Electronic Supplementary Material (ESI) for Chemical Science.
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Supporting Information

Content:

1. Experimental Section

General procedure. All experiments and manipulations were carried out under a dry argon atmosphere using either standard *Schlenk* techniques or an MBraun LABmaster Pro glovebox. Toluene, benzene, flurobenzene, and *n*-hexane were dried using Braun solvent drying system, degassed, and stored over 4Å molecular sieve. Toluene-d_8, benzene-d_6, and THF-d_8 were dried by refluxing over NaK, distilled prior to use, and stored over 4Å molecular sieve. Commercial reagents were purchased from Aldrich, Acros, or Alfa-Aesar Chemical Co. and used as received. L(Cl)GaPCO (L = HC[C(Me)N(Ar)]$_2$, Ar = 2,6-*i*Pr$_2$C$_6$H$_3$),[1] IMe$_4$,[2] and Fc[B(C$_6$F$_5$)$_4$][3] were prepared according to literature procedures. NMR spectra (^{1}H, ^{13}C, ^{31}P) were recorded on Bruker Avance II 500 MHz spectrometer and were referenced to internal C$_6$D$_5$H (^{1}H δ = 7.16; ^{13}C δ = 128.06), C$_7$D$_7$H (^{1}H δ = 2.08, 6.97, 7.01, 7.09; ^{13}C δ = 137.19, 129.26, 127.96, 125.96), and THF-d_8 (^{1}H δ = 1.72, 3.58; ^{13}C δ = 67.21, 25.31). ^{31}P NMR spectra are referenced to internal C$_6$D$_5$H (^{1}H δ = 7.16), C$_7$D$_7$H (^{1}H δ = 2.08, 6.97, 7.01, 7.09), and THF-d_8 (^{1}H δ = 1.72, 3.58) using chi-values (χ).[4] 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. Melting points were measured in sealed glass capillaries. Cyclic voltammetry studies were performed in a glovebox using a Metrohm Autolab PGSTAT 204 potentiostat with a three electrodes setup consisting of a Pt disc (d ¼ 1 mm) working electrode, Pt wire counter electrode, and Ag wire pseudoreference electrode, and ferrocene as internal standard. Positive feedback compensation was utilized to reduce solvent resistance effects.

Synthesis of [L(Cl)GaP]$_2$ (2a)

A toluene (10 mL) solution of L(Cl)GaPCO **1** (2.0 g, 3.44 mmol) was irradiated for 5 hours and the resulting green solid was collected by filtration, washed with toluene (2 mL) and dried. Yield: 65% (1.23 g). M.p. 120 °C (dec.). Single crystals suitable for X-ray diffraction were grown by cooling a hot toluene solution of **2a** to ambient temperature. Anal. calcd. (%) for C$_{58}$H$_{82}$Cl$_2$Ga$_2$N$_4$P$_2$ (1104.39): C, 62.89; H, 7.46; N, 5.06. Found: C, 62.83; H, 7.52; N, 5.11. ^{1}H NMR (500 MHz, C$_7$D$_8$, 298 K) δ = 0.99 (d, $^3J_{HH}$ = 6.7 Hz, 6H, CH(C*H*$_3$)$_2$), 1.13 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.19 (t, $^3J_{HH}$ = 7.2 Hz, 12H, CH(C*H*$_3$)$_2$), 1.64 (s, 6H, CC*H*$_3$), 3.04 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 3.74 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, C*H*(CH$_3$)$_2$), 4.93 (s, 1H, C*H*), 6.90-7.10 (m, 6H, C$_6$*H*$_3$). ^{13}C{^{1}H} NMR (125 MHz, C$_7$D$_8$, 298 K) δ = 23.1, 23.7, 24.1, 24.5 (CH(*C*H$_3$)$_2$), 27.1, 27.6, 28.6, 29.3 (*C*H(CH$_3$)$_2$), 97.0 (*C*H), 140.3, 142.7, 145.6, 168.9 (*C*$_6$H$_3$). ^{31}P{^{1}H} (202 MHz, C$_7$D$_8$, 298 K) δ = 761.6 ppm. ATR-IR: *v* 2957, 2908, 2851, 1552, 1454, 1432, 1379, 1309, 1256, 1170, 1013, 931, 863, 788, 774, 749, 632, 608, 525 cm^{-1}.

Synthesis of [L(Br)GaP]$_2$ (2b)

TMSBr (2 mL, 13.54 mmol) was added to a solid sample of **2a** (1.0 g, 0.902 mmol) at ambient temperature and stirred overnight. All volatiles were then removed in *vacuo* and the green residue was washed with toluene (1 mL). Yield: 99% (1.06 g). Single crystals suitable for X-ray diffraction were grown by cooling a

hot toluene solution of **2b** to ambient temperature. M.p. 123 °C (dec.). Anal. calcd. (%) for $C_{58}H_{82}Br_2Ga_2N_4P_2$ (1192.29): C, 58.22; H, 6.91; N, 4.68. Found: C, 58.33; H, 7.05; N, 4.79. ^{1}H NMR (500 MHz, C_7D_8, 298 K) δ = 0.99 (d, $^3J_{HH}$ = 6.5 Hz, 6H, CH(CH_3)$_2$), 1.13 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$), 1.22 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(CH_3)$_2$), 1.26 (d, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$), 1.63 (s, 6H, CCH_3), 3.00 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 3.68 (sept, $^3J_{HH}$ = 6.8 Hz, 2H, CH(CH$_3$)$_2$), 4.86 (s, 1H, CH), 6.90-7.08 (m, 6H, C_6H_3). ^{13}C{^{1}H} NMR (125 MHz, C_7D_8, 298 K) δ = 23.6, 24.2, 24.7, 25.0 (CH(*C*H$_3$)$_2$), 27.7, 28.2, 29.8 (*C*H(CH$_3$)$_2$), 97.6 (*C*H), 140.8, 143.3, 146.2, 169.5 (*C*$_6$H$_3$). ^{31}P{^{1}H} (202 MHz, C_7D_8, 298 K) δ = 766.8. ATR-IR: *v* 2967, 2919, 2859, 1558, 1519, 1459, 1436, 1384, 1311, 1258, 1173, 1101, 1015, 935, 867, 791, 774, 754, 710, 633, 527 cm^{-1}.

Synthesis of [L(Cl)GaP]$_2$[IMe$_4$] (3a)

To a toluene (10 mL) suspension of **2a** (100 mg, 0.09 mmol), IMe$_4$ (11 mg, 0.09 mmol) was added at ambient temperature. The initial green suspension immediately dissolved and a dark red solution formed. It was then filtered over celite and dried in *vacuo*. It was washed with *n*-hexane (2 mL), and dried to yield a red crystalline powder. Single crystals suitable for X-ray diffraction were grown by diffusing *n*-hexane to a saturated toluene solution of **3a** at ambient temperature. Yield: 95% (105 mg). M.p. 141 °C (dec.). Anal. calcd. (%) for $C_{65}H_{94}Cl_2Ga_2N_6P_2$ (1228.49): C, 63.38; H, 7.69; N, 6.82. Found: C, 63.42; H, 7.73; N, 6.87. ^{1}H NMR (500 MHz, C_7D_8, 298 K) δ = 0.45 (d, $^3J_{HH}$ = 6.4 Hz, 3H, CH(CH_3)$_2$), 0.69 (d, $^3J_{HH}$ = 6.4 Hz, 3H, CH(CH_3)$_2$), 0.92 (t, $^3J_{HH}$ = 7.1 Hz, 3H, CH(CH_3)$_2$), 1.05 (d, $^3J_{HH}$ = 6.8 Hz, 3H, CH(CH_3)$_2$), 1.09 (d, $^3J_{HH}$ = 6.7 Hz, 3H, CH(CH_3)$_2$), 1.12 (d, $^3J_{HH}$ = 6.7 Hz, 3H, CH(CH_3)$_2$), 1.16-1.28 (m, 12H, CH(CH_3)$_2$), 1.29 (t, $^3J_{HH}$ = 6.5 Hz, 6H, CH(CH_3)$_2$), 1.38-1.40 (m, 12H, CH(CH_3)$_2$), 1.40 (s, 3H, CCH_3), 1.42 (s, 3H, CCH_3), 1.51 (s, 3H, CCH_3), 1.53 (s, 3H, CCH_3), 1.58 (s, 3H, CCH_3), 1.61 (s, 3H, CCH_3), 2.77 (s, 3H, NCH_3), 3.06 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.16 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.23 (s, 3H, NCH_3), 3.23 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.29 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.38 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.58 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.80 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.95 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 4.87 (s, 1H, CH), 4.88 (s, 1H, CH), 6.86 (d, $^3J_{HH}$ = 7.8 Hz, 1H, C_6H_3), 7.05-7.08 (m, 2H, C_6H_3), 7.10-7.15 (m, 5H, C_6H_3), 7.18-7.23 (m, 2H, C_6H_3), 7.26-7.32 (m, 2H, C_6H_3). ^{13}C{^{1}H} NMR (125 MHz, C_7D_8, 298 K) δ = 7.8, 14.0 (NCH_3), 22.7, 23.2, 23.5, 23.8, 23.9, 24.0, 24.2, 24.6, 24.7, 25.0, 25.3, 25.4, 25.6, 26.2, 26.3, 26.8, 27.2, 27.5, 27.7, 27.9 (CH(*C*H$_3$)$_2$), 28.6, 29.1, 29.5, 29.9, 30.0, 31.7, 32.4, 32.6, 33.3, 33.5 (*C*H(CH$_3$)$_2$), 96.5, 97.9 (*C*H), 122.9, 123.3, 123.7, 123.9, 124.0, 124.1, 124.3, 125.0, 125.2, 125.3, 126.0, 127.0, 142.0, 143.2, 143.3, 143.5, 143.7, 144.0, 144.4, 145.0, 145.1, 145.3, 151.3, 152.5, 166.4, 166.8, 168.3, 168.8 (*C*$_6$H$_3$). ^{31}P{^{1}H} (202 MHz, C_7D_8, 298 K) δ = –85.8 (d, $^1J_{P-P}$ = 353.0 Hz), –258.5 (d, $^1J_{P-P}$ = 353.0 Hz). ATR-IR: *v* 2951, 2909, 2852, 1541, 1515, 1451, 1431, 1378, 1312, 1253, 1173, 1094, 1014, 934, 854, 792, 755, 724, 689, 635, 526 cm^{-1}.

Synthesis of [L(Br)GaP]$_2$[IMe$_4$] (3b)

Compound **3b** was synthesized following the similar protocols used for **3a** using **2b** (100 mg, 0.084 mmol) and IMe$_4$ (10 mg, 0.084 mmol). Single crystals suitable for X-ray diffraction were grown by diffusing *n*-

hexane to a saturated toluene solution of **3a** at ambient temperature. Yield: 92% (100 mg). M.p. 147 °C (dec.). Anal. calcd. (%) for $C_{65}H_{94}Br_2Ga_2N_6P_2$ (1316.39): C, 59.11; H, 7.17; N, 6.36. Found: C, 59.15; H, 7.21; N, 6.39. ^{1}H NMR (500 MHz, C_7D_8, 298 K) δ = 0.42 (d, $^3J_{HH}$ = 6.4 Hz, 3H, CH(CH_3)$_2$), 0.80 (d, $^3J_{HH}$ = 6.4 Hz, 3H, CH(CH_3)$_2$), 0.89 (t, $^3J_{HH}$ = 7.1 Hz, 3H, CH(CH_3)$_2$), 1.01 (d, $^3J_{HH}$ = 6.8 Hz, 3H, CH(CH_3)$_2$), 1.06 (m, 6H, CH(CH_3)$_2$), 1.13 (d, $^3J_{HH}$ = 6.8 Hz, 3H, CH(CH_3)$_2$), 1.15 (d, $^3J_{HH}$ = 6.8 Hz, 6H, CH(CH_3)$_2$), 1.20 (d, $^3J_{HH}$ = 6.6 Hz, 3H, CH(CH_3)$_2$), 1.21-1.24 (m, 6H, CH(CH_3)$_2$), 1.31 (d, $^3J_{HH}$ = 6.8 Hz, 3H, CH(CH_3)$_2$), 1.34-1.36 (m, 6H, CH(CH_3)$_2$),1.40 (s, 3H, CCH_3), 1.42 (s, 3H, CCH_3), 1.47 (s, 3H, CCH_3), 1.50 (s, 3H, CCH_3), 1.54 (s, 3H, CCH_3), 1.59 (s, 3H, CCH_3), 2.86 (s, 3H, NCH_3), 3.04 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.12 (s, 3H, NCH_3), 3.17 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.24 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, CH(CH$_3$)$_2$), 3.43 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.67 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.83 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.96 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 4.89 (s, 1H, CH), 4.91 (s, 1H, CH), 6.83 (d, $^3J_{HH}$ = 7.5 Hz, 1H, C$_6H_3$), 7.02-7.05 (m, 2H, C$_6H_3$), 7.06-7.12 (m, 5H, C$_6H_3$), 7.14-7.18 (m, 2H, C$_6H_3$), 7.22-7.27 (m, 2H, C$_6H_3$). ^{13}C{^{1}H} NMR (125 MHz, C_7D_8, 298 K) δ = 8.3, 14.3 (NCH_3), 23.1, 23.6, 24.0, 24.3, 24.5, 24.6, 25.1, 25.2, 25.5, 25.6, 26.8, 27.1, 27.2, 27.5, 27.8, 28.0 (CH(CH_3)$_2$), 28.8, 29.0, 29.5, 29.9, 30.3, 32.0, 33.4, 33.9 (CH(CH$_3$)$_2$), 97.2, 98.7 (CH), 123.3, 123.6, 123.9, 124.2, 124.4, 124.5, 124.7, 125.4, 125.7, 126.4, 127.6, 142.3, 142.6, 143.4, 143.6, 143.9, 144.1, 144.4, 144.5, 145.0, 145.6, 145.7, 145.8, 151.6, 152.6, 167.0, 167.4, 169.0, 169.4 (C$_6$H$_3$). ^{31}P{^{1}H} (202 MHz, C_7D_8, 298 K) δ = –77.7 (d, $^1J_{P–P}$ = 358.9 Hz), –247.5 (d, $^1J_{P–P}$ = 358.9 Hz). ATR-IR: *v* 2945, 2908, 2855, 1544, 1518, 1454, 1431, 1378, 1312, 1252, 1172, 1096, 1014, 934, 854, 791, 755, 636, 531 cm^{-1}.

Synthesis of {[L(Cl)GaP]$_2$[IMe$_4$]}[BAr$^F_4$] (4a)

To a red toluene solution (5 mL) of **3a** (50 mg, 0.04 mmol), [FeCp$_2$][BAr$^F_4$] (35 mg, 0.04 mmol) was added at room temperature. Immediately the red solution turned light orange and **4a** was obtained as orange crystals in 83% isolated yield. Yield: 64 mg. M.p.: 100 °C (dec.). Anal. calcd. (%) for $C_{89}H_{94}BCl_2F_{20}Ga_2N_6P_2$ (1907.47): C, 55.94; H, 4.96; N, 4.40. Found: C, 56.05; H, 5.01; N, 4.47. ATR-IR: *v* 2955, 2911, 2855, 1634, 1521, 1452, 1405, 1365, 1312, 1252, 1172, 1096, 1019, 976, 867, 797, 754, 661, 656 cm^{-1}.

Synthesis of {[L(Br)GaP]$_2$[IMe$_4$]}[BAr$^F_4$] (4b)

Compound **4b** was synthesized following the similar protocols used for **4a** using **3b** (50 mg, 0.038 mmol), [FeCp$_2$][BAr$^F_4$] (33 mg, 0.038 mmol). Single crystals suitable for X-ray diffraction were grown by storing a saturated toluene solution of **4b** at ambient temperature. Yield: 79% (60 mg, orange crystals). M.p.: 107 °C (dec.). Anal. calcd. (%) for $C_{89}H_{94}BBr_2F_{20}Ga_2N_6P_2$ (1999.72): C, 53.46; H, 4.74; N, 4.20. Found: C, 53.54; H, 4.83; N, 4.31. ATR-IR: *v* 2951, 2911, 2855, 1634, 1521, 1504, 1455, 1365, 1311, 1252, 1172, 1079, 1019, 974, 864, 797, 754, 681, 656 cm^{-1}.

Synthesis of [L(Cl)GaP(IMe$_4$)HPGa(Cl)L][BAr$^F_4$] (5a)

HSn(nBu)$_3$ (30 μL, 0.030 mmol; 1M solution in fluorobenzene) was added to a solution of **4a** (50 mg, 0.026 mmol) in flurobenzene (5 mL) at ambient temperature. Upon addition the solution turned colourless. Then

the mixture was stirred for **5a** min and all the volatiles were removed in *vacuo*. The colourless residue was then washed with *n*-hexane (1 mL) and dried in *vacuo* to afford **5a** as a colourless crystalline powder. Yield 73% (36 mg). Single crystals suitable for an X-ray diffraction analysis were obtained by slow diffusion of *n*-hexane to a saturated flurobenzene solution of **5a** at ambient temperature. M.p.: 153 °C (dec.). Anal. calcd. (%) for $C_{89}H_{95}BCl_2F_{20}Ga_2N_6P_2$ (1908.48): C, 55.91; H, 5.01; N, 4.40. Found: C, 56.01; H, 5.12; N, 4.47. ^{1}H NMR (300 MHz, THF-d_8, 298 K) δ = 0.25 (d, $^3J_{HH}$ = 6.3 Hz, 3H, CH(CH_3)$_2$), 0.45 (d, $^3J_{HH}$ = 6.1 Hz, 3H, CH(CH_3)$_2$), 0.80 (d, $^3J_{HH}$ = 6.6 Hz, 3H, CH(CH_3)$_2$), 0.92 (d, $^3J_{HH}$ = 6.5 Hz, 3H, CH(CH_3)$_2$), 1.00–1.06 (m, 6H, CH(CH_3)$_2$), 1.08–1.12 (m, 9H, CH(CH_3)$_2$), 1.18–1.23 (m, 9H, CH(CH_3)$_2$), 1.28 (t, $^3J_{HH}$ = 6.7 Hz, 6H, CH(CH_3)$_2$), 1.39 (t, $^3J_{HH}$ = 6.6 Hz, 6H, CH(CH_3)$_2$), 1.69 (s, 3H, CCH_3), 1.77 (s, 6H, CCH_3), 1.81 (s, 3H, CCH_3), 1.93 (s, 3H, CCH_3), 1.97 (s, 3H, CCH_3), 2.56 (s, 3H, NCH_3), 2.72 (s, 3H, NCH_3), 2.78 (sept, 2H, CH(CH$_3$)$_2$), 3.03 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, CH(CH$_3$)$_2$), 3.37 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 3.49 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 5.42 (s, 1H, CH), 5.45 (s, 1H, CH), 6.91 (d, $^3J_{HH}$ = 6.8 Hz, 1H, C$_6H_3$), 7.10–7.17 (m, 2H, C$_6H_3$), 7.19–7.27 (m, 4H, C$_6H_3$), 7.31–7.40 (m, 4H, C$_6H_3$), 7.53 (t, $^3J_{HH}$ = 7.6 Hz, 1H, C$_6H_3$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, 298 K) δ = 7.7, 8.6, 9.1, 23.9, 24.4 (CH(*C*H$_3$)$_2$), 28.3, 29.0, 29.3, 29.4, 30.3, 33.1 (*C*H(CH$_3$)$_2$), 98.8, 99.4 (*C*H), 115.9, 116.0 (N*C*), 125.0, 125.4, 126.0, 128.2, 128.8, 129.2, 131.0, 136.4, 138.0, 140.1, 145.4, 148.4, 150.0, 163.2, 164.7, 171.7, 171.9, 172.7 (*C*$_6$H$_3$). ^{31}P{^{1}H} (121 MHz, THF-d_8, 298 K) δ = –148.8 (d, $^1J_{PP}$ = 84.9 Hz), –229.1 (d, $^1J_{PP}$ = 82.0 Hz). ^{31}P (121 MHz, THF-d_8, 298 K) δ = –147.5 (dd, $^1J_{PP}$ = 25.3, 84.9 Hz), –228.0 (dd, $^1J_{PP}$ = 85.6, 180.9 Hz). ATR-IR: ν 2964, 2926, 2867, 2156, 1640, 1510, 1456, 1371, 1258, 1178, 1082, 1021, 977, 941, 871, 800, 758, 684, 659, 604, 571, 533 cm^{-1}.

Synthesis of [L(Br)GaP(IMe$_4$)HPGa(Br)L][BAr$^F_4$] (5b)

Compound **5b** was synthesized following the similar protocols used for **5a** using **4b** (50 mg, 0.025 mmol), HSn(*n*Bu)$_3$ (30 µL, 0.030 mmol; 1M solution in fluorobenzene). Yield: 70% (34 mg, colorless crystals). M.p.: 151 °C (dec.). Anal. calcd. (%) for $C_{89}H_{95}BBr_2F_{20}Ga_2N_6P_2$ (1996.37): C, 53.43; H, 4.79; N, 4.20. Found: C, 53.61; H, 4.96; N, 4.27. ^{1}H NMR (300 MHz, THF-d_8, 298 K) δ = 0.28 (d, $^3J_{HH}$ = 6.0 Hz, 3H, CH(CH_3)$_2$), 0.48 (d, $^3J_{HH}$ = 5.9 Hz, 3H, CH(CH_3)$_2$), 0.82 (d, $^3J_{HH}$ = 6.2 Hz, 3H, CH(CH_3)$_2$), 0.93 (d, $^3J_{HH}$ = 6.5 Hz, 3H, CH(CH_3)$_2$), 1.03 (t, $^3J_{HH}$ = 6.1 Hz, 6H, CH(CH_3)$_2$), 1.11–1.19 (m, 9H, CH(CH_3)$_2$), 1.18–1.23 (m, 9H, CH(CH_3)$_2$), 1.28 (br, 6H, CH(CH_3)$_2$), 1.39 (t, $^3J_{HH}$ = 6.5 Hz, 6H, CH(CH_3)$_2$), 1.69 (s, 3H, CCH_3), 1.77 (s, 3H, CCH_3), 1.78 (s, 3H, CCH_3), 1.82 (s, 3H, CCH_3), 1.94 (s, 3H, CCH_3), 1.97 (s, 3H, CCH_3), 2.51 (s, 3H, NCH_3), 2.72 (s, 3H, NCH_3), 2.86 (sept, 3H, CH(CH$_3$)$_2$), 3.09 (sept, $^3J_{HH}$ = 6.7 Hz, 2H, CH(CH$_3$)$_2$), 3.41 (sept, $^3J_{HH}$ = 6.7 Hz, 1H, CH(CH$_3$)$_2$), 5.41 (s, 1H, CH), 5.46 (s, 1H, CH), 6.89 (d, $^3J_{HH}$ = 7.4 Hz, 1H, C$_6H_3$), 7.14–7.18 (m, 2H, C$_6H_3$), 7.27–7.33 (m, 4H, C$_6H_3$), 7.35–7.40 (m, 4H, C$_6H_3$), 7.54 (t, $^3J_{HH}$ = 7.6 Hz, 1H, C$_6H_3$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, 298 K) δ = 8.8, 9.1, 24.1, 24.4 (CH(*C*H$_3$)$_2$), 27.4, 28.4, 28.7, 30.1, 30.4 (*C*H(CH$_3$)$_2$), 99.1, 99.7 (*C*H), 115.9, 116.0 (*C*N), 125.4, 125.6, 125.6, 125.9, 126.2, 126.4, 129.0, 129.2, 129.4, 129.7, 130.9, 136.4, 138.0, 138.4, 140.0, 140.4, 140.7, 141.1, 142.5, 144.1, 146.4, 148.5, 150.1, 163.1, 164.8, 171.2, 171.7, 172.0 (*C*$_6$H$_3$). ^{31}P{^{1}H} (121 MHz, THF-d_8, 298 K) δ = –142.5 (d, $^1J_{PP}$ = 87.9 Hz), –225.5 (d, $^1J_{PP}$ = 87.2 Hz). ^{31}P (121 MHz, THF-d_8, 298 K) δ = –142.4 (dd, $^1J_{PP}$ = 24.7, 87.9 Hz), –225.3 (dd, $^1J_{PP}$ =

88.5, 181.1 Hz). ATR-IR: *v* 2967, 2926, 2872, 2155, 1641, 1512, 1456, 1367, 1315, 1257, 1177, 1085, 1021, 979, 938, 870, 800, 757, 685, 658, 608, 571, 531 cm^{-1}.

2. Spectroscopic Characterization

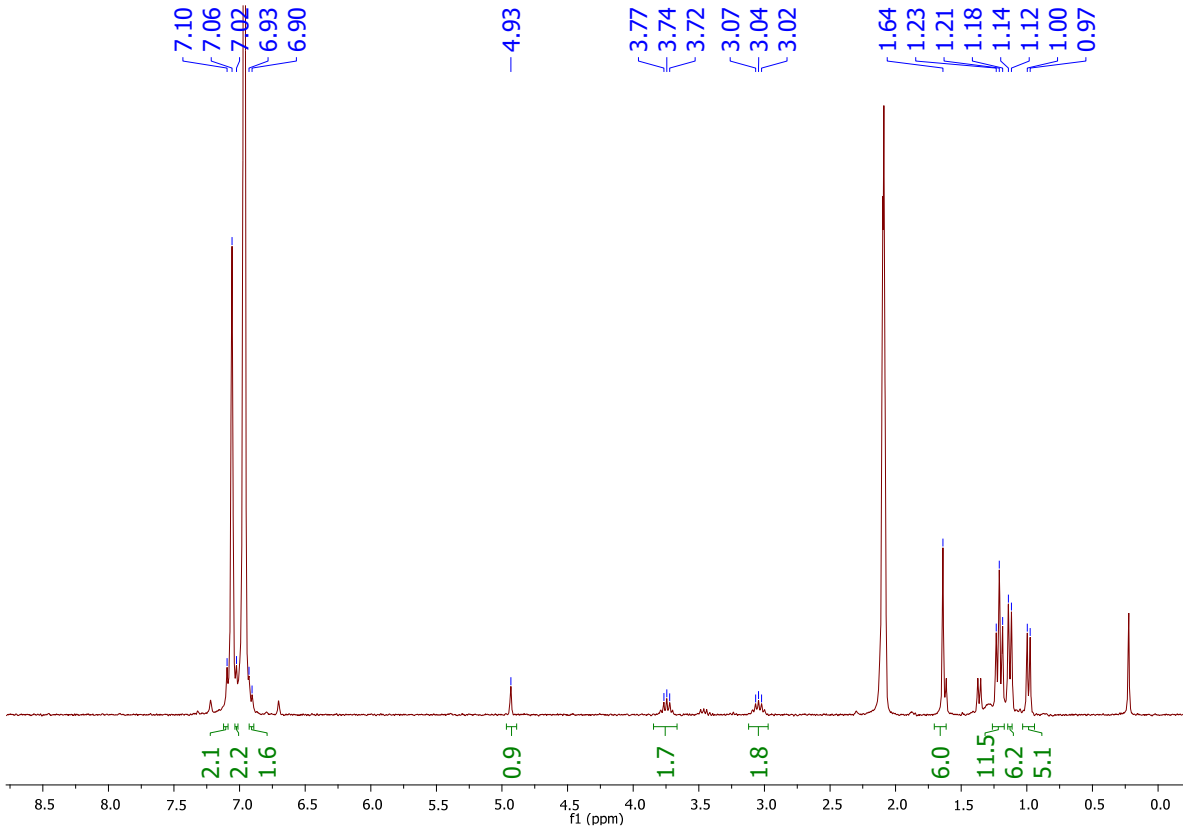


Figure S1. ^{1}H NMR (500 MHz, C_7D_8, 298 K) spectrum of compound **2a**.

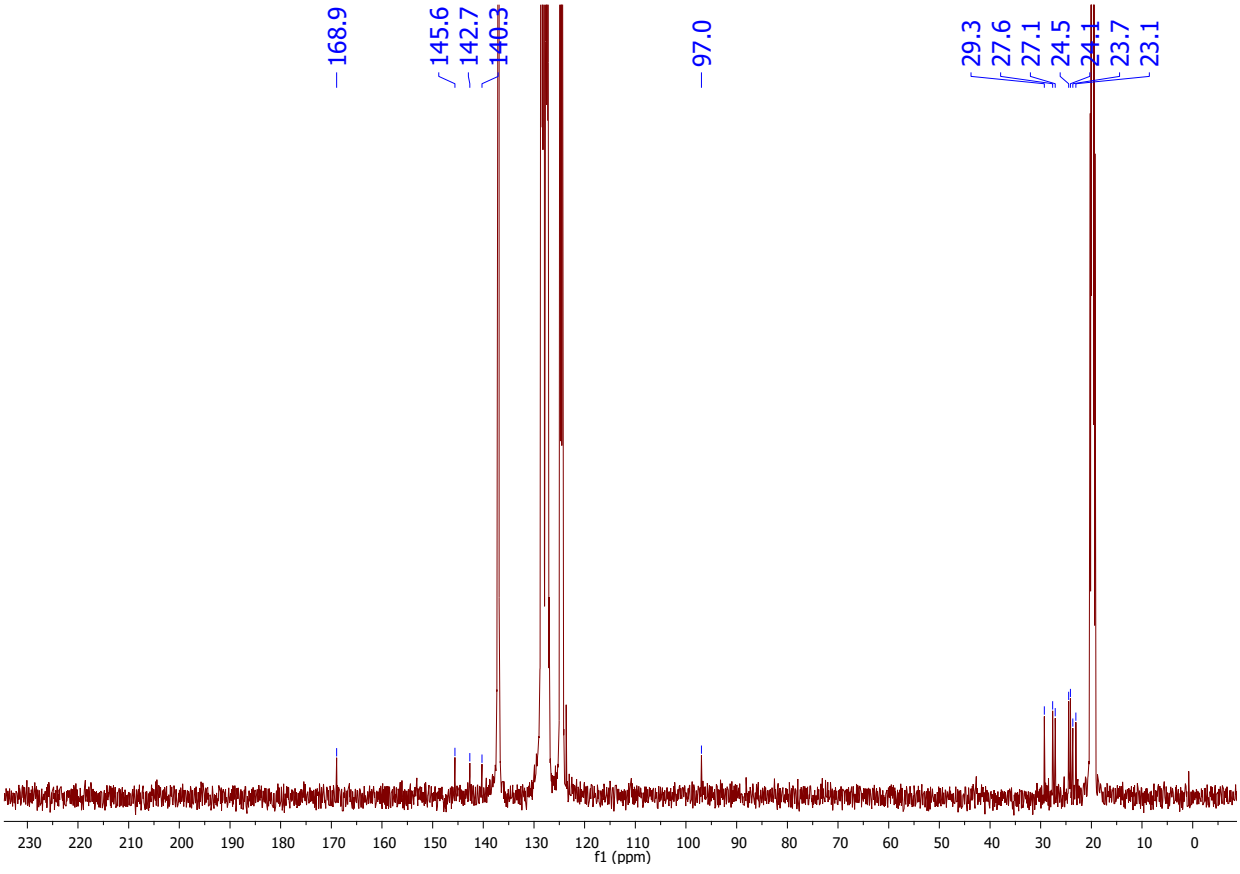


Figure S2. $^{13}C\{^{1}H\}$ NMR (125 MHz, C_7D_8, 298 K) spectrum of compound **2a**.

