800 | 3.80857200 |
| H    | -2.14725700 | 0.53658300  | 3.21996400 |
| C    | -1.69734000 | -0.93381800 | 4.68017100 |
| H    | -1.09665700 | -0.21821700 | 5.24188600 |
| H    | -1.02551500 | -1.53561800 | 4.06943900 |
| H    | -2.18715800 | -1.58523100 | 5.40546600 |
| C    | -3.69481500 | 0.60064900  | 4.68108000 |
| H    | -4.34476500 | 1.23983200  | 4.08448700 |
| H    | -3.15280700 | 1.23827600  | 5.38167000 |
| H    | -4.32667500 | -0.07652100 | 5.25911000 |
| C    | -4.83240300 | -1.09454600 | -0.74876800|
| H    | -4.75866800 | -0.00937000 | -0.80861200|
| C    | -3.79415800 | -1.67326200 | -1.71427300|
| H    | -3.96825900 | -1.32651500 | -2.73373700 |
| H    | -3.83967900 | -2.76189000 | -1.71519200 |
| H    | -2.77661400 | -1.39849100 | -1.43135500 |
| C    | -6.25114100 | -1.47231500 | -1.18346000|
| H    | -6.99835400 | -1.10573600 | -0.47816000 |
| H    | -6.37565400 | -2.55266700 | -1.26652200 |
| H    | -6.46894400 | -1.04416300 | -2.16317600 |
Absolute energy of CO\textsubscript{2} at B3LYP-D3BJ/def2-TZVP level of theory: -188.671581 au.

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

| Atom | x        | y        | z        |
|------|----------|----------|----------|
| C    | 0.0000000 | 0.0000000 | 0.0000000 |
| O    | 0.0000000 | 0.0000000 | 1.1597060 |
| O    | 0.0000000 | 0.0000000 | -1.1597060 |

Absolute energy of 2*CO\textsubscript{2} at B3LYP-D3BJ/def2-TZVP level of theory: -7320.212173 au.

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

| Atom | x        | y        | z        |
|------|----------|----------|----------|
| Cl   | 1.5350500 | 0.9086240 | 2.6849200 |
| P    | 0.0339890 | -0.4877020 | -0.6469060 |
| Ga   | 1.8837670 | 0.0322070 | 0.6652170 |
| Ga   | -2.0924030 | 0.3949130 | -0.4541600 |
| N    | 2.8355450 | -1.6650800 | 1.0845110 |
| N    | 3.4641650 | 0.9596850 | -0.0348270 |
| N    | -3.4925680 | -0.8955660 | -0.9166100 |
| N    | -3.2346200 | 1.7388930 | 0.3433740 |
| C    | 4.1259840 | -1.6243150 | 1.3862650 |
| C    | 4.9236770 | -0.4818350 | 1.2355300 |
| H    | 5.9328540 | -0.5705720 | 1.6061170 |
| C    | 4.6488180 | 0.6787460 | 0.5112100 |
| C    | 4.8205530 | -2.8511850 | 1.9196950 |
| H    | 4.7537750 | -2.8622040 | 3.0087940 |
| H    | 5.8738300 | -2.8374760 | 1.6490080 |
| H    | 4.3654980 | -3.7678310 | 1.5543700 |
| C    | 5.7836060 | 1.6568050 | 0.3468370 |
| H    | 6.7366620 | 1.1841720 | 0.5702880 |
| H    | 5.6385280 | 2.4857570 | 1.0423560 |
| H    | 5.8157820 | 2.0804030 | -0.6534430 |
| C    | 2.1051930 | -2.8981840 | 1.1558990 |
| C    | 1.6520780 | -3.3883860 | 2.3917560 |
| C    | 0.9592570 | -4.5989060 | 2.4034730 |
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
Absolute energy of 5 at B3LYP-D3BJ/def2-TZVP level of theory: -7508.905936 au.
Cartesian coordinates of the optimized geometry for 5 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| Ga      | -2.479972 | 0.565012 | 0.585535 |
| Ga      | 2.664237  | -0.473888 | 0.201770 |
| Cl      | -2.058789 | 1.557976 | 2.518662 |
| P       | -0.587655 | -0.413424 | -0.402375 |
| O       | -0.631032 | -1.861827 | 1.844418 |
| O       | 1.436716  | -1.419862 | 1.194890 |
| O       | -0.010735 | 2.101895 | -1.100268 |
| O       | 1.794717  | 0.995237 | -0.470577 |
| N       | -3.941534 | -0.717939 | 0.899258 |
| N       | -3.515354 | 1.820408 | -0.519012 |
| N       | 4.219587  | 0.036855 | 1.171543 |
| N       | 3.455904  | -1.597672 | -1.140867 |
| C       | -5.201403 | -0.302295 | 0.851013 |
| C       | -5.594588 | 0.942091 | 0.345454 |
| H       | -6.651149 | 1.149744 | 0.403983 |
| C       | -4.839072 | 1.872772 | -0.373831 |
| C       | -6.305289 | -1.194189 | 1.357107 |
| H       | -6.446673 | -1.011107 | 2.424099 |
| H       | -6.067546 | -2.247342 | 1.237495 |
| H       | -7.241385 | -0.971345 | 0.850338 |
| C       | -5.604693 | 2.986530 | -1.040425 |
| H       | -5.357721 | 3.941955 | -0.578532 |
| H       | -6.675087 | 2.820860 | -0.952461 |
| H       | -5.338988 | 3.071435 | -2.092903 |
| C       | -3.632553 | -2.087617 | 1.212700 |
| C       | -3.425335 | -2.973405 | 0.140290 |
| C       | -3.076528 | -4.289045 | 0.430534 |
| H       | -2.909068 | -4.987919 | -0.377194 |
| C       | -2.940496 | -4.718928 | 1.740985 |
| H       | -2.662142 | -5.744346 | 1.948768 |
| C       | -3.156622 | -3.833328 | 2.781769 |
| H       | -3.038839 | -4.172901 | 3.802327 |
| C       | -3.500172 | -2.504542 | 2.544305 |
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 | -1.76423300 | 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  |

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|  | X          | Y          | Z          |
|---|------------|------------|------------|
| 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
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