Supporting Information

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

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Supporting Information

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6. References
1. Experimental Section

General procedure. All experiments and manipulations were carried out under a dry argon atmosphere using either standard Schlenk or glovebox techniques. Toluene, benzene, and n-hexane were dried using an MBraun solvent drying system (SPS), degassed, and stored over 4Å molecular sieve. Deuterated solvents (CD₆, toluene-d₈) were dried by refluxing over NaK alloy, distilled prior to use, and stored over 4Å molecular sieve. Commercial reagents were purchased from Aldrich, Acros, or Alfa-Aesar Chemical Co. and used as received. LGa(Cl)PLGa 1 (L = HC[C(Me)N(Ar)]₂, Ar = 2,6-iPr₂-C₆H₃), was prepared by literature method.[1] NMR spectra (δ in ppm) were recorded using a Bruker Avance DPX 300 (¹H 300 MHz, ¹³C {¹H} 75 MHz, ³¹P {¹H} 121 MHz), a Bruker Avance II 500 (¹H 500 MHz, ¹³C {¹H} 126 MHz, ³¹P {¹H} 202 MHz), or a Bruker Avance III HD 600 (¹H 600 MHz, ¹³C {¹H} 151 MHz, ³¹P {¹H} 243 MHz) spectrometer and were referenced to internal CD₃OD (δ = 7.16; ¹³C δ = 128.06) or C₇D₇H (δ = 2.08, 6.97, 7.01, 7.09; ¹³C δ = 137.48, 128.87, 127.96, 125.13, 20.43), the ³¹P NMR spectra are referenced to internal CD₃PO (δ = 0; ³¹P δ = 21.6) or C₇D₇PO (δ = 42.2; ³¹P δ = 63.4), or a Bruker Avance III HD 600 (¹H 600 MHz, ¹³C {¹H} 151 MHz, ³¹P {¹H} 243 MHz) spectrometer and were referenced to internal CD₃OD (δ = 7.16) or C₇D₇H (δ = 2.08, 6.97, 7.01, 7.09) using chi-values (χ).[2] Elemental analyses were performed at the Elementaranalyse Labor of the University of Duisburg-Essen. IR spectra were recorded by a Bruker ALPHA-T FT-IR spectrometer equipped with a single-reflection ATR sampling module.

Synthesis of 2: N,N'-diisopropylcarbodiimide (45 mg, 0.29 mmol) was added to a toluene solution (10 mL) of 1 (300 mg, 0.29 mmol). After shaking the reaction mixture at ambient temperature for one minute, all volatiles were removed under vacuum to yield a colorless crystalline solid. Yield: 99% (330 mg). M.p. 91 °C (dec.). Single crystals suitable for X-ray diffraction were grown by cooling a toluene solution of 2 at −30 °C for 12 h. Anal. calcd. (%) for C₅₆H₉₀ClGa₂N₄P (1164.56): C, 66.88; H, 8.29; N, 7.20. Found: C, 66.95; H, 8.37; N, 7.31. ¹H NMR (600 MHz, CD₆, 298 K) δ = 0.85 (d, 3JHH = 6.7 Hz, 6H, CH(CH₃)₂), 0.91 (d, 3JHH = 6.8 Hz, 6H, CH(CH₃)₂), 0.98 (d, 3JHH = 6.7 Hz, 6H, CH(CH₃)₂), 1.06 (d, 3JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.12 (d, 3JHH = 6.7 Hz, 6H, CH(CH₃)₂), 1.24 (d, 3JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.31 (s, 6H, CCH₃), 1.39 (d, 3JHH = 6.0 Hz, 6H, NCH(CH₃)₂), 1.50 (d, 3JHH = 6.7 Hz, 6H, CH(CH₃)₂), 1.52 (s, 6H, CCH₃), 1.54 (d, 3JHH = 6.7 Hz, 6H, CH(CH₃)₂), 1.61 (d, 3JHH = 6.4 Hz, 6H, NCH(CH₃)₂), 2.98 (sept, 3JHH = 6.0 Hz, 1H, NCH(CH₃)₂), 3.04 (sept, 3JHH = 6.7 Hz, 2H, CH(CH₃)₂), 3.25 (sept, 3JHH = 6.7 Hz, 2H, CH(CH₃)₂), 3.49 (sept, 3JHH = 6.8 Hz, 2H, CH(CH₃)₂), 3.54 (sept, 3JHH = 6.8 Hz, 2H, CH(CH₃)₂), 4.23 (sept, 3JHH = 6.3 Hz, 1H, NCH(CH₃)₂), 4.71 (s, 1H, CH), 4.76 (s, 1H, CH), 6.90 (t, 3JHH = 7.6 Hz, 2H, C₆H₅), 6.99-7.02 (m, 3H, C₆H₅), 7.12-7.14 (m, 2H, C₆H₅), 7.16-7.17 (m, 3H, C₆H₅), 7.19 (t, 3JHH = 7.6 Hz, 2H, C₆H₅). ¹³C {¹H} NMR (151 MHz, CD₆, 298 K) δ = 21.6, 24.5, 24.8, 24.9, 25.0, 25.4, 25.6, 25.7, 25.9, 26.6, 27.1
(CH(CH$_3$)$_2$); 28.1, 28.3, 28.4, 28.6, 29.4, 29.6 (CH(CH$_3$)$_2$); 48.7 (d, $^3$J$_{PC}$ = 5.4 Hz, NCH(CH$_3$)$_2$), 62.3 (d, $^3$J$_{PC}$ = 13.8 Hz, NCH(CH$_3$)$_2$); 98.1, 98.2 (CH); 124.0, 125.0, 125.8, 127.3, 128.8, 129.5, 138.0, 143.4, 144.0, 144.4, 144.8, 145.9 (C$_6$H$_3$); 166.8 (d, $^1$J$_{PC}$ = 38.7 Hz, CNCH(CH$_3$)$_2$); 170.1, 171.5 (C$_6$H$_3$). $^{31}$P{${}^1$H} (243 MHz, C$_6$D$_6$, 298 K) $\delta$ = −108.6 ppm. ATR-IR: $\nu$ 2960, 2921, 2864, 1573, 1524, 1463, 1386, 1314, 1254, 1209, 1168, 1106, 1018, 938, 859, 793, 757, 729, 695, 620, 581, 527 cm$^{-1}$.

**Synthesis of 3:** Compound 3 was synthesized by following the similar protocols used for 2 using $N_2$$N'$-dicyclohexylcarbodiimide (59 mg, 0.29 mmol), 1 (300 mg, 0.29 mmol), and toluene (10 mL).

Yield: 99% (358 mg, colorless solid). M.p. 93 °C (dec.). Anal. calcd. (%) for C$_{71}$H$_{104}$ClGa$_2$N$_3$P (1244.63): C, 68.36; H, 8.40; N, 6.74. Found: C, 68.47; H, 8.51; N, 6.89. $^1$H NMR (600 MHz, toluene-d$_8$, 298 K) $\delta$ = 0.89 (d, $^3$J$_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 0.95 (d, $^3$J$_{HH}$ = 6.6 Hz, 12H, CH(CH$_3$)$_2$), 1.01 (d, $^3$J$_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.10 (d, $^3$J$_{HH}$ = 6.7 Hz, 2H, CyH), 1.15 (d, $^3$J$_{HH}$ = 6.7 Hz, 2H, CyH), 1.18 (d, $^3$J$_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 1.25 (d, $^3$J$_{HH}$ = 6.7 Hz, 6H, CH(CH$_3$)$_2$), 1.31 (d, $^3$J$_{HH}$ = 12.4 Hz, 3H, CyH), 1.36 (s, 6H, C$_6$H$_3$), 1.42 (d, $^3$J$_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 1.45 (d, $^3$J$_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 1.49-1.52 (m, 3H, CyH), 1.57 (s, 6H, C$_6$H$_3$), 1.61 (d, $^3$J$_{HH}$ = 9.4 Hz, 1H, CyH), 1.76 (s, 1H, CyH), 1.88-1.94 (m, 6H, CyH), 2.69 (bs, 1H, CyH), 2.81 (d, $^3$J$_{HH}$ = 11.1 Hz, 2H, CyH), 2.96 (sept, $^3$J$_{HH}$ = 6.6 Hz, 2H, CH(CH$_3$)$_2$), 3.15 (sept, $^3$J$_{HH}$ = 6.6 Hz, 2H, CH(CH$_3$)$_2$), 3.50 (sept, $^3$J$_{HH}$ = 6.8 Hz, 4H, CH(CH$_3$)$_2$), 3.69 (t, $^3$J$_{HH}$ = 10.93 Hz, 1H, CyH), 4.79 (s, 1H, CH), 4.81 (s, 1H, CH), 6.93 (t, $^3$J$_{HH}$ = 7.3 Hz, 2H, C$_6$H$_3$), 7.00 (t, $^3$J$_{HH}$ = 6.7 Hz, 2H, C$_6$H$_3$), 7.06-7.13 (m, 6H, C$_6$H$_3$), 7.16 (t, $^3$J$_{HH}$ = 6.7 Hz, 2H, C$_6$H$_3$). $^{13}$C{${}^1$H} NMR (151 MHz, C$_6$D$_6$, 298 K) $\delta$ = 23.8, 24.0, 24.4, 24.5, 24.7, 25.0, 25.1, 25.2, 25.3, 26.3, 26.5, 26.8, 27.3, 27.6 (CH(CH$_3$)$_2$), Cy); 28.0, 28.9, 29.0, 34.2, 36.0 (CH(CH$_3$)$_2$, Cy); 57.5 (d, $^3$J$_{PC}$ = 3.6 Hz, NCH(CH$_3$)$_2$), 67.7 (d, $^3$J$_{PC}$ = 14.4 Hz, NCH(CH$_3$)$_2$); 97.0, 97.8 (CH); 123.3, 124.1, 124.4, 126.8, 127.1, 140.4, 143.0, 143.3, 143.8, 144.3, 145.2 (C$_6$H$_3$); 165.5 (d, $^1$J$_{PC}$ = 41.5 Hz, CNCH(CH$_3$)$_2$); 169.2, 170.6 (C$_6$H$_3$). $^{31}$P{${}^1$H} (243 MHz, C$_6$D$_6$, 298 K) $\delta$ = −105.3 ppm. ATR-IR: $\nu$ 2957, 2908, 2848, 1547, 1433, 1386, 1367, 1313, 1252, 1205, 1172, 1103, 1022, 936, 860, 795, 628, 556 cm$^{-1}$.

**Synthesis of 4:** Ethylisocyanate (31 μL, 0.38 mmol) was added to a toluene solution (15 mL) of 1 (400 mg, 0.38 mmol) at ambient temperature. After shaking the reaction mixture at this temperature for one minute, all volatiles were removed under vacuum to yield a colorless crystalline solid. Yield: 99% (420 mg). M.p. 141 °C (dec.). Anal. calcd. (%) for C$_{61}$H$_{87}$ClGa$_2$N$_3$OP (1109.48): C, 65.87; H, 7.88; N, 6.30. Found: C, 65.97; H, 7.93; N, 6.37. $^1$H NMR (300 MHz, toluene-d$_8$, 298 K) $\delta$ = 0.91 (d, $^3$J$_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 0.98 (t, $^3$J$_{HH}$ = 7.5 Hz, 6H, CH(CH$_3$)$_2$), 1.03-1.06 (m, 18H, CH(CH$_3$)$_2$), 1.08-1.10 (m, 9H, CH(CH$_3$)$_2$, NCH$_2$CH$_3$), 1.17 (d, $^3$J$_{HH}$ = 6.7 Hz, 6H, CH(CH$_3$)$_2$), 1.23...
(d, ^3J_{HH} = 6.7 \text{ Hz}, 6H, CH(CH_3)_2), 1.38 (s, 6H, CCH_3), 1.50 (s, 6H, CCH_3), 2.85 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.15 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 4H, CH(CH_3)_2), 3.36 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.48 (sept, ^3J_{HH} = 6.7 \text{ Hz}, 2H, NCH_2CH_3), 4.73 (s, 1H, CH), 4.83 (s, 1H, CH), 7.00-7.03 (m, 4H, C_6H_5), 7.10-7.17 (m, 6H, C_6H_5). ^13C\{^1H\} NMR (126 MHz, toluene-d_8, 298 K) \delta = 14.3, 15.4 (NCH_2CH_3); 21.3, 23.1, 24.1, 24.3, 24.4, 24.5, 24.9, 25.3, 25.6, 25.7 (CH(CH_3)_2); 27.8, 28.1, 28.3, 28.8, 29.7, 32.0 (CH(CH_3)_2); 39.3 (d, ^1J_{PC} = 2.6 \text{ Hz}, NCH_2CH_3); 97.4, 98.1 (CH); 123.9, 124.4, 124.5, 125.6, 127.4, 131.2, 142.1, 142.3, 143.3, 145.2, 145.4, 169.2, 170.8 (C_6H_5); 179.7 (d, ^1J_{PC} = 13.8 \text{ Hz}, NCO). ^31P\{^1H\} (121 MHz, C_6D_6, 298 K) \delta = -112.0 \text{ ppm. ATR-IR: } \nu 2964, 2925, 2865, 1605, 1527, 1438, 1381, 1315, 1261, 1225, 1178, 1099, 1021, 935, 867, 795, 757, 727, 633, 531 \text{ cm}^{-1}.

**Synthesis of 5:** Compound 5 was synthesized by following the similar protocols used for 4 using isopropylisocyanate (29 \mu L, 0.29 mmol), 1 (300 mg, 0.29 mmol), and toluene (10 mL). Yield: 99% (496 mg, colorless solid). M.p. 147 \text{ °C} (dec.). Anal. calcld. (%) for C_{65}H_{93}ClGa_2N_5O_3P: C, 66.12; H, 7.96; N, 6.22. Found: C, 66.20; H, 7.99; N, 6.33. \(^1H\) NMR (600 MHz, C_6D_6, 298 K) \delta = 0.95 (d, ^3J_{HH} = 6.6 \text{ Hz}, 6H, CH(CH_3)_2), 1.06-1.08 (m, 18H, CH(CH_3)_2), 1.13 (d, ^3J_{HH} = 6.8 \text{ Hz}, 6H, CH(CH_3)_2), 1.18 (d, ^3J_{HH} = 6.6 \text{ Hz}, 6H, CH(CH_3)_2), 1.24 (d, ^3J_{HH} = 6.8 \text{ Hz}, 6H, CH(CH_3)_2), 1.31 (d, ^3J_{HH} = 6.7 \text{ Hz}, 6H, CH(CH_3)_2), 1.33 (s, 6H, CCH_3), 1.43 (d, ^3J_{HH} = 6.7 \text{ Hz}, 6H, CH(CH_3)_2), 1.50 (s, 6H, CCH_3), 2.86 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.38 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.42 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.58 (sept, ^3J_{HH} = 6.8 \text{ Hz}, 2H, CH(CH_3)_2), 3.67 (sept, ^3J_{HH} = 6.5 \text{ Hz}, 2H, NCH(CH_3)_2), 4.76 (s, 1H, CH), 4.88 (s, 1H, CH), 7.01-7.03 (m, 4H, C_6H_5), 7.11-7.14 (m, 4H, C_6H_5), 7.16-7.18 (m, 4H, C_6H_5). ^13C\{^1H\} NMR (151 MHz, C_6D_6, 298 K) \delta = 21.4 (NCH(CH_3)_2); 24.0, 24.2, 24.3, 24.5, 24.6, 25.1, 25.3, 25.7, 26.5 (CH(CH_3)_2); 27.9, 28.1, 28.3, 28.7, 29.6 (CH(CH_3)_2); 46.6 (NCH(CH_3)_2); 98.3, 98.8 (CH); 124.0, 124.5, 125.0, 125.7, 127.2, 128.5, 129.3, 137.9, 141.6, 142.2, 142.7, 143.3, 145.4, 145.5, 169.3, 170.8 (C_6H_5); 180.4 (d, ^1J_{PC} = 14.9 \text{ Hz}, NCO). ^31P\{^1H\} (243 MHz, C_6D_6, 298 K) \delta = -114.8 \text{ ppm. ATR-IR: } \nu 2963, 2924, 2865, 1623, 1517, 1462, 1435, 1380, 1317, 1254, 1203, 1175, 1101, 1021, 935, 864, 795, 760, 542, 531 \text{ cm}^{-1}.

**Synthesis of 6:** Compound 6 was synthesized by following the similar protocols used for 4 using cyclohexylisocyanate (37 \mu L, 0.29 mmol), 1 (300 mg, 0.29 mmol), and toluene (10 mL). Yield: 98% (330 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown by cooling an n-hexane solution of 6 at −30 °C for 12 h. M.p. 143 \text{ °C} (dec.). Anal. calcld. (%) for C_{65}H_{93}ClGa_2N_5O_3P: C, 66.94; H, 8.04; N, 6.00. Found: C, 67.03; H, 8.11; N, 6.03. \(^1H\) NMR (600 MHz, C_6D_6, 298 K) \delta = 0.87 (t, ^3J_{HH} = 7.1 \text{ Hz}, 3H, CH(CH_3)_2), 0.92 (d, ^3J_{HH} = 6.6 \text{ Hz}, 6H, CH(CH_3)_2), 1.04-1.06 (m, 18H, CH(CH_3)_2, CH_2), 1.15 (d, ^3J_{HH} = 6.8 \text{ Hz}, 6H, CH(CH_3)_2), 1.21 (d, ^3J_{HH} = 6.8 \text{ Hz}, 6H,
Reaction of 2 with CO\(_2\): A toluene solution (5 mL) of 2 (150 mg, 0.13 mmol) in a J-Young Schlenk flask was degassed using the freeze pump-thaw method. CO\(_2\) (1 bar) gas was added, and the solution was stirred at ambient temperature for 1 h. All volatiles were then removed in vacuo to yield a colorless crystalline powder. The \(^{31}\)P\{\(^1\)H\} NMR spectrum at 25 °C shows two sharp singlets, which were assigned to the mono and double\(^{11}\) CO\(_2\) addition products. Unfortunately, due to the similar solubility of these two products, we failed to isolate a pure sample of the mono CO\(_2\) addition product. The crude \(^1\)H and \(^{31}\)P\{\(^1\)H\} NMR spectra of the mixture are provided to confirm the bulk material’s constitutions match (Figures S29-S30).

Reaction of 3 with CO\(_2\): Compound 3 also led to the mono and double\(^{11}\) CO\(_2\) addition products at room temperature, when exposed to CO\(_2\) gas (1 bar) in toluene similar to compound 2. Again, we failed to isolate a sample of the pure mono CO\(_2\) addition product due to the similar solubility of these two products. The \(^1\)H and \(^{31}\)P\{\(^1\)H\} NMR spectra of this mixture are provided to confirm the bulk material’s constitutions match (Figures S30-S31).

Synthesis of 7: A toluene solution (5 mL) of 4 (150 g, 0.13 mmol) in a J-Young Schlenk flask was degassed using the freeze pump-thaw method. CO\(_2\) (1 bar) gas was added and the solution was stirred at room temperature for 1 h. All volatiles were then removed in vacuo to yield a colorless crystalline powder of 7. Yield: 97% (150 mg). M.p. 93 °C (dec.). Anal. calcd. (%) for C\(_{66}\)H\(_{57}\)ClGa\(_2\)N\(_2\)O\(_3\)P (1153.47): C, 64.40; H, 7.58; N, 6.06. Found: C, 64.47; H, 7.66; N, 6.11. \(^1\)H NMR (500 MHz, toluene-d\(_8\), 298 K) \(\delta = 0.79\) (t, \(^3\)J\(_{HH} = 7.3\) Hz, 3H, CH\(_2\)Cl\(_3\)), 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\(_3\))\(_2\)), 1.10 (d, \(^3\)J\(_{HH} = 6.7\) Hz, 6H, CH(CH\(_3\))\(_2\)), 1.14 (d, \(^3\)J\(_{HH} = 6.8\) Hz, 6H, CH(CH\(_3\))\(_2\)), 1.22 (d, \(^3\)J\(_{HH} = 6.8\) Hz, 6H, CH(CH\(_3\))\(_2\)), 1.26 (d, \(^3\)J\(_{HH} = 6.8\) Hz, 6H, CH(CH\(_3\))\(_2\)), 1.40 (d, \(^3\)J\(_{HH} = 6.8\) Hz, 6H, CH(CH\(_3\))\(_2\)),
1.42 (s, 6H, CCH₃), 1.60 (s, 6H, CCH₃), 2.92 (sept, ³JHH = 6.8 Hz, 2H, CH(CH₃)₂), 3.01 (sept, ³JHH = 6.7 Hz, 2H, CH(CH₃)₂), 3.14 (q, ³JHH = 7.3 Hz, 2H, CH₂CH₃), 3.32 (sept, ³JHH = 6.8 Hz, 2H, CH(CH₃)₂), 3.67 (sept, ³JHH = 6.8 Hz, 2H, CH(CH₃)₂), 4.72 (s, 1H, CH), 4.86 (s, 1H, CH), 7.07-7.20 (m, 12H, C6H3). ¹³C{¹H} NMR (126 MHz, toluene-d₈, 298 K) δ = 14.3, 21.3 (NCH₂CH₃); 23.6, 24.3, 24.4, 24.7, 24.8, 24.9 (CH(CH₃)₂); 26.2, 28.2, 28.8, 29.5 (CH(CH₃)₂); 32.0, 40.0 (CH₂); 97.5, 97.6 (CH); 123.1, 124.5, 125.6, 126.9, 138.8, 142.2, 142.5, 143.8, 144.7, 146.1, 169.6, 172.0 (C₆H₃); 174.6 (d, ¹JC₆ = 28.4 Hz, OCO); 179.8 (d, ¹JC₆ = 15.6 Hz, NCO). ³¹P{¹H} (121 MHz, C₆D₆, 298 K) δ = −40.0 ppm. ATR-IR: ν 2964, 2925, 2863, 1943, 1667, 1521, 1436, 1383, 1315, 1251, 1174, 1097, 1018, 940, 867, 795, 757, 710, 636, 541 cm⁻¹.