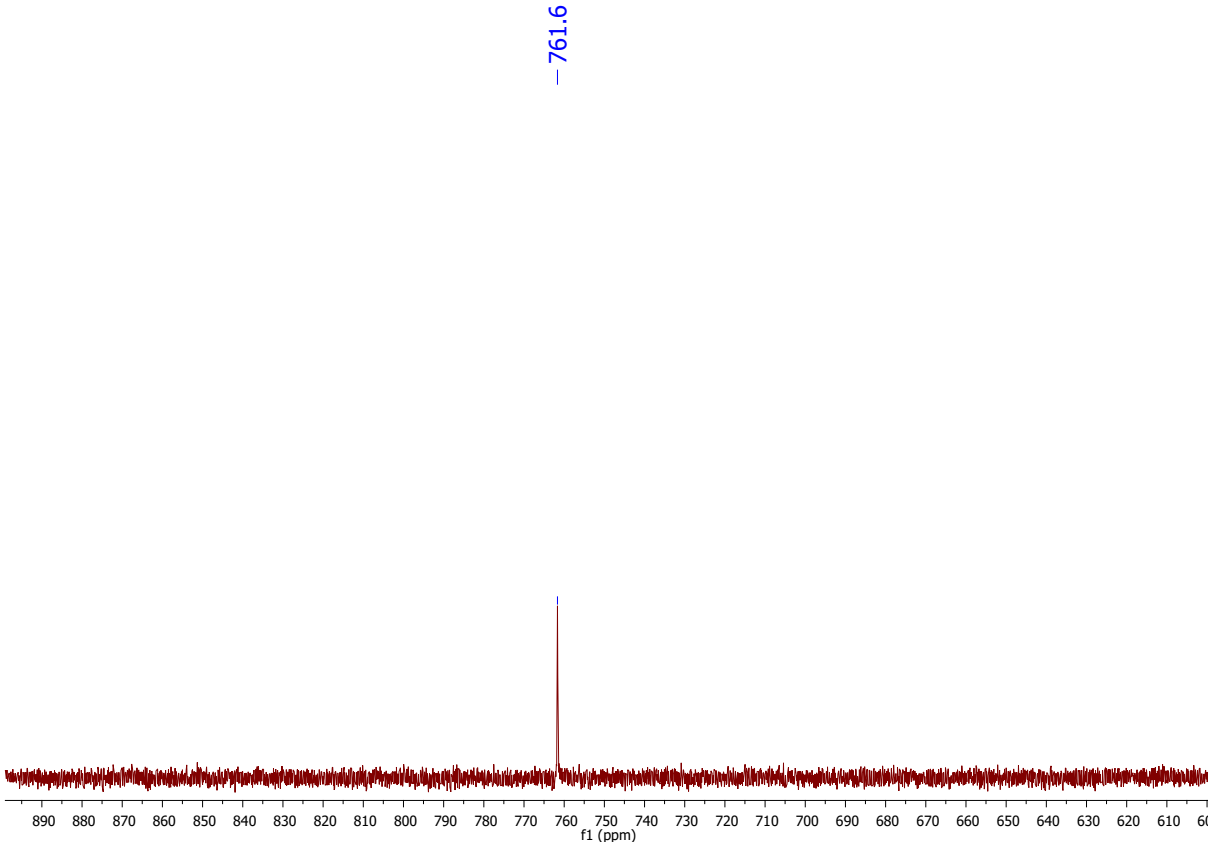


Figure S3. $^{31}P\{^{1}H\}$ NMR (202 MHz, C_7D_8, 298 K) spectrum of compound **2a**.

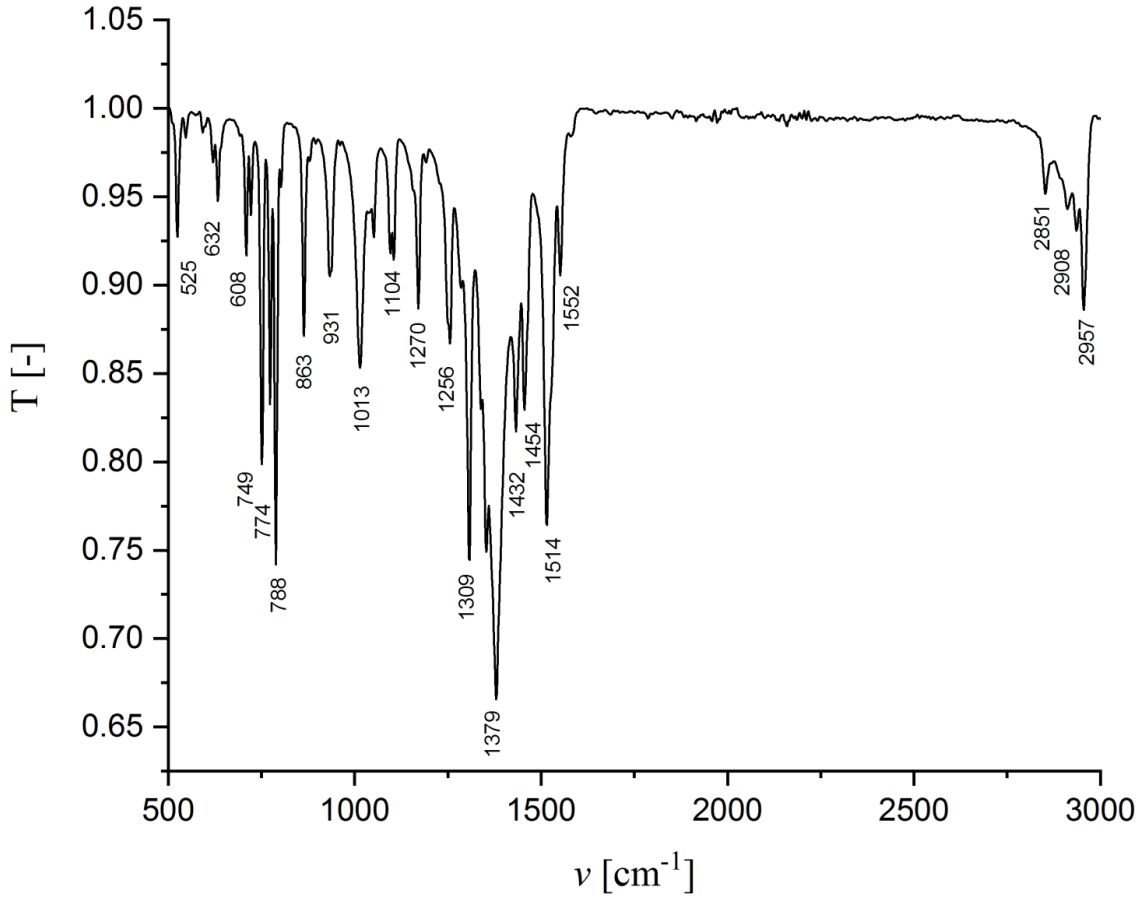


Figure S4. ATR-IR spectrum of **2a**.

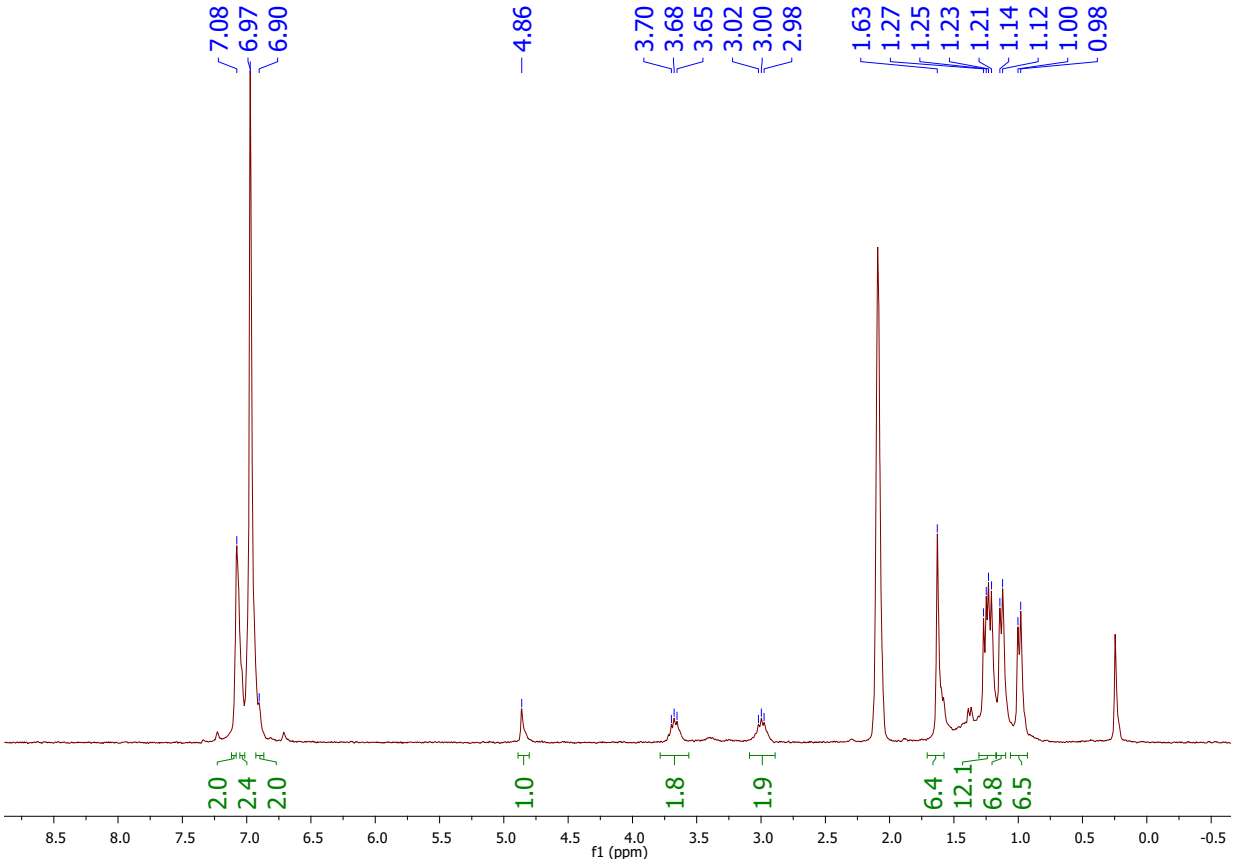


Figure S5. ^{1}H NMR (500 MHz, C_7D_8, 298 K) spectrum of compound **2b**.

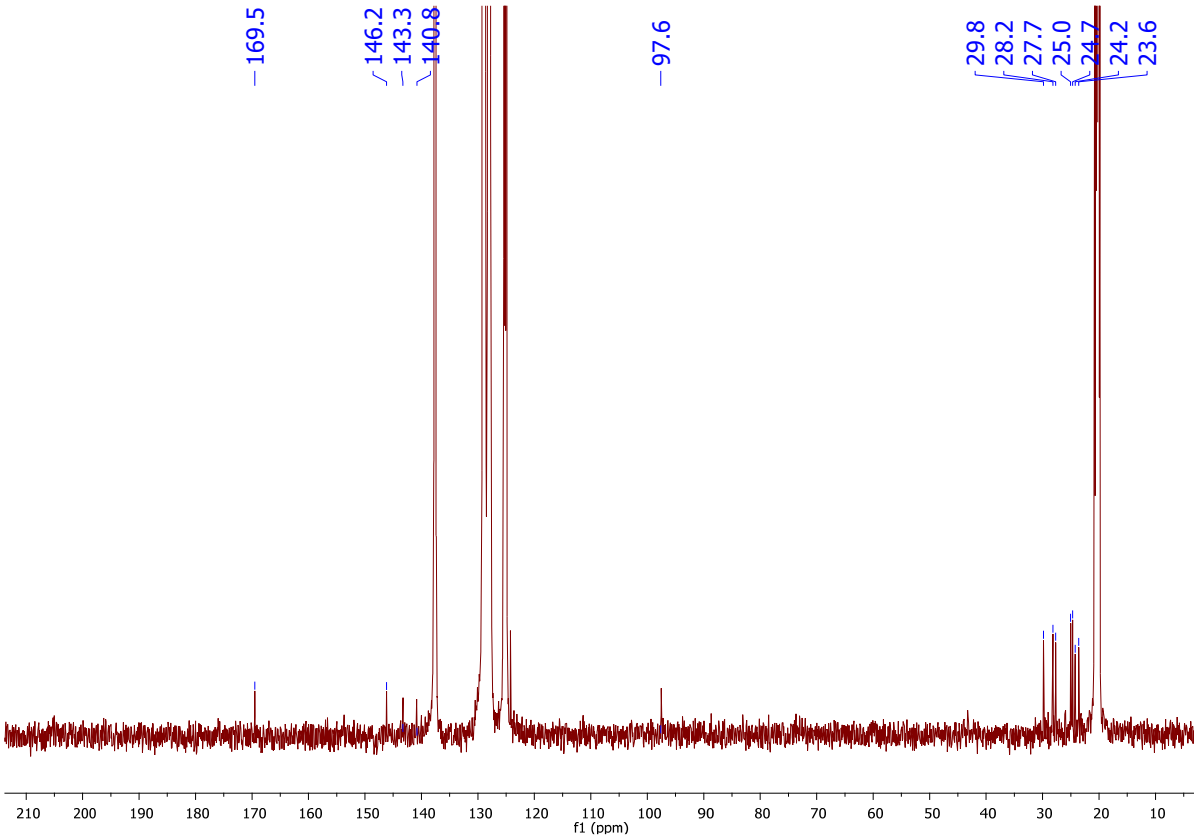


Figure S6. $^{13}C\{^{1}H\}$ NMR (125 MHz, C_7D_8, 298 K) spectrum of compound **2b**.

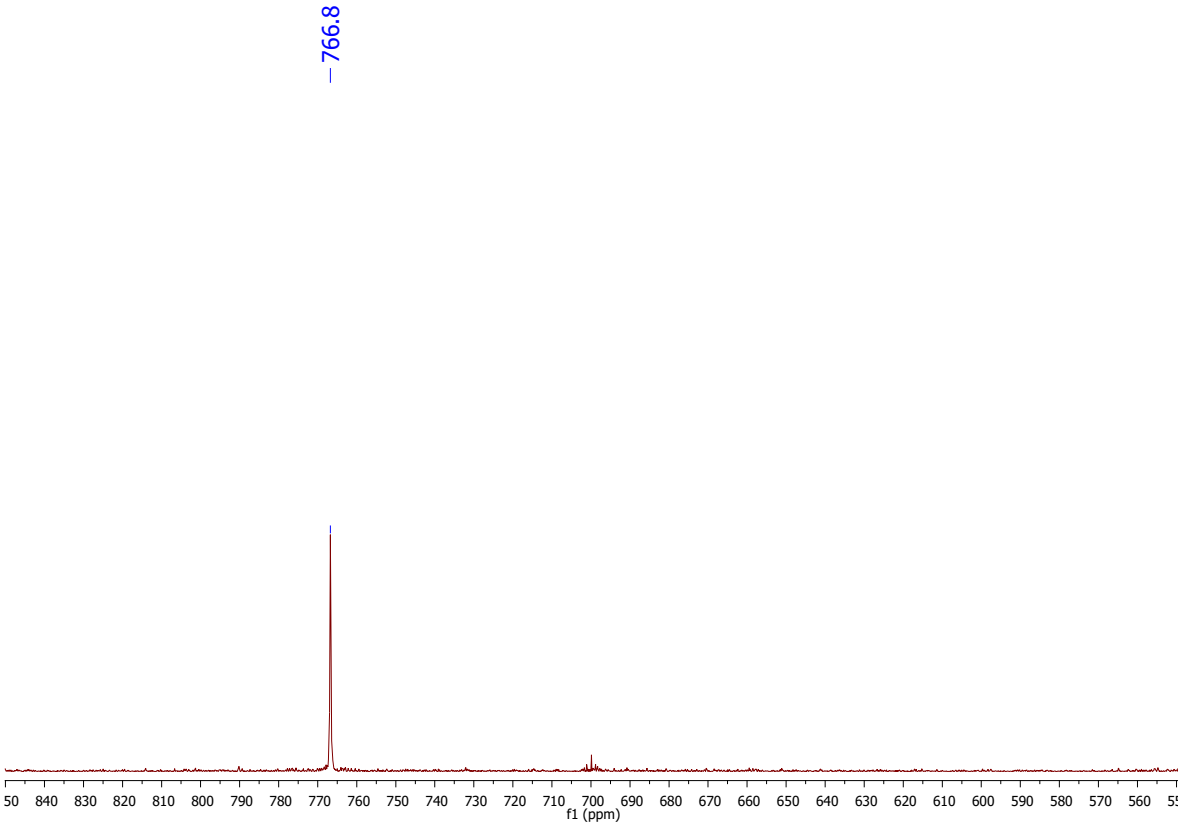


Figure S7. $^{31}P\{^{1}H\}$ NMR (202 MHz, C_7D_8, 298 K) spectrum of compound **2b**.

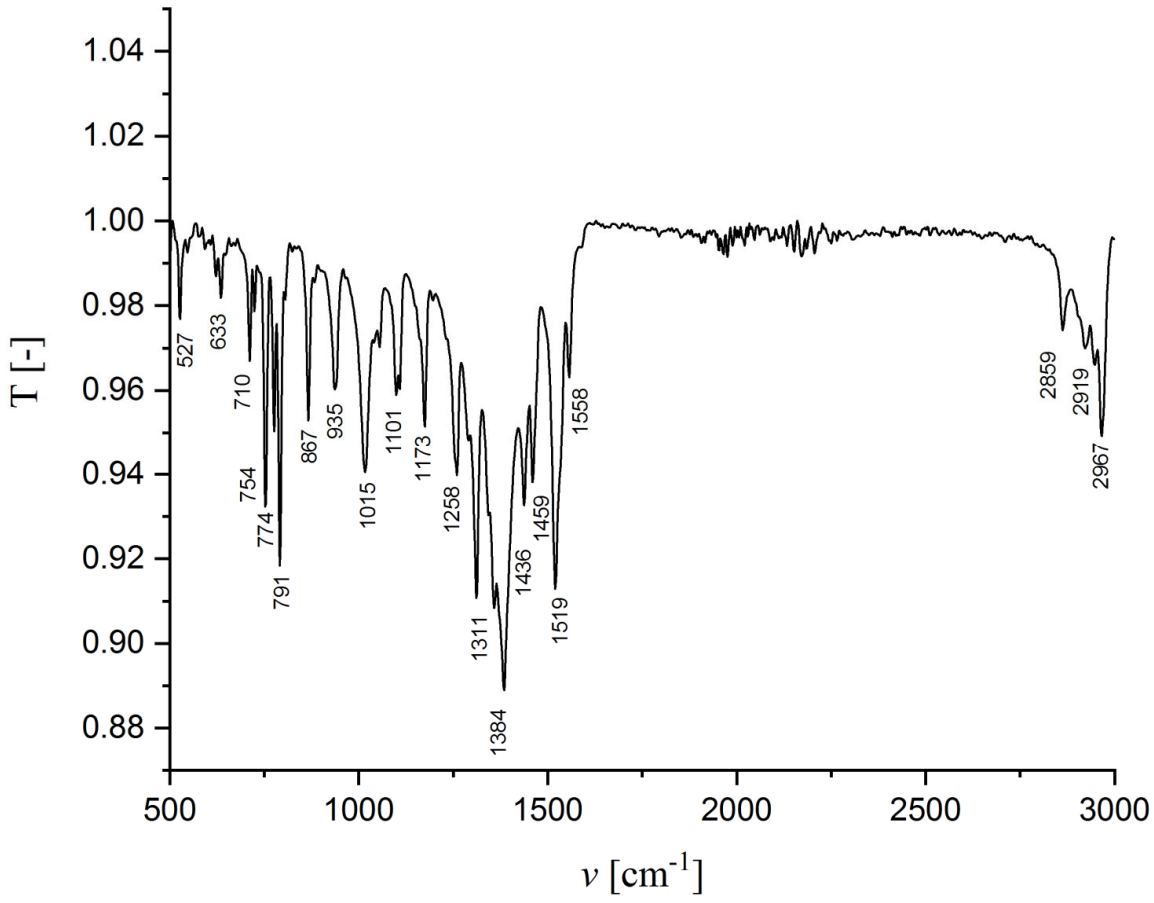


Figure S8. ATR-IR spectrum of **2b**.

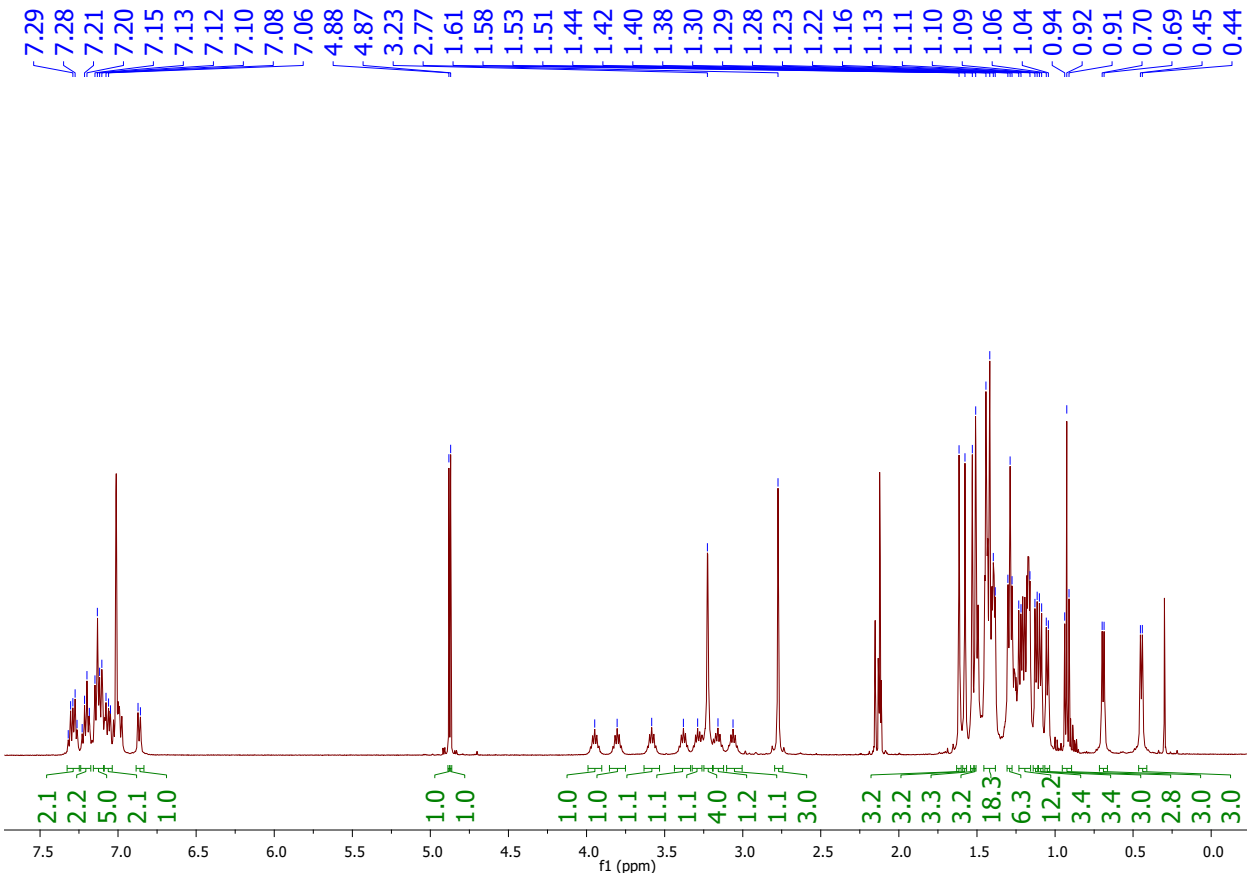


Figure S9. ^{1}H NMR (300 MHz, C_7D_8, 298 K) spectrum of compound **3a**.

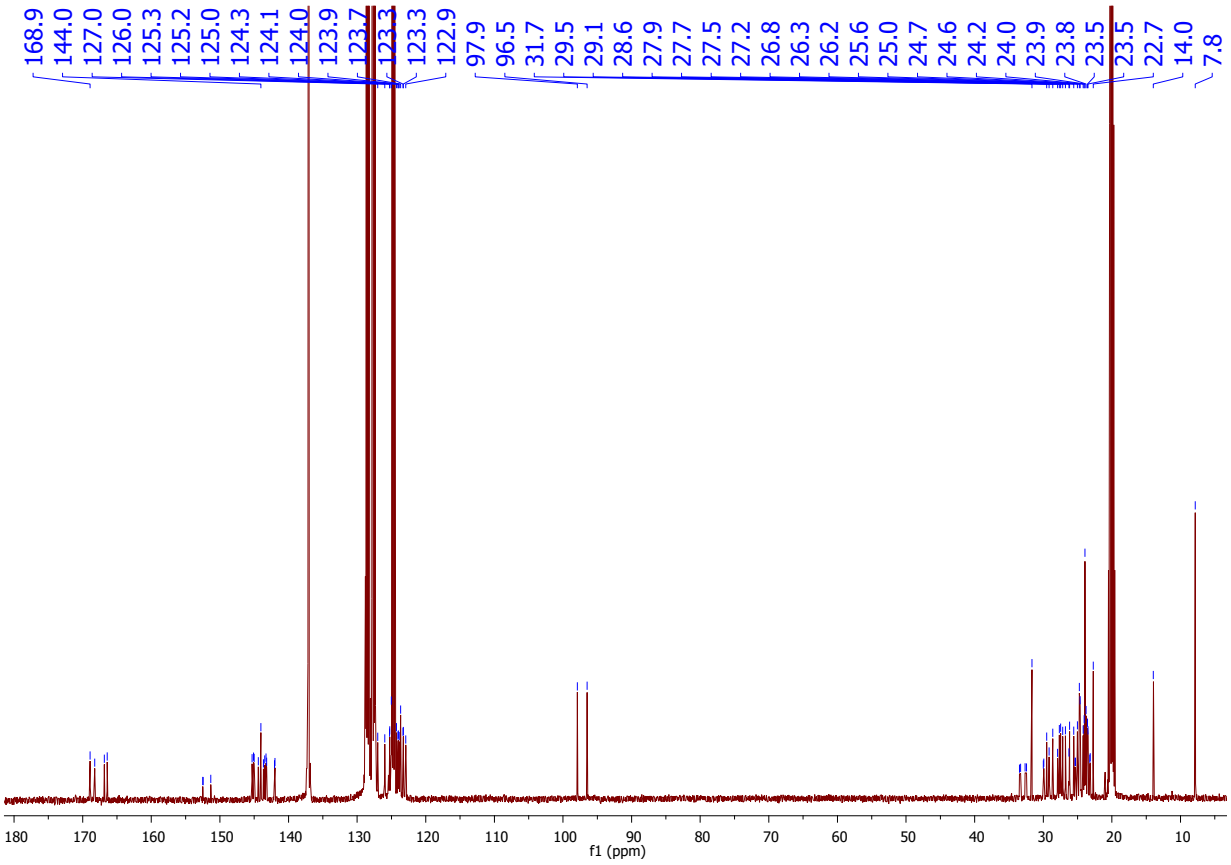


Figure S10. ^{13}C{^{1}H} NMR (150 MHz, C_7D_8, 298 K) spectrum of compound **3a**.

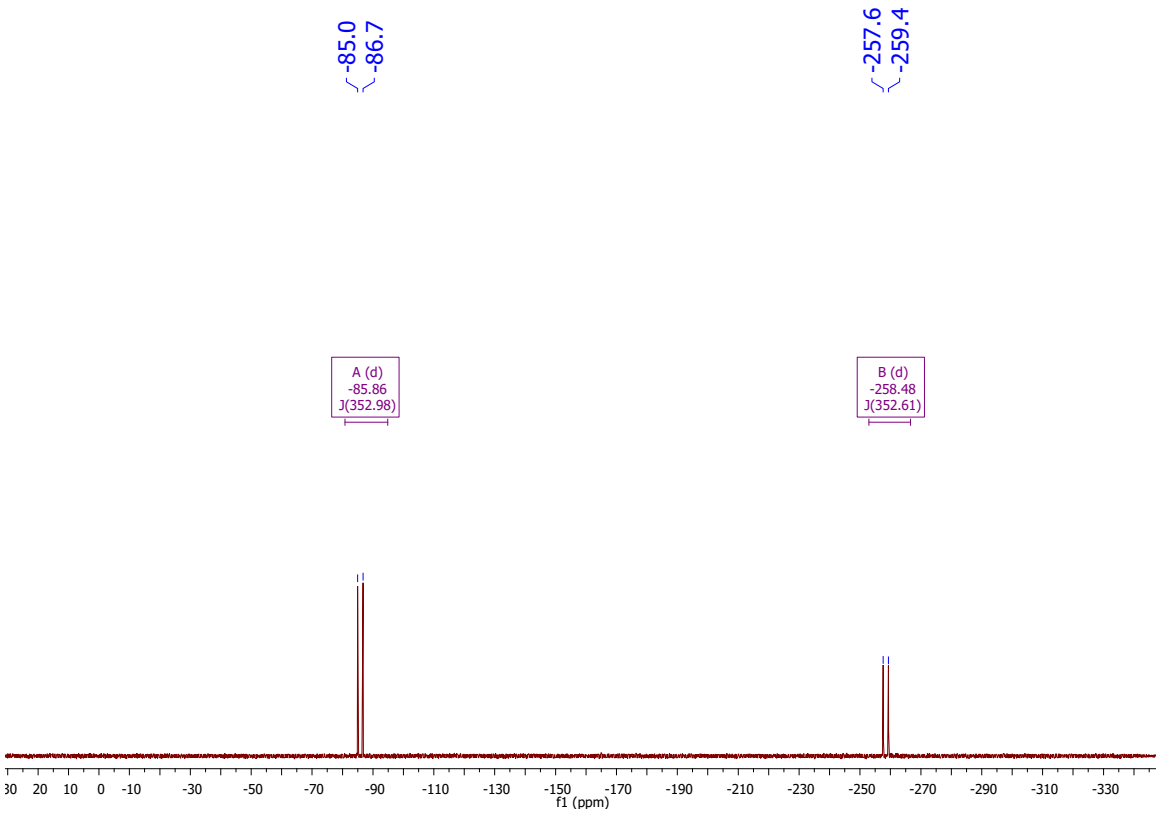


Figure S11. $^{31}P\{^{1}H\}$ NMR (161 MHz, C_7D_8, 298 K) spectrum of compound **3a**.

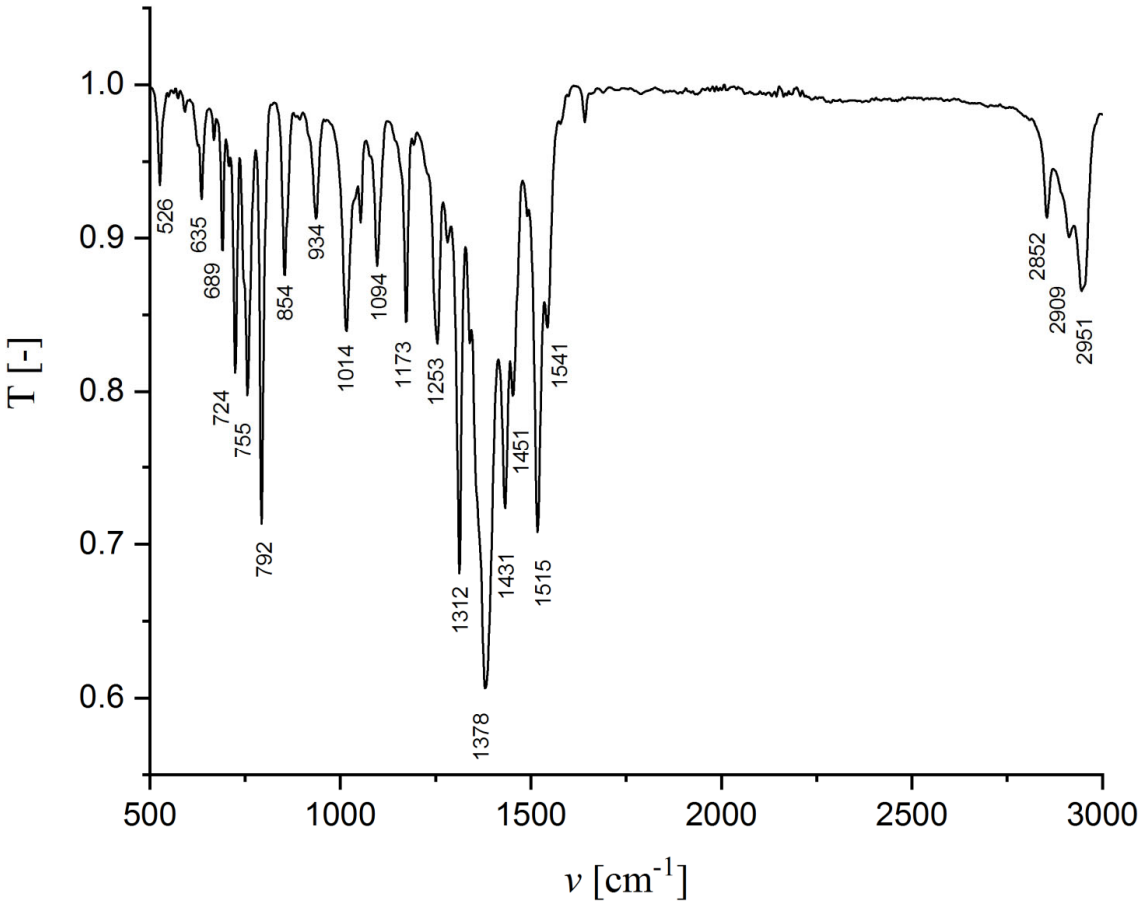


Figure S12. ATR-IR spectrum of **3a**.

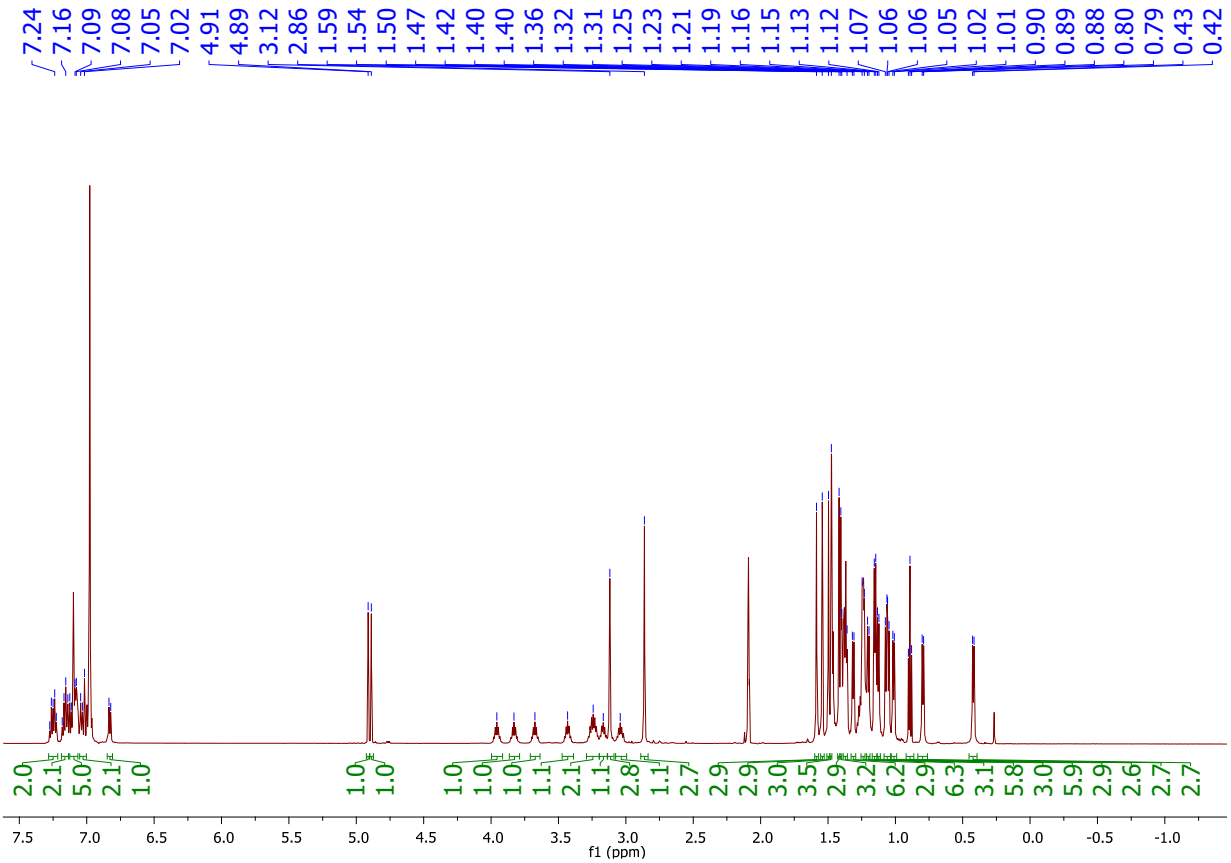


Figure S13. ^{1}H NMR (500 MHz, C_7D_8, 298 K) spectrum of compound **3b**.

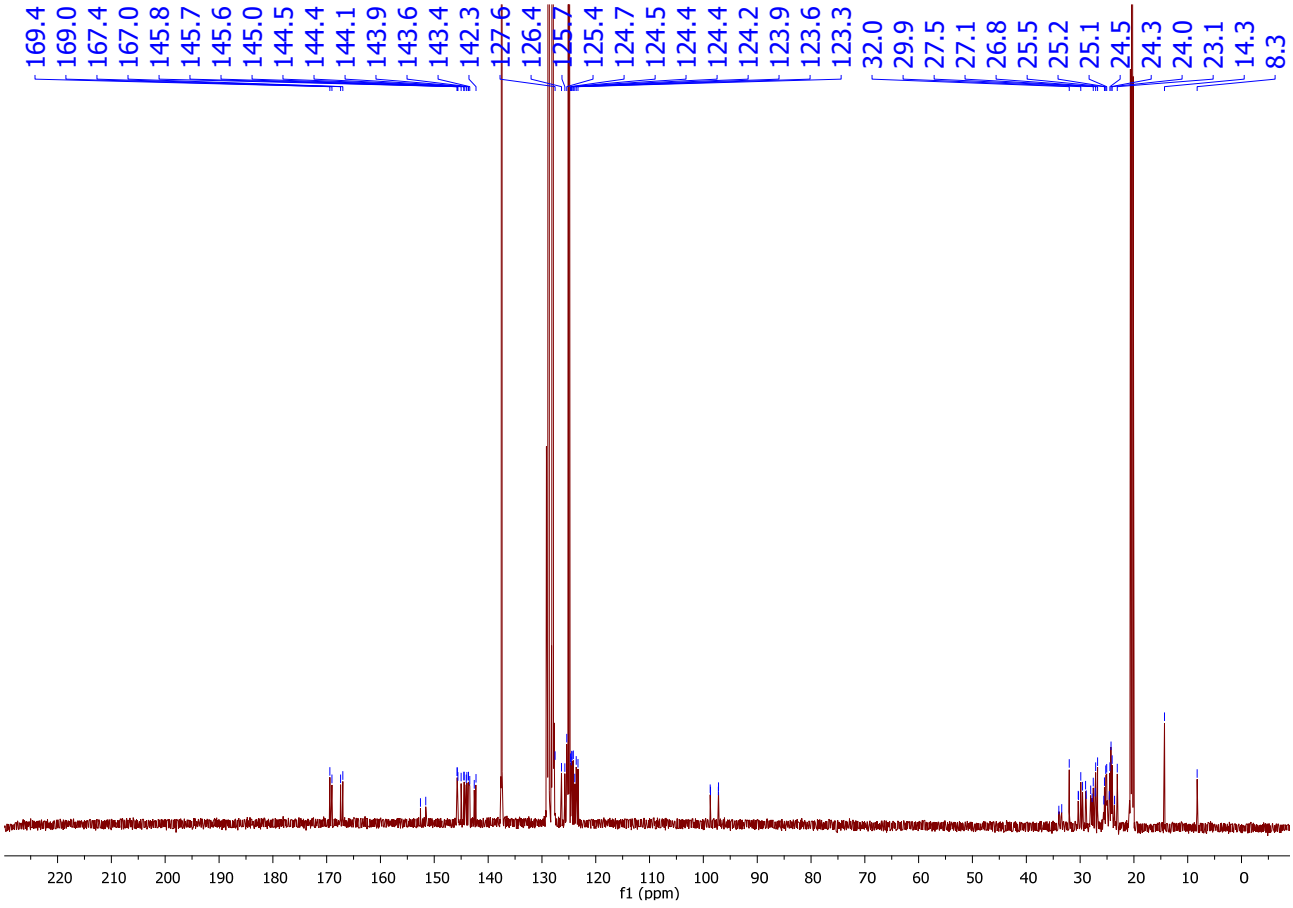


Figure S14. $^{13}C\{^{1}H\}$ NMR (125 MHz, C_7D_8, 298 K) spectrum of compound **3b**.

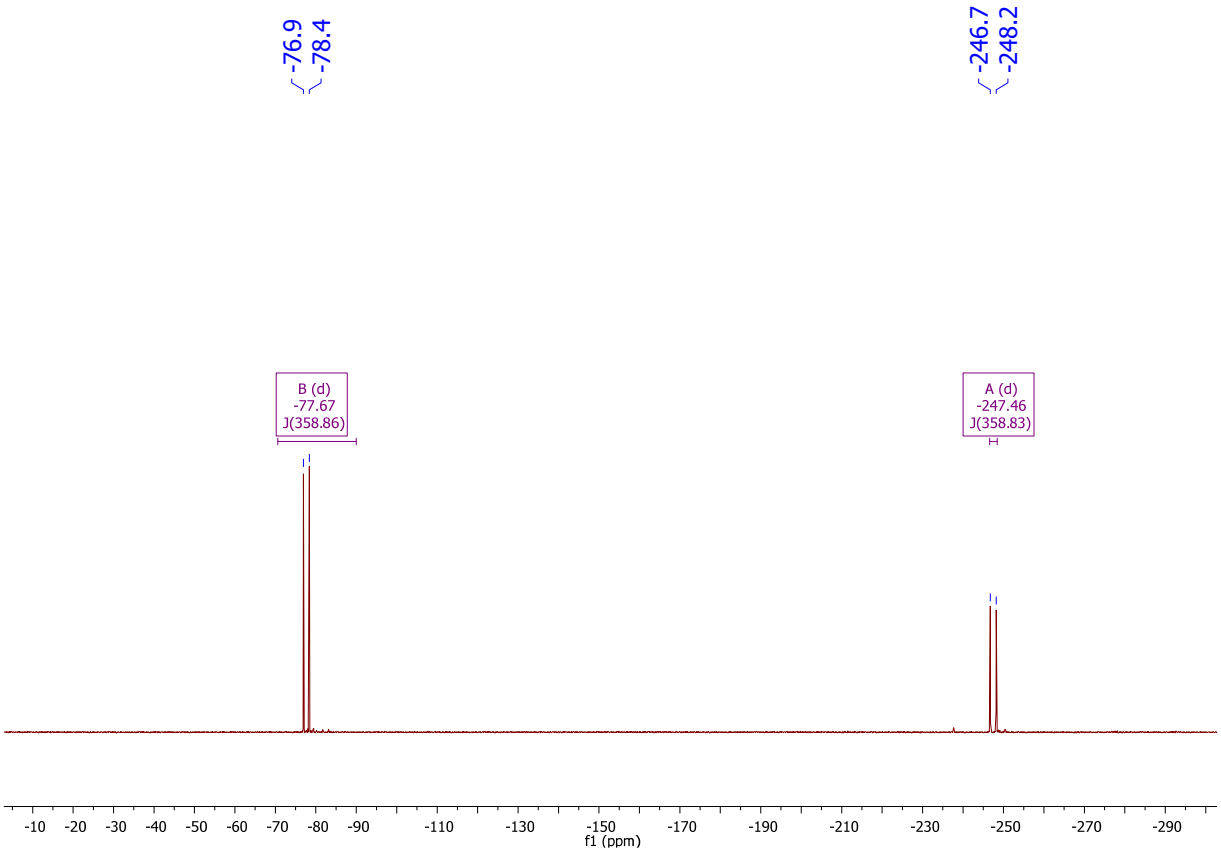


Figure S15. $^{31}P\{^{1}H\}$ NMR (202 MHz, C_7D_8, 298 K) spectrum of compound **3b**.

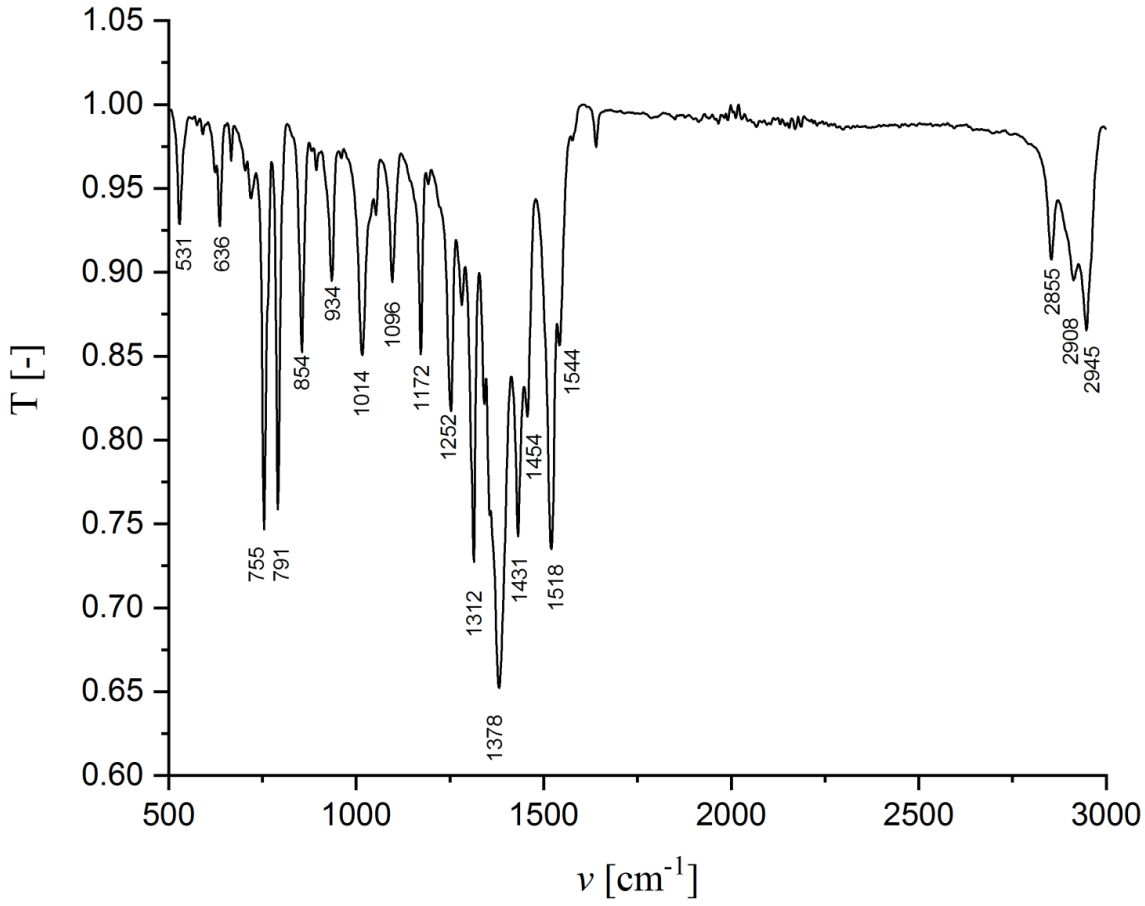


Figure S16. ATR-IR spectrum of **3b**.

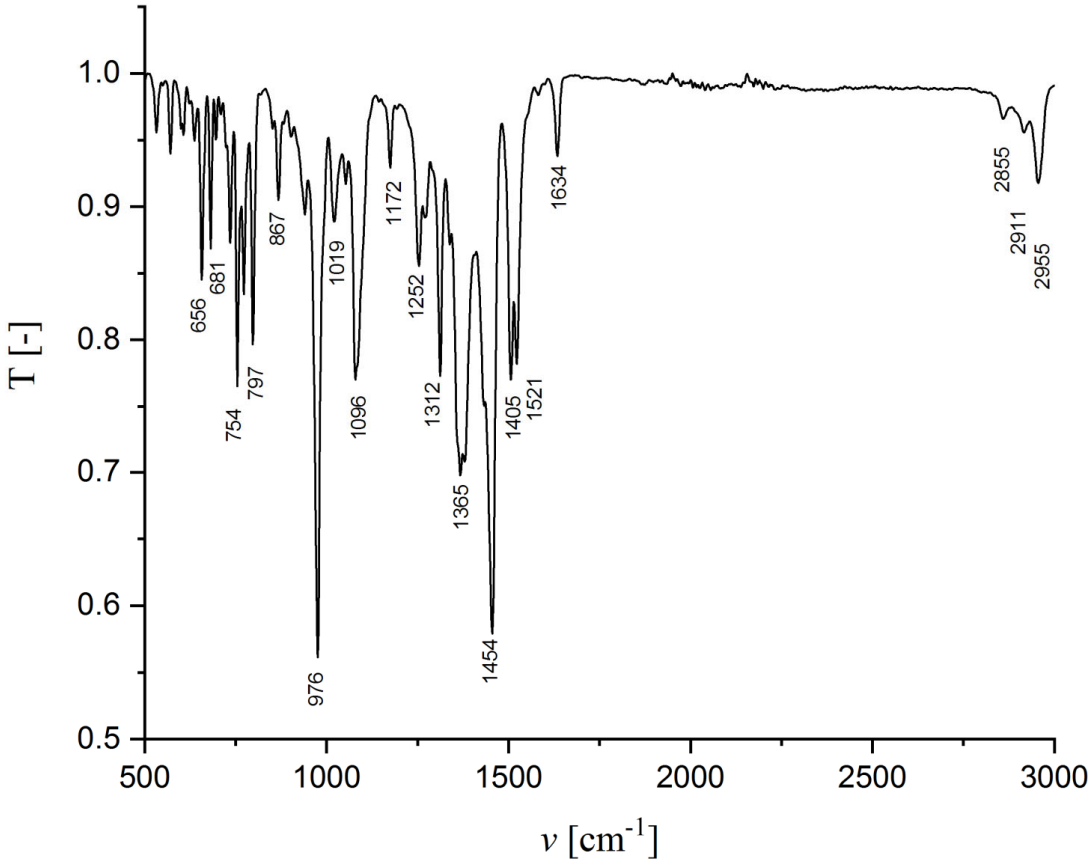


Figure S17. ATR-IR spectrum of **4a**.

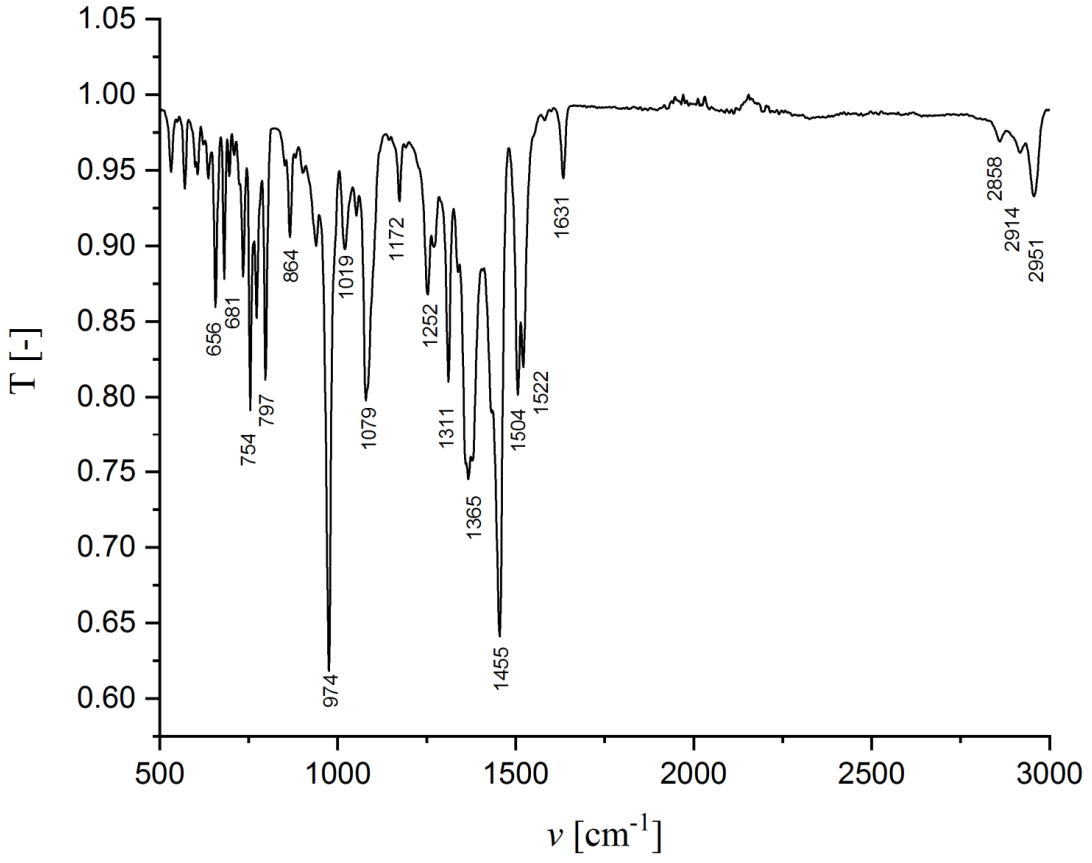


Figure S18. ATR-IR spectrum of **4b**.

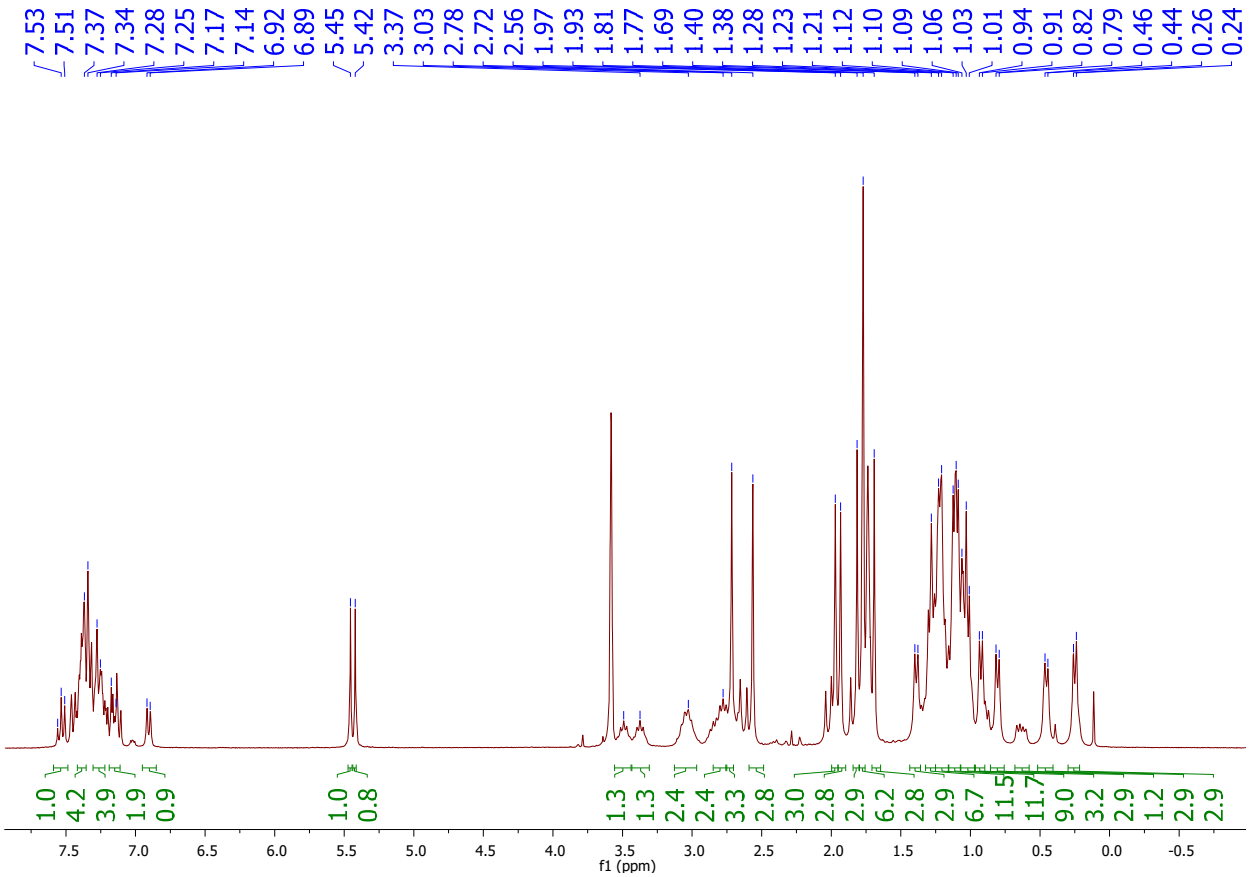


Figure S19. ^{1}H NMR (300 MHz, THF-d_8, 298 K) spectrum of compound **5a**.

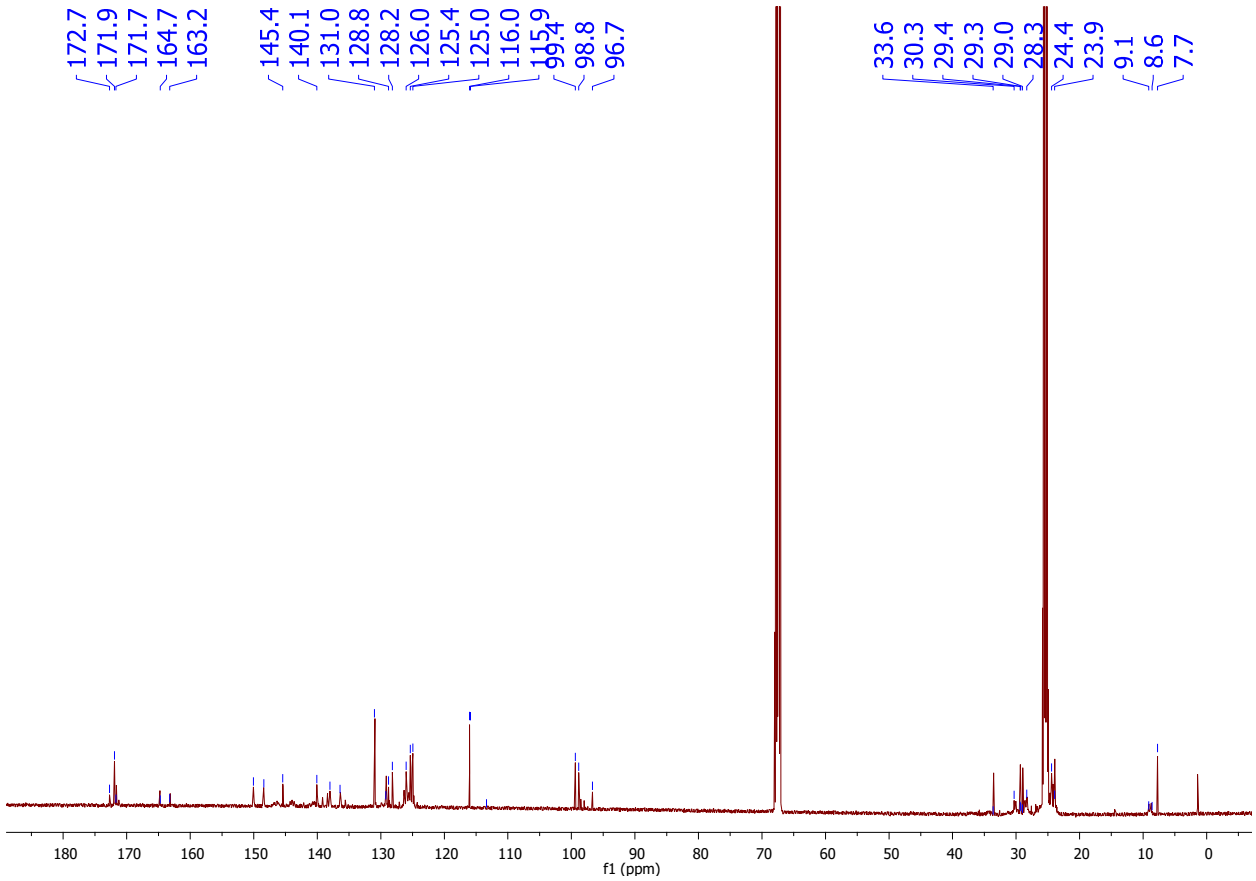


Figure S20. ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, 298 K) spectrum of compound **5a**.