**Synthesis of 8:** Compound 8 was synthesized by following the similar protocols used for 7 using compound 5 (200 mg, 0.18 mmol), CO₂ gas (1 bar), and toluene (10 mL). Yield: 98% (200 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown upon storage of saturated toluene solution of 8 at ambient temperature. M.p. 95 °C (dec.). Anal. calcld. (%) for C₆₃H₈₉ClGa₂N₅O₃P (1167.49): C, 64.66; H, 7.67; N, 5.98. Found: C, 64.71; H, 7.73; N, 5.98. ¹H NMR (600 MHz, toluene-d₈, 298 K) δ = 1.01 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.05 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.07 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.10 (d, ³JHH = 6.7 Hz, 6H, CH(CH₃)₂), 1.17 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.21 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.25 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.29 (d, ³JHH = 6.8 Hz, 6H, CH(CH₃)₂), 1.39 (s, 6H, CCH₃), 1.44 (d, ³JHH = 6.6 Hz, 6H, CH(CH₃)₂), 1.60 (s, 6H, CCH₃), 2.98 (sept, ³JHH = 6.7 Hz, 2H, CH(CH₃)₂), 3.03 (sept, ³JHH = 6.7 Hz, 2H, CH(CH₃)₂), 3.32 (sept, ³JHH = 6.8 Hz, 2H, CH(CH₃)₂), 3.61 (sept, ³JHH = 6.5 Hz, 1H, NCH(CH₃)₂), 3.69 (sept, ³JHH = 6.7 Hz, 2H, CH(CH₃)₂), 4.79 (s, 1H, CH), 4.86 (s, 1H, CH), 7.01-7.03 (m, 5H, C₆H₃), 7.08 (t, ³JHH = 7.6 Hz, 3H, C₆H₃), 7.13 (t, ³JHH = 6.7 Hz, 2H, C₆H₃), 7.17 (d, ³JHH = 6.7 Hz, 2H, C₆H₃). ¹³C{¹H} NMR (151 MHz, toluene-d₈, 298 K) δ = 12.3, 23.9, 24.3, 24.4, 24.6, 24.7, 24.9, 25.1, 25.2, 25.7, 26.4 (CH(CH₃)₂); 28.2, 28.5, 28.8, 29.4 (CH(CH₃)₂); 48.3 (NCH(CH₃)₂); 97.5, 98.8 (CH); 123.1, 124.5, 126.9, 139.3, 142.1, 142.5, 143.6, 144.9, 146.0, 169.5, 171.9 (C₆H₃); 174.4 (d, ¹JC₆ = 27.4 Hz, OCO); 180.6 (d, ¹JC₆ = 15.3 Hz, NCO). ³¹P{¹H} (121 MHz, toluene-d₈, 298 K) δ = −34.5 ppm. ATR-IR: ν 2963, 2925, 2861, 1671, 1577, 1522, 1439, 1384, 1314, 1238, 1173, 1149, 1103, 1018, 937, 864, 795, 757, 730, 695, 642, 531 cm⁻¹.

**Synthesis of 9:** Compound 9 was synthesized by following the similar protocols used for 7 using compound 7 (200 mg, 0.17 mmol), CO₂ gas (1 bar), and toluene (10 mL). Yield: 98% (200 mg, colorless solid). Single crystals suitable for X-ray diffraction were grown upon storage of saturated toluene solution of 9 at ambient temperature. M.p. 93 °C (dec.). Anal. calcld. (%) for C₆₃H₈₉ClGa₂N₅O₃P (1207.52): C, 65.49; H, 7.74; N, 5.79. Found: C, 65.57; H, 7.82; N, 5.83. ¹H
NMR (600 MHz, toluene-ds, 298 K) δ = 1.00 (d, 3JHH = 6.8 Hz, 6H, CH(CH3)2), 1.10 (td, 3JHH = 7.2 Hz, 12H, CH(CH3)2), 1.22 (td, 3JHH = 6.7 Hz, 12H, CH(CH3)2), 1.25 (d, 3JHH = 6.7 Hz, 6H, CH(CH3)2), 1.29 (d, 3JHH = 6.8 Hz, 6H, CH(CH3)2), 1.39 (s, 6H, CCH3), 1.40 (d, 3JHH = 6.8 Hz, 6H, CH(CH3)2), 1.43-1.54 (m, 5H, CH2), 1.59 (s, 6H, CCH3), 1.66 (m, 1H, CH2), 1.74 (br, 2H, CH2), 1.94 (br, 1H, CH2), 2.96 (sept, 3JHH = 6.8 Hz, 2H, CH(CH3)2), 3.08 (sept, 3JHH = 6.7 Hz, 2H, CH(CH3)2), 3.32 (sept, 3JHH = 6.8 Hz, 2H, CH(CH3)2), 3.39 (br, 1H, CH), 3.70 (sept, 3JHH = 6.8 Hz, 2H, CH(CH3)2), 4.85 (s, 2H, CH), 7.00-7.04 (m, 4H, C6H5), 7.07-7.12 (m, 6H, C6H5), 7.16 (d, 3JHH = 6.4 Hz, 2H, C6H5). 13C{1H} NMR (151 MHz, toluene-ds, 298 K) δ = 23.9, 24.3, 24.4, 24.6, 24.9, 25.2, 25.4, 25.6, 26.3, 26.8, 27.0 (CH(CH3)2); 28.2, 28.6, 29.4 (CH(CH3)2); 32.7, 57.1 (NCy); 97.5, 98.8 (CH); 123.2, 124.6, 124.7, 124.8, 125.4, 126.9, 139.2, 142.2, 142.5, 143.8, 144.7, 146.1, 169.5, 171.7 (C6H5); 174.1 (d, 1JC = 28.3 Hz, OCO); 181.1 (d, 1JC = 14.7 Hz, NCO). 31P{1H} (121 MHz, toluene-ds, 298 K) δ = −35.0 ppm. ATR-IR: ν 2958, 2925, 2865, 1663, 1577, 1518, 1436, 1384, 1317, 1251, 1235, 1176, 1098, 1024, 938, 864, 795, 757, 734, 695, 649, 531 cm⁻¹.

Scheme S1. Reactions of compounds 2 and 3 with CO2.
2. Spectroscopic Characterization

Figure S1. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 2. *trace impurities.

Figure S2. $^{13}$C {$^1$H} NMR (151 MHz, C$_6$D$_6$, 298 K) spectrum of compound 2.
Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR (243 MHz, C$_6$D$_6$, 298 K) spectrum of compound 2. *trace impurities.

Figure S4. ATR-IR spectrum of 2.
Figure S5. $^1$H NMR (600 MHz, toluene-d$_8$, 298 K) spectrum of compound 3.

Figure S6. $^{13}$C{$^1$H} NMR (151 MHz, toluene-d$_8$, 298 K) spectrum of compound 3.
Figure S7. $^{31}$P{$_1^1$H} NMR (121 MHz, toluene-d$_8$, 298 K) spectrum of compound 3. *trace impurity.

Figure S8. ATR-IR spectrum of 3.
Figure S9. $^1$H NMR (300 MHz, toluene-d$_8$) spectra of the temperature-dependent reversible reaction of DIC and gallaphosphene 1; 1) compound 2; 2) compound 2 after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2$^{nd}$ time to 90 °C.

Figure S10. $^{31}$P($^1$H) NMR (121 MHz, toluene-d$_8$) spectra tracking the temperature dependent reversible reaction of DIC and gallaphosphene 1; 1) compound 2; 2) compound 2 after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2$^{nd}$ time to 90 °C.
Figure S11. $^1$H NMR (300 MHz, toluene-d$_8$) spectra of the temperature dependent reversible reaction of DCC and gallaphosphene 1; 1) compound 3; 2) compound 3 after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.

Figure S12. $^{31}$P{$^1$H} NMR (121 MHz, toluene-d$_8$) spectra tracking the temperature dependent reversible reaction of DCC and gallaphosphene 1; 1) compound 3; 2) compound 3 after heating at 90 °C; 3) after cooling to ambient temperature; 4) after heating 2nd time to 90 °C.
Figure S13. Stacked variable temperature (VT) $^1$H NMR (300 MHz, toluene-d$_8$) spectra of compound 2.

Figure S14. Stacked variable temperature (VT) $^{31}$P NMR (121 MHz, toluene-d$_8$) spectra of compound 2.
Figure S15. Stacked variable temperature (VT) $^1$H NMR (300 MHz, toluene-d$_8$) spectra of compound 3.

Figure S16. Stacked variable temperature (VT) $^{31}$P NMR (121 MHz, toluene-d$_8$) spectra of compound 3.
Figure S17. $^1$H NMR (600 MHz, toluene-d$_8$, 298 K) spectrum of compound 4.

Figure S18. $^{13}$C{$^1$H} NMR (151 MHz, toluene-d$_8$, 298 K) spectrum of compound 4.
Figure S19. $^{31}$P-$^1$H NMR (121 MHz, C$_6$D$_6$, 298 K) spectrum of compound 4.

Figure S20. ATR-IR spectrum of 4.
Figure S21. $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.

Figure S22. $^{13}$C{$^1$H} NMR (151 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.
**Figure S23.** $^{31}$P {$^1$H} NMR (243 MHz, C$_6$D$_6$, 298 K) spectrum of compound 5.

**Figure S24.** ATR-IR spectrum of 5.
**Figure S25.** $^1$H NMR (600 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.

**Figure S26.** $^{13}$C{$^1$H} NMR (151 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6.
Figure S27. $^{31}$P/$^1$H NMR (243 MHz, C$_6$D$_6$, 298 K) spectrum of compound 6. *trace impurity.

Figure S28. ATR-IR spectrum of 6.
Figure S29. $^1$H NMR (300 MHz, toluene-d$_8$, 298 K) spectrum of reaction of 2 with CO$_2$.

Figure S30. $^{31}$P$^\{^1^H\}$ NMR (121 MHz, toluene-d$_8$, 298 K) spectrum of reaction of 2 with CO$_2$. 
Figure S31. $^1$H NMR (300 MHz, toluene-$d_8$, 298 K) spectrum of reaction of 3 with CO$_2$.

Figure S32. $^{31}$P{$^1$H} NMR (121 MHz, toluene-$d_8$, 298 K) spectrum of reaction of 3 with CO$_2$. 
**Figure S33.** $^1$H NMR (500 MHz, toluene-$d_8$, 298 K) spectrum of compound 7. *trace impurities.*

**Figure S34.** $^{13}$C-$^1$H) NMR (126 MHz, toluene-$d_8$, 298 K) spectrum of compound 7.
Figure S35. $^{31}$P{$^1$H} NMR (121 MHz, C$_6$D$_6$, 298 K) spectrum of compound 7.

Figure S36. ATR-IR spectrum of 7.
Figure S37. $^1$H NMR (300 MHz, C$_6$D$_6$, 298 K) spectrum of compound 8.

Figure S38. $^{13}$C{$^1$H} NMR (151 MHz, toluene-d$_8$, 298 K) spectrum of compound 8.
Figure S39. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, toluene-d$_8$, 298 K) spectrum of compound 8.

Figure S40. ATR-IR spectrum of 8.
**Figure S41.** $^1$H NMR (600 MHz, toluene-$d_8$, 298 K) spectrum of compound 9. *trace impurities.*

**Figure S42.** $^{13}$C\{$^1$H} NMR (151 MHz, toluene-$d_8$, 298 K) spectrum of compound 9.
Figure S43. $^{31}\text{P}\left\{{}^1\text{H}\right\}$ NMR (121 MHz, toluene-d$_8$, 298 K) spectrum of compound 9.

Figure S44. ATR-IR spectrum of 9.
Figure S45. $^1$H NMR (300 MHz, toluene-d$_8$) spectra of the temperature dependent reversible reaction of CO$_2$ and compound 4; 1) compound 7; 2) compound 7 after heating at 90 °C; 3) after cooling to ambient temperature.

Figure S46. $^{31}$P{$^1$H} NMR (121 MHz, toluene-d$_8$) spectra of the temperature dependent reversible reaction of CO$_2$ and compound 4; 1) compound 7; 2) compound 7 after heating at 90 °C; 3) after cooling to ambient temperature. #unidentified impurity.
Figure S47. $^1$H NMR (300 MHz, toluene-d$_8$) spectra of the temperature dependent reversible reaction of CO$_2$ and compound 5; 1) compound 8; 2) compound 8 after heating at 90 °C; 3) after cooling to ambient temperature.

Figure S48. $^{31}$P{$^1$H} NMR (121 MHz, toluene-d$_8$) spectra tracking the temperature dependent reversible reaction of CO$_2$ and compound 5; 1) compound 8; 2) compound 8 after heating at 90 °C; 3) after cooling to ambient temperature.
Figure S49. $^1$H NMR (300 MHz, toluene-$d_8$) spectra of the temperature dependent reversible reaction of CO$_2$ and compound 6; 1) compound 9; 2) compound 9 after heating at 90 °C; 3) after cooling to ambient temperature.

Figure S50. $^{31}$P{$^1$H} NMR (121 MHz, toluene-$d_8$) spectra tracking the temperature dependent reversible reaction of CO$_2$ and compound 6; 1) compound 9; 2) compound 9 after heating at 90 °C; 3) after cooling to ambient temperature.
3. X-Ray Crystallographic Analysis

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

CCDC-2089048 (2), -2089049 (6), -2089050 (8), and -2089051 (9) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.
Table S1. Crystal data and structure refinement of 2 and 6.

| Compound | 2          | 6          |
|----------|------------|------------|
| Emp. formula | C_{72}H_{104}ClGa_{2}N_{4}P | C_{68}H_{100}ClGa_{2}N_{3}OP |
| Formula weight | 1259.47 | 1209.38 |
| Temperature [K] | 100(2) | 100(2) |
| Crystal system | monoclinic | orthorhombic |
| Space group | P 2₁ | P 2₁ 2₁ 2₁ |
| a [Å] | 12.3792(15) | 13.2671(8) |
| b [Å] | 12.7475(15) | 14.3515(9) |
| c [Å] | 21.578(3) | 68.902(4) |
| α [°] | 90 | 90 |
| β [°] | 92.262(3) | 90 |
| γ [°] | 90 | 90 |
| V [Å³] | 3402.5(7) | 13119.1(1) |
| Z | 2 | 8 |
| ρ [Mgm⁻³] | 1.229 | 1.225 |
| μ [mm⁻¹] | 0.899 | 1.942 |
| F(000) | 1344 | 5160 |
| Crystal size [mm] | 0.411 × 0.215 × 0.130 | 0.162 × 0.096 × 0.057 |
| θ max [°] | 33.448 | 78.458 |
| Index ranges | -19 ≤ h ≤ 19 | -16 ≤ h ≤ 15 |
| | -19 ≤ k ≤ 19 | -18 ≤ k ≤ 18 |
| | -33 ≤ l ≤ 33 | -87 ≤ l ≤ 86 |
| No. of reflect. collected | 147001 | 482739 |
| Unique reflect. | 26323 | 27953 |
| Rint | 0.0306 | 0.1205 |
| Data / restraints / params. | 24791/223/830 | 25967/25/1497 |
| Goodness-of-fit on F² | 1.013 | 1.069 |
| R1 [I>2σ(I)] | 0.0214 | 0.0554 |
| wR2 [I>2σ(I)] | 0.0515 | 0.1288 |
| R1 [all data] | 0.0242 | 0.0608 |
| wR2 [all data] | 0.0522 | 0.1321 |
| x(Flack) | 0.115(3) | 0.058(13) |
| Largest diff. peak and hole max./min.[e·Å⁻³] | 0.389/-0.253 | 1.630/-0.613 |
Table S2. Crystal data and structure refinement of 8 and 9.