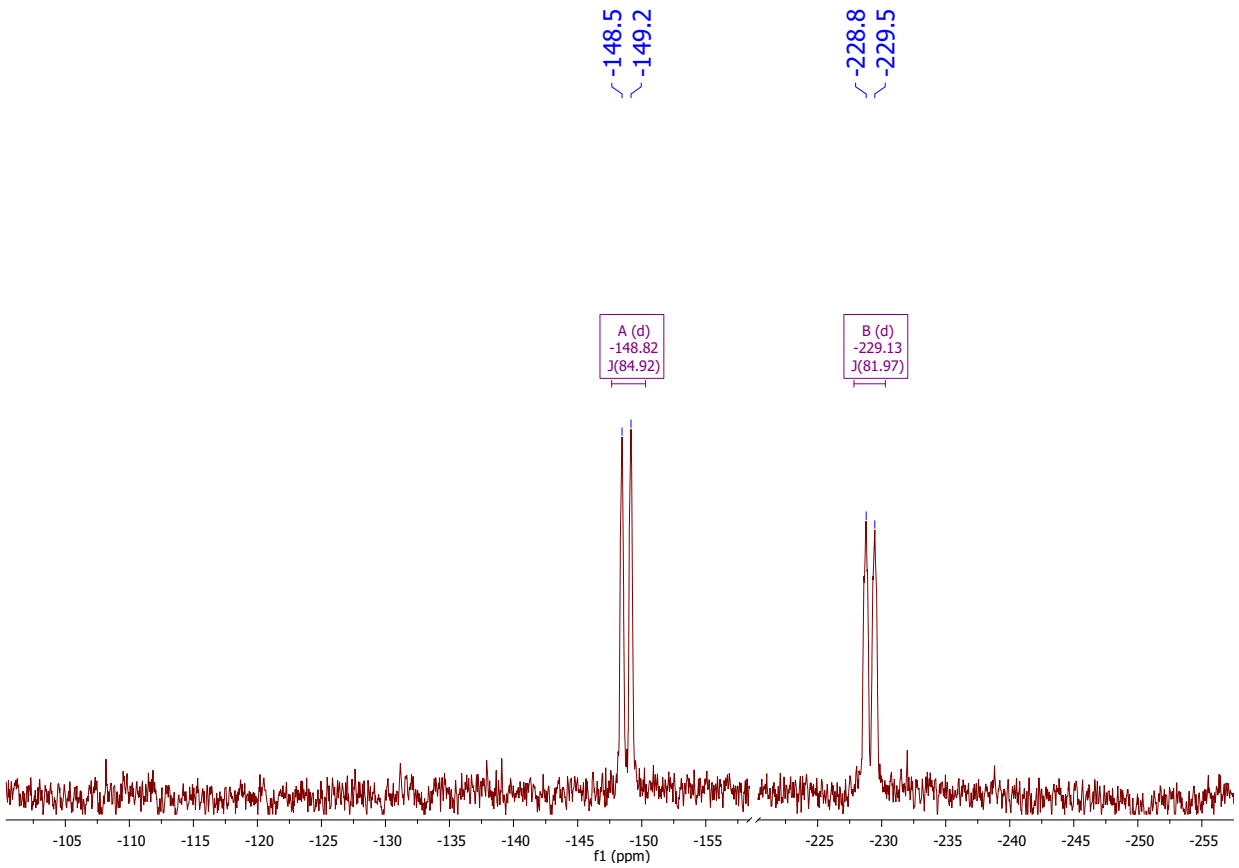


Figure S21. $^{31}P\{^{1}H\}$ NMR (121 MHz, THF-d_8, 298 K) spectrum of compound **5a**.

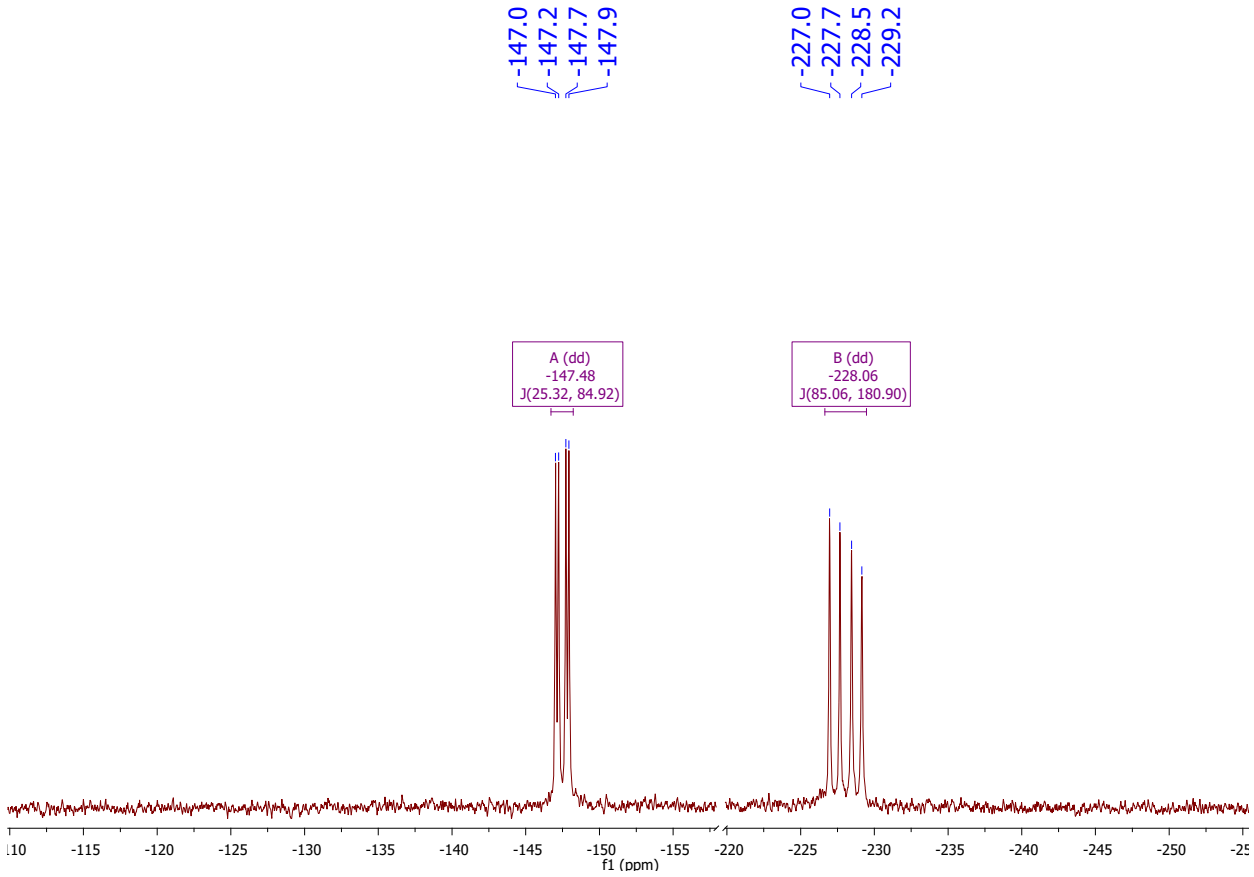


Figure S22. ^{31}P NMR (121 MHz, THF-d_8, 298 K) spectrum of compound **5a**.

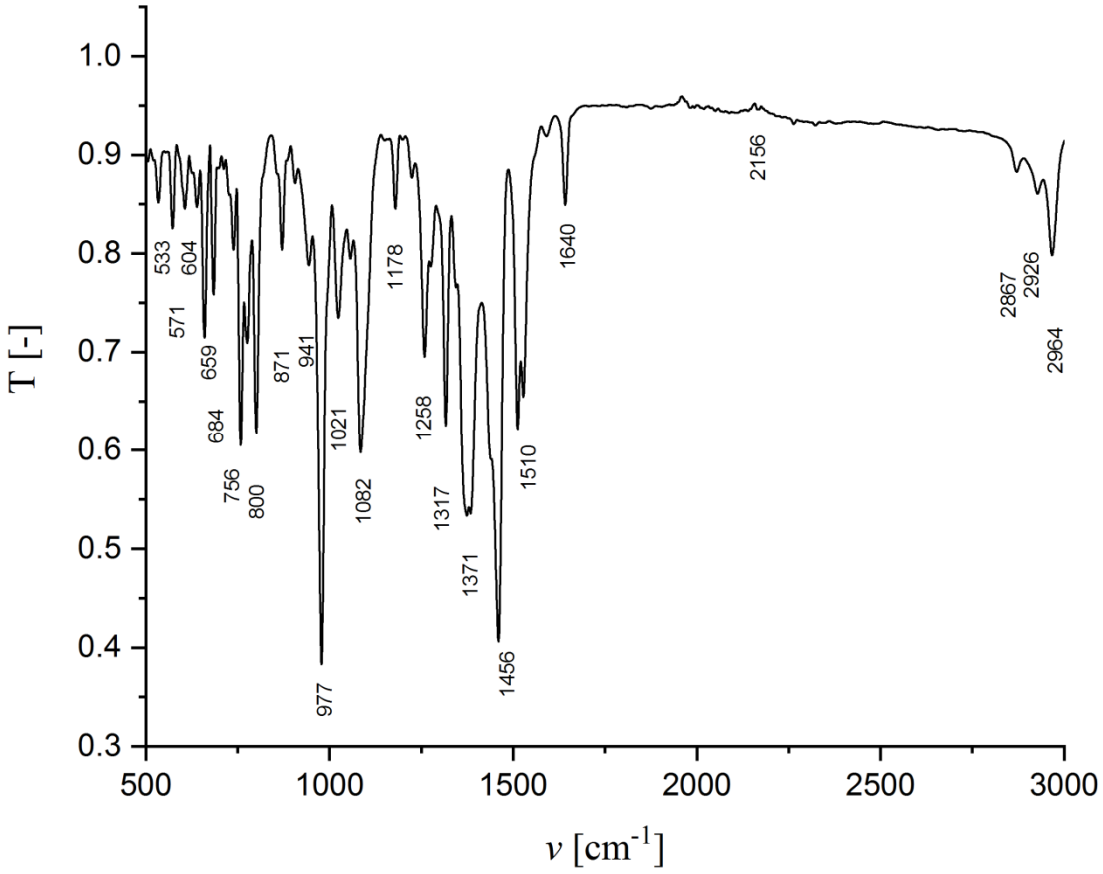


Figure S23. ATR-IR spectrum of **5a**.

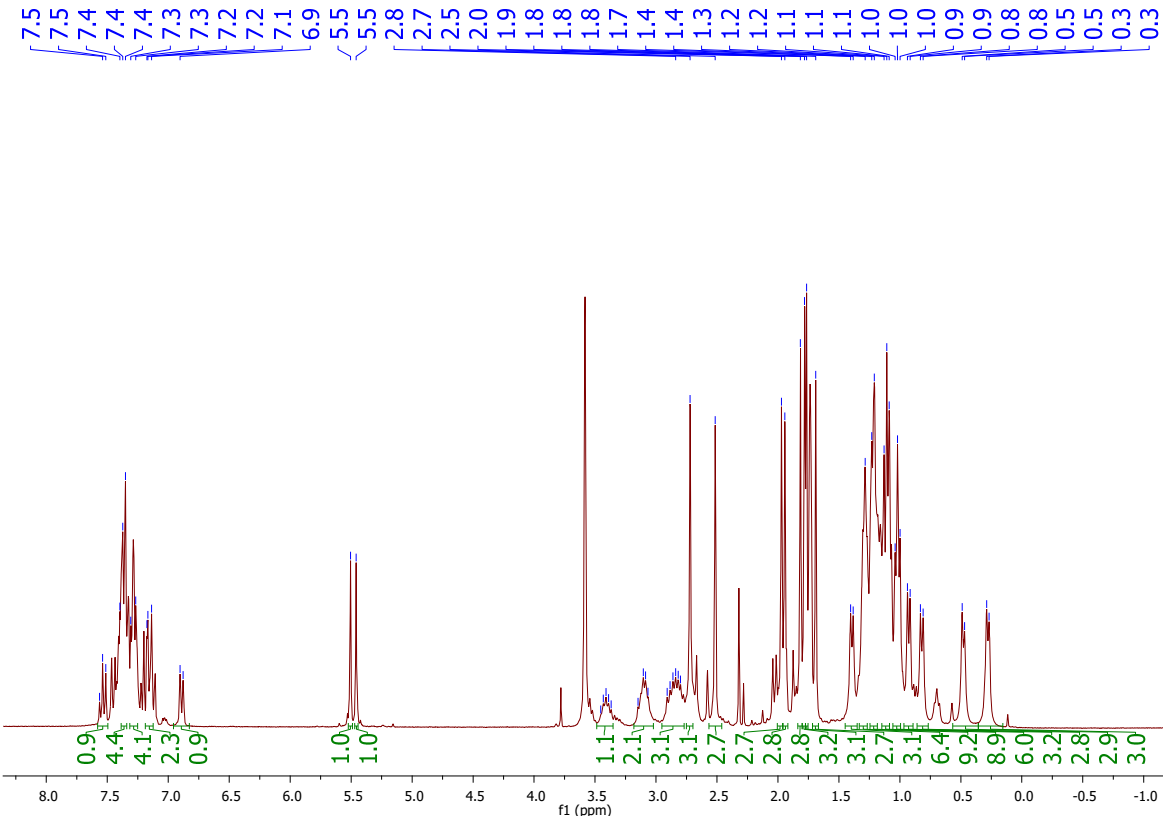


Figure S24. ^{1}H NMR (300 MHz, THF-d_8, 298 K) spectrum of compound **5b**.

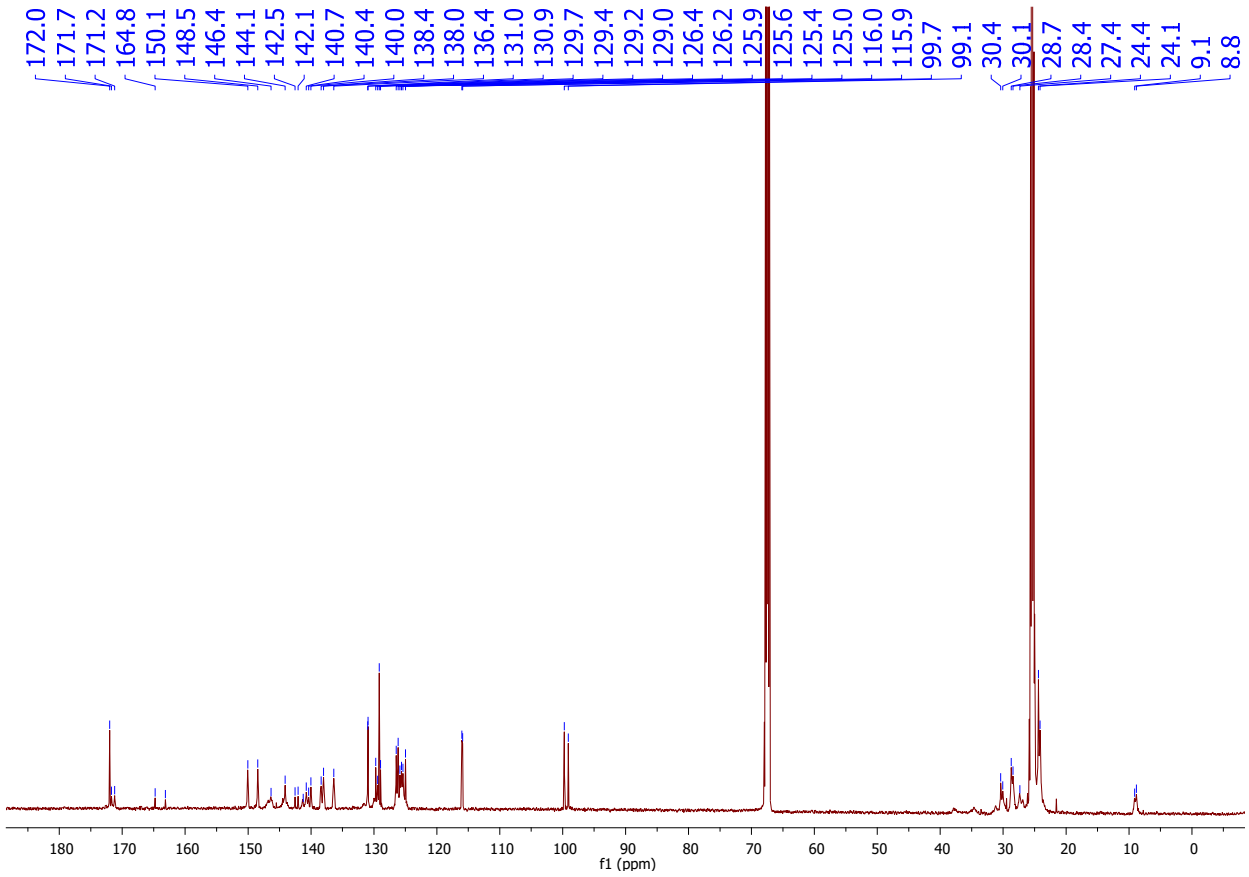


Figure S25. $^{13}C\{^{1}H\}$ NMR (125 MHz, THF-d_8, 298 K) spectrum of compound **5b**.

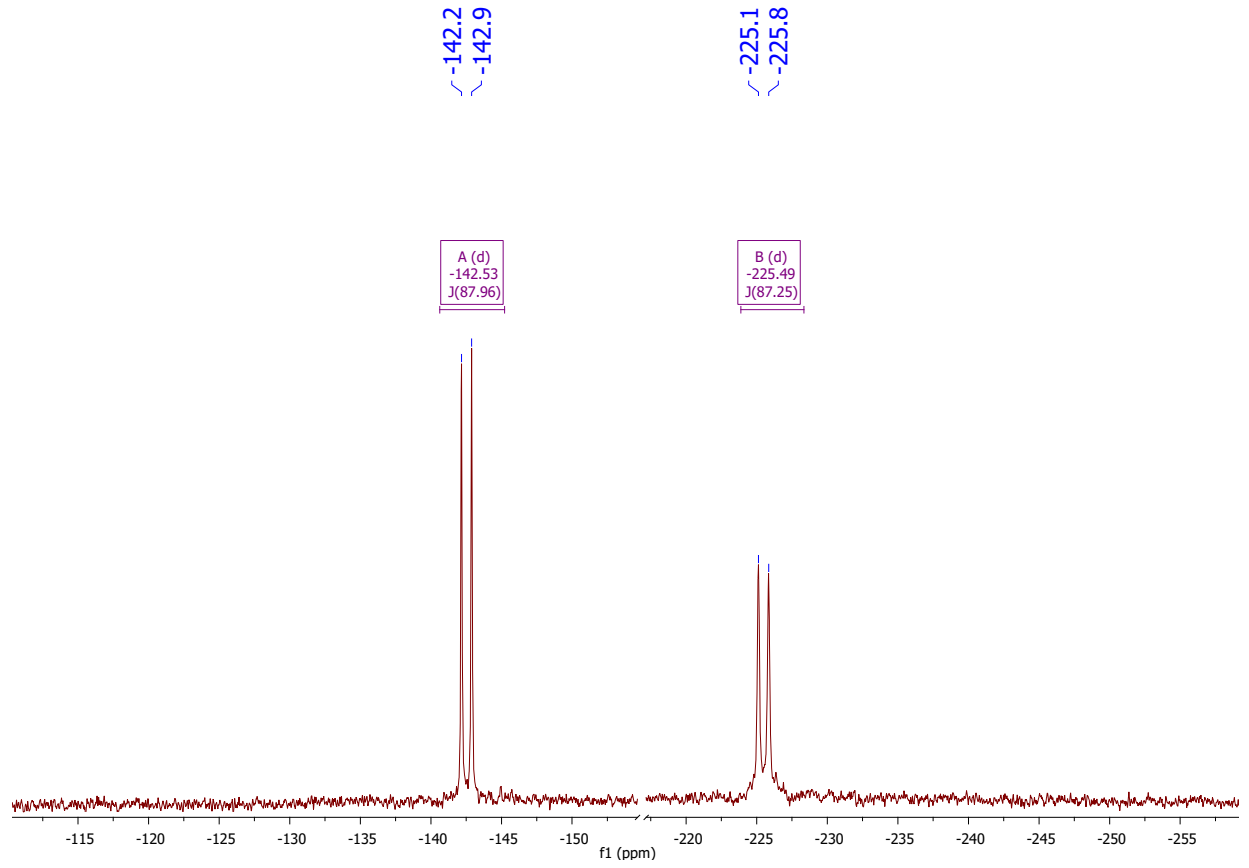


Figure S26. $^{31}P\{^{1}H\}$ NMR (121 MHz, THF-d_8, 298 K) spectrum of compound **5b**.

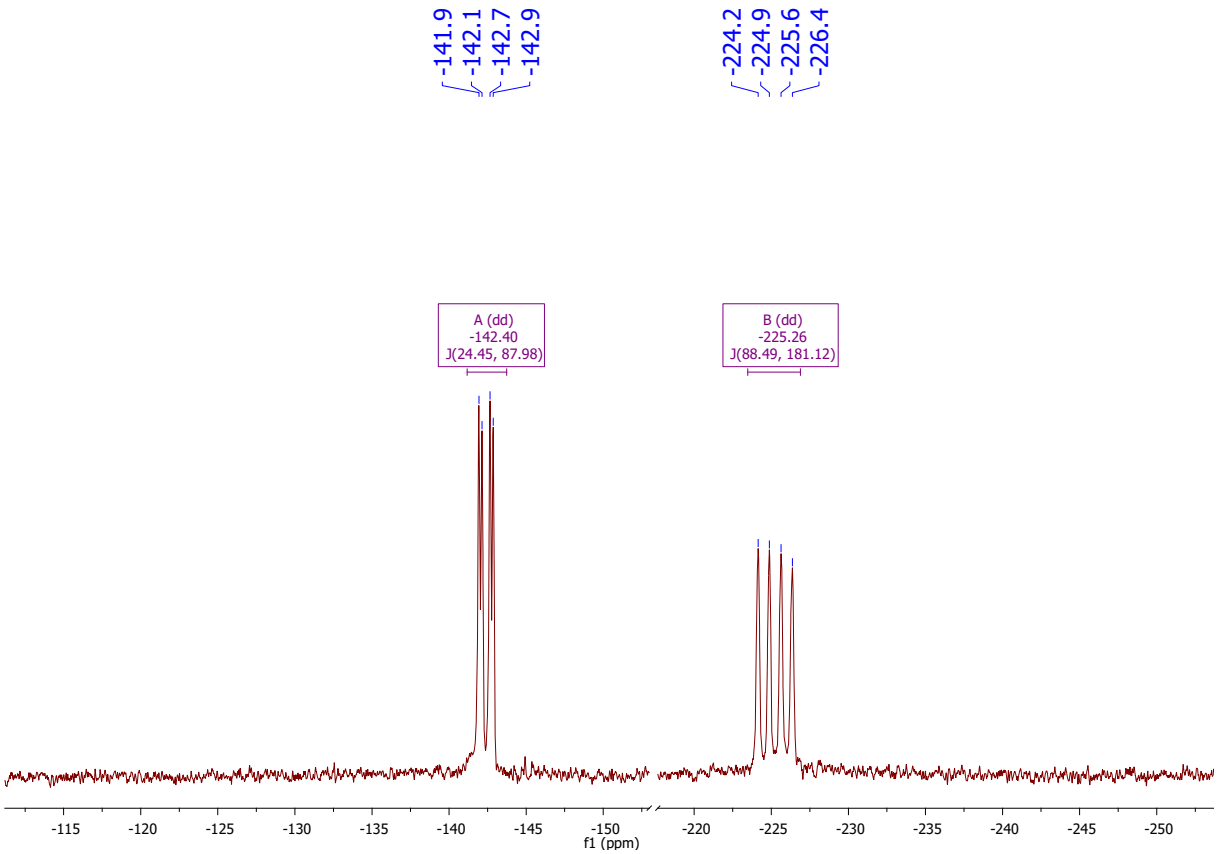


Figure S27. ^{31}P NMR (121 MHz, THF-d_8, 298 K) spectrum of compound **5b**.

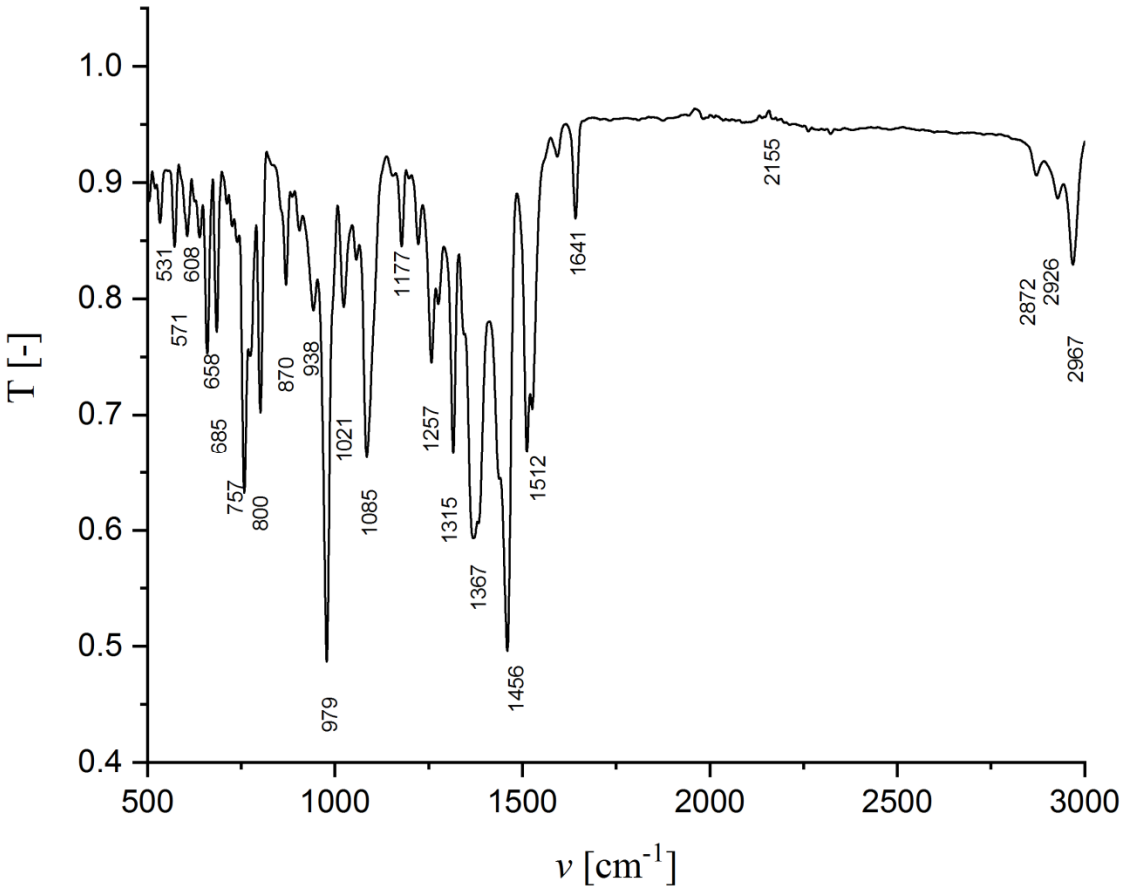


Figure S28. ATR-IR spectrum of **5b**.

3. Cyclic Voltammetry

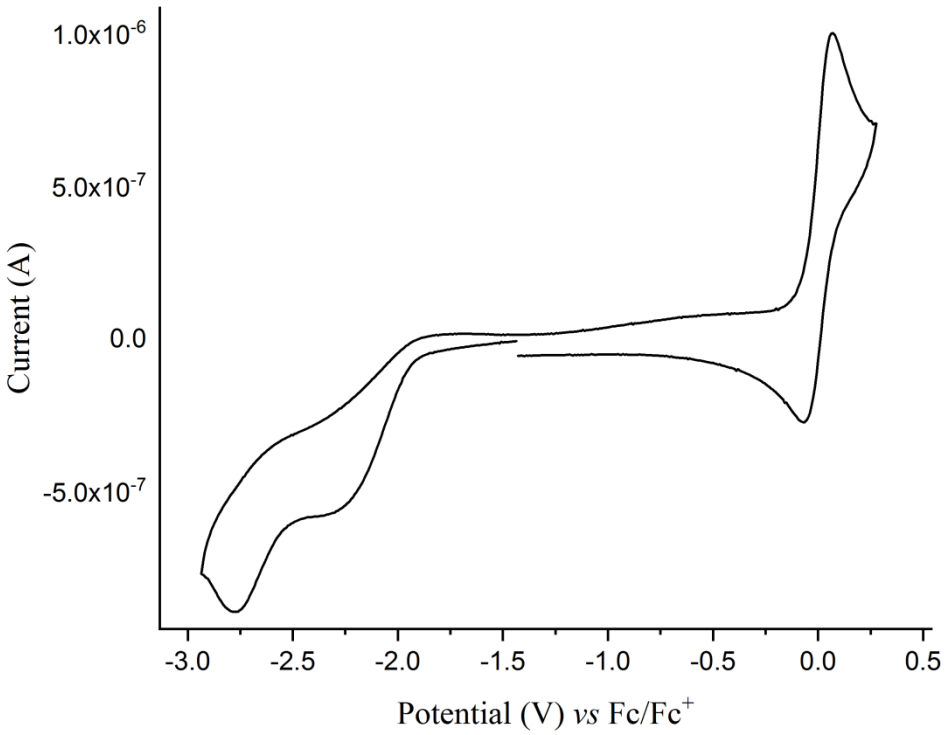


Figure S29a. Cyclic voltammogram of **2a** in THF (0.01 M *n*-$Bu_4N[PF_6]$) as a supporting electrolyte, $0.1Vs^{-1}$, *vs* Fc/Fc^+).

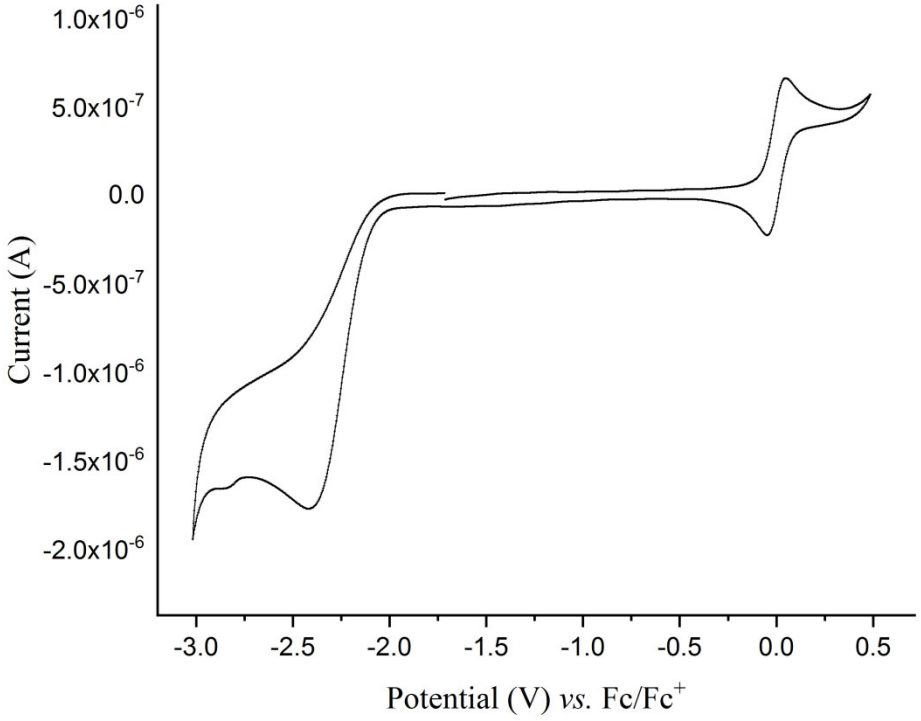


Figure S29b. Cyclic voltammogram of **2a** in THF (0.01 M *n*-$Bu_4N[B(C_6F_5)_4]$) as a supporting electrolyte, $0.1Vs^{-1}$, *vs* Fc/Fc^+).

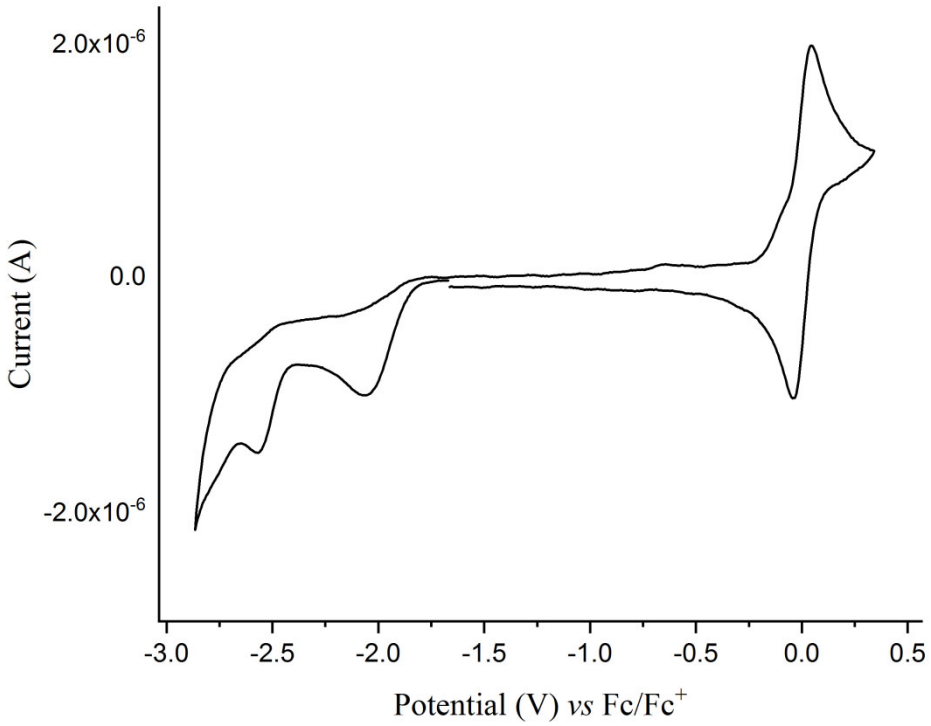


Figure S30a. Cyclic voltammogram of **2b** in THF (0.01 M *n*-$Bu_4N[PF_6]$) as a supporting electrolyte, $0.1Vs^{-1}$, *vs* Fc/Fc^+).

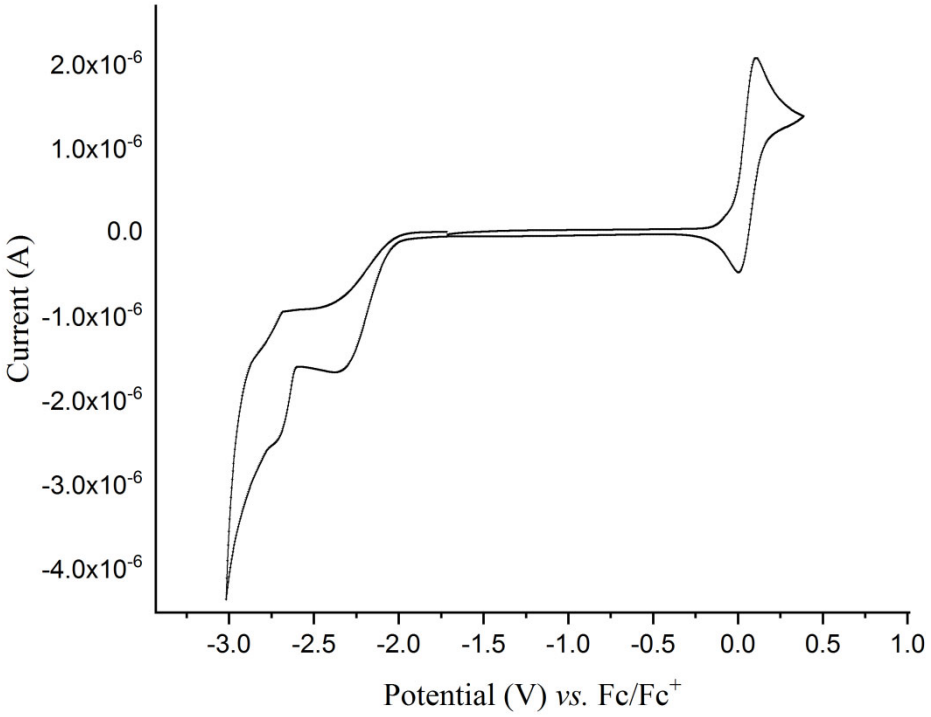


Figure S30b. Cyclic voltammogram of **2b** in THF (0.01 M *n*-$Bu_4N[B(C_6F_5)_4]$) as a supporting electrolyte, $0.1Vs^{-1}$, *vs* Fc/Fc^+).

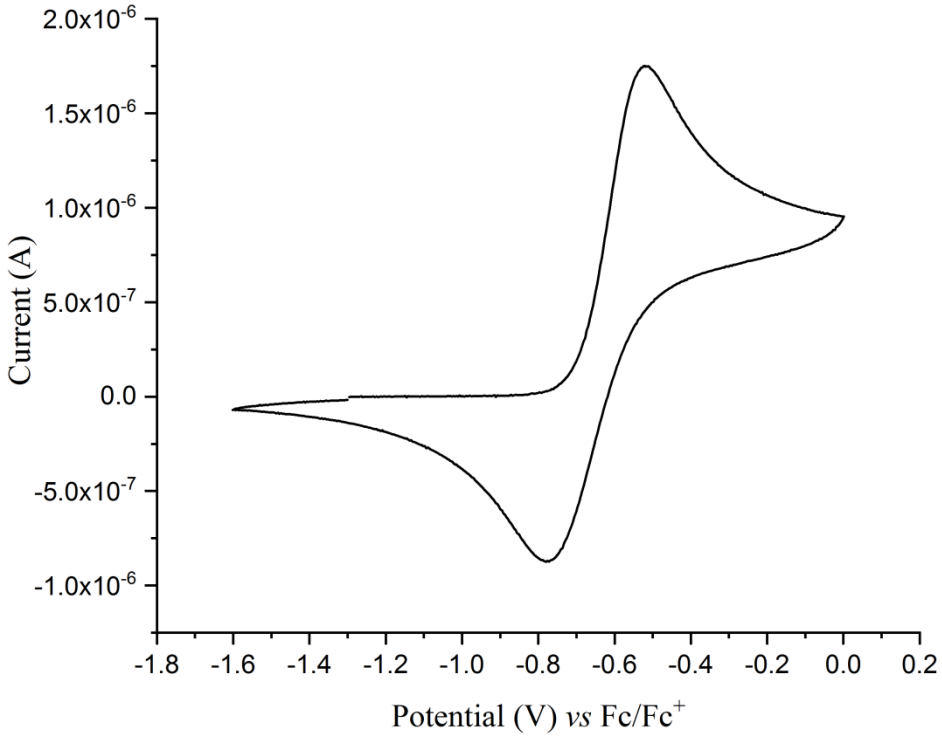


Figure S31. Cyclic voltammogram of **3a** in THF (0.01 M *n*-$Bu_4N[B(C_6F_5)_4]$) as a supporting electrolyte, $0.05Vs^{-1}$, *vs* Fc/Fc^+). The cycle for Fc/Fc^+ couple has been removed for clarity.

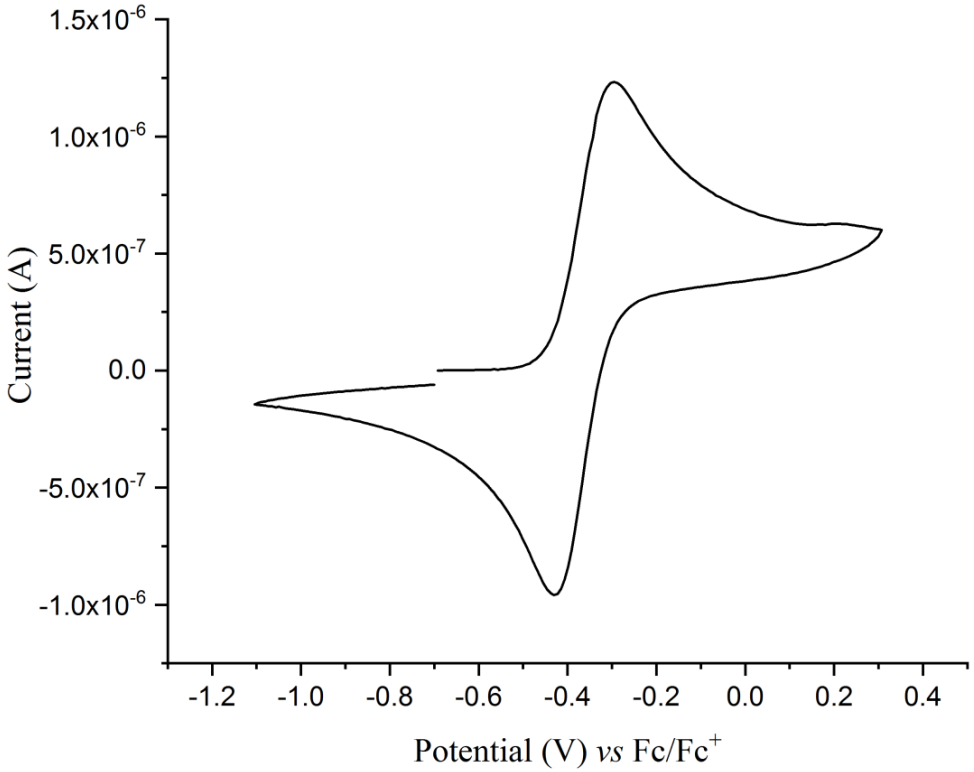


Figure S32. Cyclic voltammogram of **3b** in THF (0.01 M *n*-$Bu_4N[B(C_6F_5)_4]$) as a supporting electrolyte, $0.1Vs^{-1}$, *vs* Fc/Fc^+). The cycle for Fc/Fc^+ couple has been removed for clarity.

4. UV-vis Spectroscopy

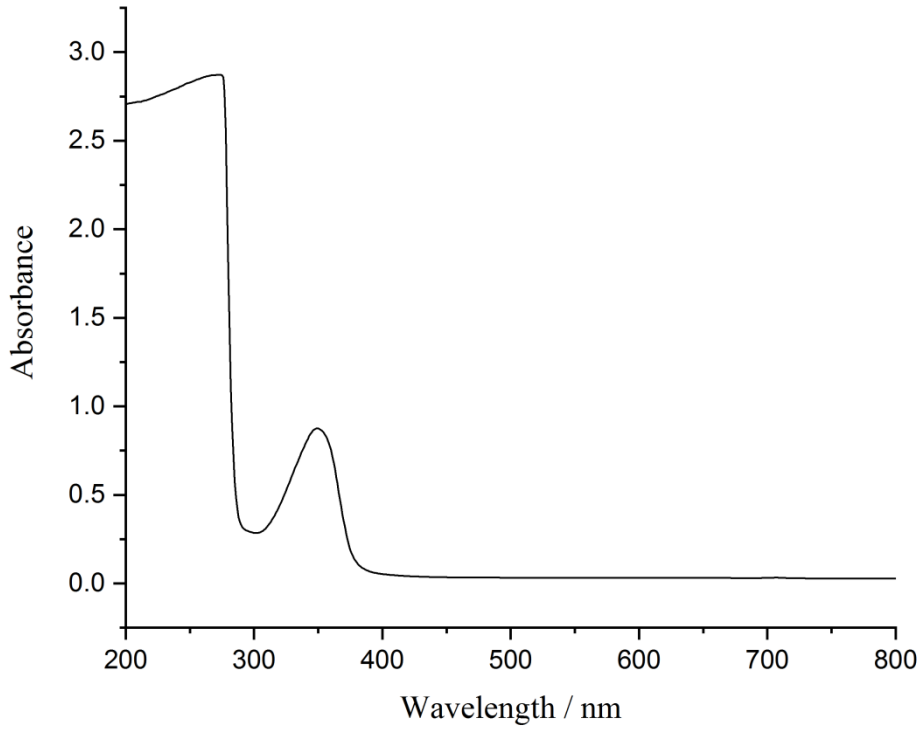


Figure S33. UV-visible spectrum of **2a** (10^{-4} M) recorded in flurobenzene.

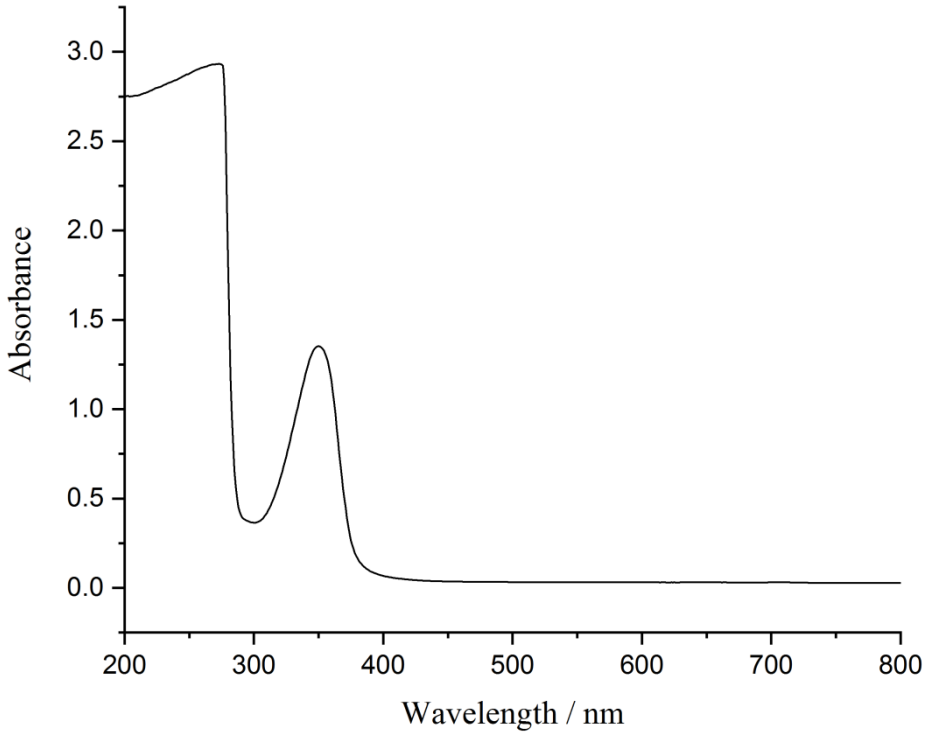


Figure S34. UV-visible spectrum of **2b** (10^{-4} M) recorded in flurobenzene.

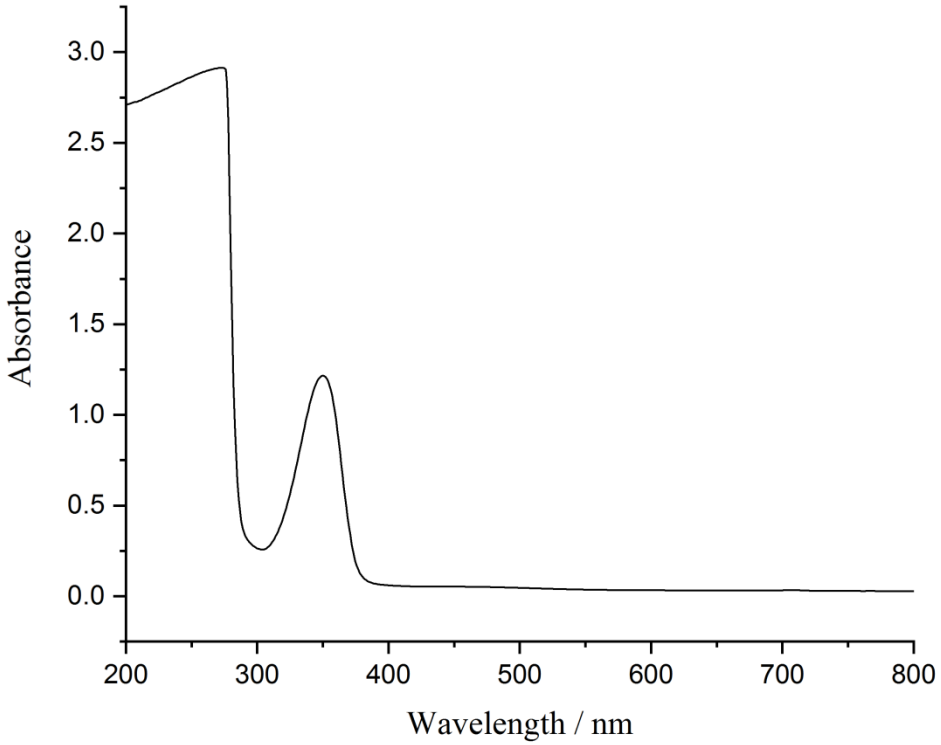


Figure S35. UV-visible spectrum of **3a** (10^{-4} M) recorded in flurobenzene.

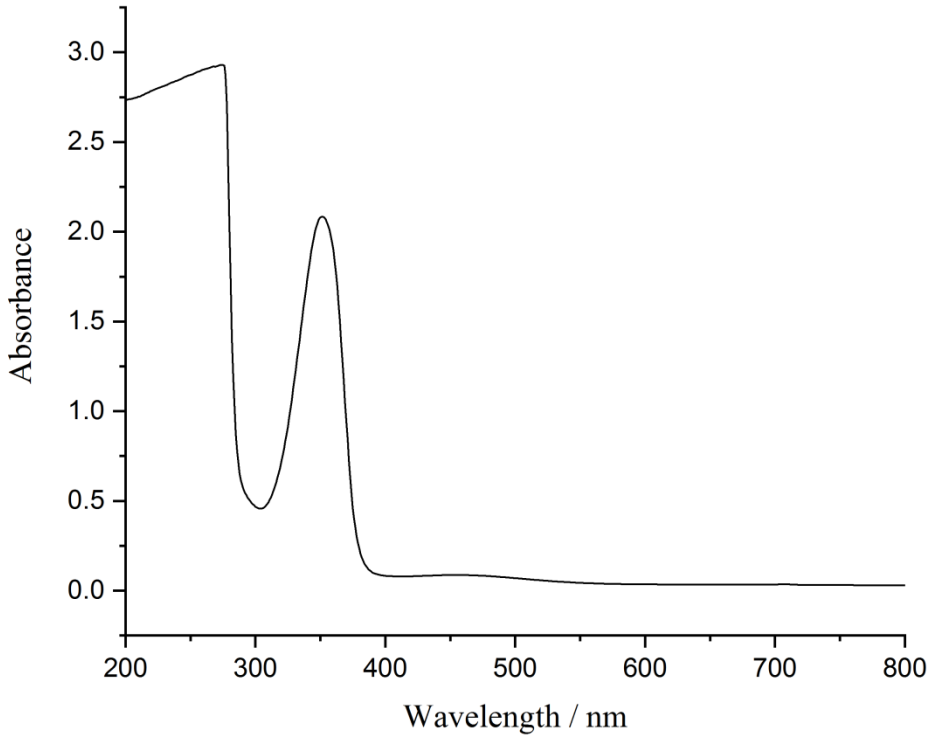


Figure S36. UV-visible spectrum of **3b** (10^{-4} M) recorded in flurobenzene.

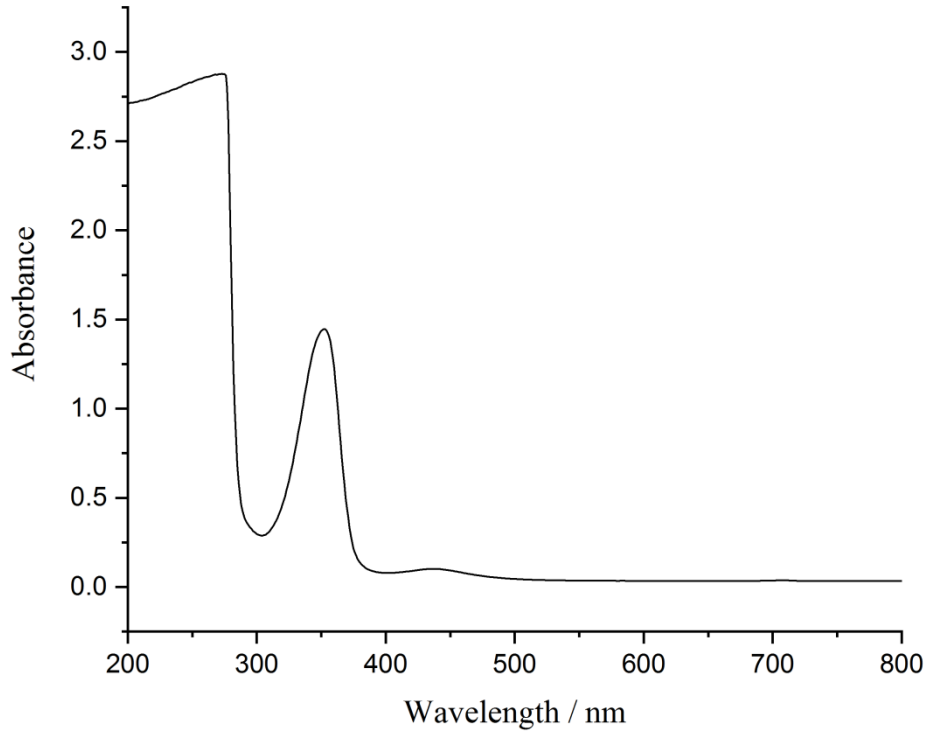


Figure S37. UV-visible spectrum of **4a** (10^{-4} M) recorded in flurobenzene.

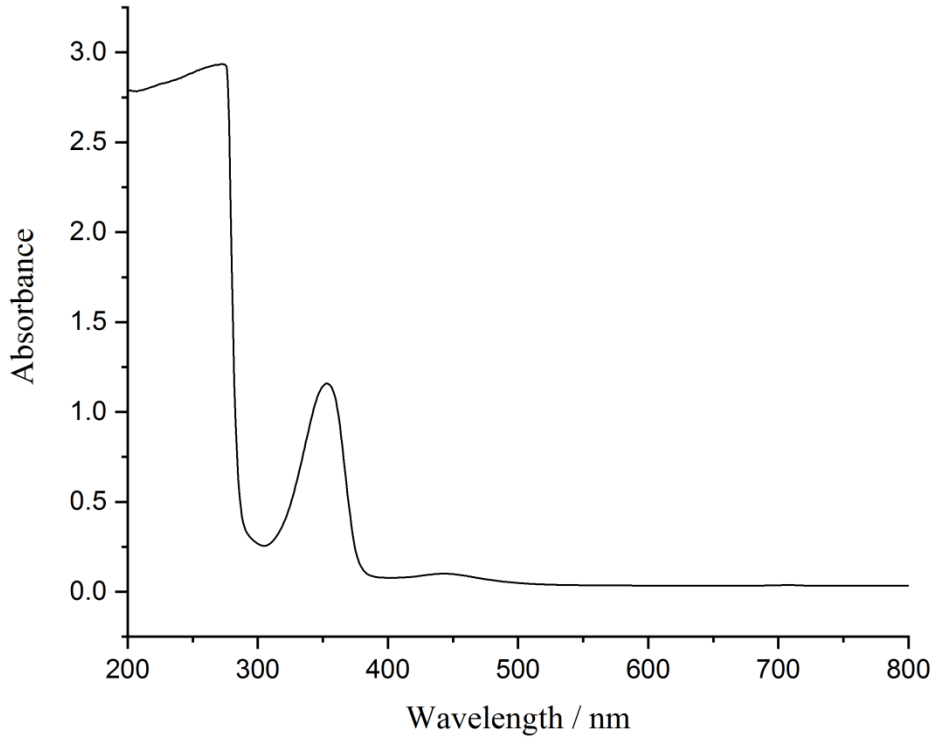


Figure S38. UV-visible spectrum of **4b** (10^{-4} M) recorded in flurobenzene.

5. X-Ray Crystallographic Analysis

The crystals were mounted on nylon loops in inert oil. Data of **2a**, **3a**, and **3b** were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (monochromated Mo_{Ka} radiation, λ = 0.71073 Å) at 100(2) K while those of **2b**, **4a**, **4b**, **5a**, and **5b** were collected on a Bruker AXS D8 Venture diffractometer with Photon II detector (monochromated Cu_{Ka} radiation, λ = 1.54178 Å, microfocus source) at 100(2) K. The structures were solved by Direct Methods (SHELXS-2013)[5] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017).[6-8] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups.

In **2a** an isopropyl group is disordered over two positions. The structure of **3a** contains highly disordered solvent – possibly *n*-hexane. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* (**1990**), 194–201). Since the nature and amount of the solvent is not clear it was not included in the sum formula. In **3b** an isopropyl group is disordered over two positions. All its corresponding bond lengths and angles were restrained to be equal (SADI). RIGU and SIMU restraints were applied to its atoms' anisotropic displacement parameters. The solvent molecule is disordered over a centre of inversion. Its bond lengths and angles were restrained to be equal (SADI) and RIGU restraints were used for the displacement parameters. Due to their close proximity C3_1 and C3_2 were refined with common displacement parameters (EADP). The central core of the cation of **4a** is disordered over two positions. The corresponding bond lengths and angles were restrained to be equal (SADI) and RIGU restraints were applied to the displacement parameters. Due to their close proximity C60 and C60' as well as C61 and C61' were refined with additional SIMU restraints. The toluene molecule is disordered over two positions. RIGU restraints were used for the refinement of its atoms' displacement parameters. In **4b** a second orientation of the central Br–Ga–P–P–Ga–Br chain could be identified and refined. Hints on the missing carbene of this component can be found in the residual electron density but due to the low occupancy (approx. 5%) the second orientation of the carbene could not be identified completely nor refined. RIGU and SIMU restraints were used to refine the displacement parameters of the minor component. For Ga2' and Br2' an additional ISOR (σ = 0.003) restraint was necessary. In **5a** the PH hydrogen atoms were refined freely with their P–H bond lengths restrained to be equal (SADI). The central Ga(Cl)–PH–P(carbene)–Ga(Cl) moiety is disordered over two positions. For Ga1 and Cl1 a third orientation can be found but a refinement failed due to the low occupancy. The corresponding bond lengths of the carbene were restrained to be equal (SADI) and RIGU restraints were applied to its displacement parameters. For atoms in close proximity additional SIMU restraints were used. The structure contains highly disordered solvent – fluoro benzene or toluene. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* (**1990**), 194–201). Since the nature and amount of the solvent is not clear it was not included in the sum formula. In **5b** the PH hydrogen atoms could not be identified in the residual electron density. Their positions were taken from the isomorphous chloro compound. The H atom of the larger disorder component was refined freely, the co-ordinates of the

one of the smaller were refined by a riding model (AFIX 3) and its displacement parameter was refined freely. The P–H bond lengths were restrained to be equal to 1.42 Å (DFIX). The proper assignment of these hydrogen atoms should be confirmed by other means. The central Ga(Br)–PH–P(carbene)–Ga(Br) moiety is disordered over two positions. The corresponding bond lengths of the carbene were restrained to be equal (SADI) and RIGU restraints were applied to its displacement parameters. For atoms in close proximity additional SIMU restraints were used. The alternate positions of N5 were refined with common displacement parameters (EADP). The structure also contains highly disordered solvent – possibly fluoro benzene or toluene. The final refinement was done with a solvent free dataset from a PLATON/SQUEEZE run. (For details see: A. L. Spek, *Acta Cryst. A46* (**1990**), 194–201). Since the nature and amount of the solvent is not clear, it was not included in the sum formula. The crystal was a very thin plate and diffracted rather poorly, esp. at higher angles. In addition, the highly anisotropic shape of the crystal hampered the absorption correction. This leads to a rather high R_{int}. Due to the weak data quantitative results should be carefully scrutinized and may be unreliable.