| Compound | 8 | 9 |
|----------|---|---|
| Emp. formula | $\text{C}_{66.50}\text{H}_{93}\text{ClGa}_2\text{N}_5\text{O}_3\text{P}$ | $\text{C}_{80.10}\text{H}_{109}\text{ClGa}_2\text{N}_5\text{O}_3\text{P}$ |
| Formula weight | 1216.31 | 1394.58 |
| Temperature [K] | 100(2) | 100(2) |
| Crystal system | triclinic | triclinic |
| Space group | $P\overline{1}$ | $P\overline{1}$ |
| $a$ [Å] | 12.7138(13) | 12.4401(7) |
| $b$ [Å] | 22.680(2) | 12.7679(7) |
| $c$ [Å] | 23.894(2) | 23.7801(12) |
| $\alpha$ [°] | 82.361(5) | 88.165(3) |
| $\beta$ [°] | 88.926(5) | 83.535(3) |
| $\gamma$ [°] | 76.638(5) | 85.239(3) |
| $V$ [Å$^3$] | 6643.2(11) | 3739.1(4) |
| $Z$ | 4 | 2 |
| $\rho$ [Mgm$^{-3}$] | 1.216 | 1.239 |
| $\mu$ [mm$^{-1}$] | 1.946 | 1.794 |
| $F$(000) | 2580 | 1484 |
| Crystal size [mm] | $0.220 \times 0.119 \times 0.042$ | $0.095 \times 0.074 \times 0.051$ |
| $\theta$ max [°] | 75.564 | 81.135 |
| Index ranges | $-15 \leq h \leq 15$ | $-15 \leq h \leq 14$ |
| | $-28 \leq k \leq 28$ | $-16 \leq k \leq 16$ |
| | $-29 \leq l \leq 29$ | $-30 \leq l \leq 30$ |
| No. of reflect. collected | 247431 | 208100 |
| Unique reflect. | 27202 | 16280 |
| $R_{int}$ | 0.2748 | 0.0714 |
| Data / restraints / params. | 17943/0/1396 | 13586/732/982 |
| Goodness-of-fit on $F^2$ | 1.076 | 1.024 |
| $R1 [I>2\sigma(I)]$ | 0.0806 | 0.0335 |
| $wR2 [I>2\sigma(I)]$ | 0.2175 | 0.0810 |
| $R1$ [all data] | 0.1266 | 0.0441 |
| $wR2$ [all data] | 0.2516 | 0.0880 |
| Largest diff. peak and hole max./min.[e·Å$^{-3}$] | 1.360/-1.459 | 0.608/-0.414 |
Figure S51. Molecular structure of 2 with thermal ellipsoids at 50% probability level. The hydrogen atoms and solvent molecules (toluene) are omitted for clarity. Selected bond length (Å) and angels (°): Ga1-N1 1.9511(11), Ga1-N2 1.9861(11), Ga1-Cl1 2.1967(4), Ga1-P1 2.3084(4), Ga2-N5 1.9279(11), Ga2-N4 1.9668(11), Ga2-N3 1.9704(12), Ga2-P1 2.3115(4), P1-C59 1.8860(13), N5-C59 1.3882(17), N6-C59 1.2834(17); N1-Ga1-N2 95.57(5), N1-Ga1-Cl1 108.52(3), N2-Ga1-Cl1 106.61(3), N1-Ga1-P1 128.82(4), N2-Ga1-P1 110.66(3), Cl1-Ga1-P1 104.915(14), N5-Ga2-N4 116.74(5), N5-Ga2-N3 116.42(5), N4-Ga2-N3 97.34(5), N5-Ga2-P1 75.96(4), N4-Ga2-P1 142.51(4), N3-Ga2-P1 108.21(4), C59-P1-Ga1 121.55(4), C59-P1-Ga2 75.66(4), Ga1-P1-Ga2 130.987(17), C59-N5-Ga2 101.82(8), N5-C59-P1 105.66(9).
Figure S52. Molecular structure of 6 with thermal ellipsoids at 50% probability level. The hydrogen atoms, a solvent molecule (n-hexane) and the alternate positions of the disordered parts are omitted for clarity. Selected bond length (Å) and angles (°): Ga1-N2 1.949(5), Ga1-N1 1.949(5), Ga1-Cl1 2.2102(17), Ga1-P1 2.296(2), Ga2-N4 1.937(4), Ga2-N3 1.961(5), Ga2-N5 2.005(4), Ga2-P1 2.266(2), P1-C59 1.904(7), O1-C59 1.234(8), N5-C59 1.366(8); N2-Ga1-N1 95.9(2), N2-Ga1-Cl1 107.14(16), N1-Ga1-Cl1 105.83(15), N2-Ga1-P1 105.32(16), N1-Ga1-P1 135.06(16), Cl1-Ga1-P1 104.99(8), N4-Ga2-N3 95.92(19), N4-Ga2-N5 113.34(18), N3-Ga2-N5 112.03(18), N4-Ga2-P1 148.61(15), N3-Ga2-P1 107.98(15), N5-Ga2-P1 76.64(13), C59-P1-Ga2 75.9(2), C59-P1-Ga1 115.8(3), Ga2-P1-Ga1 132.96(11), O1-C59-N5 126.3(6), O1-C59-P1 124.1(5), N5-C59-P1 107.5(4).
**Figure S53.** Molecular structure of 8 with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. Selected bond length (Å) and angels (°): Ga1-N1 1.944(4), Ga1-N2 1.962(4), Ga1-Cl1 2.2015(14), Ga1-P1 2.3272(15), Ga2-O2 1.840(4), Ga2-N5 1.887(5), Ga2-N4 1.917(4), Ga2-N3 1.942(5), P1-C63 1.861(5), P1-C59 1.863(6), O1-C59 1.240(7), O2-C63 1.322(7), O3-C63 1.187(7); N1-Ga1-N2 95.93(16), N1-Ga1-Cl1 106.70(14), N2-Ga1-Cl1 104.62(14), N1-Ga1-P1 118.95(15), N2-Ga1-P1 113.13(13), Cl1-Ga1-P1 115.08(5), O2-Ga2-N5 107.17(19), O2-Ga2-N4 100.45(19), N5-Ga2-N4 124.8(2), O2-Ga2-N3 114.54(19), N5-Ga2-N3 110.2(2), N4-Ga2-N3 99.73(19), C63-P1-C59 109.2(2), C63-P1-Ga1 107.9(2), C59-P1-Ga1 95.26(18), C63-O2-Ga2 127.5(4).
Figure S54. Molecular structure of 9 with thermal ellipsoids at 50% probability level. The hydrogen atoms and a solvent molecule (toluene) are omitted for clarity. Selected bond length (Å) and angels (°): Ga1-N1 1.9432(14), Ga1-N2 1.9604(14), Ga1-Cl1 2.1961(4), Ga1-P1 2.3215(5), Ga2-O2 1.8337(12), Ga2-N5 1.8963(14), Ga2-N3 1.9142(14), Ga2-N4 1.9407(13), P1-C66 1.8524(18), P1-C59 1.8563(18), O1-C59 1.228(2), O2-C66 1.323(2), O3-C66 1.214(2); N1-Ga1-N2 97.20(6), N1-Ga1-Cl1 104.46(4), N2-Ga1-Cl1 104.15(4), N1-Ga1-P1 125.76(4), N2-Ga1-P1 108.44(4), Cl1-Ga1-P1 113.815(18), O2-Ga2-N5 107.31(6), O2-Ga2-N3 102.60(6), N5-Ga2-N3 123.62(6), O2-Ga2-N4 110.11(6), N5-Ga2-N4 112.61(6), N3-Ga2-N4 99.79(6), C66-P1-C59 109.84(8), C66-P1-Ga1 99.52(5), C59-P1-Ga1 103.16(5), C66-O2-Ga2 125.50(11).
4. Computational Details

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

**Influence of the Dipp groups on the reaction behavior**

In order to determine the influence of the sterically demanding Dipp groups on the observed reaction behavior, the [2+2] cycloaddition of the reference system (RS) RS\textsubscript{1}, in which the Dipp groups in 1 are replaced by small methyl substituents, to the corresponding heterocycles RS\textsubscript{2}–RS\textsubscript{5} were studied (Scheme S2). In a second step, the energetic parameters of the cycloaddition reaction of the four-membered metallaheterocycles 2, 4, 10, 12 and RS\textsubscript{2}–RS\textsubscript{5} with CO\textsubscript{2} to the six-membered metallaheterocycles 7, 13–15 and RS\textsubscript{6}–RS\textsubscript{9} were calculated (Scheme S2). A comparison between the data for the gallaphosphenes 1 and RS\textsubscript{1} reveals, that only in the case of the carbodiimides a strong deviation from one another is found. For the addition of DMC to 1 and RS\textsubscript{1}, almost the same values are found, while this is not the case for the cycloaddition of the larger carbodiimide DIC. The reaction of DIC with RS\textsubscript{1} is energetically more favorable than that of DMC with RS\textsubscript{1}; in the case of 1, the order is reversed. This demonstrates the influence of the Dipp groups of the β-diketiminate ligands: the large isopropyl groups lead to steric repulsive interactions making the formation of 2 (R = Dipp) approx. 4 kcal/mol less favorable than that of RS\textsubscript{5} (R = Me).

The calculated Gibbs free energies (\(\Delta G\)) for the addition to the reference system RS\textsubscript{1} show the same trend as the calculated energies (\(\Delta E\)): CO\textsubscript{2} addition is by far the most unfavorable, then EtNCO and DMC additions follow, and the addition of DIC exhibits the energetically most favored value. A different order is found for gallaphosphene 1. Here, the addition of DIC is even less favorable than that of EtNCO. This means that starting from 1 the formation of 2 is less favorable than the formation of 4 due to entropic reasons. Presumably, the free
rotation of the large groups in 2 is severely restricted and the entropy loss during the cycloaddition is correspondingly high.

\[ X = \text{inversion} \]

\[ \begin{align*}
\text{RS1} & \quad \text{Ve} \quad O \quad O & \quad \text{RS2} & \quad -12.2 \quad \text{c.} \\
\text{RS1} & \quad \text{Ve} \quad \text{EtN} \quad \text{VeN} & \quad \text{RS3} & \quad -26.3 \quad \text{c.} \\
\text{RS1} & \quad \text{Ve} \quad \text{MeN} \quad \text{VeN} & \quad \text{RS4} & \quad -35.2 \quad \text{c.} \\
\text{RS1} & \quad \text{Ve} \quad \text{H}-\text{N} \quad \text{H}-\text{N} & \quad \text{RS5} & \quad -57.8 \quad \text{c.} \\
1 \quad \text{Dipp} & \quad O \quad O & \quad 10 & \quad -5.4 \quad \text{c.} \\
1 \quad \text{Dipp} & \quad \text{EtN} \quad \text{VeN} & \quad 4 & \quad -3.1 \quad \text{c.} \\
1 \quad \text{Dipp} & \quad \text{MeN} \quad \text{VeN} & \quad 12 & \quad -35.7 \quad \text{c.} \\
1 \quad \text{Dipp} & \quad \text{H}-\text{N} \quad \text{H}-\text{N} & \quad 2 & \quad -33.4 \quad \text{c.}
\end{align*} \]

\[ X = \text{rotation} \]

\[ \begin{align*}
\text{RS2} & \quad \text{Ve} \quad O \quad O & \quad \text{RS6} & \quad -12.3 \quad \text{c.} \\
\text{RS3} & \quad \text{Ve} \quad \text{EtN} \quad \text{VeN} & \quad \text{RS7} & \quad -13.7 \quad \text{c.} \\
\text{RS4} & \quad \text{Ve} \quad \text{MeN} \quad \text{MeN} & \quad \text{RS8} & \quad -5.6 \quad \text{c.} \\
\text{RS5} & \quad \text{Ve} \quad \text{H}-\text{N} \quad \text{H}-\text{N} & \quad \text{RS9} & \quad -5.8 \quad \text{c.} \\
10 \quad \text{Dipp} & \quad O \quad O & \quad 13 & \quad -13.9 \quad \text{c.} \\
12 \quad \text{Dipp} & \quad \text{EtN} \quad \text{VeN} & \quad 7 & \quad -13.4 \quad \text{c.} \\
2 \quad \text{Dipp} & \quad \text{MeN} \quad \text{MeN} & \quad 14 & \quad -5.5 \quad \text{c.} \\
2 \quad \text{Dipp} & \quad \text{H}-\text{N} \quad \text{H}-\text{N} & \quad 15 & \quad -6.2 \quad \text{c.}
\end{align*} \]

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

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

|     | E         | G         |
|-----|-----------|-----------|
| CO₂ | -188.671581 | -188.680564 |
| EtN=C=O | -247.420958 | -247.372101 |
| MeN=C=NMMe | -227.501536 | -227.441922 |
| i-PrN=C=Ni-Pr | -384.847226 | -384.683500 |
| RS1 | -5420.153444 | -5419.823496 |
| 1   | -7131.516108 | -7130.348273 |
| RS2 | -5608.844510 | -5608.504329 |
| 10  | -7320.212730 | -7319.031643 |
| RS6 | -5797.535601 | -5797.16198 |
| 13  | -7508.905936 | -7507.721369 |
| RS3 | -5667.621040 | -5667.217459 |
| 4   | -7378.986696 | -7377.736580 |
| RS7 | -5856.314385 | -5855.899541 |
| 7   | -7567.679568 | -7566.425322 |
| RS4 | -5647.711040 | -5647.295424 |
| 12  | -7359.044646 | -7357.813111 |
| RS8 | -5836.397975 | -5835.971878 |
| 14  | -7547.756456 | -7546.491359 |
| RS5 | -5805.060938 | -5804.538370 |
| 2   | -7516.416505 | -7515.045034 |
| RS9 | -5993.733767 | -5993.199743 |
| 15  | -7705.096392 | -7703.716865 |
| 11  | -7378.975817 | -7377.727521 |

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

|     | E¹  | G²  | E³  |
|-----|-----|-----|-----|
| CO₂ | -188.582581 | -188.591707 | -188.671227 |
| EtN=C=O | -247.315618 | -247.266333 | -247.420578 |
| 1   | -7126.709669 | -7125.521419 | -7131.508923 |
| TS₁₋₁₀ | -7315.300074 | -7314.101426 | -7320.177414 |
| 10  | -7315.325668 | -7314.129424 | -7320.204522 |
| TS₁₋₄ | -7374.051336 | -7372.786884 | -7378.942449 |
| 4   | -7374.090857 | -7372.824263 | -7378.980314 |

* B3LYP-D3BJ/6-31G*.  ** B3LYP-D3BJ/def2-TZVP//B3LYP-D3BJ/6-31G*.

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

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

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

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -1.36084900 | -0.06937300 | -0.00004500 |
Cartesian coordinates of the optimized geometry for MeN=C=NMe at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):
N   -1.15290000  0.40013900  -0.37850000
N    1.15255700  0.39858700   0.37923500
C   -0.00011700  0.32117800   0.00022100
C    2.28924100 -0.35503500  -0.11874500
H    3.04375600  0.34083500  -0.48810000
H    2.73411200 -0.92027800   0.70131800
H    2.02251700 -1.04604800   0.70331300
H   -2.28896300 -0.35562000  -0.11874500
C   -2.28896300 -0.35562000   0.11874500
H   -3.04348100  0.33878000  -0.49023200
H   -2.73421800 -0.91854000  -0.70331300
H   -2.02124800 -1.04896300   0.91934100

Cartesian coordinates of the optimized geometry for i-PrN=C=Ni-Pr at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):
N   -1.16163100  0.55712800  -0.35515100
N    1.16165000  0.55724600   0.35492800
C   -0.00000200  0.48622800  -0.00004300
C    2.27882700 -0.22607800   0.18811700
H    1.91232200 -0.88058300   0.98714400
H    3.21707600 -0.45700300  -1.74279000
H    3.71083600 -1.66938000  -0.54711200
H   -2.12056400 -1.77707200  -1.31858100
C   -3.31097900  0.73194000  -0.77217300
H   -4.15758600  1.33234800  -1.57104200
H   -3.67746000  1.40796200  -0.00226600
C    2.27885300 -0.22606300  -0.18815200
H    3.74612500  1.26225400  -0.63579700
C    4.22670400  0.00016500  -1.00936300

Cartesian coordinates of the optimized geometry for RS1 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):
Cl   0.00000030  0.00017800  -1.39219600
P    0.00000800  -0.00035100  2.33073900
Ga   1.47543700  -0.00010300   0.64121800
Ga  -1.47538100 -0.00010300  -0.64121800
N    2.67792300 -1.45122800   0.12459500
N    2.67792300 -1.45122800   0.12459500
N   -2.67792300  1.45122800  -0.12459500
C    3.74612500  1.26225400  -0.63579700
C    4.22670400  0.00016500  -1.00936300
Cartesian coordinates of the optimized geometry for 1 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Atomic Symbol | x     | y     | z     |
|---------------|-------|-------|-------|
| 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 |
| C             | -3.26851000 | -1.60217000 | 0.37982100 |
| C             | -3.20010000 | 0.95289400 | 0.94558700 |
| C             | 4.45837100 | -0.48143900 | 0.89056500 |
| C             | 4.90750000 | 0.73799000 | 0.37428100 |
| H             | 5.95223400 | 0.94234500 | 0.49621700 |
| C             | 4.20837600 | 1.63564200 | -0.44706000 |
| C             | 5.50887900 | -1.37552400 | 2.50115400 |
| H             | 6.00313000 | -0.95102400 | 1.36635500 |
| H             | 5.48596800 | -2.37304200 | 1.06537700 |
| C             | 5.05298400 | 2.68814800 | -1.12297900 |
| H             | 6.09750000 | 2.36736700 | -1.17049900 |
| H             | 5.01117600 | 3.61691300 | -0.55333900 |
| H             | 4.69886900 | 2.90886600 | -2.12685200 |
| C             | 2.92768100 | -2.27445400 | 1.13154900 |
| H             | 2.72142900 | -2.70136800 | 2.45245500 |
| C             | 2.58053000 | -4.06658200 | 2.69394100 |
| H             | 2.42744500 | -4.41198000 | 3.70789900 |
| C             | 2.62954100 | -4.98724500 | 1.66127500 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 2.52570900| -6.04461400| 1.86992700 |
| C       | 2.78579400| -4.54673500| 0.35712500 |
| H       | 2.79963600| -5.26691400| -0.45012600|
| C       | 3.02932500| -3.92596000| 0.06656400 |
| C       | 3.13149600| -2.74873100| -1.37049100|
| H       | 2.98810200| -1.67099800| 1.40069900 |
| C       | 4.56437200| -3.03071100| 1.84154400 |
| H       | 4.69651100| -2.71139400| 2.87701000 |
| H       | 4.79873600| -4.09832100| 1.78548100 |
| C       | 2.10661700| -3.37329000| 2.32025700 |
| H       | 3.20025000| 2.48910200  | -2.90567900|
| C       | 2.07859500| 3.83150800  | 1.28704090 |
| C       | 1.55595300| 4.67348800  | 2.26827900 |
| H       | 2.45753800| 5.71151600  | 0.02724400 |
| C       | 2.26765100| 4.20651500  | 3.53709000 |
| H       | 4.85960600| 4.87592700  | 2.84678000 |
| C       | 1.48943600| 2.87325500  | 3.84695100 |
| C       | 1.25081000| 2.51335200  | 4.83752200 |
| H       | 2.86076800| 3.63215000  | 0.09986000 |
| C       | 3.20149500| 5.65797400  | 0.75540000 |
| C       | 3.45544000| 9.90667000  | 1.09452400|
| H       | 4.04553200| 6.98451300  | 0.37081100|
| H       | 4.41558900| 5.51868200  | 0.48645700 |
| C       | 1.01460000| 4.66815400  | 0.81263600 |
| C       | 0.39582100| 3.77684700  | 0.85904700 |
| H       | 0.45471400| 5.44833100  | 0.29289500 |
| C       | 1.19095100| 4.99887400  | 1.83771900 |
| C       | 2.30559800| 0.54985100  | 3.27460100 |
| H       | 2.13122900| -0.04720000 | 2.38132600 |
| C       | 3.77059700| 0.35593100  | 3.68830600 |
| C       | 4.45754400| 0.58741100  | 2.87623200 |
| H       | 4.01826800| 0.99548400  | 4.53873500 |
| H       | 3.94494800| -0.60483900| 3.98314600 |
| C       | 1.37234200| 0.00389100  | 4.35340500 |
| C       | 1.50750600| -1.07405600| 4.46601700 |
| H       | 1.57543800| 0.44466600  | 5.33198700 |
| C       | 0.33157300| 0.18847600  | 4.09795300 |
| C       | -4.56225400| -1.56777000| 0.11023000 |
| C       | -5.17237500| -0.50630500| 0.57109600 |
| H       | -6.23707300| -0.59169300| 0.78306000 |
| C       | -4.59105900| 0.61867500  | 1.60288900 |
| C       | -5.94596000| 2.67699400  | 0.59684800 |
| H       | -4.97613400| 3.64765700  | 0.49214000 |
| C       | -5.56778700| 2.54106400  | 1.65916900 |
| H       | -6.39901300| 2.67363500  | 0.56976000 |
| 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       | -2.75997800| 2.55373800  | 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 |
| C       | -3.99165600| 0.82042100  | 2.52547200 |
| C       | -4.40548600| 1.81970000  | 4.35755800 |
| H       | -3.89166400| 2.30917800  | 5.18645600 |
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| 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 | -4.61304100 |
| C     | -2.06917200 | -3.87183300 | 0.97596600  |
| H     | -2.45146600 | -2.94180000 | 1.39118400  |
| C     | -2.99249300 | -5.00218000 | 1.45168800  |
| H     | -2.66186400 | -5.96500300 | 1.05670700  |
| H     | -3.98394900 | -4.06562800 | 2.54181800  |
| C     | -0.65008700 | -4.06554000 | 1.50880500  |
| H     | -0.65002400 | -4.05185300 | 2.59989700  |
| H     | 0.00775600  | -3.27411400 | 1.15463100  |
| C     | -2.84456200 | 2.26637500  | 1.34227200  |
| H     | -2.70110500 | 3.25246700  | 0.35698400  |
| C     | -2.98394900 | -5.06562800 | 2.54181800  |
| H     | -2.09730500 | 4.81587400  | 2.09929800  |
| C     | -1.79760500 | 5.81258500  | 2.39572100  |
| H     | -2.22791400 | 3.82017700  | 3.05614200  |
| C     | -2.03565100 | 4.05499400  | 4.09322600  |
| H     | -2.78564200 | 1.44246600  | 3.74747500  |
| C     | -3.56361100 | 0.76508900  | 3.39186600  |
| H     | -4.10653300 | 0.61988800  | 3.89263200  |
| C     | -1.66166000 | -0.21275200 | 4.58734700  |
| H     | -0.68313800 | 1.22335300  | 4.25705300  |
| C     | -1.81125000 | 0.20175200  | 2.93834600  |
| H     | -3.24272000 | 1.97174700  | 5.10838300  |
| H     | -3.47816300 | 1.13587600  | 5.76927100  |
| C     | -4.13238500 | 2.59845500  | 5.02116300  |
| H     | -2.46345200 | 2.55931100  | 5.59647300  |
| C     | -2.94336200 | 2.97148900  | -1.11612000 |
| H     | -3.27897800 | 1.93893000  | -1.21450900 |
| C     | -4.05639000 | 3.85719300  | -1.68912100 |
| H     | -3.77833600 | 4.91222300  | -1.66060000 |
| H     | -4.24990600 | 3.59291000  | -2.73056700 |
| H     | -4.98788500 | 3.74308300  | -1.13174800 |
| C     | -1.65157700 | 3.11636100  | -1.92566000 |
| H     | -0.87424100 | 2.44581000  | -1.56038200 |
| H     | -1.83012800 | 2.87901700  | -2.97574000 |
| C     | -1.26636200 | 4.13431800  | -1.87448100 |
| H     | 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     | 3.47758000  | -1.29716400 | 5.55136400  |
| H     | 3.18358500  | -3.01504400 | 5.26844000  |
| H     | 4.54358600  | -2.20025900 | 4.50090300  |