CCDC-2184009 (**2a**; mks_001m), -2184010 (**2b**; mks_005m), -2184011 (**3a**; mks_037am_sq), -2184012 (**3b**; mks_049m), -2184320 (**4a**; mks_057m), -2184142 (**4b**; mks_056m), -2184019 (**5a**; mks_073), and -2184020 (**5b**; mks_077) contain 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 **2a**, **2b**, and **3a**.

Compound	**2a**	**2b**	**3a**
Emp. formula	$C_{58}H_{82}Cl_2Ga_2N_4P_2$	$C_{58}H_{82}Br_2Ga_2N_4P_2$	$C_{65}H_{94}Cl_2Ga_2N_6P_2$
Formula weight	1107.55	1196.47	1231.74
Temperature [K]	100(2)	100(2)	0.152 × 0.098 × 0.094
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/n$	P-1
a [Å]	13.7010(18)	13.6417(6)	14.863(2)
b [Å]	13.8715(16)	13.9614(6)	20.330(5)
c [Å]	15.7041(18)	15.7579(7)	25.712(6)
α [°]	90	90	83.603(4)
β [°]	105.336(6)	105.1021(15)	75.258(6)
γ [°]	90	90	72.565(4)
V [Å^3]	2878.3(6)	2897.6(2)	7163(3)
Z	2	2	4
ρ [Mgm^{-3}]	1.278	1.371	1.142
μ [mm^{-1}]	1.124	3.569	0.910
F (000)	1168	1240	2608
Crystal size [mm]	0.452 *x* 0.402 *x* 0.368	0.151 × 0.136 × 0.096	0.152 × 0.098 × 0.094
θ max [°]	40.215	80.790	30.528
Index ranges	$-16 \le h \le 24$ $-25 \le k \le 25$ $-28 \le l \le 27$	$-17 \le h \le 17$ $-17 \le k \le 17$ $-20 \le l \le 19$	$-21 \le h \le 21$ $-29 \le k \le 29$ $-36 \le l \le 36$
No. of reflect. collected	72672	113993	264320
Unique reflect.	18029	6312	43665
R_{int}	0.0346	0.0431	0.0782
Data / restraints / params.	18029 / 0 / 347	6312 / 0 / 317	43665 / 0 / 1435
Goodness-of-fit on F^2	1.043	1.032	1.032
$R1$ [$I>2\sigma(I)$]	0.0330	0.0228	0.0436
$wR2$ [$I>2\sigma(I)$]	0.0822	0.0593	0.1016
$R1$ [all data]	0.0495	0.0243	0.0756
$wR2$ [all data]	0.0910	0.0593	0.1119
Largest diff. peak and hole max./min.[e·Å^{-3}]	1.096 and –0.610	0.502 and –0.377	1.550 and –0.921

Table S2. Crystal data and structure refinement of **3b**, **4a**, and **4b**.

Compound	**3b**	**4a**	**4b**
Emp. formula	$C_{68}H_{101}Br_2Ga_2N_6P_2$	$C_{96}H_{102}BCl_2F_{20}Ga_2N_6P_2$	$C_{89}H_{94}BBr_2F_{20}Ga_2N_6P_2$
Formula weight	1363.74	2002.92	1999.71
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	monoclinic	triclinic	monoclinic
Space group	$P2_1/n$	P-1	$P2_1/c$
a [Å]	14.7131(10)	12.6151(10)	21.557(2)
b [Å]	25.5509(18)	16.6393(13)	20.432(2)
c [Å]	18.5397(13)	23.1348(18)	20.684(2)
α [°]	90	77.844(3)	90
β [°]	99.6843(16)	77.731(3)	20.684(2)
γ [°]	90	86.897(3)	90
V [Å^3]	6870.4(8)	4638.6(6)	8979.6(16)
Z	4	2	4
ρ [Mgm^{-3}]	1.318	1.434	1.479
μ [mm^{-1}]	2.037	2.344	2.888
F (000)	2852	2062	4068
Crystal size [mm]	0.477 × 0.204 × 0.122	0.326 × 0.149 × 0.080	0.130 × 0.112 × 0.096
θ max [°]	33.212	80.659	81.277
Index ranges	$-22 \le h \le 22$ $-39 \le k \le 39$ $-28 \le l \le 28$	$-16 \le h \le 16$ $-21 \le k \le 21$ $-29 \le l \le 29$	$-27 \le h \le 27$ $-26 \le k \le 25$ $-26 \le l \le 26$
No. of reflect. collected	228807	283933	405733
Unique reflect.	26297	20142	19684
R_{int}	0.0514	0.0434	0.0949
Data / restraints / params.	20984 / 117 / 799	18999 / 266 / 1392	16685 / 39 / 1178
Goodness-of-fit on F^2	1.043	1.171	1.011
$R1$ [$I>2\sigma(I)$]	0.0314	0.0382	0.0281
$wR2$ [$I>2\sigma(I)$]	0.0641	0.0850	0.0665
$R1$ [all data]	0.0501	0.0407	0.0369
$wR2$ [all data]	0.0703	0.0862	0.0706
Largest diff. peak and hole max./min.[e·Å^{-3}]	0.774 and –0.463	0.580 and –0.506	0.430 and –0.708

Table S3. Crystal data and structure refinement of **5a**, and **5b**.

Compound	**5a**	**5b**
Emp. formula	$C_{89}H_{95}BCl_2F_{20}Ga_2N_6P_2$	$C_{89}H_{95}BBr_2F_{20}Ga_2N_6P_2$
Formula weight	1911.79	2000.71
Temperature [K]	100(2)	100(2)
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a [Å]	12.5203(3)	12.5498(4)
b [Å]	16.6728(5)	16.6890(7)
c [Å]	23.1865(7)	23.2672(9)
α [°]	78.0634(15)	77.921(2)
β [°]	77.1747(12)	77.403(2)
γ [°]	87.3124(14)	87.595(2)
V [Å^3]	4617.3(2)	4650.5(3)
Z	2	2
ρ [Mgm^{-3}]	1.375	1.429
μ [mm^{-1}]	2.327	2.789
F (000)	1964	2036
Crystal size [mm]	0.261 x 0.171 x 0.142	0.144 x 0.124 x 0.015
θ max [°]	2.71 to 79.55	1.988 to 75.216
Index ranges	$-15 \le h \le 15$ $-21 \le k \le 21$ $-29 \le l \le 29$	$-15 \le h \le 15$ $-20 \le k \le 20$ $-29 \le l \le 29$
No. of reflect. collected	267036	234649
Unique reflect.	18937	14631
R_{int}	0.0426	0.1279
Data / restraints / params.	20020 / 200 / 1274	19037 / 195 / 1263
Goodness-of-fit on F^2	1.230	1.192
*R*1 [$I>2\sigma(I)$]	0.0584	0.0793
*wR*2 [$I>2\sigma(I)$]	0.1201	0.1684
*R*1 [all data]	0.0610	0.1015
*wR*2 [all data]	0.1212	0.1771
Largest diff. peak and hole max./min.[Å^{-3}]	1.084 and –0.641	0.577 and –0.795

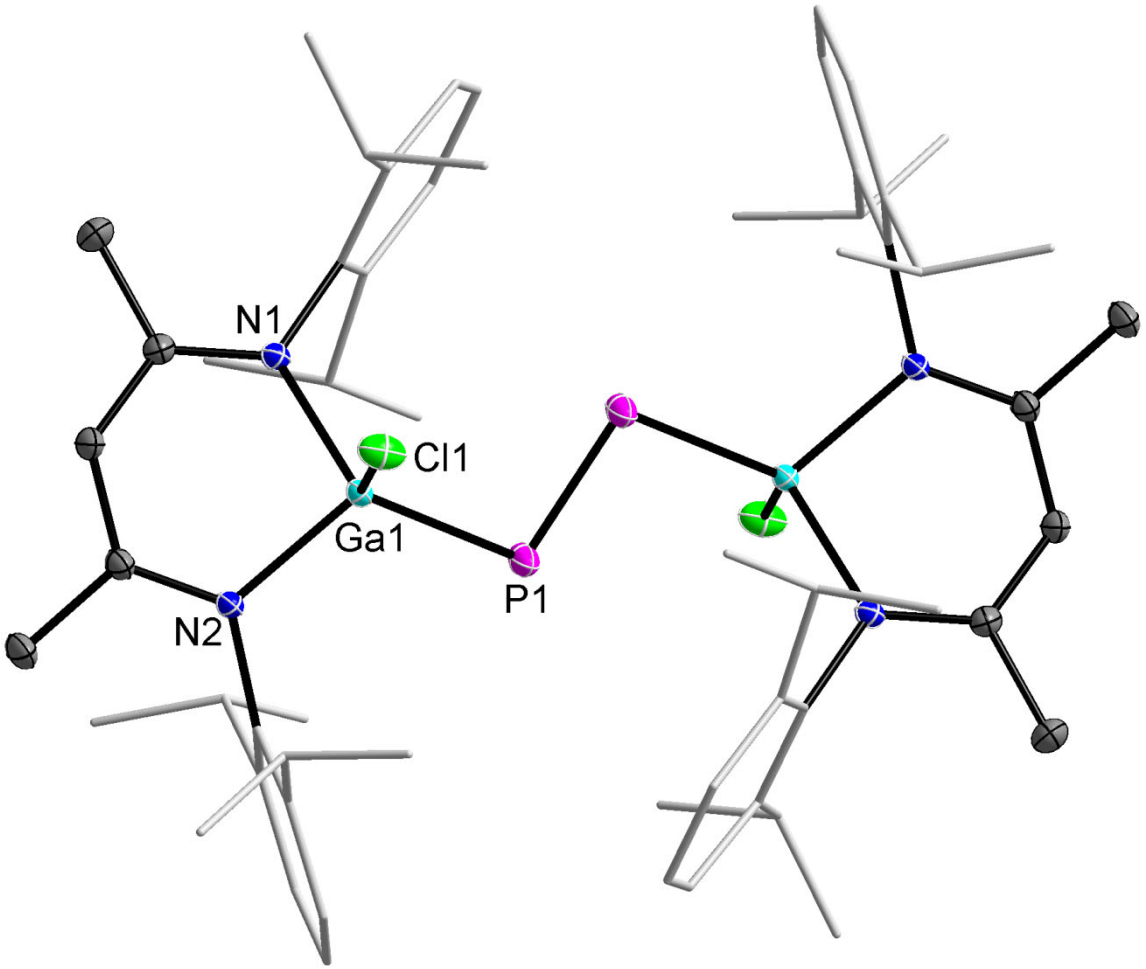


Figure S39. Molecular structure of **2a** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)–N(2) 1.9363(7), Ga(1)–N(1) 1.9436(7), Ga(1)–Cl(1) 2.2207(3), Ga(1)–P(1) 2.3131(3), P(1)–P(1)$^{\#1}$ 2.0381(5); N(2)–Ga(1)–N(1) 97.40(3), N(2)–Ga(1)–Cl(1) 105.39(2), N(1)–Ga(1)–Cl(1) 103.88(2), N(2)–Ga(1)–P(1) 111.98(2), N(1)–Ga(1)–P(1) 118.22(2), Cl(1)–Ga(1)–P(1) 117.464(13), P(1)$^{\#1}$–P(1)–Ga(1) 95.182(18) $^{\#1}$coordinates used to generate equivalent atoms: -x,-y,-z+1.

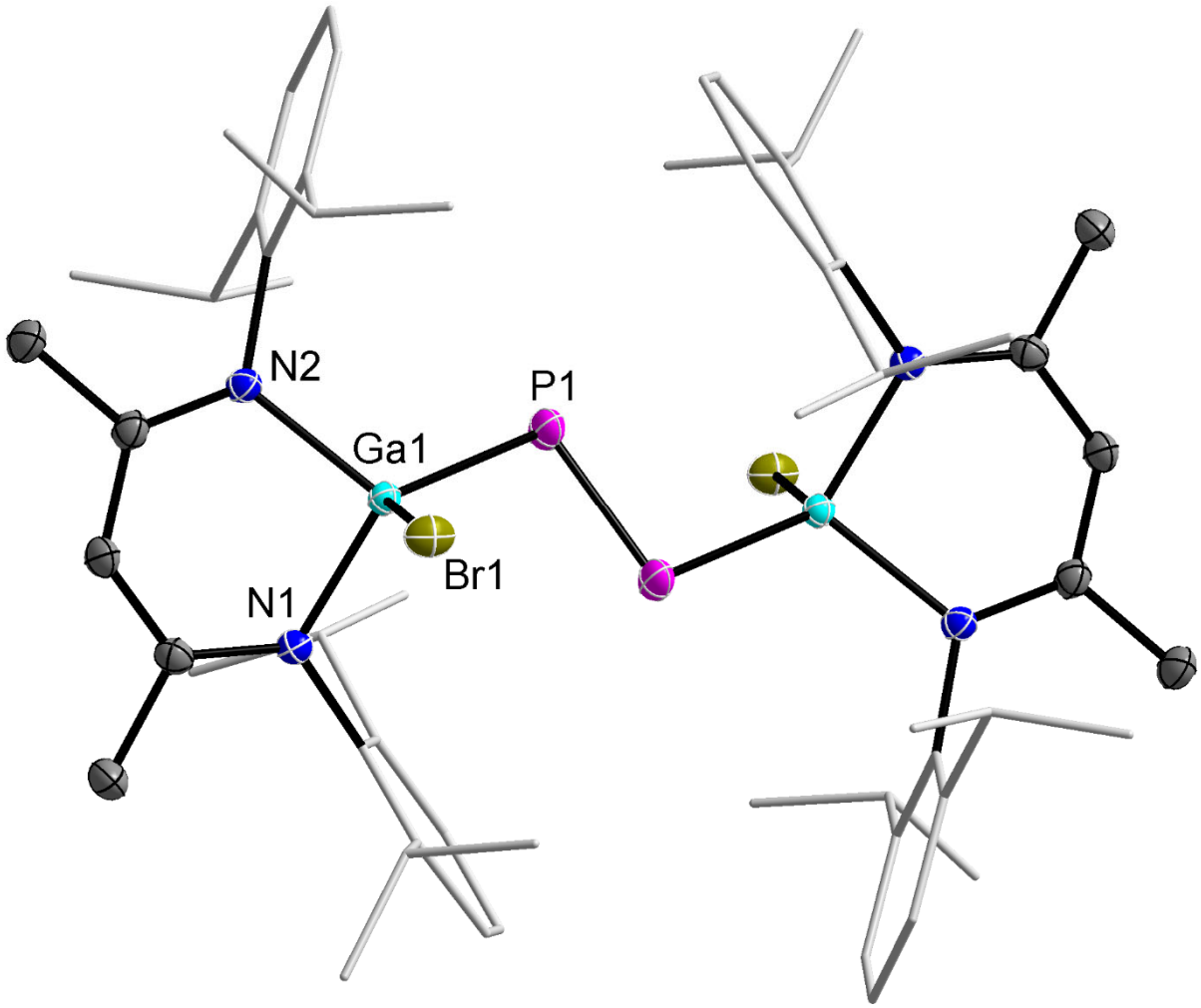


Figure S40. Molecular structure of **2b** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. Selected bond length (Å) and angels (°): Br(1)–Ga(1) 2.3680(2), Ga(1)–N(2) 1.9331(12), Ga(1)–N(1) 1.9439(12), Ga(1)–P(1) 2.3120(4), P(1)–P(1)$^{\#1}$ 2.0282(8); N(2)–Ga(1)–N(1) 97.58(5), N(2)–Ga(1)–P(1) 112.51(3), N(1)–Ga(1)–P(1) 117.80(3), N(2)–Ga(1)–Br(1) 105.41(3), N(1)–Ga(1)–Br(1) 104.03(3), P(1)–Ga(1)–Br(1) 117.114(13), P(1)$^{\#1}$–P(1)–Ga(1) 94.92(2).

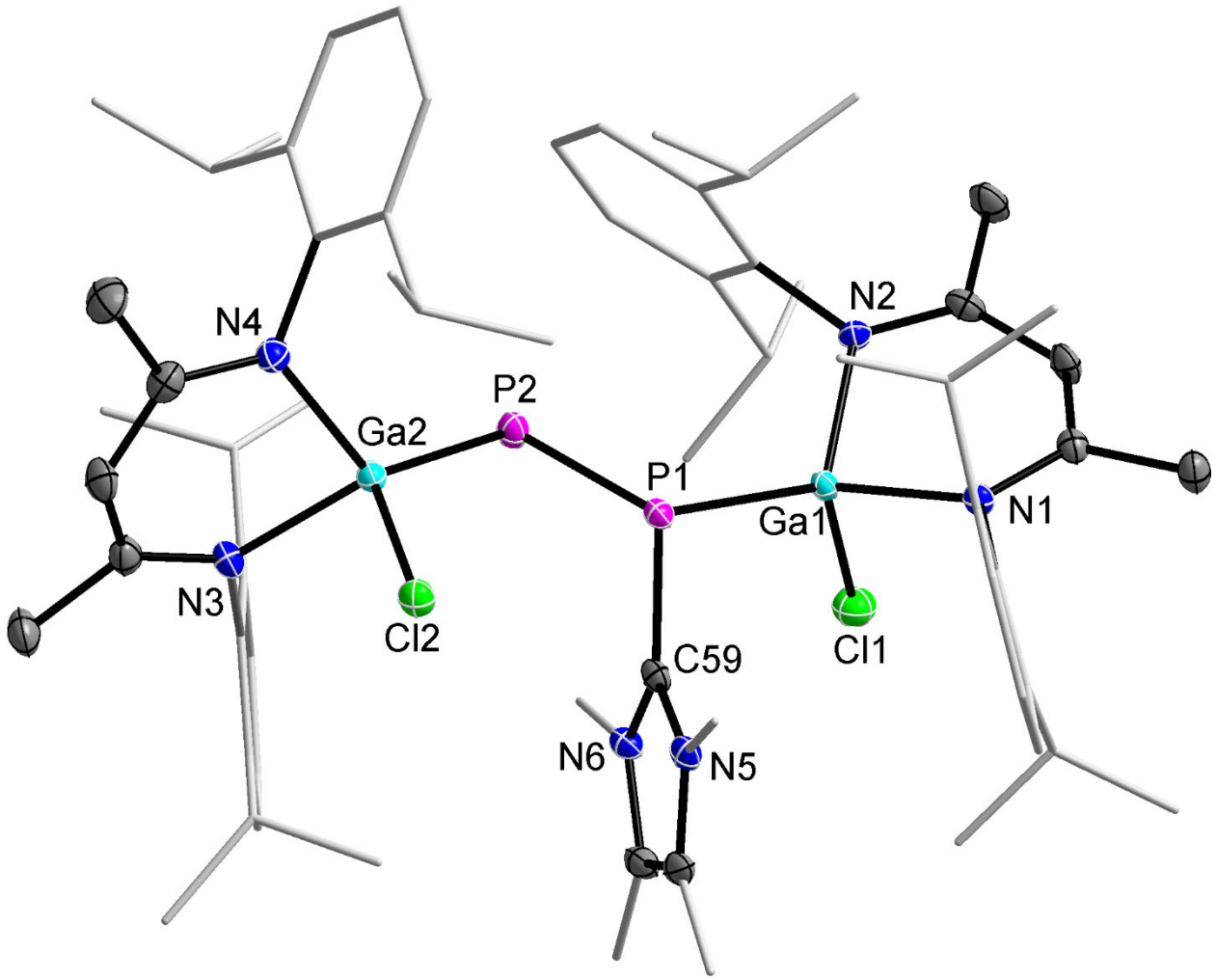


Figure S41. Molecular structure of **3a** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. Selected bond length (Å) and angels (°): (**molecule 1**) Ga(1)–N(1) 1.9506(16), Ga(1)–N(2) 1.9722(17), Ga(1)–Cl(1) 2.2249(6), Ga(1)–P(1) 2.3328(7), Ga(2)–N(3) 1.9851(17), Ga(2)–N(4) 2.0167(17), Ga(2)–Cl(2) 2.2590(7), Ga(2)–P(2) 2.2747(6), P(1)–C(59) 1.862(2), P(1)–P(2) 2.1871(8); N(1)–Ga(1)–N(2) 96.53(7), N(1)–Ga(1)–Cl(1) 101.43(5), N(2)–Ga(1)–Cl(1) 97.97(5), N(1)–Ga(1)–P(1) 120.93(5), N(2)–Ga(1)–P(1) 116.64(5), Cl(1)–Ga(1)–P(1) 118.81(2), N(3)–Ga(2)–N(4) 92.72(7), N(3)–Ga(2)–Cl(2) 101.85(5), N(4)–Ga(2)–Cl(2) 98.33(5), N(3)–Ga(2)–P(2) 121.02(5), N(4)–Ga(2)–P(2) 118.33(5), Cl(2)–Ga(2)–P(2) 119.33(2), C(59)–P(1)–P(2) 110.67(7), C(59)–P(1)–Ga(1) 95.21(6), P(2)–P(1)–Ga(1) 103.70(3), P(1)–P(2)–Ga(2) 95.93(3); (**molecule 2)** Ga(1)–N(2) 1.9551(16), Ga(1)–N(1) 1.9714(15), Ga(1)–Cl(1) 2.2113(6), Ga(1)–P(1) 2.3433(6), Ga(2)–N(4) 2.0023(17), Ga(2)–N(3) 2.0113(16), Ga(2)–Cl(2) 2.2579(6), Ga(2)–P(2) 2.2695(7), P(1)–C(59) 1.864(2), P(1)–P(2) 2.1835(8); N(1)–Ga(1)–N(2) 96.53(7), N(1)–Ga(1)–Cl(1) 101.43(5), N(2)–Ga(1)–Cl(1) 97.97(5), N(1)–Ga(1)–P(1) 120.93(5), N(2)–Ga(1)–P(1) 116.64(5), Cl(1)–Ga(1)–P(1) 118.81(2), N(3)–Ga(2)–N(4) 92.72(7), N(3)–Ga(2)–Cl(2) 101.85(5), N(4)–Ga(2)–Cl(2) 98.33(5), N(3)–Ga(2)–P(2) 121.02(5), N(4)–Ga(2)–P(2) 118.33(5), Cl(2)–Ga(2)–P(2) 119.33(2), C(59)–P(1)–P(2) 110.67(7), C(59)–P(1)–Ga(1) 95.21(6), P(2)–P(1)–Ga(1) 103.70(3), P(1)–P(2)–Ga(2) 95.93(3).

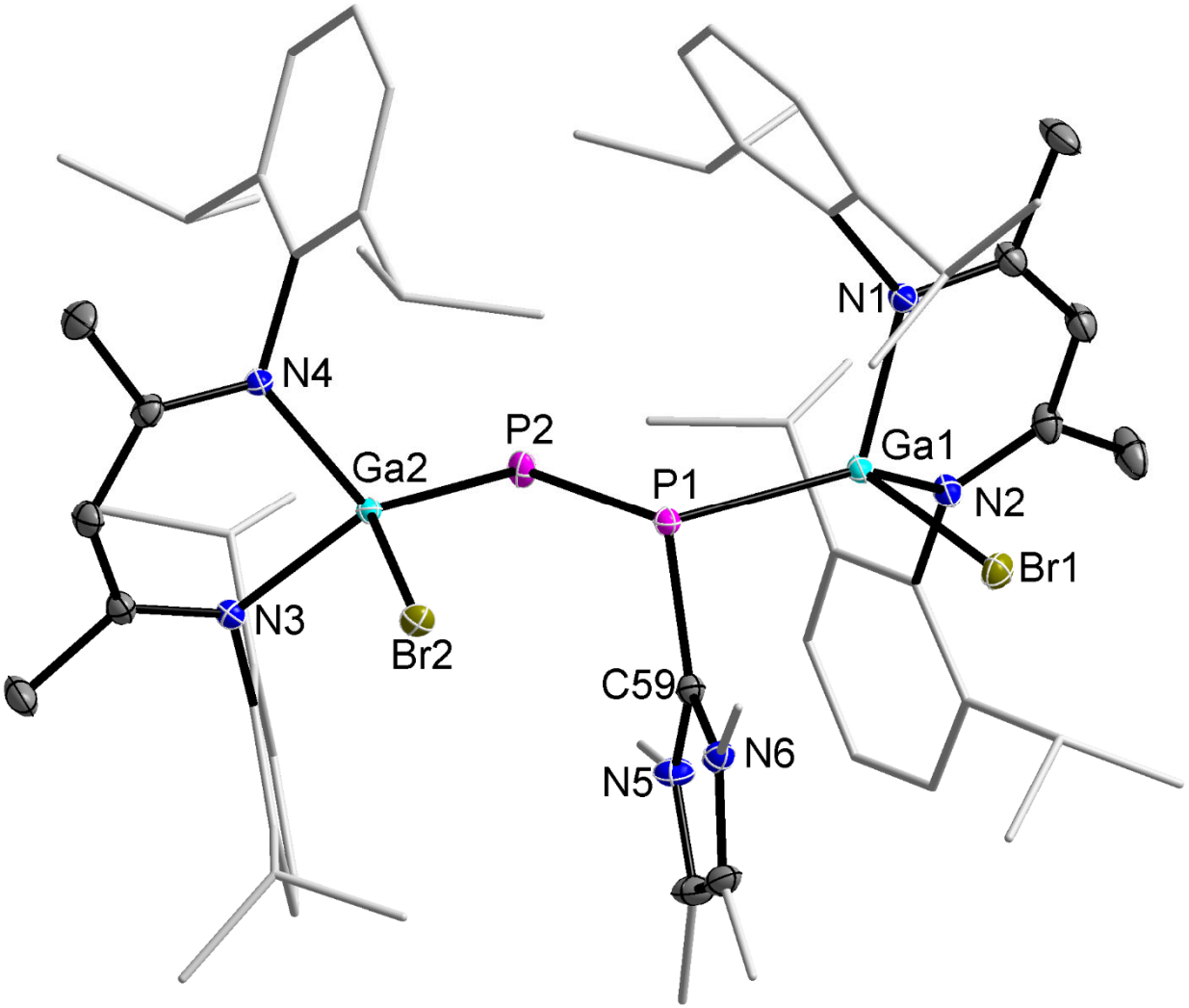


Figure S42. Molecular structure of **3b** with thermal ellipsoids at 50% probability level. The hydrogen atoms, and the alternate position of the disordered part are omitted for clarity. Selected bond length (Å) and angels (°): Br(1)–Ga(1) 2.3981(2), Br(2)–Ga(2) 2.4083(2), Ga(1)–N(1) 1.9513(11), Ga(1)–N(2) 1.9732(11),Ga(1)–P(1) 2.3205(4), Ga(2)–N(4) 1.9751(11), Ga(2)–N(3) 2.0028(11), Ga(2)–P(2) 2.2664(4), P(1)–C(59) 1.8570(13), P(1)–P(2) 2.1623(5); N(1)–Ga(1)–N(2) 96.36(5), N(1)–Ga(1)–P(1) 114.82(3), N(2)–Ga(1)–P(1) 134.28(4), N(1)–Ga(1)–Br(1) 102.46(4), N(2)–Ga(1)–Br(1) 100.16(4), P(1)–Ga(1)–Br(1) 104.349(11), N(4)–Ga(2)–N(3) 93.36(5), N(4)–Ga(2)–P(2) 121.61(3), N(3)–Ga(2)–P(2) 117.42(3), N(4)–Ga(2)–Br(2) 101.94(3), N(3)–Ga(2)–Br(2) 99.17(3), P(2)–Ga(2)–Br(2) 118.447(12), C(59)–P(1)–P(2) 110.55(5), C(59)–P(1)–Ga(1) 96.46(4), P(2)–P(1)–Ga(1) 113.099(18), P(1)–P(2)–Ga(2) 94.977(17).

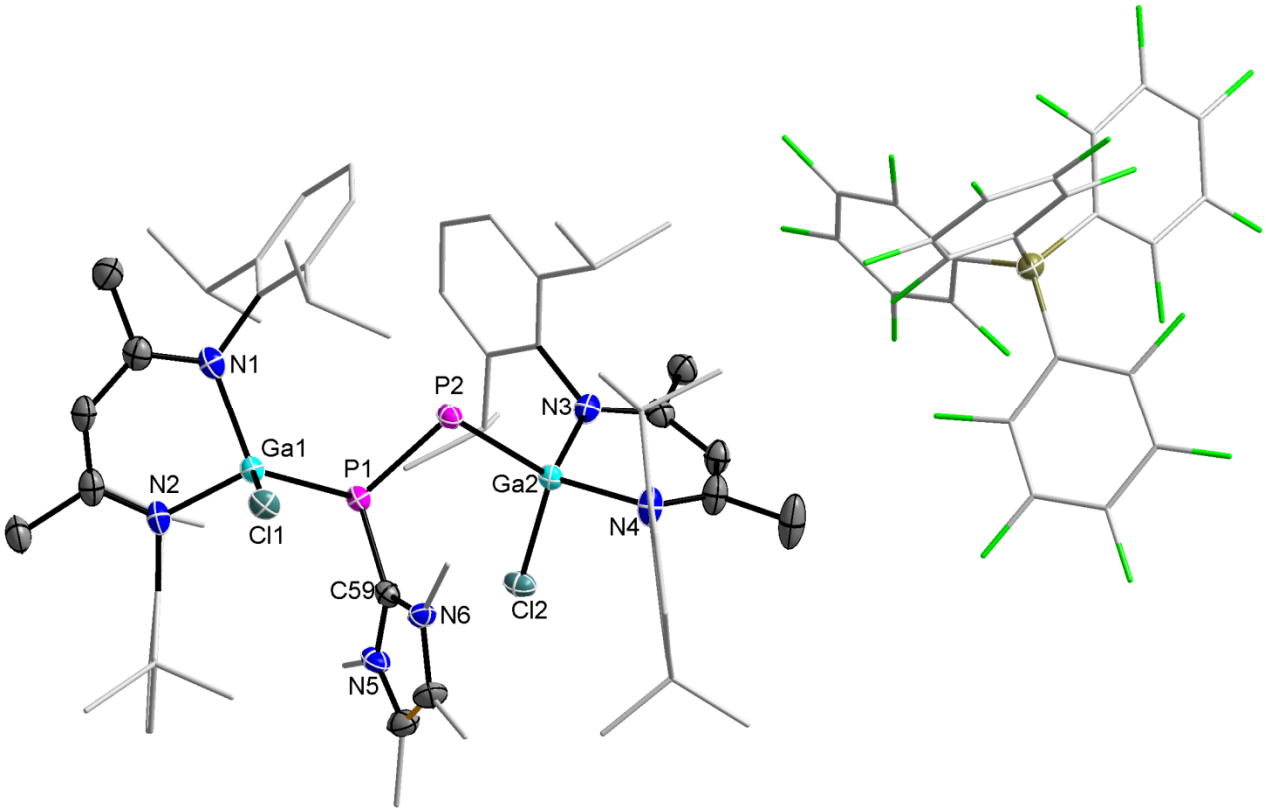


Figure S43. Molecular structure of **4a** with thermal ellipsoids at 50% probability level. The hydrogen atoms, a disordered solvent molecule (toluene), and the alternate position of the disordered part are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)–N(2) 1.9261(19), Ga(1)–N(1) 1.983(2), Ga(1)–Cl(1) 2.2021(10), Ga(1)–P(1) 2.3479(13), Ga(2)–N(3) 1.8686(18), Ga(2)–N(4) 1.9669(18), Ga(2)–Cl(2) 2.2074(10), Ga(2)–P(2) 2.3456(10), P(1)–C(59) 1.823(3), P(1)–P(2) 2.1423(8); N(2)–Ga(1)–N(1) 96.57(8), N(2)–Ga(1)–Cl(1) 106.28(6), N(1)–Ga(1)–Cl(1) 105.95(7), N(2)–Ga(1)–P(1) 112.02(7), N(1)–Ga(1)–P(1) 118.73(6), Cl(1)–Ga(1)–P(1) 115.17(6), N(3)–Ga(2)–N(4) 99.03(8), N(3)–Ga(2)–Cl(2) 105.72(6), N(4)–Ga(2)–Cl(2) 101.77(6), N(3)–Ga(2)–P(2) 108.10(6), N(4)–Ga(2)–P(2) 124.00(6), Cl(2)–Ga(2)–P(2) 115.82(5), C(59)–P(1)–P(2) 110.32(11), C(59)–P(1)–Ga(1) 102.17(9), P(2)–P(1)–Ga(1) 110.25(4), P(1)–P(2)–Ga(2) 100.12(3).

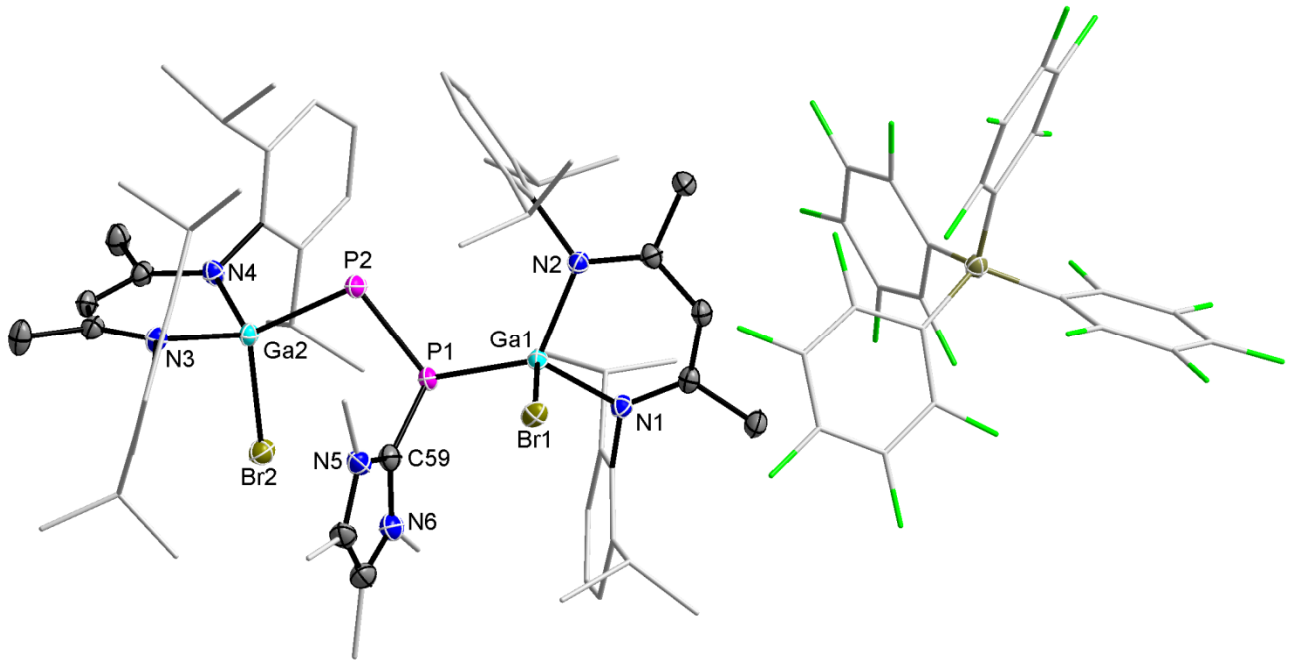


Figure S44. Molecular structure of **4b** with thermal ellipsoids at 50% probability level. The hydrogen atoms and the alternate position of the disordered part are omitted for clarity. Selected bond length (Å) and angels (°):Br(1)-Ga(1) 2.3498(5), Br(2)-Ga(2) 2.3403(6), Ga(1)-N(2) 1.9308(15), Ga(1)-N(1) 1.9422(15), Ga(1)-P(1) 2.3591(8), Ga(2)-N(4) 1.9336(15), Ga(2)-N(3) 1.9553(15), Ga(2)-P(2) 2.3522(7), P(1)-C(59) 1.8262(19), P(1)-P(2) 2.1336(7); N(2)-Ga(1)-N(1) 97.57(6), N(2)-Ga(1)-Br(1) 108.74(5), N(1)-Ga(1)-Br(1) 104.00(5), N(2)-Ga(1)-P(1) 119.49(5), N(1)-Ga(1)-P(1) 111.16(5), Br(1)-Ga(1)-P(1) 113.71(3), N(4)-Ga(2)-N(3) 96.91(6), N(4)-Ga(2)-Br(2) 105.42(5), N(3)-Ga(2)-Br(2) 104.47(5), N(4)-Ga(2)-P(2) 111.79(5), N(3)-Ga(2)-P(2) 120.45(5), Br(2)-Ga(2)-P(2) 115.40(2), C(59)-P(1)-P(2) 111.85(6), C(59)-P(1)-Ga(1) 100.18(6), P(2)-P(1)-Ga(1) 113.07(3), P(1)-P(2)-Ga(2) 101.59(3).

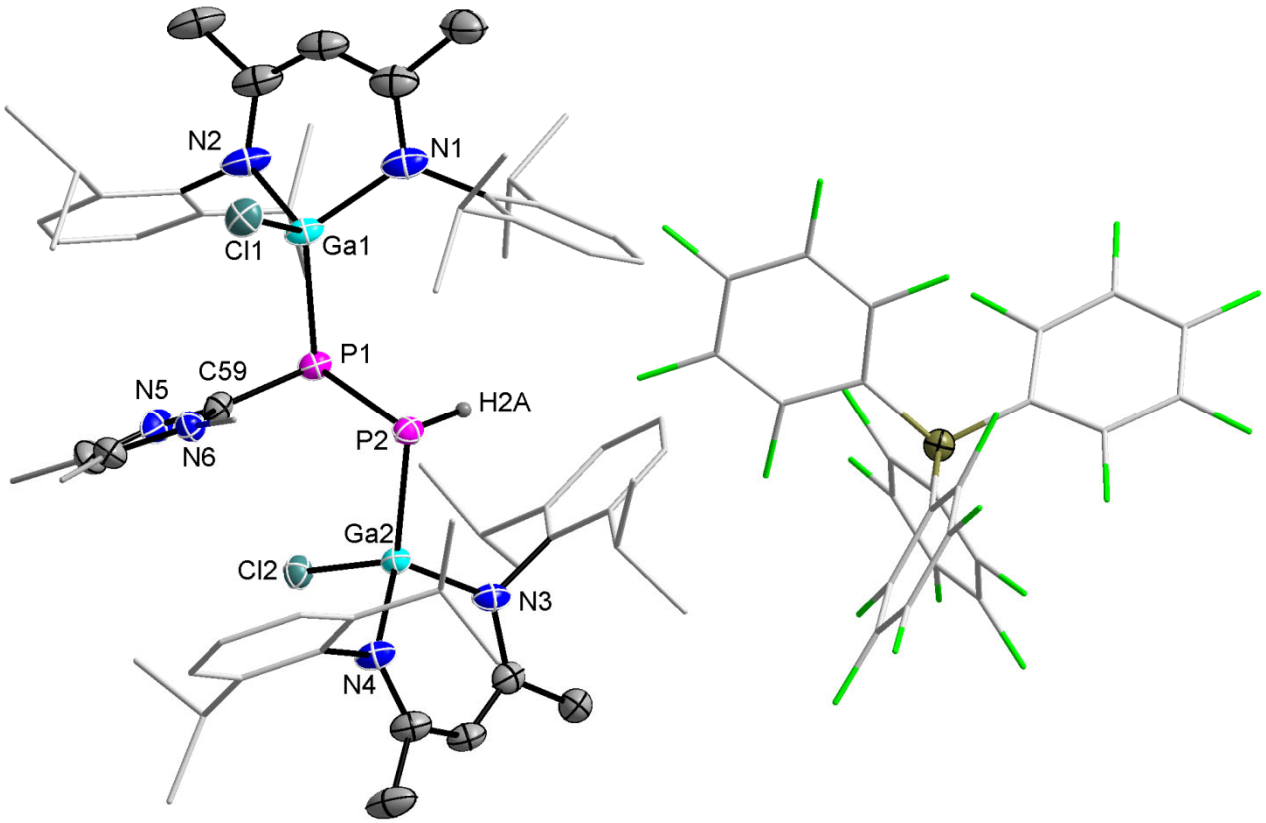


Figure S45. Molecular structure of **5a** with thermal ellipsoids at 50% probability level. The hydrogen atoms and the alternate position of the disordered part are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)-N(2) 1.913(3), Ga(1)-N(1) 1.991(3), Ga(1)-Cl(1) 2.2000(14), Ga(1)-P(1) 2.3655(16), Ga(2)-N(3) 1.860(3), Ga(2)-N(4) 1.988(3), Ga(2)-Cl(2) 2.2032(15), Ga(2)-P(2) 2.3466(16), P(1)-C(59) 1.838(4), P(1)-P(2) 2.2227(14), N(5)-C(59) 1.351(5), N(5)-C(60) 1.378(8), N(5)-C(62) 1.468(6), N(6)-C(59) 1.348(6); N(2)-Ga(1)-N(1) 96.48(14), N(2)-Ga(1)-Cl(1) 105.43(10), N(1)-Ga(1)-Cl(1) 104.99(10), N(2)-Ga(1)-P(1) 110.68(10), N(1)-Ga(1)-P(1) 118.85(9), Cl(1)-Ga(1)-P(1) 117.68(7), N(3)-Ga(2)-N(4) 98.82(12), N(3)-Ga(2)-Cl(2) 106.26(10), N(4)-Ga(2)-Cl(2) 102.64(9), N(3)-Ga(2)-P(2) 114.16(9), N(4)-Ga(2)-P(2) 118.06(10), Cl(2)-Ga(2)-P(2) 114.93(7), C(59)-P(1)-P(2) 103.18(16), C(59)-P(1)-Ga(1) 99.66(14), P(2)-P(1)-Ga(1) 107.23(6), P(1)-P(2)-Ga(2) 99.12(5), N(6)-C(59)-P(1) 132.6(4), N(5)-C(59)-P(1) 121.3(4).

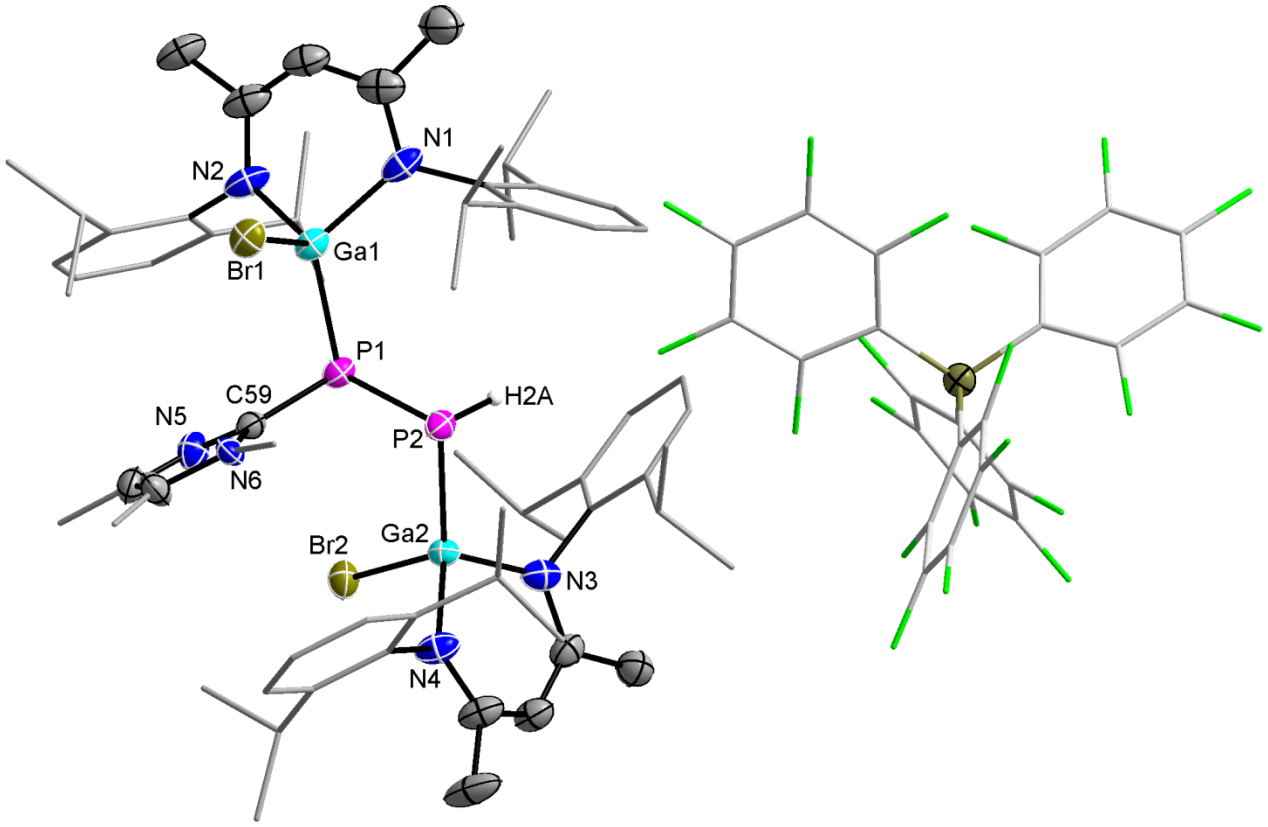


Figure S46. Molecular structure of **5b** with thermal ellipsoids at 50% probability level. The hydrogen atoms and the alternate position of the disordered part are omitted for clarity. Selected bond length (Å) and angels (°): Ga(1)-N(2) 1.914(5), Ga(1)-N(1) 2.007(6), Ga(1)-Br(1) 2.356(2), Ga(1)-P(1) 2.367(3), Ga(2)-N(3) 1.859(6), Ga(2)-N(4) 2.004(6), Ga(2)-P(2) 2.339(3), Ga(2)-Br(2) 2.354(2), P(1)-C(59) 1.829(8), P(1)-P(2) 2.223(3), N(5)-C(59) 1.340(10), N(5)-C(60) 1.387(10), N(5)-C(62) 1.452(9), N(6)-C(59) 1.54(9); N(2)-Ga(1)-N(1) 96.3(2), N(2)-Ga(1)-Br(1) 105.73(17), N(1)-Ga(1)-Br(1) 104.58(17), N(2)-Ga(1)-P(1) 110.26(19), N(1)-Ga(1)-P(1) 118.78(17), Br(1)-Ga(1)-P(1) 118.34(11), N(3)-Ga(2)-N(4) 98.9(2), N(3)-Ga(2)-P(2) 113.78(18), N(4)-Ga(2)-P(2) 117.50(19), N(3)-Ga(2)-Br(2) 106.04(19), N(4)-Ga(2)-Br(2) 102.13(18), P(2)-Ga(2)-Br(2) 116.34(13), C(59)-P(1)-P(2) 104.1(3), C(59)-P(1)-Ga(1) 98.9(3), P(2)-P(1)-Ga(1) 107.51(11), P(1)-P(2)-Ga(2) 99.43(11), N(5)-C(59)-P(1) 121.2(6), N(6)-C(59)-P(1) 131.9(6).

6. Computational Details

All quantum chemical calculations were performed using the program package ORCA 5.03. The structural optimizations were done using the B3LYP (12-15) functional and a def2-TZVP basis set[9-16] while the subsequent spin and EPR analyses included relativistic effects using the Zero Order Regular Approximation (ZORA)[17]. The calculations include atom pairwise dispersion correction[18,19] Natural Population Analysis was performed using the NBO7.0 Program (NBO7.0) in combination with ORCA4.2.1.[20]

Table S4. Calculated (selected) bond distances (Å) and angles (°) of compounds **2a-b**, **3a-b**, and **4a-b**.

Bond/Angle	**2a**	**2b**	**3a**	**3b**	**4a**	**4b**
P1=P2	2.040	2.040	2.158	2.158	2.130	2.133
Ga1–P1	2.332	2.333	2.325*	2.327*	2.358*	2.359*
Ga2–P2	2.334	2.333	2.280	2.280	2.354	2.357
P1–C59			1.852	1.852	1.816	1.817
Ga1–P1–P2	95.8	95.3	111.6*	111.0*	119.5*	118.1*
P1–P2–Ga2	94.9	95.3	93.7	94.0	99.6	100.3
Ga1–P1–C59			96.0	96.5	99.5	99.9
*carbene side						

Table S5. Mayer and Löwdin bond orders (in parenthesis) of compounds **2a-b**, **3a-b**, and **4a-b**.

Bond	**2a**	**2b**	**3a**	**3b**	**4a**	**4b**
P1=P2	1.8810 (2.0810)	1.8830 (2.0849)	1.2075 (1.4480)	1.2193 (1.4461)	1.2938 (1.4820)	1.2534 (1.4746)
Ga1–P1	0.9573 (1.2032)	0.9632 (1.2067)	0.9295* (1.1291*)	0.9346* (1.1275*)	0.8369* (1.0189*)	0.8718* (1.0194*)
Ga2–P2	0.9506 (1.2093)	0.9628 (1.2066)	1.1797 (1.4726)	1.1647 (1.4728)	0.9554 (1.1927)	0.9781 (1.1920)
P1–C59			1.0712 (1.2002)	1.0670 (1.1960)	1.0013 (1.1979)	1.0268 (1.2004)
*carbene side						

Table S6. Natural population analysis (NPA) atomic charges of compounds **2a-b**, **3a-b**, and **4a-b**.

atom	2a	2b	3a	3b	4a	4b
P1	–0.31175	–0.30720	–0.09235*	–0.09188*	–0.04921*	–0.04625*
P2	–0.31816	–0.30720	–0.84128	–0.83266	–0.33600	–0.32474
Ga1	1.41333	1.33854	1.45620*	1.39219*	1.48556*	1.41174*
Ga2	1.41224	1.33854	1.37116	1.30478	1.42213	1.34646
C (carbene)			0.16318	0.16437	0.16668	0.16319
N1 (carbene)			–0.31110	–0.31191	–0.30599	–0.30681
N2 (carbene)			–0.30965	–0.30810	–0.28370	–0.28485
*carbene side						

Table S7. FMO energies as well as the HOMO-LUMO gap of compounds **2a**, **2b**, **3a**, and **3b** calculated at M06-2X/def2-TZVPP//def2-SVP level of theory.

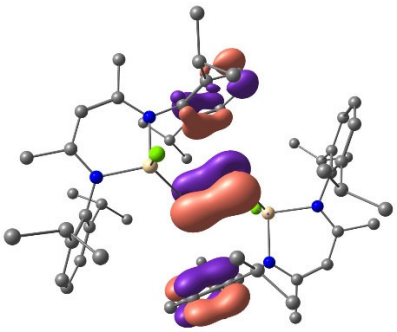
Orbital	**Energy / eV**			
	2a	**2b**	**3a**	**3b**
HOMO	–5.22	–5.26	–3.91	–3.95
LUMO	–2.37	–2.44	–1.34	–1.37
HOMO-LUMO gap	–7.60	–7.70	–5.25	–5.32

Table S8. Calculated *g*-tensor and hyperfine coupling constants (A in MHz) for the radical cations **4a** and **4b** calculated at the ZORA B3LYP D3BJ def2-tzvp level of theory.

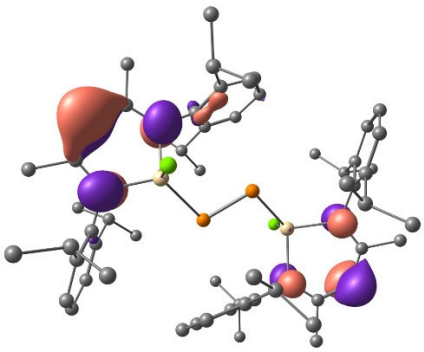
	4a				**4b**			
	x	*y*	*z*	iso	*x*	*y*	*z*	iso
g-tensor	1.997	2.004	2.019	2.006	2.000	2.002	2.016	2.006
A(P1)	263.1	274.7	426.9	321.6	263.2	275.1	421.3	319.9
A(P2)	–126.9	–145.8	594.7	107.4	–129.0	–147.8	598.8	107.3
A(Ga1)	83.2	84.2	97.4	88.3	84.1	84.8	97.5	88.8
*A(*Ga2)	–26.8	–43.0	–46.1	-38.6	–29.7	–45.7	–48.9	-41.4

Table S9. Mulliken spin populations of the radical cations **4a** and **4b**.

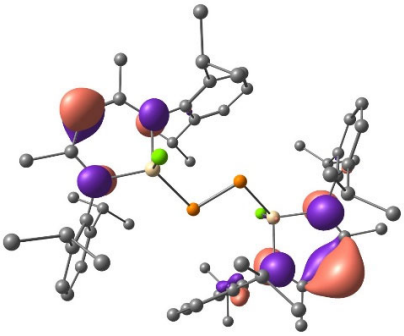
	4a	**4b**
P1	0.122	0.117
P2	0.797	0.804
Ga1	0.016	0.015
Ga2	–0.006	–0.007
$C59_{NHC}$	0.019	0.019
$N1_{NHC}$	0.004	0.004
$N2_{NHC}$	0.010	0.010



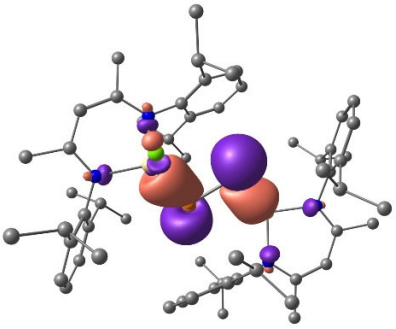
HOMO−3 (-0.2291 au)



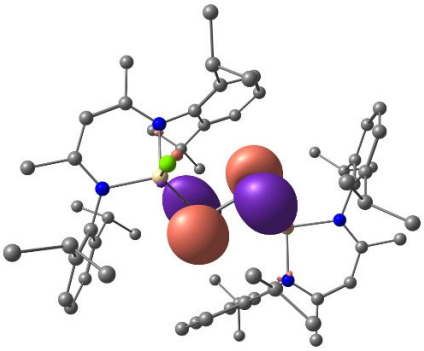
HOMO−2 (-0.2149 au)



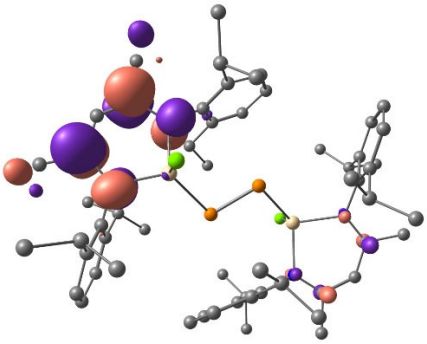
HOMO−1 (-0.2139 au)



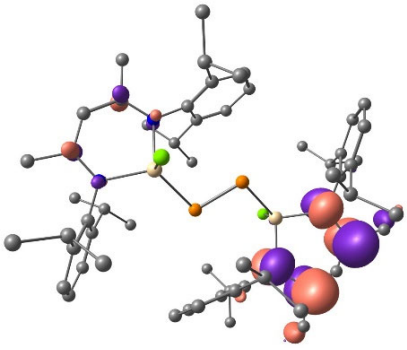
HOMO (-0.1919 au)



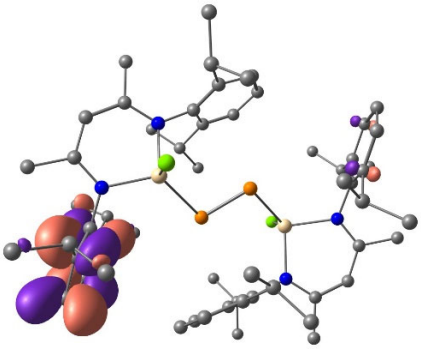
LUMO (-0.0873 au)



LUMO+1 (-0.0499 au)

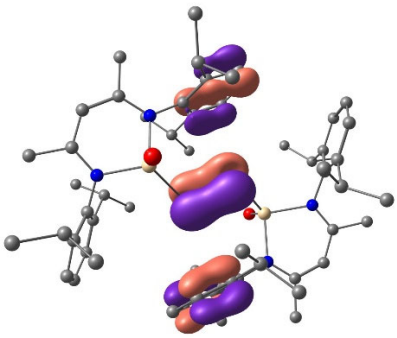


LUMO+2 (-0.0495 au)

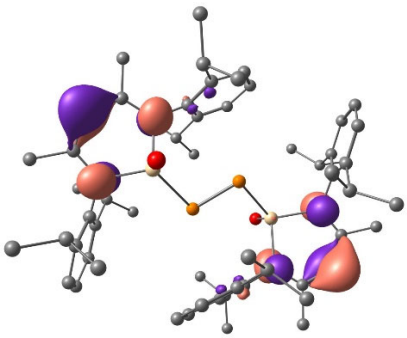


LUMO+3 (-0.0129 au)

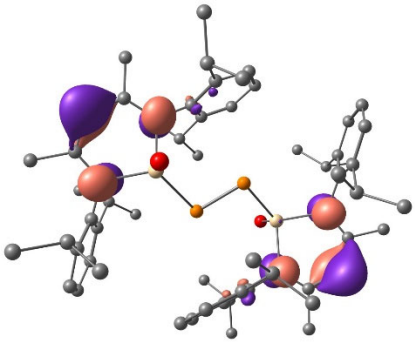
Figure S47. Selected molecular orbitals (from HOMO−3 to LUMO+3) of compound **2a** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.



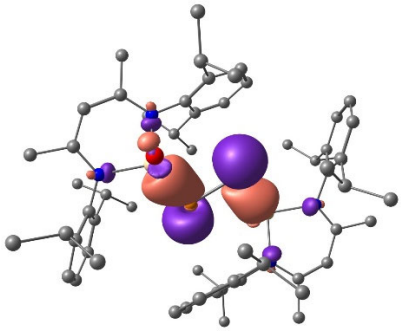
HOMO−3 (-0.2309 au)



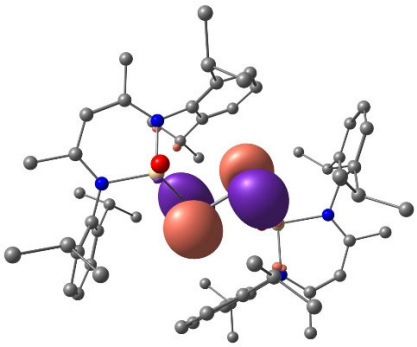
HOMO−2 (-0.2154 au)



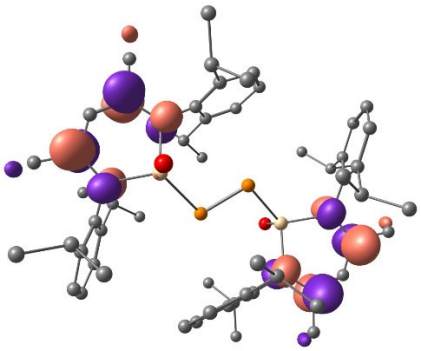
HOMO−1 (-0.2145 au)



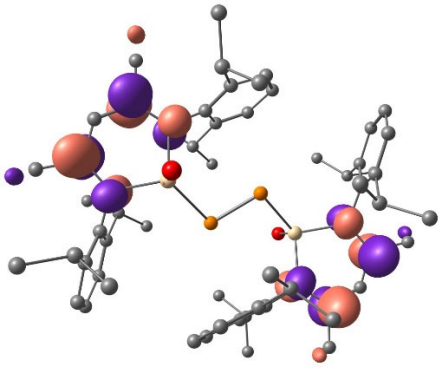
HOMO (-0.1932 au)



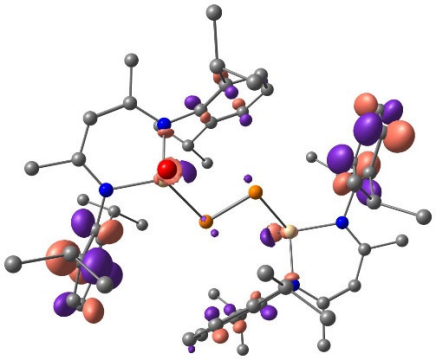
LUMO (-0.0898 au)



LUMO+1 (-0.0510 au)

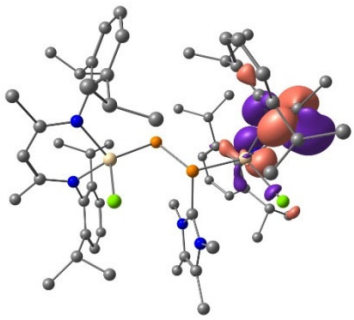


LUMO+2 (-0.0506 au)

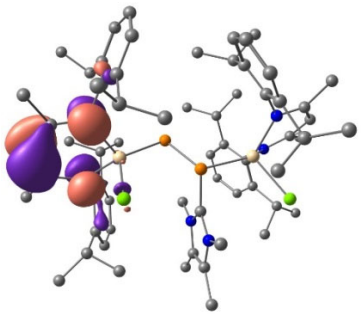


LUMO+3 (-0.0143 au)

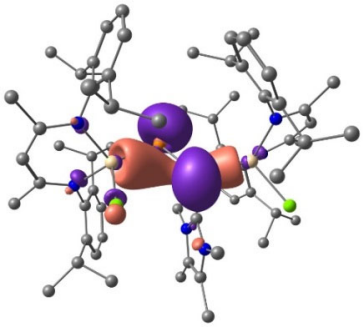
Figure S48. Selected molecular orbitals (from HOMO−3 to LUMO+3) of compound **2b** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.