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

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C1    | 0.87142800 | -2.09710200 | -1.63002300 |
| P     | 0.17845100 | 1.42019900  | -0.14733000 |
| Ga    | 1.68133400 | -0.31741400 | -0.56199500 |
| Ga    | -1.87274400 | 0.45763300  | 0.29628600  |
| N     | 3.22553800 | 0.30417100  | -1.57586300 |
| N     | 2.65379600 | -0.86039600 | 2.02889300  |
| N     | -3.50439300 | 1.41651900  | -0.11525100 |
| N     | -2.61667900 | -1.32045200 | 0.29505100  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 4.31670300 | 0.70849600 | -0.93842000 |
| C    | 4.53925000 | 0.51346600 | 0.43064700  |
| H    | 5.44096400 | 0.95301100 | 0.82588800  |
| C    | 3.78538800 | -0.24542700 | 1.34030600  |
| H    | 5.92776400 | 0.74957700 | -2.46798500 |
| H    | 6.19078000 | 1.75046300 | -1.05908900 |
| C    | 4.31285400 | -0.36384300 | 2.74350900  |
| H    | 5.21252700 | 0.23216200 | 2.86991600  |
| H    | 4.54942000 | -1.40051700 | 2.99194800  |
| H    | 3.55613300 | -0.01772900 | 3.45082400  |
| C    | -4.59702400 | 0.79640700 | -0.54374500 |
| C    | -4.71766100 | -0.59633600 | -0.63703800 |
| H    | -5.65161600 | -0.95980200 | -1.03491900 |
| C    | -3.81539100 | -1.58087200 | -0.20968300 |
| C    | -5.78853500 | 1.62175500 | -0.94975800 |
| H    | -5.52844300 | 2.31133500 | -1.75548300 |
| H    | -6.14241500 | 2.22718500 | -0.11271600 |
| C    | -6.60401300 | 0.98738200 | -1.28569400 |
| C    | -4.26319000 | -3.01453800 | -0.31198200 |
| C    | -5.20441900 | -3.08671800 | -0.85007200 |
| H    | -4.40380300 | -3.44758300 | 0.68096300  |
| O    | -3.51486700 | -3.62028500 | -0.82542200 |
| O    | -1.18727100 | 0.83102900 | 2.07127000  |
| C    | 0.04983300 | -0.48770200 | -0.64690600 |
| O    | 0.93354100 | 1.41027200 | 2.56747700  |
| C    | -1.78183100 | -2.39331200 | -0.82896700 |
| H    | -1.31346000 | -2.97431900 | -0.03281200 |
| H    | -0.99272800 | -1.94712400 | 1.42875700  |
| H    | -2.35179300 | -3.05907000 | 1.47810800  |
| C    | -3.46788100 | 2.87118500 | -0.00323300 |
| H    | -4.18691300 | 3.23635200 | 0.73415900  |
| H    | -2.47395300 | 3.17447500 | 0.31899000  |
| H    | -3.67276800 | 3.35974500 | -0.95880200 |
| C    | 3.07274900 | 0.51641000 | -3.00833100 |
| H    | 2.19900500 | -0.03343400 | -3.35275800 |
| H    | 2.92800400 | 1.57430200 | -3.24907000 |
| H    | 3.93412600 | 0.15065900 | -3.57080800 |
| C    | 1.96695200 | -1.69427400 | 2.00681100  |
| H    | 1.47815500 | -1.08841600 | 2.77361700  |
| H    | 1.21265100 | -2.28219600 | 1.48782500  |
| H    | 2.64889600 | -2.39527800 | 2.49035400  |

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

| Atom | X    | Y    | Z    |
|------|------|------|------|
| Cl   | 1.53505000 | 0.90862400 | 2.68492000 |
| P    | 0.03398900 | -0.48770200 | -0.64690600 |
| Ga   | 1.88376700 | 0.03220700 | 0.66521700  |
| Ga   | -2.09240300 | 0.39491300 | -0.45416000 |
| N    | 2.83554500 | -1.66508000 | 1.08451100  |
| N    | 3.46416500 | 0.95968500 | -0.03482700 |
| N    | -3.49256800 | -0.89556600 | -0.91661000 |
| N    | -3.23462000 | 1.73889300 | -0.34337400 |
| C    | 4.12598400 | -1.62431500 | 1.38626500  |
| C    | 4.92367700 | -0.48183500 | 1.23533000  |
| H    | 5.93285400 | -0.50757200 | 1.60611700  |
| C    | 4.64881800 | 0.67874600 | 0.51121000  |
| C    | 4.82055300 | -2.85118500 | 1.91969500  |
| H    | 4.75377500 | -2.86220400 | 3.00879400  |
| H    | 5.87383000 | -2.83747600 | 1.64900800  |
| C    | 4.36549800 | -3.76783100 | 1.55437000  |
| C    | 5.78306000 | 1.65680500 | 0.34683700  |
| C    | 6.73666200 | 1.18417200 | 0.57028800  |
| C    | 5.63852800 | 2.48575700 | 1.04235600  |
| H    | 5.81578200 | 2.08040300 | -0.65344300 |

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

|     | X         | Y         | Z         |
|-----|-----------|-----------|-----------|
| C   | -3.02741800 | -3.20699100 | -0.27322700 |
| C   | -2.73340700 | -1.45398800 | -3.69340600 |
| H   | -2.89619700 | -0.48375600 | -3.23028300 |
| C   | -3.89325600 | -1.70893600 | -4.66560900 |
| H   | -3.78881100 | -2.68032000 | -5.15406100 |
| H   | -3.91053300 | -0.94140400 | -5.44188800 |
| C   | -4.85879500 | -1.69277400 | -4.15821500 |
| C   | -3.39175900 | -2.90115200 | 1.16786100  |
| H   | -3.88454200 | -1.92979200 | 1.19700600  |
| C   | -4.36953100 | -3.92266100 | 1.75827800  |
| H   | -3.91408000 | -4.91053000 | 1.84391100  |
| H   | -5.26571500 | -4.02341200 | 1.14355200  |
| C   | -2.12616600 | -2.80228100 | 2.02337000  |
| C   | -2.65217300 | 2.82790000  | 1.08645700  |
| C   | -2.18903000 | 3.96462400  | 0.40594600  |
| C   | -1.67366300 | 5.01194900  | 1.16765900  |
| H   | -1.31804400 | 5.90187400  | 0.66616500  |
| C   | -1.59232900 | 4.92806000  | 2.54624500  |
| C   | -1.17280200 | 5.74761000  | 3.11534800  |
| C   | -2.03884700 | 3.78883700  | 3.19730700  |
| C   | -1.96509000 | 3.72848000  | 4.27448300  |
| C   | -2.58964600 | 2.72684000  | 2.48652700  |
| C   | -3.09323100 | 1.49652400  | 3.22135400  |
| C   | -3.74688800 | 0.94462900  | 2.54597000  |
| C   | -1.92789200 | 0.57175600  | 3.58233300  |
| H   | -2.29076800 | 0.32965900  | 4.07891200  |
| C   | -1.22363000 | 1.07187600  | 4.24799200  |
| C   | -1.36568500 | 0.27618600  | 2.69805100  |
| C   | -3.92088500 | 1.84216700  | 4.46326000  |
| C   | -4.35906400 | 0.93501100  | 4.88355400  |
| C   | -4.73143800 | 2.53409500  | 4.22723000  |
| C   | -3.30936300 | 2.29918900  | 5.24264700  |
| C   | -2.24793800 | 4.10167000  | 1.10533100  |
| C   | -2.63221900 | 3.17321300  | 1.51956100  |
| C   | -3.19678900 | 5.22974000  | 1.53142600  |
| C   | -2.85369400 | 6.19828700  | 1.61857000  |
| C   | -3.24659100 | 5.28609600  | 2.62048000  |
| C   | -4.20971300 | 5.07140100  | 1.15741500  |
| C   | -0.85372400 | 4.31282600  | 1.70650500  |
| C   | -0.16177200 | 3.52973500  | 1.40715100  |
| C   | -0.90863600 | 4.29593400  | 2.79573000  |
| C   | -0.43031200 | 5.27223300  | 1.40170600  |
| C   | 1.87831600  | 2.65634000  | 3.70311100  |
| C   | 2.50964600  | 1.79143800  | 3.50782600  |
| C   | 0.55744900  | 2.12322000  | 4.26851700  |
| C   | 0.73918200  | 1.55529500  | 5.18278900  |
| C   | 0.07036500  | 1.46010100  | 3.55984300  |
| C   | 0.12550500  | 2.94206800  | 4.50424000  |
| C   | 2.57874900  | 3.53852400  | 4.74531000  |
| C   | 2.83318900  | 2.94724700  | 5.62695500  |
| C   | 1.93147600  | 4.35447000  | 5.07291500  |
| C   | 3.49434600  | 3.98378600  | 4.35618400  |
| O   | -1.42384000 | 1.14139100  | -2.10908500 |
| C   | -0.15068200 | 0.77242000  | -2.06836100 |
| O   | 0.69372900  | 1.10776200  | -2.85807200 |
Cartesian coordinates of the optimized geometry for 13 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ga      | -2.47997200 | 0.56501200 | -0.63432800 |
| Ga      | -2.76423700 | -0.74788000 | 0.20177100 |
| Cl      | -2.05878900 | -0.55979600 | 2.51866200 |
| P       | -0.58765500 | -1.05342400 | -0.40237500 |
| O       | -0.63103200 | -0.86970800 | 2.44297800 |
| O       | -0.47278100 | -0.53868200 | 0.86491400 |
| O       | -0.18712500 | 0.53542100 | 0.85506100 |
| C       | 3.15147400 | -2.79818300 | -0.62368000 |
| C       | 2.22850300 | -2.71687100 | -1.19016400 |
| H       | 3.90256300 | -3.27252400 | -1.25846200 |
| H       | 2.94753300 | -3.47348400 | 0.23660700 |
| C       | 3.14994800 | 2.79375800 | -0.64372800 |
| C       | 3.90086400 | 3.26397300 | -1.28177100 |
| H       | 2.22714600 | 2.70785900 | -1.20982800 |
| H       | 2.94549000 | 3.43905600 | 0.21194000 |
| C       | -2.44458800 | -0.00865700 | 2.64050200 |
| H       | -1.40545700 | -0.00696800 | -2.32020900 |
| H       | -2.60330200 | -0.89840500 | -3.25333800 |
| C       | -3.84619600 | 0.00971600 | 2.82455500 |
| H       | -2.77828100 | 0.01011300 | 3.03406000 |
| H       | -4.27712400 | 0.89876400 | 3.29017300 |
| H       | -4.27764100 | -0.87586200 | 3.29626100 |
N  -3.51535400  1.82040800  -0.51901200
N   4.21958700  0.03685500   1.17154300
N   3.45590400  -1.59767200  -1.14086700
C  -5.20140300  -0.30229500   0.85101300
C  -5.59458800   0.94209100   0.34545400
H  -6.65114900   1.14974400   0.40398300
C  -4.83907200   1.87277200  -0.37383100
C  -6.30528900  -1.19418900   1.35710700
H  -6.44667300  -1.01110700   2.42409900
H  -6.06754600  -2.24734200   1.23749500
H  -7.24138500  -0.97134500   0.85033800
C  -5.60469300   2.98653000  -1.04042500
H  -5.35772100   3.94195500  -0.57853200
H  -6.67508700   2.82086000  -0.95246100
C  -3.63255300  -2.08761700   1.94876800
C  -3.42533500  -2.97340500   0.43053400
H  -2.90906800   4.98791900  -0.37719400
C  -2.94049600   4.71892800   1.74095000
C  -3.15662200  -3.83328800  -2.78176900
C  -3.50172200  -3.03839000   3.80232700
C  -3.53044600  -1.53709300  -1.29942600
C  -5.66783000  -2.85863200  -1.76117100
C  -5.81270000  -2.37226400  -1.33189800
C  -5.24904800  -3.93506600   1.72561000
C  -5.22259200  -2.51970000  -2.78754600
C  -2.61357600  -3.12102300  -2.27141700
H  -1.59898400  -2.85976200  -1.98707700
H  -2.78519200  -2.72309200  -3.27280200
H  -2.68683800  -4.20800700  -2.33859800
C  -3.63589900  -3.36640000   3.72353400
C  -3.96975300  -0.58851600   3.33792900
C  -4.82640700  -2.05223500   4.64476500
C  -5.01472800  -1.31518900   5.42810400
C  -4.56002800  -2.99206000   5.13250000
H  -5.75686600  -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
C  -2.55279100  -0.66316700   5.32213300
C  -2.89026800   2.73257700  -1.44314500
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
C  -1.37453500   5.16947800  -4.01833800
H  -2.00163600   4.89024500  -1.98374700
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  -3.83001000
H  -5.08290800   0.98230600  -3.16215500
H  -4.44040800  -0.35310500  -4.11699000
H  -4.33626100  -1.30242100  -4.73059100
C  -1.78947600   0.27042700  -4.03396200
H  -1.76424300   0.73588000  -5.02110600
H  -1.94194100  -0.79925400  -4.17838100
H  -0.81548700   0.40755900  -3.56698000
H  -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
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H  -2.95156800  6.31556600  0.05858400
C  -1.26698900  4.65910000  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  -0.26687600  1.87388500
H   6.95809100   0.69323900  1.57784600
H   7.31167700  -1.02314700  1.80428200
H   6.21842400  -0.16610000  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   3.93436100   3.48954400  3.56440500
Cartesian coordinates of the optimized geometry for RS3 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| Cl   | 1.14727600 | -1.66660000 | 1.92489400 |
| P    | 0.13175600 | -0.28555400 | -1.52790400 |
| Ga   | 1.78116900 | -0.55956600 | 0.07287900  |
| N    | 3.30357100 | -1.58987000 | -0.59475200 |
| N    | 2.77693100 | 1.02347900 | -0.66223800 |
| N    | -3.52458300 | -0.56923700 | -1.20389000 |
| C    | 4.55361300 | -1.16741000 | -0.49136900 |
| C    | 4.91928200 | 0.08176800  | -0.02820000 |
| H    | 5.97623900 | 0.29343100 | -0.03283600 |
| C    | 0.40955880 | 1.10509900  | 0.51815400  |
| C    | 5.66832000 | -0.06386000 | -0.96832900 |
| H    | 5.63083100 | -3.03086400 | -0.46293000 |
| C    | 6.63602000 | -1.61017000 | -0.78197100 |
| H    | 5.57701600 | -2.25743100 | -0.20384900 |
| C    | 4.77367100 | 2.37779900  | 0.95286200  |
| H    | 5.84961500 | 2.30945700  | 0.81895000  |
| C    | 4.56729300 | 2.59137600  | 2.00362400  |
| C    | 4.40340200 | 3.22591000  | 0.37341200  |
| C    | -4.48554900 | -1.15412000 | -0.50313700 |
| C    | -4.47142900 | -1.26917600 | 0.89362900  |
| H    | -5.30720800 | -1.79296300 | 1.32934600  |
| H    | -5.34285900 | -0.73465400 | 1.50302800  |
| H    | -5.67217100 | -1.72743000 | -1.23149800 |
| H    | -5.35609700 | -2.47375900 | -1.96317100 |
| C    | -6.20337100 | -0.94705900 | -1.78063500 |
| H    | -6.36627000 | -2.19338500 | -0.53755200 |
| C    | -3.83234600 | -0.93827600 | 3.26761900  |
| H    | -4.71738700 | -1.55243200 | 3.40887600  |
| H    | -3.99725300 | 0.02143600  | 3.76226600  |
| H    | -2.98009900 | -1.41607900 | 3.76782000  |
| C    | -0.09783400 | 1.62704200  | -1.54324200 |
| O    | 0.69718300  | 2.46797800  | -1.83414300 |
| N    | 1.34631100  | 1.84694900  | -0.93899500 |
| C    | 1.86904200  | 3.20374300  | -0.87180200 |
| H    | 1.48132100  | 3.77255200  | -1.72043500 |
| C    | 2.95629500  | 3.15263800  | -0.97432000 |
| C    | 1.50755400  | 3.91965900  | 0.42710200  |
| H    | 1.93253700  | 4.92603100  | 0.44876700  |
| H    | 0.42491900  | 3.37231300  | 1.29193000  |
| C    | 2.00810300  | 2.15505600  | 1.11962000  |
| H    | 2.30325900  | 2.47049400  | 2.13643000  |
| H    | 2.09933300  | 3.02541200  | 0.46871700  |
| H    | 0.95626300  | 1.88469000  | 1.13914600  |
| C    | 3.00408000  | -2.90292500 | -1.14957100 |
| H    | 1.92714600  | -2.99292000 | -1.28122200 |
| C    | 3.47009000  | -3.05260300 | -2.12570600 |
| H    | 3.32617400  | -3.70686600 | -0.48175800 |
| C    | -1.58505800 | 0.50140600  | 2.47642500  |
| H    | 2.14563100  | 1.15547700  | 3.14790600  |
| H    | 1.07136700  | -0.26381900 | 3.05865600  |
| C    | 1.82288700  | 1.10232800  | 1.98896200  |
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| Cl   | -1.51423300 | 0.95822400 | -2.83290200 |
| P    | -0.14305800 | -0.71048700 | 0.39277200  |
| Ga   | -1.88089300 | 0.34251500  | -0.71037600 |
| Ga   | 2.06216700  | 0.00749300  | 0.36483700  |
| N    | -3.32016800 | -1.02009200 | -0.93597300 |
| N    | -3.08238700 | 1.71751900  | 0.01682300  |
| N    | 3.15978800  | -1.58544300 | 0.86885900  |
| N    | 3.46905000  | 0.93404700  | -0.59730000 |
| C    | -4.55504200 | -0.62367700 | -1.18836600 |
| C    | -4.96334800 | 0.71878200  | -1.11815400 |
| H    | -5.96643400 | 0.91708100  | -1.46288000 |
| C    | -4.31573500 | 1.78449400  | -0.49803000 |
| C    | -5.61378800 | -1.62255000 | -1.57104000 |
| H    | -6.58769400 | -1.67637000 | -2.65889700 |
| H    | -6.55802000 | -1.30894700 | -1.18921200 |
| C    | -5.38719200 | -2.61880000 | -1.20299800 |
| C    | -5.07932800 | 3.08418400  | -0.41696800 |
| H    | -6.13523900 | 2.92654400  | -0.59119200 |
| H    | -4.69498600 | 3.75903500  | -1.18763000 |
| C    | -4.93656300 | 3.58120200  | 0.53982200  |
| C    | -2.95951200 | -2.40750500 | -0.92404100 |
| C    | -2.72907100 | -3.09477900 | -2.12593900 |
| C    | -2.33474800 | -4.43138900 | -2.05211000 |
| H    | -2.15327100 | -4.97907600 | -2.96776700 |
| C    | -2.16486300 | -5.06405300 | -0.83417000 |
| H    | -1.85394400 | -6.10073500 | -0.79903000 |
| C    | -2.38300900 | -4.36479300 | 0.34372400  |
| H    | -2.22694400 | -4.85986000 | 1.29130600  |
| C    | -2.77882700 | -3.03238700 | 0.32538400  |
| H    | -3.03030600 | -2.27952400 | 1.61873600  |
| H    | -2.74039200 | -1.24273500 | 1.45153300  |
| C    | -4.52075300 | -2.27893400 | 1.98368000  |
| C    | -5.12814900 | -1.80969000 | 1.21060400  |
| H    | -4.68116800 | -1.72896100 | 2.91268100  |
| H    | -4.88175600 | -3.30005800 | 2.12608300  |
| H    | -2.18535900 | -7.76830000 | 2.78979800  |
| H    | -2.51605200 | -3.75583900 | 3.14515800  |
| H    | -2.26365200 | -2.07357100 | 3.61844800  |
| H    | -1.13616400 | -2.84603900 | 2.50891000  |
| C    | -2.62956500 | 2.75131200  | 0.90881300  |
| C    | -1.96051100 | 3.87270200  | 0.39766400  |
| C    | -1.50649200 | 4.83985000  | 1.29418000  |
| H    | -0.97599300 | 5.70466300  | 0.91766400  |
| C    | -1.73763100 | 4.71608100  | 2.65206000  |
| C    | -1.37887900 | 5.47441700  | 3.33649600  |
| C    | -2.42754700 | 3.61521600  | 3.13828400  |
| C    | -2.59671100 | 3.52826500  | 4.20148900  |
| C    | -2.88214800 | 2.61071300  | 2.28939400  |
| C    | -1.74804300 | 4.07429900  | -1.09017200 |
| H    | -2.29102300 | 3.29535100  | -1.61941200 |
| H    | -2.29251300 | 5.42550200  | -1.57064000 |
| H    | -2.22493800 | 5.48956900  | -2.65852900 |
| H    | -1.72201100 | 6.25823400  | -1.15472800 |
| H    | -3.33576600 | 5.56620300  | -1.28423700 |
| C    | -0.27526400 | 3.93238100  | -1.47109200 |
| H    | 0.13903300  | 2.98414600  | -1.13147500 |
| H    | 0.31705800  | 4.73513400  | -1.03276000 |
| H    | -0.15391100 | 3.97142400  | -2.55276900 |
| C    | -3.64840600 | 1.42024900  | 2.84835100  |
Cartesian coordinates of the optimized geometry for RS7 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Ga   | -2.40950400| -0.00109100| -0.23309000|
| Ga   | 2.32426700 | -0.11207400| 0.25593400 |
| Cl   | -1.46907600| -0.25743500| -2.24420700|
| P    | -0.82498900| 0.62571700 | 1.38745300 |
| O    | -0.49857700| 2.73739100 | -0.13940200|
| O    | -0.68087100| -1.91786500| 2.09430500 |
| N    | -3.90468400| 1.22579800 | -0.36317900|
| N    | -3.40923400| -1.61960200| 0.13183900 |
| N    | 3.07034800 | -0.98696900| -1.28138200|
| N    | 3.94563800 | 0.20053100 | 1.24520600 |
| C    | -5.10701000| 0.88361900 | 0.07796700 |
| C    | -5.44177100| -0.39330300| 0.55116800 |
| H    | -6.45088500| -0.50616800| 0.91402800 |
| C    | -4.67232900| -1.56612200| 0.52677300 |
| C    | -6.20225900| 1.91737600 | 0.06598800 |
| H    | -6.37935100| 2.28160000 | -0.94795600|
| H    | -5.92609400| 2.78251500 | 0.67213400 |
| H    | -7.12972500| 1.50350100 | 0.45198300 |
| C    | -5.35165300| -2.84062000| 0.95324500 |
| C    | -5.44788800| -3.52847700| 0.11021800 |
| H    | -6.34547900| -2.63698700| 1.34269400 |
| C    | -4.76829200| -3.35194300| 1.72072400 |
| C    | 4.36554800 | -1.26220200| -1.37081300|
| C    | 5.31385200 | -0.90865600| -0.39892000|
| H    | 6.32935300 | -1.20021200| -0.61407000|
| C    | 5.12453200 | -0.23133500| 0.81301800 |
| C    | 4.86600700 | -1.99277900| -2.58719600|
| H    | 4.35516700 | -2.95089500| -2.70022200|
| H    | 5.93499600 | -2.17306000| -2.51978300|
| C    | 4.66754100 | -1.41689300| -3.49351600|
| C    | 6.34086900 | 0.01644600 | 1.66350000 |
| H    | 6.21756200 | -0.42500300| 2.65443800 |

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

| Symbol | X       | Y       | Z       |
|--------|---------|---------|---------|
| Ga     | 2.56739700 | 0.64157700 | -0.57765700 |
| Ga     | -2.52540600 | -0.54517100 | -0.33280500 |
| Cl     | 2.30772400 | 1.52032800 | -2.59543500 |
| P      | 0.65223500 | -0.31846900 | 0.38322400 |
| O      | 0.96561200 | -1.68637800 | -1.86924600 |
| O      | -0.06507100 | 2.15664200 | 1.12382400 |
| N      | 4.08471100 | -0.61602100 | -0.71875200 |
| N      | 3.50742800 | 1.99089700 | 0.50733800 |
| C      | 5.32572100 | -0.15373200 | -0.63739400 |
| C      | 5.65224800 | 1.13743400 | -2.06535000 |
| H      | 6.70298100 | 1.37922600 | -2.03612000 |
| H      | 6.23626000 | 2.08555600 | 0.34311000 |
| C      | 6.48624200 | -1.03684500 | -1.01821500 |
| H      | 6.72829800 | -0.86703700 | -2.06927800 |
| H      | 6.25534200 | -2.09150400 | -0.90114300 |
| C      | 7.36587900 | -0.78859100 | -0.42830600 |
| C      | 5.52819300 | 3.27085600 | 1.03294500 |
| C      | 5.24738400 | 4.18665400 | 0.51352500 |
| C      | 6.07172200 | 3.15286000 | 0.97929300 |
| C      | 5.23217000 | 3.39980000 | 0.20730220 |
| C      | 3.82674900 | -2.01155400 | -0.94745400 |
| C      | 3.57727500 | -2.82242400 | 0.17431800 |
| C      | 3.24600100 | -4.15751200 | -0.03804300 |
| H      | 3.04692000 | -4.79958400 | 0.80867300 |
| C      | 3.17079000 | -4.67909100 | -1.32008200 |
| H      | 2.90499300 | -5.71835200 | -1.46761700 |
| C      | 3.44242400 | -3.86966900 | -2.40956000 |
| C      | 3.38392400 | -4.28354500 | -3.40771000 |
| C      | 3.77290800 | -2.52593200 | -2.25068400 |
| H      | 3.74390500 | -2.28717700 | 1.58695400 |
| H      | 3.64388800 | -1.20449100 | 1.54205300 |
| C      | 5.15618700 | -2.58536300 | 2.11092000 |
## Cartesian coordinates of the optimized geometry for RS4 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Atom | X            | Y            | Z            |
|------|--------------|--------------|--------------|
| H    | -5.36366900  | 1.01253500   | 0.54128500   |
| C    | -4.84554200  | 2.97578700   | 1.18718900   |
| H    | -5.04844000  | 4.01870000   | 0.93811600   |
| H    | -3.76840300  | 2.80867800   | 1.13476500   |
| H    | -5.17488300  | 2.80867800   | 2.21357900   |
| C    | -7.10022400  | 2.22678000   | 0.33703200   |
| H    | -7.38991600  | 3.24735900   | 0.08131100   |
| H    | -7.43179000  | 2.03542400   | 1.35945600   |
| H    | -7.65483900  | 1.55174200   | -0.32350400  |
| C    | -2.75618800  | 0.58000500   | -3.77498200  |
| H    | -2.85221300  | -0.36952300  | -3.26069700  |
| H    | -2.48392100  | -0.44050600  | -5.66352200  |
| H    | -3.01678400  | 1.22694900   | -5.84566200  |
| C    | -2.51553200  | -1.86562000  | 2.26626100   |
| C    | -2.49076800  | -0.86412200  | 3.25533500   |
| C    | -1.67868600  | -1.06008600  | 4.36870800   |
| C    | -1.64101200  | -0.30247400  | 5.13737700   |
| C    | -0.90890000  | -2.20289700  | 4.50650600   |
| C    | -0.93619100  | -3.16956500  | 3.51952700   |
| C    | -0.32162400  | -4.05305700  | 3.62387400   |
| C    | -1.72409600  | -3.02125000  | 2.37899000   |
| C    | -3.15635700  | 0.37929900   | 3.16347500   |
| H    | -3.55379100  | 0.57256100   | 2.11164700   |
| C    | -2.66950900  | 1.62743300   | 3.72222700   |
| H    | -1.71455400  | 1.80978800   | 3.23053300   |
| H    | -2.50106700  | 1.55278000   | 4.79778000   |
| C    | -3.29817900  | 2.50123900   | 3.55643700   |
| C    | -4.70822600  | 0.13660500   | 3.84932100   |
| H    | -5.34642400  | 1.01790100   | 3.76280900   |
| H    | -5.56914200  | -0.07826000  | 4.91103800   |
| H    | -5.23750200  | -0.70717600  | 3.40513200   |
| C    | -1.68183800  | -4.11302900  | 1.32606500   |
| H    | -2.27295900  | -3.78267300  | 0.47305600   |
| C    | -0.25087800  | -4.36158100  | 0.83782200   |
| H    | -0.23962800  | -5.12190700  | 0.05736600   |
| H    | 0.38241500   | -4.71629600  | 1.65083600   |
| H    | 0.20226000   | -3.46009900  | 0.43346100   |
| C    | -2.28813000  | -5.42371800  | 1.84799600   |
| C    | -3.29927100  | -5.26594000  | 2.22852900   |
| C    | -1.68359300  | -5.83201100  | 2.56011300   |
| H    | -2.32073900  | -6.16928500  | 1.05086600   |
| C    | 0.08199200   | -1.24969000  | -1.14210300  |
| C    | -0.49002400  | 1.14193600   | 0.62552000   |
| N    | -1.23532400  | -1.51197300  | -1.32111500  |
| C    | -1.58571600  | -2.33924300  | -2.48843100  |
| H    | -1.09002700  | -2.90817100  | -3.37127300  |
| H    | -2.66361200  | -2.25740600  | -2.63621100  |
| C    | -1.21277900  | -3.81068100  | -2.37028400  |
| H    | -2.14648200  | -3.92498000  | -2.19101600  |
| H    | -1.76431800  | -4.29587500  | -1.56617500  |
| H    | -1.46276600  | -4.31976300  | -3.30397300  |
| O    | -1.77444900  | 0.98930400   | 0.34607500   |

Cartesian coordinates of the optimized geometry for RS4 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):
Cartesian coordinates of the optimized geometry for 12 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga
-1.87698600 -0.18671800 0.21768900
Ga
2.28363500 0.21095300 0.04361200
Cl
-1.89589700 -0.35774500 -2.00075400
P
0.14064800 0.77372400 0.73965600
N
-2.78050900 -1.75996400 0.96562800
N
-3.31179800 1.11922700 0.73894300
N
3.13209200 1.79056500 -0.78123500
N
3.35270700 -1.13783200 -0.90691200
N    2.33601700   0.12791400   1.97177500
N    -3.70422000  -1.64138000  -1.92203300
C    -4.30271400  -0.43944300   2.28588200
H    -5.03047800  -0.50256600   3.08039500
C    -4.20990200   0.81880900   1.67016700
C    -4.13653800  -2.86879400   2.68178500
H    -5.08625800  -2.69771400   3.44047500
H    -3.38624700  -3.09904400   3.44047500
H    -4.21912200  -3.74135700   2.03910100
C    -5.20938600   1.83663200   2.14273700
H    -6.21228800   1.41519100   2.08069900
H    -5.17505500   2.75837000   1.57277000
H    -5.02020600   2.06454200   3.19258000
C    -2.42981200  -3.06347400   0.47304200
C    -3.15661000  -3.58096900  -0.61626300
C    -2.82300800  -4.84918100  -1.08371200
H    -3.36961200  -5.26963700  -1.91662800
C    -1.79109800  -5.57737500  -0.51001600
H    -2.67118000  -5.61189800   0.98740100
C    -1.38918600  -3.78930300   1.06994700
C    -4.30514500  -2.81230100  -1.24772600
C    -5.65733900  -3.25710900  -0.67315100
H    -6.46942800  -2.69443600  -1.13873300
H    -5.71350600  -3.09358600   0.40236200
H    -5.82939800  -4.31922400  -0.86209800
C    -4.31537100  -2.90660600  -2.77495600
H    -4.55960000  -3.91318000  -3.11985200
H    -3.35022700  -2.62105000  -3.18910700
H    -5.07056200  -2.23103400  -3.18070100
C    -0.60659200  -3.25725000   2.25372300
H    -1.03421200  -2.29831400   2.53934200
C    -0.68658300  -4.18844000   3.46954200
H    -1.71670700  -4.41957900   3.74340500
H    -0.19956800  -3.72090400  -4.32687800
H    -0.17850900  -5.13529200   3.27420100
C    -0.85169200  -3.01387600   1.87367000
H    -1.34504500  -3.94331800   1.59132900
H    -1.37822400  -2.56436600   2.70822900
H    -0.91749500  -2.32347800   1.03013700
C    -3.32142800   2.40192500   0.08390700
C    -4.00599100   2.52297000  -1.14096400
C    -3.96552800   3.74814600  -1.80137200
H    -4.48225500   3.85948600  -2.74439300
C    -3.26898000   4.82419100  -1.27620400
H    -3.23899800   5.76502800  -1.81158700
H    -2.61445700   4.69318400  -0.06435900
H    -2.07700100   5.53726800   0.34560200
C    -2.63121200   3.49306600   0.64543300
C    -4.83230200   1.38532600  -1.71705500
C    -4.45749500   0.45738600  -1.29232600
C    -6.30731300   1.51928800  -1.31174300
H    -6.88743100   0.68549000   1.71343100
H    -6.73246000   2.44673500  -1.70200200
H    -6.43231900   1.52502900  -0.23044400
C    -4.71494300   1.26627300  -3.23803600
H    -5.15469900   0.34153600  -3.57353400
H    -3.67304000   1.23559200  -3.55011000
H    -5.20943400   2.09502300  -3.74894100
C    -1.97026400   3.44625200   2.01263400
H    -1.93069900   2.40669300   2.32913600
C    -2.78695500   4.23061000   3.04929200
H    -3.82086400   3.89649400   3.11138400
H    -2.80265100   5.29562400   2.79740400
H    -2.33654100   4.13043100   4.03811500
Cartesian coordinates of the optimized geometry for RS8 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga  -2.20042100  -0.47646900  0.02499400
Ga   2.36625400  -0.01785700 -0.20617000
Cl  -1.29910800  -2.06139700  1.30428900
P  -0.74707400   0.40262200 -1.59004000
N  -2.96697700   0.81025300  1.25713400
N  -3.84419300  -1.13340100 -0.76389700
N   3.14463200  -0.91265100  1.30570700
N   1.19125100   1.37557900  0.23343700
N  -0.49559800   2.83374000 -0.31760800
C  -4.26248100   1.09270300  1.25123700
C  -5.01716700  -0.58836100 -0.48642600
C  -4.77474000   2.14268500  2.01240000
H  -5.83554500   2.32065200  2.04719000
H  -4.23684400   3.08295300  2.06585200
H  -4.62304100   1.83429000  3.23765900
C  -6.24467400  -1.12247700 -1.17638200
H  -7.13813600  -0.60807100 -0.83483000
H  -6.36145000  -2.19103700 -0.98519000
H  -6.16524400  -0.99782400  2.25837200
C   5.19136100   0.29943800 -0.57334400
C   5.40400800  -0.44823100  0.59306100
C   6.43603400  -0.61556700  0.85670200
C   4.45929000  -1.00913800  1.46437500
C   6.40742500   0.78780000 -1.31330700
C   6.40906300   0.41934700 -2.34113300
H   7.31929300   0.45646100 -0.82458500
H   6.41819200   1.87865500 -1.36430700
C   4.98696300  -1.76460600  2.65419800
H   4.63134700  -1.32013300  3.58587700
H   6.07322100  -1.76573200  2.66310800
H   4.63688900  -2.79864500  2.64084800
C   0.04723000   1.68110600 -0.46453200
O   1.54561500  -1.21266500  1.35504300
C   0.28170400  -1.16457600 -1.71521300
O  -0.28883800  -2.10111800 -2.23296300
C  -3.72848900  -2.24672800 -1.70395000
H  -4.18616400  -3.15489500 -1.30251300
H  -4.19856900  -2.05119000 -2.66186300
H  -2.67557800  -2.44883800 -1.89068200
C  -2.07062300   1.43886300  2.22325300
H  -1.96444700   2.50947800  2.04125000
H  -2.41184800   1.27875700  3.24854600
H  -1.08362300   0.99308500  2.12753500
C   3.84145100   1.38394300 -2.27031800
H   4.23748800   0.85829600 -3.14267100
Cartesian coordinates of the optimized geometry for 14 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga  2.51899400 -0.20800400 -0.00612500
Ga -2.85473700  0.52118400 -0.20092500
Cl  2.98703100  0.30375700  2.09413700
P   0.38040800  0.76373200 -0.30944800
N   2.89367900 -2.07771200 -0.95168000
N   -3.44988300  2.20207800  0.58138100
N  -4.55387500 -0.42396000 -0.15844400
N  -1.91740500  0.70625300 -1.81373500
N  -0.04442300  0.43515800 -3.10405800
C   3.68132600 -2.34001000 -1.58151000
C   4.34305700 -1.36567300 -2.34700000
H   4.83937500 -1.73263600 -3.23166900
C   4.59215700 -0.03610100 -2.01869900
C   3.96804500 -3.76923600 -1.97258900
H   4.18260500 -3.82851400 -3.03773600
H   3.15901800 -4.44782400 -1.72511600
H   4.85685900 -4.10842400 -1.43729600
C   5.51573300  0.73846000 -2.92461000
H   5.99598500  0.08235800 -3.64865000
H   6.27722900  1.27755900 -2.36543600
H   4.93252900  1.48610900 -3.46558900
C   2.29015600 -3.18259700  0.15715100
C   2.94393600 -3.75235000  1.25524800
C   3.26991100 -4.87944600  1.84419000
H   2.86094700 -5.34221100  2.69011100
C   1.18177400 -5.40856400  1.37225800
C   0.75392300 -6.28541800  1.84162900
C   0.52178200 -4.97283400  0.31847300
H  -0.43071700 -5.18208800 -0.01368600
C   1.05264100 -3.66605200 -0.29969100
C   4.22567600 -3.17920800  1.83136600
H   4.42897700 -2.23897700  1.32306000
C   5.42719000 -4.10346200  1.60195900
H   6.33634200 -3.65165400  2.00451600
H   5.59111300 -4.29966100  0.54182700
H   5.28308300 -5.06510600  2.90853600
C   4.06726400 -2.86091100  3.32250300
H   3.93806200 -3.77171600  3.91075400
H   3.20806300 -2.21419800  3.48839300
H   4.95557100 -2.34675400  3.69280300
C   0.28825800 -2.96182200 -1.40558900
H   0.58324900 -1.91566200 -1.37646700
C   0.67202000 -3.47516800 -2.81331300
H   1.65538800 -3.30062500 -3.08713200
H  -0.00534300 -2.95705400 -3.54539900
H   0.41873600 -4.54678300 -2.89186500
C  -1.22320700 -3.00716100 -1.18679000
H  -1.64454200 -3.97815600 -1.44921900
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -1.69857800 | -2.2646500 | -1.82402500 |
| H    | -1.49192600 | -2.79096300 | -0.15623900 |
| C    | 4.74425200  | 1.71652600  | 0.37022400  |
| C    | 5.89107300  | 1.49032200  | -0.41583100 |
| H    | 6.59114000  | 2.59481000  | -0.84529000 |
| C    | 7.48007300  | 2.44291800  | 1.44298700  |
| C    | 6.16317400  | 3.88681000  | 0.57814400  |
| C    | 5.00592100  | 4.08804100  | 0.15361300  |
| H    | 4.65976400  | 5.09654000  | -0.33929900 |
| C    | 6.16317400  | 3.88681000  | 0.57814400  |
| H    | 6.72295200  | 4.73216000  | 0.95540400  |
| C    | 6.59114000  | 2.59481000  | -0.84529000 |
| H    | 7.48007300  | 2.44291800  | 1.44298700  |
| C    | 6.16317400  | 3.88681000  | 0.57814400  |
| C    | 5.00592100  | 4.08804100  | 0.15361300  |
| H    | 4.65976400  | 5.09654000  | -0.33929900 |
| C    | 6.16317400  | 3.88681000  | 0.57814400  |
| C    | 5.00592100  | 4.08804100  | 0.15361300  |
| H    | 4.65976400  | 5.09654000  | -0.33929900 |
| C    | 6.16317400  | 3.88681000  | 0.57814400  |
| C    | 5.00592100  | 4.08804100  | 0.15361300  |
| H    | 4.65976400  | 5.09654000  | -0.33929900 |
Cartesian coordinates of the optimized geometry for RS5 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

|   |   |   |
|---|---|---|
| C | -1.51594800 | 4.17549600 | -2.32539300 |
| H | -0.99904000 | 3.22481500 | -2.21381300 |
| H | -0.77783700 | 4.97588300 | -2.25041600 |
| H | -1.94724300 | 4.21784100 | -3.32723300 |
| C | -4.52736600 | -1.86787400 | -0.17195500 |
| C | -4.29115700 | -2.53276600 | 1.04741400 |
| C | -4.23828800 | -3.92387000 | 1.03636600 |
| H | -4.05389300 | -4.45299400 | 1.96088700 |
| C | -4.41826300 | -4.64153000 | -0.13496700 |
| H | -4.37246400 | -5.72300700 | -0.12156700 |
| C | -4.70978400 | -2.57876400 | -1.36800400 |
| H | -3.95701000 | -1.79297200 | 2.36851100 |
| C | -5.48330400 | -1.83943000 | 3.14625100 |
| H | -5.75939700 | -2.86880700 | 3.39103800 |
| H | -6.30465700 | -4.40534700 | 2.57577000 |
| C | -2.90431500 | -1.68006100 | 4.11821900 |
| C | -4.99924500 | -1.90221500 | -2.69573900 |
| H | -4.93150000 | -0.82537900 | -2.54239900 |
| C | -6.41482300 | -2.23133500 | -3.19302900 |
| H | -6.64049800 | -1.66600900 | -4.09570000 |
| H | -7.17376600 | -1.99942300 | -2.44724900 |
| H | -6.50341200 | -3.29282400 | -3.43193000 |
| C | -3.97665000 | -2.28394800 | -3.77249600 |
| H | -2.95052000 | -2.06390400 | -3.45918900 |
| H | -4.17587400 | -1.73420600 | -4.69413900 |
| H | -4.03059500 | -3.34908400 | -4.00395300 |
| C | -0.55132800 | 0.53532800 | -1.93667800 |
| O | -1.75355600 | -0.42393400 | 0.94652100 |
| O | -0.44280800 | -0.47553400 | 0.82794200 |
| C | -2.27566000 | -1.24012400 | 1.48903600 |
| C | -2.65137800 | 0.92275600 | -3.05535600 |
| H | -2.52025900 | 1.78210000 | -3.59612600 |
| H | -2.58502800 | 0.06884400 | -3.72874300 |
| H | -3.70134800 | 1.10993500 | -2.82255500 |
| C | -1.36207400 | 0.26531000 | -3.33592100 |
| H | 1.88422500 | -1.22585000 | -3.39530200 |
| H | 1.86017800 | -0.33878500 | -2.57340700 |
| H | 1.51054800 | -0.23909000 | -4.29218200 |
Cartesian coordinates of the optimized geometry for 2 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| Ga    | -1.8928850| 0.2274250 | 0.1520080 |
| Ga    | 2.25067300| 0.2623200 | -0.0456550|
| Cl    | -1.9653910| -0.4167230| -2.0549560|
| P     | 0.10857900| 0.7858040 | 0.66493700|
| N     | -2.7265380| -1.8397660| 0.90643200|
| N     | -3.3833830| 1.0135660 | 0.65072900|
| N     | 2.99540300| 1.8640110 | -0.96079000|
| N     | 3.29860000| -1.0931380| -1.04409300|
| N     | 2.34207200| 0.2060430 | 1.90142700|
| N     | 0.59682800| 0.3036980 | 3.46768600|

C    | -5.5849950| -1.7546450| -1.6033430 |
H    | -6.5148900| -1.6767000| -1.0467200 |
H    | -5.4531030| -2.7905640| -1.9215290 |
H    | -5.6741600| -1.1492280| -2.5080530 |
C    | 4.5778040  | -0.7815800| -1.1146430 |
C    | 4.6035320  | -1.7177410|  0.9899390 |
H    | 5.4529152  | -2.3819470| -3.0881080 |
C    | 3.7001060  | -1.8647490|  0.9899390 |
C    | 5.7513870  | -0.7652640| -2.0577610 |
H    | 6.4685840  | -1.5395130| -1.7994920 |
H    | 6.2592410  |  0.2011170| -2.0257470 |
C    | 4.0299100  | -2.9016320|  1.1198000 |
H    | 5.4529000  | -2.3819470| -3.0881080 |
H    | 5.4529152  | -2.3819470| -3.0881080 |
H    | 5.4529152  | -2.3819470| -3.0881080 |
C    | 0.0682960  |  3.0978400|  0.5985340 |
C    | 1.7918170  |  2.8863690|  1.1198000 |
H    | 1.5234380  |  3.8115340|  0.5985340 |
H    | 3.0682400  |  1.8601960|  1.7140780 |
C    | 3.7108010  |  3.6205480|  1.8114130 |
C    | 3.7721120  |  2.8160890|  0.2368400 |
H    | 1.3922880  |  2.9295440|  2.5024800 |
H    | 0.0566150  |  3.0093900|  2.3996080 |
H    | 1.4959950  |  3.7893900|  3.0756010 |
H    | 3.7843800  |  2.0231470|  3.0657530 |
C    | -1.9922950 |  2.8180020|  0.9155220 |
H    | -2.2178830 |  1.8156230|  1.3111810 |
C    | -1.8559920 |  3.7661260| -2.1073760 |
H    | -2.7882800 |  3.8217910| -2.6749300 |
H    | -1.0647850 |  3.4218710| -2.7749690 |
H    | -1.5985240 |  4.7691210| -1.7603500 |
C    | -3.1426640 |  3.2366640| -0.0386500 |
H    | -4.0872150 |  3.2636700| -0.5516150 |
H    | -2.9050680 |  4.2277720|  0.4123210 |
H    | -3.2478540 |  2.5350300|  0.8228530 |
C    | 3.6421610  |  1.0466700| -2.3939690 |
H    | 3.6653240  |  0.5590450| -3.3720100 |
H    | 2.7504020  |  1.6688060| -2.3530510 |
H    | 4.5135590  |  1.7017470| -2.3148920 |
C    | 1.7608650  | -1.3029430|  2.3211320 |
H    | 1.1781040  |  2.2246450|  2.2791420 |
H    | 2.3517250  | -1.2863810|  3.2384220 |
H    | 1.0618050  |  0.4723960|  2.3649640 |
C    | -1.6877560 |  0.4426000|  2.3305630 |
H    | -2.0827130|  1.4015760|  2.6558300 |
H    | -1.5783350| -0.2154850|  3.1982400 |
H    | -0.7030060|  0.6369530|  1.9177380 |
C    | -2.9771970| -1.9191350| -2.6054400 |
H    | -3.1549380| -2.9977330| -2.6413690 |
H    | -3.6126020| -1.4368300| -3.3508120 |
H    | -1.9418730| -1.7390020| -2.8894960 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -3.60332700 | -1.73746800 | 1.90518900 |
| C       | -4.20395200 | -0.54154000 | 2.29739200 |
| H       | -4.87178500 | -0.61435100 | 3.14227000 |
| C       | -4.19073200 | 0.70602500  | 1.65332600 |
| C       | -3.97876800 | -2.96708600 | 2.69078200 |
| H       | -4.97283500 | -2.86317500 | 3.11920200 |
| H       | -4.26897900 | -3.08881800 | 3.51169600 |
| C       | -5.17864800 | 1.71463500  | 2.18189400 |
| H       | -6.13866000 | 1.23893400  | 2.37495900 |
| H       | -5.30244100 | 2.54946400  | 1.50346900 |
| C       | -4.80825700 | 2.10353400  | 3.13227200 |
| C       | -2.34299300 | -3.12361400 | 0.38330600 |
| C       | -3.06462100 | -3.65129400 | -0.70474100|
| H       | -3.53945900 | 2.22643400  | 1.90518900 |
| C       | -4.30273900 | 2.17110700  | -1.29643400|
| C       | -4.37653700 | 3.31091000  | -2.09143500|
| C       | -4.95075300 | 3.28380100  | -3.00641600|
| C       | -3.72219400 | 4.79311100  | -1.73583100|
| C       | -3.79505700 | 5.35152200  | -2.37459600|
| C       | -3.00398100 | 4.52705600  | -0.55605600|
| C       | -2.50829800 | 5.44546300  | -0.27203100|
| C       | -2.90321300 | 3.41689000  | 0.28254100 |
| C       | -5.09167800 | 0.93296700  | -1.68457900|
| C       | -4.59444000 | 0.07608000  | -1.23852700|
| C       | -6.51618000 | 0.98849400  | -1.11408200|
| C       | -7.06745300 | 0.08519000  | -1.38472700|
| C       | -7.05854300 | 1.84918200  | -1.51991100|
| C       | -6.51579000 | 1.06676800  | -0.02846700|
| C       | -5.13909300 | 0.69550000  | -3.19458900|
| C       | -5.60744500 | -0.26701900 | -3.40159900|
| C       | -4.13744300 | 0.68346500  | -3.62074800|
| C       | -5.72961600 | 1.45680600  | -3.70765800|
| C       | -2.17431400 | 3.57826600  | 1.60397500 |
| C       | -2.06523100 | 2.59235300  | 2.05054700 |
| C       | -2.97962900 | 4.46359700  | 2.56851700 |
| C       | -8.99533500 | 4.10227300  | 2.71772300 |
| C       | -3.04693900 | 5.48312900  | 2.18326200 |
| C       | -4.24823600 | 4.50538300  | 3.54069600 |
| C       | -0.77766500 | 4.17310100  | 1.42607000 |
| C       | -0.82721900 | 5.19719200  | 1.05656300 |
|   |    X     |    Y     |    Z     |
|---|---------|---------|---------|
| H | -0.18422600 | 3.58435900 | 0.73400400 |
| H | -0.25446700 | 4.19872100 | 2.38268000 |
| C | 4.13866400  | 1.79672600 | -1.63359900 |
| C | 4.79320100  | 0.59835500 | -1.93761900 |
| H | 5.70228300  | 0.70590700 | -2.50670200 |
| C | 4.34963800  | -0.71782700 | 1.78118200 |
| C | 4.79320100  | 3.06737100 | -2.68700200 |
| H | 5.61263600  | 2.82762100 | -2.80581800 |
| C | 5.14633700  | 3.65888300 | -1.31633900 |
| H | 5.10384400  | -1.74003200 | -2.60143200 |
| C | 5.17024300  | -2.71103100 | -2.12607900 |
| C | 5.10384400  | 5.62208000 | -1.09637600 |
| C | 5.06084700  | 6.59498400 | -1.16269300 |
| C | 2.02398900  | 5.37336400 | -0.12710200 |
| C | 2.28965400  | 6.15350300 | 0.57348400 |
| C | 6.23929600  | 4.12750900 | -0.02458100 |
| C | 1.79695400  | 2.27201100 | -4.12897300 |
| C | 1.43932500  | 1.55360300 | -4.86773300 |
| H | 2.81907500  | 1.99178000 | -3.87264200 |
| H | 1.81377900  | 3.25838100 | -4.59810300 |
| C | -0.58345000 | 2.43044100 | -3.35904200 |
| C | -0.71322700 | 3.29865300 | -4.00849400 |
| C | -1.26518200 | 2.52572900 | -2.51588200 |
| C | 3.62622500  | 3.88797800 | 1.09743200 |
| C | 4.13941100  | 2.95423700 | 0.88416900 |
| C | 4.69148300  | 4.98282400 | 1.21693100 |
| C | 4.25806000  | 5.93083400 | 1.54053600 |
| C | 5.20278100  | 5.16019200 | 0.26949900 |
| C | 5.43966500  | 4.69598400 | 1.95834700 |
| C | 2.87738900  | 3.71872800 | 2.42521600 |
| C | 2.14541200  | 2.91605700 | 2.36847600 |
| C | 2.34956900  | 4.63872000 | 2.68385500 |
| C | 3.57425100  | 3.48982400 | 3.23362000 |
| C | 2.96630600  | -2.50174100 | -1.06528700 |
| C | 2.00524900  | -2.97562800 | -1.97707000 |
| C | 1.82491500  | -4.35592900 | -2.07174800 |
| C | 1.08726800  | -4.75023800 | -2.75169900 |
| C | 2.56559300  | -5.23779300 | -1.30649100 |
| C | 2.41665600  | -6.30487600 | -1.41263300 |
| C | 3.46611600  | -4.75006700 | -0.37701200 |
| C | 4.00427100  | -5.44467100 | 0.25076800 |
| C | 3.66696500  | -3.38136400 | -0.21682900 |
| C | 1.15085800  | -2.04719500 | -2.83293000 |
| C | 0.78305900  | -1.25065600 | -2.17975300 |
| C | 1.92064600  | -1.38496400 | -3.98399800 |
| C | 2.39715590  | -2.14030900 | -4.61338900 |
| C | 2.67944400  | -0.68762500 | -3.64094600 |
| C | 1.22432900  | -0.82396100 | -4.60820600 |
| C | -0.07875600 | -2.74865300 | -3.41312100 |
| C | -0.67578600 | -3.23461300 | -2.64322100 |
| C | 0.20604900  | -3.49442800 | -4.15919400 |
| C | -0.71154700 | -2.01462500 | -3.90265000 |
| C | 4.58155600  | -2.88423400 | 0.89360000 |
| C | 4.13041600  | -1.96294300 | 1.25730000 |
| C | 6.01566500  | -2.55871000 | 0.44934400 |
| C | 6.62729400  | -2.39059000 | 1.32501200 |
| C | 6.06739600  | -1.69025000 | -0.20947900 |
| C | 6.46708800  | -3.41120100 | -0.06280400 |
| Atoms | x      | y      | z      |
|-------|--------|--------|--------|
| C     | 4.652450 | -3.856326 | 2.076347 |
| H     | 3.663232  | -4.157885 | 2.909949 |
| H     | 5.217521  | -4.755699 | 1.823932 |
| C     | 1.012053  | 0.338529  | 2.262787 |
| C     | 3.359074  | 0.285171  | 2.956502 |
| H     | 3.098056  | 1.140946  | 3.587487 |
| C     | 4.735182  | 0.536575  | 2.351676 |
| H     | 5.047077  | -0.280792 | 1.702952 |
| H     | 5.481582  | 0.633625  | 3.141786 |
| C     | 4.752202  | 1.449933  | 1.762095 |
| C     | 3.780750  | -0.938059 | 3.875757 |
| H     | 3.098056  | 1.140946  | 3.587487 |
| C     | 4.735182  | 0.536575  | 2.351676 |
| H     | 5.047077  | -0.280792 | 1.702952 |
| H     | 5.481582  | 0.633625  | 3.141786 |
| C     | 4.752202  | 1.449933  | 1.762095 |
| C     | 3.780750  | -0.938059 | 3.875757 |

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

Ga  -2.661388  -1.077447  0.208031
Ga   2.684069  -0.175807  0.194632
Cl  -2.945760  -3.250831  0.500932
P  -0.401404  -0.714260 -0.329723
N   -3.604165  -0.056570  1.563397
N   -3.817315  -0.647815 -1.309002
N    3.639984  -1.318146 -1.031255
N    4.174913   0.426876  1.257974
N    1.587768   1.127793 -0.618280
N   -0.480606   2.128664 -0.737391
C   -4.672397   0.672473  1.273785
C    5.250430   0.771936 -0.000398
H   -6.120518   1.405405 -0.065729
H   -4.871451   0.142100 -1.194257
C   -5.324799   1.462301  2.377461
H   -6.176266   2.022793  2.001775
H   -4.614413   2.162708  2.821003
C   -5.667335   0.803438  3.177637
C   -5.723889   0.399768 -2.408370
H   -6.540213   1.076457 -2.174166
H   -6.145606  -0.534203 -2.788144
H   -5.129564   0.834035 -3.213964
C    4.965097  -1.345644 -1.062127
C    5.790812  -0.639884 -0.173257
H    6.850704  -0.759589 -0.307410
C    5.429117   0.144038  0.930072
C    5.646385  -2.184302 -2.109735
H    5.355250  -3.232013 -2.018197
H    6.726810  -2.117445 -2.019139
H    5.360015  -1.859118 -3.112065
C    6.541225   0.683264  1.788399
H    6.495001   1.772743  1.845160
H    7.511460   0.396374  1.392787
H    6.458623   0.305750  2.809700
C    0.207960   1.077839 -0.528084
C    2.176340   2.371573 -1.144707
H   1.453613   2.763399  1.862058
C    3.480341   2.077319 -1.881461
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 4.261590   | 1.708024   | -1.212209  |
| H    | 3.860435   | 2.990274   | -2.343430  |
| H    | 3.325095   | 1.335835   | -2.666422  |
| C    | 2.367326   | 3.433160   | -0.062110  |
| H    | 1.426676   | 3.606215   | 0.457463   |
| H    | 2.698050   | 4.377592   | -0.501487  |
| H    | 3.121686   | 3.119648   | 0.662258   |
| C    | -1.916740  | 2.202970   | -0.710752  |
| H    | -2.360335  | 1.247778   | -0.427790  |
| C    | -3.530984  | 2.563013   | -2.098560  |
| C    | -3.139259  | -1.207693  | 1.331848   |
| O    | -0.346816  | -1.692459  | 2.204520   |
| H    | -1.764310  | 0.876261   | 3.272572   |
| C    | -3.848526  | -0.480795  | 3.626960   |
| C    | 2.855868   | -2.100398  | 1.985059   |
| C    | 3.032720   | -3.171960  | -1.866280  |
| C    | 1.797643   | -1.912553  | -1.812406  |
| C    | 3.084422   | -1.823736  | -2.796650  |
| C    | 2.806543   | 0.517274   | 0.166796   |
| C    | -2.872445  | 0.037732   | -2.279965  |
| P    | -0.389513  | 0.789371   | 0.237598   |
| N    | -2.771155  | -2.111018  | 0.619242   |
| N    | 4.506251   | -0.413137  | -0.140029  |
| N    | 1.903652   | 0.691381   | 3.043180   |
| N    | 0.21904    | 0.923543   | 3.043180   |
| C    | -3.592011  | -2.273583  | 1.650323   |
| C    | -3.308710  | -1.244427  | 2.260189   |
| C    | -4.834357  | -1.523625  | 3.172128   |
| C    | -4.418570  | 0.012465   | 1.756164   |
| C    | 2.411094   | 0.012465   | 3.651071   |
| H    | -4.016247  | -3.586999  | 3.287231   |
| C    | -3.645889  | -4.352341  | 2.011326   |
| H    | -4.758070  | -4.048850  | 1.762418   |
| C    | -5.649051  | 0.836723   | 2.523910   |
| H    | -6.105021  | 0.256931   | 3.322366   |
| H    | -6.428504  | 1.233790   | 1.877634   |
| H    | -5.135728  | 1.695170   | 2.963263   |
| C    | -2.121468  | 3.275312   | 0.063140   |
| C    | -2.721116  | -3.956095  | -1.003818  |
| C    | -2.123667  | -5.132296  | -1.455869  |
| H    | -2.579439  | -5.676052  | 2.272541   |
| C    | -0.959273  | -5.611322  | -0.883934  |

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

Ga  -2.476678  -0.291324  -0.123549
Ga   2.806543  0.517274  0.166796
Cl  -2.872445  0.037732 -2.279965
P   -0.389513  0.789371  0.237598
N   -2.771155  2.116080  0.619242
N   -4.119010  0.029760  0.301739
N    3.235071  2.075900 -0.726413
N    4.506251  0.413137 -0.140290
N   -0.036200  0.823543  3.043180
C   -3.592011 -2.273583  1.650323
C   -4.308710 -1.244427  2.260189
C   -4.834357 -1.523625  3.172128
C   -4.418570  0.012465  1.756164
C    2.411094  0.012465  3.651071
H   -4.016247 -3.586999  3.287231
H   -3.645889 -4.352341  2.011326
H   -4.758070 -4.048850  1.762418
C   -5.649051  0.836723  2.523910
H   -6.105021  0.256931  3.322366
H   -6.428504  1.233790  1.877634
H   -5.135728  1.695170  2.963263
C   -2.121468  3.275312  0.063140
C   -2.721116 -3.956095  1.003818
C   -2.123667 -5.132296 -1.455869
H   -2.579439 -5.676052  2.272541
C  -0.959273 -5.611322  0.883934
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -0.51152200 | -6.52833500 | -1.24546700 |
| C    | -0.35168800 | -4.89428600 | 0.54972700  |
| H    | 0.58122300  | -5.24957900 | -1.68696300 |
| C    | -0.90668800 | -3.71363300 | 0.61818900  |
| C    | -3.98176600 | -3.46187500 | -1.24546700 |
| H    | -4.19857200 | -2.46607900 | -1.30917200 |
| C    | -5.18601010 | -3.94877700 | -1.85704500 |
| C    | -5.38054600 | -4.40103100 | -0.29685000 |
| H    | -5.20768000 | -3.75703000 | -1.71986800 |
| H    | -3.77914900 | -3.32720000 | -3.20058900 |
| H    | -3.62185300 | -4.30721400 | -3.66917000 |
| H    | -2.92086300 | -2.69983000 | -3.41927100 |
| C    | -0.17785500 | -2.93887000 | 1.70154000  |
| H    | -0.53702100 | -1.91131400 | 1.67247600  |
| H    | -0.45090300 | -3.44849300 | 3.10956900  |
| H    | -1.49995000 | -3.41269900 | 3.38849300  |
| C    | -1.28170000 | -2.92370100 | 3.84538800  |
| H    | -1.05758500 | -4.53529400 | 3.17491400  |
| C    | 1.33487800  | -2.91006100 | 1.46077900  |
| H    | 1.79391000  | -3.86940600 | 1.70376600  |
| H    | 1.78988400  | -2.15487100 | 2.09962900  |
| H    | 1.57948100  | -2.67937400 | 0.42751100  |
| C    | -4.85212700 | 1.52071900  | -0.08343600 |
| C    | -5.90734500 | 1.09834600  | -0.91688000 |
| C    | -6.62735900 | 2.06290800  | -1.61405600 |
| C    | -7.44416900 | 1.75634300  | -2.25320600 |
| C    | -6.30690700 | 3.40829200  | -1.52040600 |
| C    | -6.87317800 | 4.14281400  | -2.07884700 |
| C    | -5.25505800 | 3.80412100  | -0.71482400 |
| C    | -5.00136800 | 4.85388000  | -0.64688800 |
| C    | -4.51759200 | 2.87597200  | 0.01984900  |
| C    | -6.28085300 | -0.36584200 | -1.07153600 |
| C    | -5.45040200 | -0.95701800 | -0.69290300 |
| C    | -7.52006700 | -0.73044500 | -0.24267300 |
| C    | -7.76393900 | -1.78710200 | -0.37235100 |
| C    | -8.38477800 | -0.14273000 | -0.55910800 |
| C    | -7.36444900 | -0.55285200 | 0.82096100  |
| C    | -6.48606800 | -0.75761700 | -2.53735200 |
| C    | -6.64903400 | -1.83339800 | -2.61482900 |
| C    | -5.61229100 | -0.49738500 | -3.13218300 |
| C    | -7.35998700 | -0.26667400 | -2.96885900 |
| C    | -3.39185300 | 3.36750600  | 0.90313000  |
| C    | -2.99436400 | 2.50754000  | 1.43798400  |
| C    | -3.89197000 | 4.37857500  | 1.94223500  |
| C    | -6.68426900 | 3.95763700  | 2.56289000  |
| H    | -4.29071400 | 5.27241000  | 1.45985200  |
| H    | -3.07710100 | 4.69050800  | 2.59667600  |
| C    | -2.55175000 | 3.96441600  | 0.07112800  |
| H    | -2.58157900 | 4.87055900  | -0.44406600 |
| H    | -1.89517000 | 3.26217800  | -0.67775600 |
| C    | -1.41000300 | 4.22604900  | 0.70771900  |
| C    | 4.50830700  | 2.53014600  | -0.94244800 |
| C    | 5.58912400  | 1.67159700  | -0.70845200 |
| C    | 6.56164500  | 2.09442900  | -0.90870200 |
| C    | 5.58488600  | 0.29111000  | -0.48232200 |
| C    | 4.84377700  | 3.89123100  | 1.49335800  |
| C    | 4.15924300  | 4.17666800  | -2.28908400 |
| C    | 5.86311800  | 3.91097500  | -1.86939300 |
| C    | 4.75145300  | 4.64320400  | -0.70938900 |
| C    | 6.91016000  | 0.39422700  | -0.71196000 |
| C    | 6.90066400  | -1.44236900 | -0.43617700 |
| H    | 7.68318300  | 0.12009100  | -0.13799100 |
| H    | 7.18661300  | -0.31501200 | -1.76227300 |
| C    | 2.19149300  | 3.10809900  | -1.16452000 |
| C    | 1.55028700  | 2.84896800  | -2.38984000 |
| C    | 0.58393100  | 3.74952600  | -2.83086400 |
Cartesian coordinates of the optimized geometry for 11 at B3LYP-D3BJ/def2-TZVP level of theory (number of imaginary frequencies = 0):

Ga 1.84270400 0.21633200 0.12488000
Ga -2.26851500 -0.21537700 -0.09823500
Cl 1.76498100 0.40040600 -2.09130200
P -0.16619400 -0.76712200 0.66584800
N 2.73360300 1.79357900 0.87581900
N -3.15715800 -1.80073400 -0.83625700
N -3.42853900 1.11869400 2.97442900
C 1.71203500 -0.78309900 1.56111800
C 3.66148000 1.67304300 1.82450300
C 4.26620800 0.47088800 2.18449400
C 4.99925400 0.53467900 2.97442900
C 4.11528200 -0.78309900 1.56111800
C 4.11528200 -0.78309900 1.56111800
C 5.06907800 2.72232100 3.05524100
H 3.37640500 3.14075800 3.34126800
H 4.19878700 3.76876800 1.92752300
H 5.19107200 -1.79532300 2.02147900
H 6.18973300 -1.36233500 1.96045100
H 5.16627600 -2.71205200 1.44325100
H 5.00819800 -2.03493700 3.06964400
H 2.37935800 -0.78309900 1.56111800
C 3.07891900 3.61768100 -0.71071500
H 2.74923200 4.89368700 -1.15927100
H 3.27509400 5.31195400 -2.00637400
C 1.74856100 5.63347000 -0.54673600
H 1.49981800 6.61953100 -0.91832900
C 1.06474600 5.10673000 0.53462900
H 0.27904100 5.68224700 1.00418200
C 1.37178500 3.84123000 1.03510600
C 4.20027100 2.84005000 1.03510600
H 4.05738000 1.78968100 -1.13707800
C 5.57123700 3.25466000 -0.82649300
H 6.36405000 2.68481300 -1.31600100
C 5.64622100 3.07539200 0.24565000
H 5.75721400 4.31623300 -1.00468200
C 4.17856600 2.95449500 -2.90412000
C 4.42915300 3.96205900 -3.24150800
H 3.20069500 2.68704900 -3.30537000
C 4.91543100 2.27447300 3.33510800
C 0.62694300 3.31703200 2.24615900
C 1.07040100 2.36376400 2.52554200
C 0.74043800 4.26047800 3.45052600
C 1.77628800 4.50859600 3.68515500
H 0.29026100 3.79495300 4.32907400
H 0.21170300 5.19766100 3.26696900
H -0.84281000 3.06332000 1.92027200
H -1.34873000 3.98934400 1.65345800
H -1.34918100 2.61754100 2.77357000
H -0.93759300 2.37874900 -0.03496100
C 3.30775300 -2.36096000 0.74601800
C 3.97733500 -2.45976500 -1.26982900
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 3.96679000 | -3.68530300 | -1.93014600 |
| H       | 4.47371000 | -3.78061000 | -2.88017200 |
| C       | 3.31482700 | -4.78366200 | -1.39353300 |
| H       | 3.31007500 | -5.72598500 | -1.92660900 |
| C       | 2.67044300 | -4.67185200 | -0.17455800 |
| H       | 2.16607200 | -5.53292100 | 0.24198400  |
| C       | 2.65500300 | -3.47051700 | 0.53382400  |
| C       | 4.75894300 | -1.29537200 | -1.85407500 |
| H       | 4.35648700 | -0.38044400 | -1.42687300 |
| C       | 6.24016000 | -1.37527700 | -0.37745200 |
| H       | 6.78809600 | -0.52351300 | -1.86458800 |
| H       | 6.69553700 | -2.28934100 | -1.84900400 |
| H       | 6.37077400 | -1.37527700 | -0.37745200 |
| C       | 4.62248200 | -1.18065700 | -3.37367000 |
| H       | 5.07351700 | -0.24722800 | -3.71439300 |
| H       | 3.57638400 | -1.17755300 | -3.67349700 |
| H       | 5.32877000 | -1.99602000 | -3.90017000 |
| C       | 1.99420400 | -3.44313100 | 1.90234500  |
| H       | 1.94076800 | -2.40638700 | 2.22872600  |
| H       | 2.84339200 | -5.29005000 | 2.67334200  |
| C       | 2.36372300 | -4.13924200 | 3.92294900  |
| C       | 0.56930000 | -4.00046600 | 1.87503200  |
| H       | 0.56625300 | -5.07129200 | 1.66945800  |
| H       | -0.03615500| -3.50452500 | 1.12347400  |
| C       | -4.26614000| -1.73383700 | 2.56192000  |
| C       | -4.87350100| -0.53129700 | 1.93827800  |
| H       | -5.75855600| -0.62917100 | -2.54594700 |
| C       | -4.48759800| 0.77773100  | -1.65188900 |
| C       | -4.94060600| -3.00348800 | -2.01090200 |
| H       | -4.22273900| -3.73318800 | -2.37821100 |
| H       | -5.67390800| -2.79349800 | -2.78542000 |
| H       | -5.45398300| -3.46307600 | -1.65228800 |
| C       | -5.36141000| 1.86360800  | -2.22586000 |
| H       | -6.03059200| 2.25107300  | -1.45802700 |
| C       | -5.96728600| 1.46690400  | -3.03693500 |
| H       | -4.77402900| 2.70257000  | -2.59048000 |
| C       | -2.56702200| -3.08990400 | -0.59215200 |
| C       | -1.55796600| -3.53715200 | -1.46382500 |
| C       | -1.08068200| -4.83405000 | -1.29610900 |
| H       | -0.30618600| -5.20455800 | -1.95179800 |
| C       | -1.56776800| -5.65172100 | -0.28736900 |
| C       | -1.18857500| -6.59928000 | -0.17830800 |
| H       | -2.50079800| -5.16169500 | 0.60904200  |
| H       | -2.83439200| -5.78622200 | -3.84720800 |
| C       | -3.00872400| -3.86874400 | 0.48592500  |
| H       | -0.99583700| -2.64160500 | -2.55620000 |
| C       | -1.07806700| -1.61094500 | -2.20668000 |
| C       | -1.79529300| -2.74403600 | -3.86204100 |
| H       | -1.34483700| -2.10915200 | -4.62732800 |
| H       | -2.82973400| -2.42754000 | -3.73712300 |
| C       | -1.79629700| -3.77207200 | -4.23256100 |
| C       | 0.48844200 | -2.89655200 | -2.81812300 |
| H       | 0.88469900 | -2.12110400 | -3.47224440 |
| C       | 0.65685400 | -3.85968100 | -3.30334600 |
| H       | 1.06321600 | -2.87622100 | -1.89495200 |
| C       | -3.97206300| -3.33840400 | 1.53247900  |
| H       | -4.30647300| -2.35070500 | 1.21687800  |
| C       | -5.21249700| -4.22475500 | 1.69582200  |
| C       | -4.94826400| -5.21119300 | 2.08143200  |
| H       | -5.73829700| -4.37099800 | 0.75110700  |
| C       | -5.90851400| -3.77024300 | 2.40328200  |
| C       | -3.25388600| -3.16584000 | 2.87798100  |
| C       | -2.39708800| -2.50311500 | 2.78729900  |
| C       | -2.90896600| -4.12984300 | 3.25859900  |
| H       | -3.93065100| -2.73041600 | 3.61518500  |
**Cartesian coordinates of the optimized geometry for CO\(_2\) at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):**

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | -3.20080300 | 2.51779200 | -0.65711300 |
| C    | -2.22808800 | 3.19341700 | -1.41733100 |
| C    | -2.07713000 | 4.56199100 | -1.20886900 |
| H    | -1.33489100 | 5.10782700 | -1.77014100 |
| C    | -2.85255100 | 5.23743900 | -0.27867300 |
| H    | -2.71980300 | 6.30263100 | -0.13674000 |
| C    | -3.77397000 | 4.54553100 | 0.48616100 |
| H    | -4.35187600 | 5.07410300 | 1.23238700 |
| C    | -3.96472100 | 3.17420800 | 0.32114600 |
| C    | -1.36362200 | 2.46370600 | -2.43652000 |
| H    | -1.04552800 | 1.52062700 | -1.98158500 |
| C    | -2.12356000 | 2.11823100 | -3.72568500 |
| H    | -2.51335400 | 3.02444400 | -4.19539400 |
| H    | -2.95362900 | 1.43689700 | -3.55404000 |
| H    | -1.44863000 | 1.63814000 | -4.32924000 |
| C    | -0.08909500 | 3.22652200 | -2.79038900 |
| H    | -0.30918400 | 4.19468800 | -1.90428500 |
| H    | 0.54584800  | 2.60092100 | -3.41425100 |
| C    | -4.96732900 | 2.45689500 | 1.21075700 |
| C    | -5.09698600 | 1.44341600 | 0.83245000 |
| C    | -6.34286800 | 3.13800000 | 1.20601100 |
| C    | -7.06459100 | 2.52347200 | 1.74694400 |
| C    | -6.72358600 | 3.29924000 | 0.19640400 |
| C    | -6.30632300 | 4.10991400 | 1.70111100 |
| C    | -4.44123400 | 2.34009100 | 2.64820200 |
| C    | -3.52886600 | 1.74386800 | 2.68635800 |
| C    | -5.18841200 | 1.85484500 | 3.32824600 |
| C    | -4.23799800 | 3.32875300 | 3.06561100 |
| C    | -1.11446800 | -0.18267800 | 2.19382400 |
| C    | 0.64874200  | -0.15129800 | 3.73954300 |
| H    | 1.27772100  | -0.37467100 | 2.86300100 |
| H    | 1.02002900  | 0.79231200  | 4.15425100 |
| C    | 0.83309900  | -1.25127800 | 4.77865600 |
| H    | 1.88460000  | -1.34664600 | 5.05971600 |
| H    | 0.24971200  | -1.02914400 | 5.67292400 |
| H    | 0.49141700  | -2.20880500 | 4.38487400 |
| O    | -2.39894400 | -0.07955600 | 1.81705100 |

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

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| C    | -3.20080300 | 2.51779200 | -0.65711300 |
| O    | 0.00000000  | 0.00000000 | 0.00000000 |
| N    | 0.00000000  | 0.00000000 | 1.16912200 |
| O    | 0.00000000  | 0.00000000 | -1.16912200 |

**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   | -1.04817900 | -1.76883200 | 2.35783400 |
| P    | -0.16137300 | 0.65776100  | -0.72027000 |
| Ga   | -1.52793900 | -0.67708600 | 0.45603700 |

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| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 4.57711700 | 0.28302700 | 1.05093300 |
| C    | 4.67452800 | 3.77170700 | -0.52403500 |
| H    | 4.04586900 | 4.61881000 | -0.23669800 |
| H    | 4.73980600 | 3.77170700 | -1.61681000 |
| C    | 5.67561100 | 3.91198400 | -0.11736000 |
| C    | 5.72644400 | -0.58054200 | 1.52365600 |
| H    | 6.64801400 | 0.00246700 | 1.56228800 |
| H    | 5.87127300 | -1.41753400 | 0.83243700 |
| C    | 2.08601700 | 3.03697800 | -1.26877500 |
| C    | 2.15950500 | 2.74753300 | -2.64504000 |
| H    | 5.72644400 | -0.58054200 | 1.52365600 |
| H    | 1.33717000 | 3.47266200 | -3.51177700 |
| C    | 3.09706800 | 1.67755400 | -3.19200500 |
| C    | 4.08302300 | 2.25962500 | -4.21804000 |
| H    | 3.55962200 | 2.63155900 | -5.10680000 |
| C    | 4.65777000 | 3.09371100 | -4.98074000 |
| C    | 0.42611700 | 4.72833300 | -1.66476000 |
| H    | 0.47009700 | 4.48998800 | -3.02763900 |
| H    | 1.22774900 | 4.02634000 | -0.76002000 |
| C    | 3.09706800 | 1.67755400 | -3.19200500 |
| H    | 3.68777200 | 1.28094000 | -2.36060900 |
| C    | 3.01070400 | -0.29222400 | -4.11713000 |
| H    | 1.33717000 | 3.47266200 | -3.51177700 |
| C    | 1.15482500 | 4.32935300 | -0.72764000 |
| H    | 1.56522200 | 5.78370200 | 1.02937000 |
| H    | 0.85938300 | 6.49002500 | 0.56400800 |
| C    | 2.86099900 | 6.01818200 | 0.65831500 |
| C    | 0.42611700 | 4.72833300 | -1.66476000 |
| H    | -0.23982100 | 4.02426700 | 1.28828500 |
| H    | -0.24362800 | 4.12463800 | 2.37861000 |
| C    | -0.55965000 | 3.01369800 | 1.02569000 |
| H    | 3.20995700 | -1.64116500 | 1.34887000 |
| C    | 3.27411900 | -2.60485500 | 0.32912500 |
| H    | 3.51759000 | -3.95308100 | 0.70388200 |
| C    | 3.31475900 | -4.71859500 | -0.06383000 |
| C    | 3.15281800 | -4.32256100 | 2.03857900 |
| C    | 3.13190400 | -5.37393300 | 2.31047300 |
| C    | 0.54594000 | -3.48144000 | 0.30113000 |
| H    | 2.96275100 | -3.65467000 | 4.06657000 |
| C    | 3.09015200 | -1.98943500 | 2.71136800 |
| C    | 3.05126700 | -0.90121500 | 3.78014900 |
| H    | 3.86819500 | -0.20074000 | 3.56435200 |
| C    | 4.74657300 | -0.09706900 | 3.70852100 |
| H    | 1.79001700 | 0.77508400 | 4.36967900 |
| H    | 0.89011300 | -0.71442000 | 3.97908200 |
| C    | 1.57308600 | 0.25372200 | 2.68893200 |
| C    | 3.27524500 | -1.41964800 | 5.20473900 |
| C    | 3.32416900 | -0.57546300 | 5.90070400 |
| C    | 4.20858500 | -1.98688200 | 5.29223200 |
| H    | 2.45104700 | -2.06393600 | 5.53079200 |
| C    | 3.36140100 | -2.22466400 | -1.14286300 |
| H    | 3.43099100 | -1.13565000 | -1.22428000 |
| C    | 4.62507500 | -2.79457800 | -1.80823300 |
| H    | 4.61728400 | -3.89027100 | -1.80992000 |
| C    | 4.68575400 | -2.46166900 | -2.85066600 |
| H    | 5.53585000 | -2.46750300 | -1.29347100 |
| H    | 2.09883200 | -2.66788100 | -1.89554300 |
| C    | 1.19237100 | -2.21979500 | -1.48006400 |
| H    | 2.16130000 | -2.37189900 | -2.94730300 |
| H    | 1.98305200 | -3.75484200 | -1.86351400 |
| C    | -2.63310100 | 1.27539300 | 3.62576200 |
Cartesian coordinates of the optimized geometry for TS$_{1\rightarrow10}$ at B3LYP-D3BJ/6-$31G^*$ level of theory (number of imaginary frequencies = 1):

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Cl   | -1.58512700| -0.53035600| 2.36424100 |
| P    | 0.15006000 | 0.47891300 | -0.98808900|
| Ga   | -1.61963000| 0.55640200 | 0.41212000 |
| N    | -2.04788500| 2.44586500 | 0.92724500 |
| N    | 3.47368900 | -0.36855200| -0.77497700|
| N    | 2.16794400 | -2.58079000| 0.57426400 |
| C    | -3.30262800| 2.86926000 | 1.08499800 |
| C    | -4.43597100| 2.10565000 | 0.77511700 |
| H    | -5.38724800| 2.57353200 | 0.99035000 |
| C    | -4.49644700| 0.91417100 | 0.04586700 |
| C    | -3.57758600| 4.26818400 | 1.59583000 |
| H    | -3.53017700| 4.28785100 | 3.68436000 |
| H    | -4.57706600| 4.59033300 | 1.29679800 |
| H    | -2.84580400| 4.98810800 | 1.22715100 |
| C    | -5.87171100| 0.50062400 | -0.42898400|
| C    | -6.59354400| 1.29841100 | -0.24688700|
| H    | -2.13130000| -0.39688800| 0.09065600 |
| Cl   | -5.86239800| 0.26802600 | -1.49628900|
| C    | -0.98184700| 3.38251100 | 1.16532400 |
| C    | -0.59203000| 3.69519200 | 2.48584700 |
| C    | 0.39426000 | 4.67057300 | 2.66967800 |
| H    | 0.70014700 | 4.92953700 | 3.67896800 |
| C    | 0.99581200 | 5.30423200 | 1.58769100 |
| H    | 1.76182700 | 6.05741200 | 1.75343200 |
| C    | 0.61536200 | 4.96790400 | 0.29259500 |
| H    | 1.08552200 | 5.46388000 | -0.55005900|
| C    | -0.38345300| 4.01803900 | 0.05556200 |
| C    | -0.88093000| 3.78787900 | -1.36470300|
| H    | -1.40342900| 2.83041600 | -1.38704300|
| C    | -1.90189000| 4.87086600 | -1.75831300|
| H    | -2.78579900| 4.84563200 | -2.11335000|
| H    | -2.23748800| 4.72238400 | -2.79087100|
| C    | -1.45692000| 5.87037600 | -1.68578400|
| C    | 0.25882500 | 3.71485600 | -2.38890000|
| C    | 0.71453900 | 4.69684400 | -2.56459700|
| H    | -0.12839800| 3.35797500 | -3.35043000|
| H    | 1.03644200 | 3.02501700 | -2.05819800|
| C    | -3.62735600| -0.89733700| -1.22783600|
| C    | -4.13423800| -2.11981700| -0.73772900|
| C    | -4.36483800| -3.15495900| -1.65065300|
| H    | -4.74956600| -4.10448200| -1.29111000|
| C    | -4.10960100| -2.98403200| -3.00450800|
| H    | -4.29406500| -3.79561700| -3.70215400|
| C    | -3.61444000| -1.76911000| -3.47035700|
| H    | -3.41646000| -1.65815100| -4.52867000|
| C    | -3.36009400| -0.69925200| -2.60573500|
| C    | -4.43663500| -2.35447500| 0.73912800 |
| C    | -4.35498100| -1.40103100| 1.26612200 |
| C    | -5.85164900| -2.91684800| 0.96864600 |
| H    | -6.07324500| -2.94509500| 2.04149900 |
| H    | -5.93876000| -3.94180100| 0.59042700 |
| H    | -6.62819200| -2.32260800| 0.47594700 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -3.40373400| -3.29655400| 1.36992800  |
| H    | -2.39297800| -2.91285000| 1.24745400  |
| H    | -2.39297800| -2.91285000| 1.24745400  |
| H    | -3.45878500| -4.29374000| 0.91707600  |
| C    | -3.58694400| -3.40129700| 2.44530800  |
| H    | -2.81292500| 0.62447300 | -2.63622700 |
| C    | -3.73281500| 1.83830300 | -2.90908200 |
| H    | -3.76570900| 2.14316100 | -1.86502500 |
| H    | -4.75518500| 1.63267200 | -3.24845200 |
| C    | -3.36435800| 2.69459800 | -3.48440700 |
| C    | -2.48306700| 0.58219800 | -4.65485800 |
| C    | -1.99765100| 1.52266800 | -4.93778000 |
| C    | -3.39174300| 0.48714200 | -5.26224000 |
| C    | -1.80337100| -0.23175900| -4.90722900 |
| C    | 4.51890100 | -1.18827800| -0.74317500 |
| C    | 4.44072300 | -2.51385400| -0.28379900 |
| C    | 3.37216100 | -3.14133300| 0.35797500  |
| C    | 5.87471000 | -0.67598800| -1.16255100 |
| C    | 6.16264500 | 0.17692000 | -0.53898200 |
| C    | 5.85973700 | -0.31613100| -2.19378000 |
| C    | 6.63471100 | -1.45473300| -1.06912600 |
| C    | 3.62308700 | -4.52711400| 0.90372100  |
| C    | 4.60361800 | -4.89053700| 0.59209000  |
| C    | 2.85752800 | -5.22821900| 0.56166600  |
| C    | 3.58043900 | -4.52650900| 1.99752900  |
| C    | 3.65725300 | 1.00873100 | -1.16282100 |
| C    | 3.63949600 | 1.38571200 | -2.52014700 |
| C    | 3.80036200 | 2.74042000 | -2.82785800 |
| C    | 3.78421100 | 3.05115100 | -3.86265000 |
| C    | 3.95696700 | 3.69636700 | -1.82932400 |
| C    | 4.07018700 | 4.74457600 | -2.09157800 |
| C    | 3.95076400 | 3.30661200 | -0.49465500 |
| C    | 4.05004700 | 4.05471200 | 0.28566600  |
| C    | 3.80800700 | 1.96187000 | -0.13952700 |
| C    | 3.39492200 | 0.39111000 | -3.64650800 |
| C    | 3.30747700 | -0.60705300| -3.21169900 |
| C    | 4.54691800 | 0.36564300 | -4.66599400 |
| C    | 4.65781200 | 1.33417800 | -5.16007700 |
| C    | 4.35060060 | -0.38637100| -5.43823500 |
| C    | 5.50814200 | 0.12455600 | -4.19884000 |
| C    | 2.66083300 | 0.70522700 | -4.35797300 |
| C    | 1.24971700 | 0.80600000 | -3.63956500 |
| H    | 1.81108900 | -0.08999200| -5.06755100 |
| C    | 2.13377700 | 1.64582200 | -4.91711900 |
| C    | 3.79466600 | 1.57094300 | 1.32930300  |
| C    | 3.72914900 | 0.48106000 | 3.40496400  |
| C    | 5.09047700 | 1.98222400 | 2.04776800  |
| C    | 5.21972100 | 3.07028500 | 2.04880200  |
| C    | 5.97292700 | 1.54164600 | 1.56944300  |
| C    | 5.06727300 | 1.64928100 | 3.09189700  |
| C    | 2.56639400 | 2.17563500 | 2.01679000  |
| C    | 2.50372800 | 1.84903700 | 3.05758700  |
| C    | 1.63979900 | 1.89916600 | 1.50517300  |
| C    | 2.61966900 | 3.26596300 | 2.01340000  |
| C    | 3.24054100 | -3.27341700| 1.34633600  |
| C    | 3.10334000 | -4.17140100| 0.88410000  |
| C    | 0.55819600 | -4.83225300| 1.75831900  |
| C    | -1.28561300| -5.52942500| 1.35561200  |
| C    | -0.51804500| -4.59702800| 3.12833500  |
| C    | -1.21563800| -5.10594400| 3.78727500  |
| C    | 0.41934600 | -3.71332100| 3.65454000  |
| C    | 0.45126900 | -3.53975500| 4.72563700  |
| C    | 1.32679800 | -3.05171300| 2.82343500  |
| C    | 2.37631300 | -2.12097200| 3.41236800  |
| C    | 3.12137900 | -1.91207400| 2.63866300  |
| C    | 1.73901300 | -0.78274200| 3.80125900  |
| C    | 2.49641600 | -0.08630000| 4.17733200  |
Cartesian coordinates of the optimized geometry for 10 at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Cl   | 1.61952000 | 1.16711300 | 2.94759000 |
| P    | 0.23072100 | -0.67231400| -0.23568600|
| Ga   | 1.79883700 | 0.65229800 | 0.78237500 |
| Ga   | -2.05642500| -0.42594000| -0.20340400|
| N    | 3.46046600 | -0.40778600| 0.83546100 |
| N    | 3.46046600 | -0.40778600| 0.83546100 |
| N    | -2.84831000| -2.15741700| -0.66476000|
| N    | -3.69003700| 0.38819500 | 0.40939300 |
| C    | 4.61493800 | 0.21566900 | 1.03442200 |
| C    | 4.74430100 | 1.61880900 | 0.99190700 |
| H    | 5.69783700 | 2.01554500 | 1.31652900 |
| C    | 3.84980600 | 2.53718500 | 0.43802600 |
| C    | 5.86985200 | -0.57983800| 0.30504900 |
| H    | 5.96565700 | -0.77654200| 2.37868100 |
| H    | 6.75286100 | -0.02352000| 0.98355300 |
| H    | 5.84717000 | -1.54541100| 0.79678100 |
| C    | 4.29342600 | 3.98025100 | 0.35927400 |
| H    | 5.32642100 | 0.88724000 | 0.69505500 |
| C    | 3.64938200 | 4.59359300 | 1.00040400 |
| H    | 4.20573000 | 4.38139100 | -0.65178000|
| C    | 3.36744700 | -1.83822300| 0.77815000 |
| C    | 3.33254300 | -2.59961500| 1.96178600 |
| C    | 3.18679900 | -3.98828800| 1.84434100 |
| H    | 3.16393700 | -4.59519700| 2.74494500 |
| C    | 3.06545600 | -4.59757300| 0.60133800 |
| H    | 2.95627400 | -5.67675100| 0.53183600 |
| C    | 3.07997500 | -3.82299400| 0.55668800 |
| H    | 2.96089400 | -3.02014000| 1.52159400 |
| C    | 3.21470900 | -2.43566200| 0.49239300 |
| C    | 3.23322800 | -1.58755900| 1.75627100 |
| H    | 2.76838000 | -0.62886100| 1.51133500 |
| C    | 4.67395300 | -1.29012100| -2.20680400|
| H    | 5.21994600 | -0.71171100| 1.45597300 |
| H    | 4.66962800 | -0.70926500| 3.13551500 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 5.2232  | -2.2213 | 0.00    |
| C    | 2.4098  | -2.1782 | 0.00    |
| H    | 2.8874  | -3.0648 | 0.00    |
| H    | 2.3007  | -1.4315 | 0.00    |
| H    | 1.4106  | 3.1354  | -0.93    |
| C    | 1.0729  | 4.0685  | -0.39    |
| H    | 0.7255  | 5.0301  | 1.09    |
| C    | -1.3877 | 6.0779  | 1.52    |
| C    | -0.5191 | 3.1563  | 1.29    |
| C    | -0.3962 | 2.1695  | 0.83    |
| H    | -1.3876 | 3.6252  | 0.83    |
| C    | 3.2644  | 2.1024  | 2.89    |
| C    | 3.1997  | 1.2056  | 2.27    |
| C    | 4.7238  | 2.5957  | 2.84    |
| C    | 5.1019  | 2.6829  | 1.82    |
| C    | 4.8223  | 3.5718  | 3.34    |
| C    | 5.3735  | 1.8878  | 3.37    |
| C    | 2.9101  | 1.6989  | 4.33    |
| H    | 3.5208  | 0.8387  | 4.63    |
| C    | 3.1258  | 2.5048  | 5.04    |
| C    | 1.8568  | 1.4211  | 4.41    |
| C    | 4.1406  | -0.3288 | 0.50    |
| C    | -5.1025 | -1.4455 | 0.27    |
| H    | -6.1272 | -1.3821 | 0.13    |
| C    | -4.8900 | 0.3289  | 1.82    |
| C    | -4.6233 | 0.8607  | 0.27    |
| C    | -4.4732 | 0.0267  | 1.67    |
| C    | -4.0690 | -1.0971 | 0.81    |
| C    | -5.6894 | 0.8423  | 0.17    |
| C    | -6.1059 | 0.5347  | 0.81    |
| C    | -7.0106 | 0.6512  | 0.65    |
| H    | -6.2068 | 1.4954  | 0.30    |
| H    | -6.0212 | 1.8846  | 1.98    |
| C    | -1.9107 | 3.1747  | 0.57    |
| C    | -1.5708 | -2.4175 | 0.24    |
| C    | -0.6253 | -2.7519 | 0.71    |
| C    | -0.3490 | -3.7932 | 0.17    |
| C    | -0.0236 | -1.7750 | 0.07    |
| H    | 0.7186  | -2.0567 | 0.20    |
| C    | -0.3678 | -0.4367 | 0.19    |
| C    | 0.1206  | 0.3220  | 0.03    |
| C    | -1.3193 | -0.0532 | 0.00    |
| C    | -2.2256 | -0.3515 | 0.00    |
| H    | -2.8073 | -3.0521 | 0.00    |
| H    | -3.1911 | -4.3537 | 0.00    |
| H    | -2.6576 | -4.8437 | 0.00    |
| H    | -3.6599 | -5.1357 | 0.00    |
| H    | -3.9898 | -3.7455 | 0.00    |
| C    | -1.1955 | -4.4363 | 0.00    |
| H    | -0.4861 | -3.8822 | 0.00    |
| H    | -1.7129 | -5.1478 | 0.00    |
| H    | -0.6323 | -5.0189 | 0.00    |
| C    | -1.6853 | -1.4172 | 0.00    |
| H    | -2.4844 | 1.4985  | 0.00    |
| C    | -2.2178 | 2.0148  | 0.00    |
Cartesian coordinates of the optimized geometry for TS$_{14}$ at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 1):

C  1.72649900  -1.04684500   2.44577800
P  0.15367100   0.44846000   0.91534700
Ga -1.84580900  -0.33821600   0.31806000
Ga  1.80392800   0.05037800   0.04720200
N  -3.34602000   0.99635700   0.41382000
N  -3.00503300  -1.72145900  -0.50916000
N  3.04206700   1.57773000  -0.33979000
N  2.92381900  -0.85824000   1.25542300
C  -4.62833000   0.63494700   0.39060800
C  -5.07324000  -0.66871900   0.12780600
H  -6.14519800  -0.82379100   0.19826200
C  -4.33095600  -1.74374400  -0.50916000
C  -5.71255700   1.66645800   0.62460700
H  -5.44516900   2.63845900   0.20768900
Cartesian coordinates of the optimized geometry for 4 at B3LYP-D3BJ/6-31G* level of theory (number of imaginary frequencies = 0):

Cl   -1.44763700  1.13148900  -2.94253400
P    -0.02520570 -0.71364200  0.31797400
Ga   -1.76611300  0.57093200 -0.80067700
Ga   -0.20114450 -0.26862000  0.31764800
N    -3.39468100 -0.53756700  0.98266400
N    -2.73169600  2.09231200 -0.03678800
N    -2.83824700 -1.95564500  0.94276900
N    -3.57146400  0.42748900 -0.57919100
C    -4.55340700  0.04460000 -1.26345100
C    -4.73543100  1.44198000 -1.22922400
H    -5.67709600  1.80656500 -1.61985000
C    -3.91515300  2.38641200 -0.61042200
C    -5.78683600  0.97641200 -2.69759100
H    -6.68021100 -0.27002300 -1.34337700
C    -5.73460400 -1.76222000 -1.12016700
C    -4.41502100  3.81265900 -0.55822900
C    -5.42307500  3.88632500 -0.97065000
H    -3.74800100  4.45426400 -1.14574600
C    -4.41923400  4.20891900  0.45864800
C    -3.25855800 -1.96506600 -0.93482400
C    -3.13280500 -2.71070800 -2.12282800
C    -2.94511500 -4.09480000 -2.01311600
C    -2.85070700 -4.68630000 -2.91767700
C    -2.86826500 -4.71523700 -0.77226400
H    -2.72133300 -5.79033200 -0.70859000
C    -2.97685500 -3.95682300  0.39143700
C    -2.89487200 -4.44434300  1.35596800
C    -3.16278000 -2.57471200  0.33634500
C    -3.29935400 -1.74836700  1.60700700
C    -2.83708900 -0.77655800  1.41668800
C    -4.77784400 -2.49145000  1.94671400
C    -5.27520400 -0.90816600  1.16658900
C    -4.86066600 -0.93067600  2.88415600
C    -5.31921400 -2.43740500  2.06728300
C    -2.55606900 -2.34044500  2.80738800
C    -3.04502600 -3.24553000  3.18942600
C    -2.52873200 -1.60418600  3.61528300
C    -1.52579900 -2.58795900  2.54267600
C    -2.17627400  3.04162500  0.89119900
C    -1.28220200  4.02181000  0.42332300
C    -0.79841900  4.97148300  1.32882500
H    -0.10333100  5.73194800  0.98651500
C    -1.21055000  4.96020600  2.65755000
H    -0.83382800  5.70782400  3.35077700
C    -2.09571600  3.98251600  3.10341900
C    -2.39745400  3.97548600  4.14552500
C    -2.58963700  2.99901000  2.24056700
C    -0.83543200  4.01567000 -1.02632700
H    -1.58292800  3.47693400 -1.60991800
C    -0.71306100  5.41535400 -1.64198400
H    -0.48397400  5.33060700 -2.71007500
H    -0.09266100  5.99920700 -1.18182500
H    -1.64323300  5.98552600 -1.53534800
C    0.48811300  3.25485200 -1.15884900
| Atom | x       | y       | z       |
|------|---------|---------|---------|
| H    | 0.45033000 | 2.29244800 | -0.63957900 |
| H    | 1.29853800 | 3.83498500 | -0.71825100 |
| H    | 0.72615000 | 3.05865700 | -2.20504200 |
| C    | -3.56092300 | 1.93927900 | 2.74957300 |
| H    | -3.40974800 | 1.05269700 | 2.13196100 |
| C    | -5.03284200 | 2.37015900 | 2.59689800 |
| H    | -5.33369900 | 2.45936300 | 1.55112200 |
| H    | -5.21169900 | 3.33242000 | 3.09226000 |
| C    | -3.29904300 | 1.53606000 | 4.20816900 |
| H    | -3.90633900 | 0.65886700 | 4.45858800 |
| H    | -3.58491100 | 2.33168800 | 4.90718100 |
| C    | 4.14308500  | -2.17345100 | 0.90333200 |
| C    | 5.06200900  | -1.25362900 | 0.36002400 |
| C    | 6.10185700  | -1.54911000 | 0.41408200 |
| C    | 4.79147200  | -0.11999400 | -0.40564700 |
| H    | 4.91362300  | -4.12271300 | 0.47370300 |
| H    | 4.04727500  | -4.04438800 | 2.00862100 |
| H    | 5.67625100  | -3.33601400 | 1.85807700 |
| C    | 5.96815200  | 0.48199800  | -1.14172400 |
| H    | 6.85219200  | -0.14560800 | -1.02010800 |
| C    | 6.20309400  | 1.48476800  | -0.77907300 |
| C    | 5.74510300  | 0.57490600  | -2.20823700 |
| C    | 1.93438400  | -3.02154200 | 1.29235900 |
| C    | 1.52329300  | -3.19938200 | 2.62686900 |
| C    | 0.63713600  | -4.24706700 | 2.90568100 |
| H    | 0.31749200  | -4.40982100 | 3.93014000 |
| C    | 0.14912100  | -5.07063900 | 1.89745600 |
| C    | 0.54967600  | -4.86313400 | 0.58183000 |
| C    | 0.15032600  | -5.49161000 | -0.20772900 |
| C    | 1.44681100  | -3.84404100 | 0.25661100 |
| C    | 2.04071010  | -3.33438700 | 3.76748200 |
| C    | 2.58427500  | -1.49258400 | 3.33034300 |
| C    | 3.02394500  | -3.11485200 | 4.66005100 |
| C    | 2.53152300  | -3.98070400 | 5.11791900 |
| H    | 3.39397200  | -4.47355900 | 5.46843600 |
| C    | 3.88914700  | -3.48137300 | 4.09939500 |
| C    | 0.89529700  | -1.76693400 | 4.62182300 |
| C    | 0.18535800  | -1.19340100 | 4.02425700 |
| C    | 1.29335900  | -1.10478500 | 5.39649000 |
| C    | 0.34698900  | -2.56582900 | 5.13398900 |
| C    | 1.85531300  | -3.64162000 | -1.19281900 |
| C    | 2.51945200  | -2.77319900 | 1.24321500 |
| C    | 2.65408500  | -4.84436400 | -1.72843700 |
| C    | 2.03796300  | -5.75069300 | -1.73816300 |
| C    | 3.53690600  | -5.05012200 | -1.11367400 |
| H    | 2.98929100  | -4.65590500 | -2.75499700 |
| C    | 0.64755400  | -3.35069200 | -2.08775400 |
| H    | 0.97814400  | -3.08554200 | -3.09755700 |
| H    | 0.04835000  | -2.53101900 | -1.69219900 |
| H    | -0.01216700 | -4.22027500 | -2.16944400 |
| C    | 3.44208600  | 1.51188800  | -1.51891200 |
| C    | 3.87662700  | 2.80112700  | -1.15022300 |
| C    | 3.81703000  | 3.81617800  | -2.11061100 |
| H    | 4.14445900  | 4.81745200  | -1.84886700 |
| C    | 3.33649900  | 3.56415900  | -3.38976700 |
| C    | 3.29932900  | 4.36320900  | -4.12477200 |
| C    | 2.88047700  | 2.29168700  | -3.72471600 |
| H    | 2.48284600  | 2.11835300  | -4.71708900 |
| C    | 2.91500400  | 1.24090200  | -2.80192700 |
| C    | 2.40516300  | -0.15041400 | -3.17936300 |
| H    | 1.73875000  | -0.49254900 | -2.37512600 |
| C    | 1.96529000  | -0.16253400 | -4.46233100 |
| C    | 1.12284400  | -1.15426900 | -4.59680300 |
| H    | 2.18035300  | 0.04391700  | -5.34652400 |
H 0.74766400 0.55895700 -4.41764700
C 3.55057500 -1.17100200 -3.32482300
H 3.15146700 -2.13202600 -3.66740700
H 4.08400200 -1.35190600 -2.39108800
H 4.27280100 -0.82635500 -4.07463900
C 4.35794600 3.12035800 0.26095900
H 4.58964900 2.17789200 0.76526300
C 5.62600000 3.98873800 0.28568700
H 5.42823500 5.00109000 -0.08324200
H 5.99416400 4.08369100 1.31315000
H 6.43029300 3.56631400 -0.32670700
C 3.23510800 3.78986900 1.06867800
H 2.34422500 3.16117300 1.08593600
H 3.55428100 3.96436200 2.10219600
H 2.96128400 4.75694800 0.63085100
C -3.18317500 -2.07144600 -3.50428800
H -3.43211600 -1.01417600 -3.3818400
C -1.80619400 -2.12245200 -4.18472400
H -1.84514800 -1.62476500 -5.16030700
H -1.06336700 -1.60486800 -3.57756800
H -1.47705000 -3.15689300 -4.33818800
C -4.25031700 -2.72251600 -4.40113800
H -4.33648000 -2.17394600 -5.34602000
H -3.90036000 -3.75876700 -4.64539700
H -5.23450600 -2.73656800 -3.92118700
C 0.05211900 0.33424100 1.89170800
O -0.79799600 0.53506500 2.75566800
N 1.37688600 0.67286800 1.91417800
C 1.97622000 1.28033100 3.10556200
H 2.01635000 0.54669800 3.92049300
H 3.01594800 1.51243400 2.84663800
C 1.26105000 2.53572600 3.60979300
H 1.09769400 3.25581200 2.80586800
H 0.28331400 2.27892400 4.01570800
H 1.86027600 3.01668600 4.39298000
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