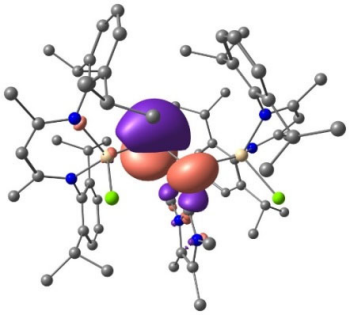
HOMO−3 (-0.2134 au)



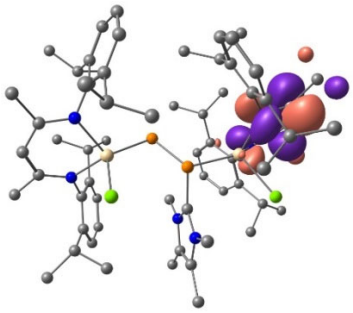
HOMO−2 (-0.2000 au)



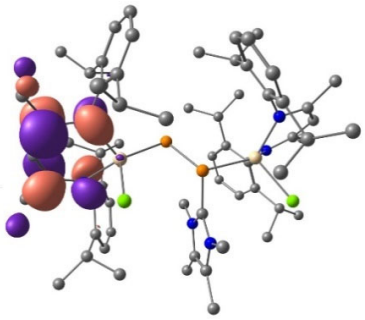
HOMO−1 (-0.1828 au)



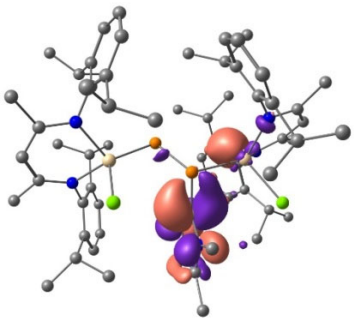
HOMO (-0.1440 au)



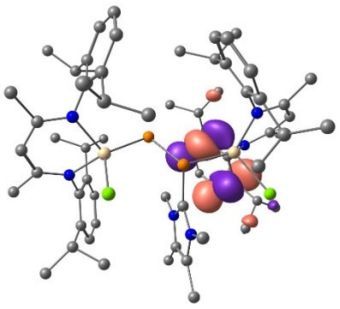
LUMO (-0.0492 au)



LUMO+1 (-0.0359 au)

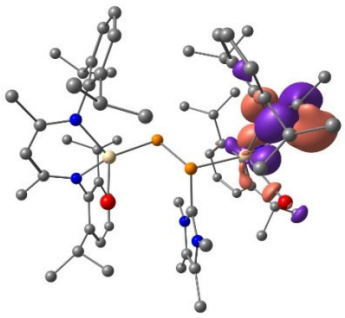


LUMO+2 (-0.0197 au)

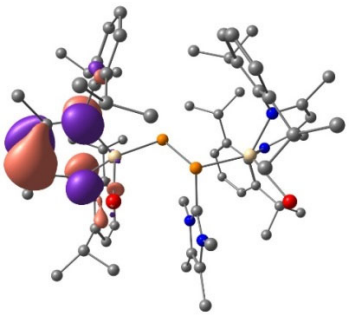


LUMO+3 (-0.0138 au)

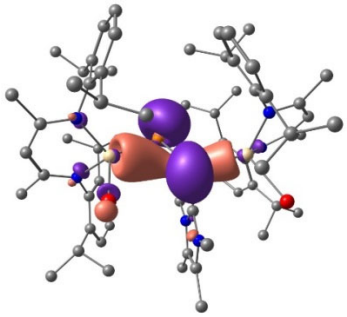
Figure S49. Selected molecular orbitals (from HOMO−3 to LUMO+3) of compound **3a** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.



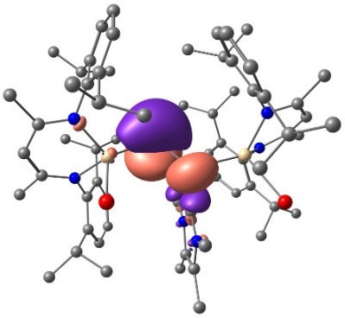
HOMO−3 (-0.2141 au)



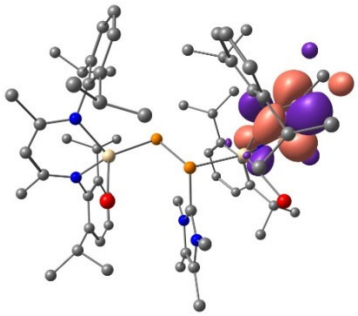
HOMO−2 (-0.2006 au)



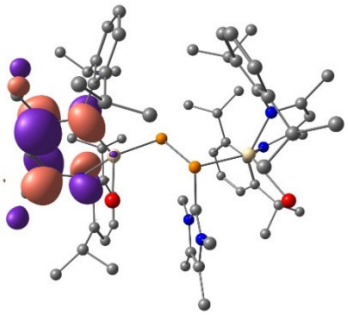
HOMO−1 (-0.1847 au)



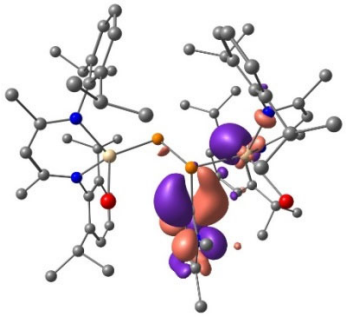
HOMO (-0.1453 au)



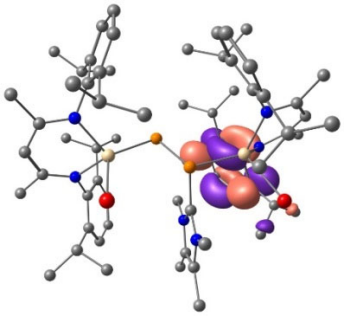
LUMO (-0.0504 au)



LUMO+1 (-0.0372 au)

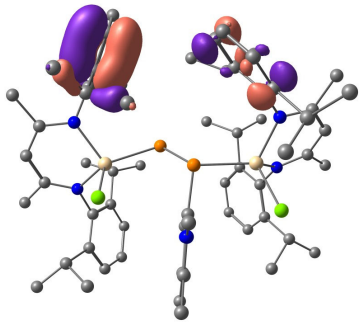


LUMO+2 (-0.020 au)

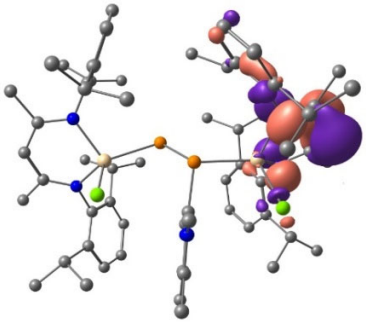


LUMO+3 (-0.0148 au)

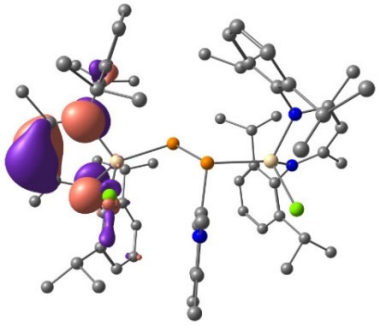
Figure S50. Selected molecular orbitals (from HOMO−3 to LUMO+3) of compound **3b** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.



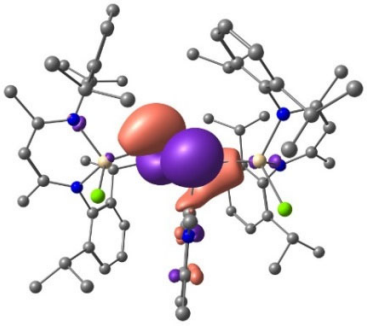
SOMO–3 (-0.3087 au)



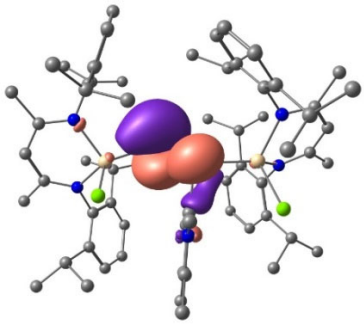
SOMO–2 (-0.2980 au)



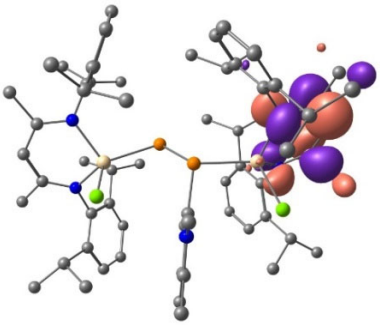
SOMO–1 (-0.2928 au)



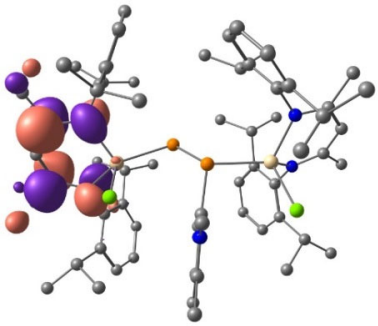
SOMO (α-spin, -0.2818 au)



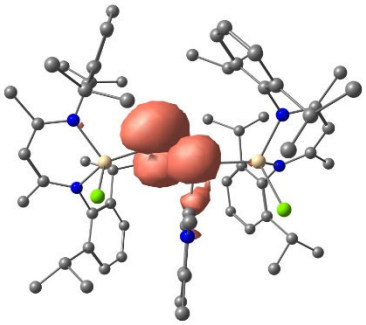
SOMO (β-spin, -0.1969 au)



LUMO (-0.1331 au)

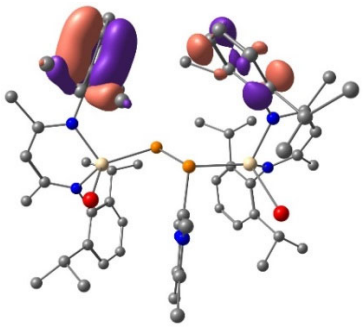


LUMO+1 (-0.1290 au)

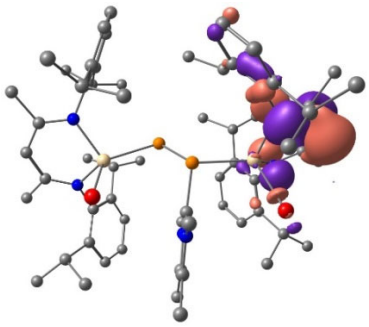


Spin density

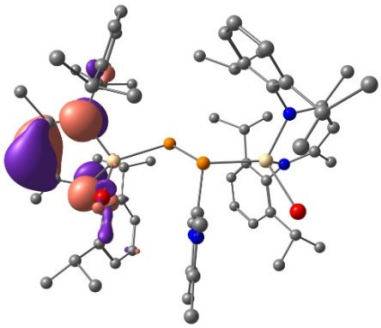
Figure S51. Selected molecular orbitals (from SOMO−3 to LUMO+1) and spin density plot of compound **4a** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.



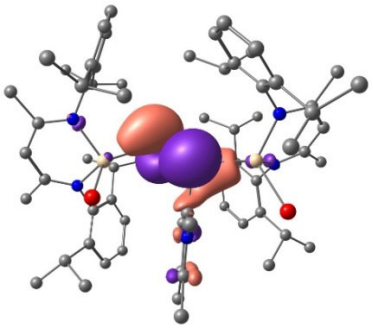
SOMO–3 (-0.3089 au)



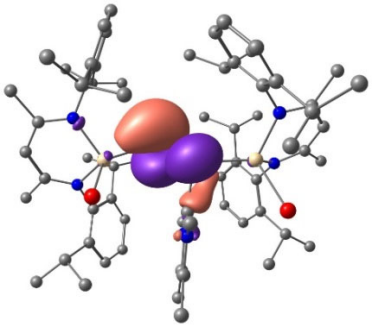
SOMO–2 (-0.2980 au)



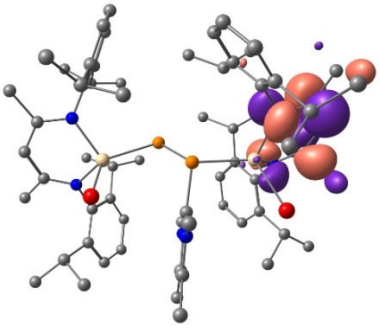
SOMO–1 (-0.2929 au)



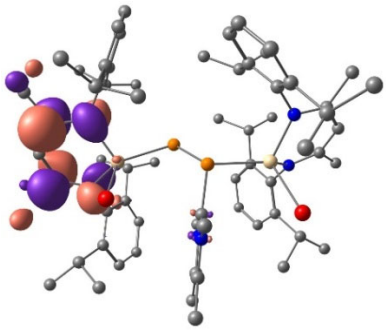
SOMO (α-spin, -0.2837 au)



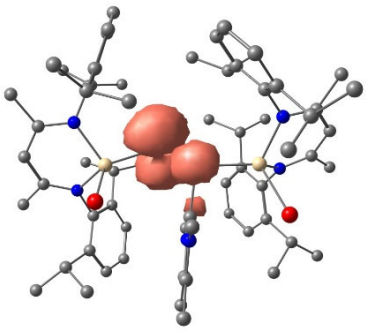
SOMO (β-spin, -0.1987 au)



LUMO (-0.1339 au)



LUMO+1 (-0.1298 au)



spin density

Figure S52. Selected molecular orbitals (from SOMO−3 to LUMO+1) and spin density plot of compound **4b** calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.0432. Hydrogen atoms were omitted for clarity reasons.

6. EPR Spectroscopy

X-band CW EPR spectra were obtained using an X-band Bruker Elexsys E500 EPR spectrometer equipped with a ER4116DM dual mode resonator and an ESR 900 He cryostat. EPR spectra at 290 K were obtained using a microwave frequency of ~9.64 GHz, microwave power of 20 mW, 100 mT field sweep centered at 340 mT, a Lock-In modulation amplitude of 0.1 mT, a time constant of 40.96 ms, a sweep time of 83.89 s with 10 averages and a modulation frequency of 100 KHz. The temperature was stabilized at 80 K for low temperature measurements using a He flow cryostat (Oxford Instruments). The EPR spectra at 80 K were obtained under identical conditions using same parameters with an exception of 120 mT sweep width, 0.3 mT of modulation amplitude and 5 averages.

Q-band pulse EPR measurements were performed using a Bruker Elexsys E580 EPR X-band Spectrometer with homebuilt Q-band extension capable to deliver 34 GHz microwave pulses up to 10W. The experiments were conducted in a homebuilt Q-band Pulse-ENDOR resonator.[21] Electron spin echo (ESE)-detected field-swept spectra were measured at 40 K using the pulse sequence: t_p–τ – 2t_p– τ –echo with typical values t_p=20 ns, τ=240 ns, repetition time 5ms.

W-band pulse EPR measurements were performed using a Bruker ELEXSYS E680 spectrometer equipped with a homebuilt W-band extension and a cryogen free Cryogenic 6 T magnet with a variable temperature insert. ESE-detected field-swept spectra were measured at 32 K using the pulse sequence: t_p–τ –2t_p– τ –echo with typical values tp=20 ns, τ=260 ns, repetition time 5ms. Small hyperfine couplings were detected using the Mims ENDOR sequence t_p–τ –t_p–T_{RF}–t_p– τ –echo. With T_{RF} = 20 µs. ELDOR detected NMR experiments aimed at uncovering large hyperfine couplings were performed at 32 K using the sequence T_{HTA}- t_p–τ –2t_p– τ –echo, with T_{HTA} (variable ELDOR frequency pulse) of 800 ns. However, the phosphorus couplings were larger than the bandwidth of the resonator, and no clear resonance signals could be observed.

All the simulations were obtained using Easyspin[22] 5.2.30 with the function “pepper” and “garlic” for low temperature and room temperature spectra, respectively. Both complexes **4a** and **4b** showed identical X-band CW EPR spectra with a small variation in their line widths and therefore were simulated using identical spin Hamiltonian parameters. The negative signs were introduced to the hyperfine coupling values in spin-Hamiltonian parameters from the complementary computational calculations (Table S8) and to match the isotropic values obtained from liquid solution simulations. The discrepancy in the simulation parameters between RT and 80 K results from fact that the low temperature simulations require a very large number of parameters, which are strongly correlated. Therefore, it may be difficult to obtain a unique solution. Nevertheless, the spin-Hamiltonian parameters obtained from the simulations are in good agreement with the parameters calculated using computational calculations (Table S9).

Table S10. Spin Hamiltonian parameters obtained from the simulation of X-band EPR spectra and calculated from the computational calculations for the radicals **4a** and **4b**.

		4a				**4b**			
		x	*y*	*z*	iso	*x*	*y*	*z*	iso
g-tensor	DFT	1.997	2.004	2.019	2.006	2.000	2.002	2.016	2.006
	Exp (80 K)				2.017				2.017
	Exp (290 K)				2.015				2.015
A(P1) /MHz	DFT	263.1	274.7	426.9	321.6	263.2	275.1	421.3	319.9
	Exp (80 K)	229.9	255.9	352.0	279.3	229.9	255.9	352.0	279.3
	Exp (290 K)				298.7				298.7
A(P2) /MHz	DFT	–126.9	–145.8	594.7	107.4	–129.0	–147.8	598.8	107.3
	Exp (80 K)	-55.3	-114.4	595.0	141.8	-55.3	-114.4	595.0	141.8
	Exp (290 K)				192.7				192.7
A(Ga1) /MHz	DFT	83.2	84.2	97.4	88.3	84.1	84.8	97.5	88.8
	Exp (80 K)	72.2	72.6	104.3	83.1	72.2	72.6	104.3	83.1
	Exp (290 K)				92.6				92.6
A(Ga2) /MHz	DFT	–26.8	–43.0	–46.1	-38.6	–29.7	–45.7	–48.9	-41.4
	Exp (80 K)	-21.2	-95.3	-98.1	-71.5	-21.2	-95.3	-98.1	-71.5
	Exp (290 K)				-59.7				-59.7

Table S11. P1 and P2 Mulliken Spin populations (p-orbitals) of the SOMO of compound **4a**.

P1	pz	0.123207	0.085762
	px	-0.008936	
	py	-0.028509	
P2	pz	**0.327342**	0.767553
	px	0.029450	
	py	**0.410761**	

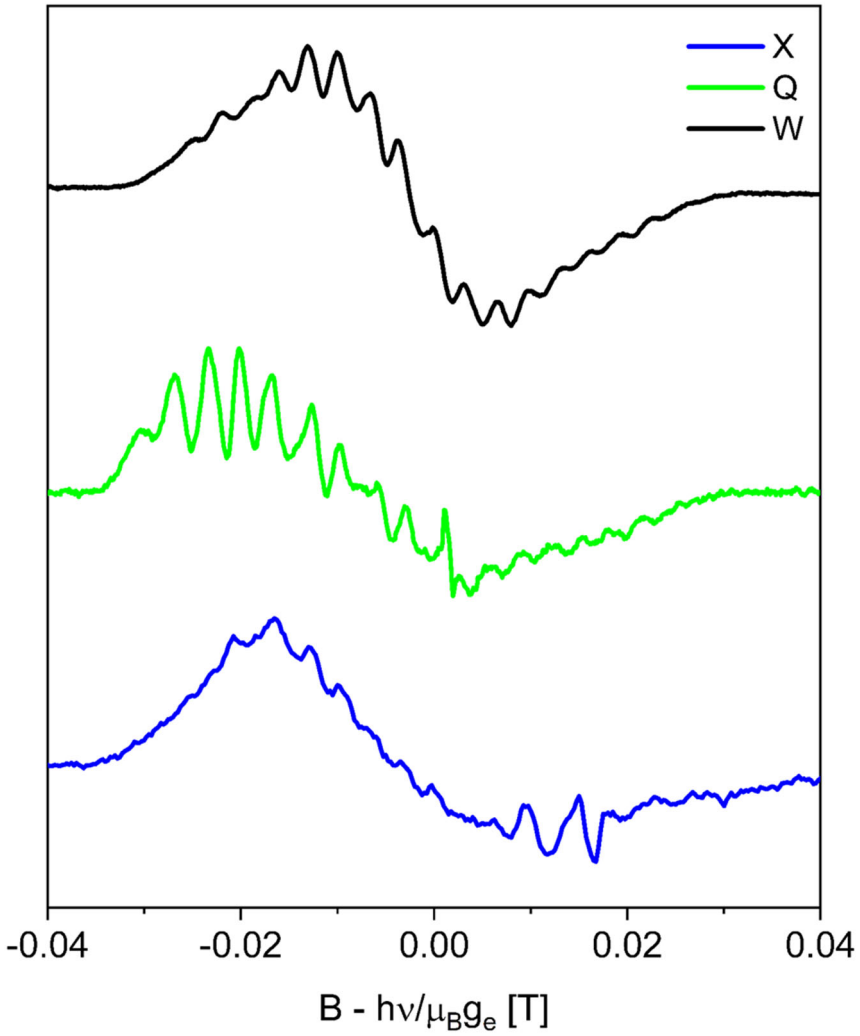


Figure S53. X-band CW (~9.64 GHz, black) EPR, Pseudo modulated Q-band (~34 GHz, green) and Pseudo modulated W-band (~94 GHz, blue) Hahn-Echo detected field sweep spectra of **4a** (1 mM 1:9 mixture of fluorobenzene and toluene) at 80 K, 40 K and 32 K, respectively.

Coordinates of all the optimized geometries:

2a

Cl	-3.635127000	7.823076000	4.184875000
Ga	-2.276410000	8.750283000	5.690977000
N	-3.349031000	10.198185000	6.495120000
C	-3.427384000	11.369828000	5.881452000
C	-2.607843000	11.747786000	4.803085000
H	-2.825186000	12.716003000	4.379407000
C	-1.462074000	11.118657000	4.304114000
C	-4.442660000	12.381861000	6.344145000
H	-4.613163000	12.316870000	7.416298000
H	-5.395635000	12.183137000	5.850001000
H	-4.130576000	13.391108000	6.085278000
H	-0.842238000	11.445955000	2.291314000
C	-4.080600000	9.902177000	7.698249000
C	-5.400554000	9.429132000	7.636893000
C	-6.025734000	9.061722000	8.829307000

H	-7.037680000	8.680162000	8.798200000
C	-5.369326000	9.143641000	10.042184000
H	-5.864151000	8.828474000	10.951542000
C	-4.061560000	9.603803000	10.086271000
H	-3.548608000	9.642474000	11.035497000
C	-3.391897000	9.985046000	8.927355000
C	-6.164419000	9.259615000	6.336636000
H	-5.517454000	9.563896000	5.515342000
C	-7.427871000	10.131374000	6.304595000
H	-8.148834000	9.806354000	7.057673000
H	-7.912230000	10.059305000	5.328380000
H	-7.204037000	11.181041000	6.498750000
C	-6.528472000	7.787406000	6.102797000
H	-5.641132000	7.159121000	6.124542000
H	-7.002959000	7.667088000	5.127075000
H	-7.222172000	7.428406000	6.866105000
H	-2.349915000	12.449117000	9.732585000
H	-2.220485000	12.369414000	7.972647000
H	-1.572922000	8.773958000	2.587995000
H	-1.235615000	8.622673000	0.168616000
H	-1.777118000	6.554455000	1.587786000
P	-2.984380000	6.607697000	7.999526000
N	-3.212266000	3.921453000	10.390811000
C	-3.609104000	1.897261000	11.706760000
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H	-4.663649000	1.974925000	11.451556000
C	-1.673077000	3.596966000	6.228583000
H	-2.336587000	3.916191000	7.035066000
C	-2.301825000	4.080546000	4.922285000
H	-1.746160000	3.731027000	4.049822000
H	-3.315518000	3.689988000	4.835361000
H	-2.365132000	5.167001000	4.880896000
C	-1.630707000	2.062141000	6.259536000
H	-2.619207000	1.654424000	6.037309000
C	-4.589419000	4.304167000	10.531349000
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C	-6.362732000	5.408753000	11.716702000
H	-6.717227000	5.950364000	12.584281000
C	-7.238692000	5.132378000	10.681622000
H	-8.271062000	5.453431000	10.741553000
C	-6.787378000	4.448716000	9.563019000
H	-7.473563000	4.245396000	8.752479000
C	-5.464203000	4.028689000	9.461554000
C	-4.107306000	5.359890000	12.817540000
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H	-3.915584000	3.343676000	8.191373000
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C	-1.195389000	9.925927000	10.216920000
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H	-0.136810000	10.170182000	10.128836000
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H	-0.769551000	12.267206000	8.962988000
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H	0.097997000	4.675867000	4.462147000
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C	1.969095000	5.091648000	9.501607000
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H	3.192293000	3.275231000	9.449367000
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H	-3.863821000	4.942039000	14.932374000
H	-3.223963000	7.123136000	13.721932000

2b

Br	-3.565077000	7.746069000	3.945188000
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C	-2.652423000	11.722164000	4.779637000
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N	-3.101399000	3.989303000	10.448158000
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H	-0.453162000	10.288514000	10.321590000
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C	2.969188000	8.631516000	4.312755000
H	3.986694000	8.274798000	4.213338000
C	2.603960000	9.396983000	5.408593000
H	3.343401000	9.634048000	6.161572000
C	1.300479000	9.862104000	5.561278000
C	-0.280562000	8.398151000	2.364502000
C	0.145980000	8.950483000	0.997902000
H	0.309703000	10.028652000	1.034309000
H	1.073398000	8.487843000	0.653843000
C	-0.477986000	6.879051000	2.296884000
H	0.445484000	6.375407000	2.001004000
H	-0.788212000	6.483820000	3.262147000
C	0.947648000	10.719199000	6.764022000
H	-0.137824000	10.768781000	6.828583000
C	1.454713000	12.157055000	6.584992000
H	1.170896000	12.771040000	7.442438000
H	1.040769000	12.620139000	5.688934000
H	2.543671000	12.176752000	6.500347000
C	1.462242000	10.122487000	8.076106000
H	1.145240000	10.740221000	8.916562000
H	2.552099000	10.076606000	8.101391000
H	1.077826000	9.114053000	8.227949000
Br	-0.542190000	6.215119000	11.269828000
Ga	-1.863405000	5.216004000	9.549985000
N	-0.691112000	3.823762000	8.779308000
C	-0.596309000	2.655253000	9.399204000
C	-1.452879000	2.239314000	10.434439000
H	-1.208818000	1.284393000	10.874187000
C	-2.661995000	2.802353000	10.856611000
C	0.480254000	1.680941000	8.995872000
H	0.782660000	1.817336000	7.960939000
H	1.359807000	1.844478000	9.622162000
H	0.148175000	0.655832000	9.146229000
H	-3.330974000	2.407312000	12.837446000
C	0.094366000	4.148861000	7.616735000
C	1.395720000	4.659524000	7.748993000
C	2.076836000	5.045031000	6.593408000
H	3.073953000	5.455351000	6.681784000
C	1.495079000	4.941048000	5.345495000
H	2.029442000	5.271473000	4.464505000
C	0.208784000	4.436983000	5.229910000
H	-0.242288000	4.371964000	4.252044000
C	-0.516943000	4.038438000	6.348890000
C	2.085682000	4.853059000	9.086120000
H	1.399739000	4.550105000	9.875116000

C	3.356901000	3.999608000	9.199272000
H	4.113590000	4.324926000	8.482228000
H	3.785784000	4.091307000	10.199517000
H	3.157966000	2.944586000	9.008688000
C	2.418083000	6.333286000	9.316885000
H	1.532504000	6.953667000	9.197658000
H	2.800675000	6.482807000	10.328002000
H	3.175752000	6.679644000	8.610725000
H	-1.401887000	1.514380000	5.557625000
H	-1.684211000	1.641312000	7.296448000
H	-2.863355000	5.123791000	12.597736000
H	-3.484334000	5.214527000	14.961269000
H	-2.856777000	7.333007000	13.642494000

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N	4.076922000	25.334970000	13.693610000
N	3.215005000	25.361122000	11.717966000
C	2.044273000	25.341575000	17.612182000
H	1.781278000	24.309503000	17.804667000
C	3.088980000	25.920267000	18.311433000
C	0.215389000	25.360721000	15.891608000
C	-0.808551000	24.696149000	16.820864000
H	-1.647980000	24.313469000	16.237077000
H	-1.200221000	25.391570000	17.564248000
H	-0.371826000	23.852822000	17.359787000
C	0.796551000	24.323607000	14.922190000
H	1.484649000	24.786294000	14.219959000
H	-0.002136000	23.859792000	14.340754000
H	1.325617000	23.537206000	15.466282000
C	8.121702000	25.002116000	12.928904000
C	8.017763000	23.935511000	13.823319000
H	7.903633000	22.931885000	13.433694000
C	8.070978000	24.133465000	15.191312000
H	8.000749000	23.290991000	15.868504000
C	8.056462000	24.708417000	11.439926000
H	8.227339000	25.636978000	10.899079000
C	9.114597000	23.685017000	11.002771000
H	9.130552000	23.605140000	9.913893000
H	8.894767000	22.692363000	11.401603000
H	10.114848000	23.957355000	11.339571000
C	6.660680000	24.214859000	11.044016000
H	6.608777000	24.055253000	9.964963000
H	5.906351000	24.950691000	11.305493000
H	6.423734000	23.271755000	11.542043000
C	3.942955000	24.011991000	13.297913000
C	3.391445000	24.027609000	12.054525000
H	5.423699000	25.101082000	15.261376000
H	3.791840000	25.625187000	15.745575000
H	2.963068000	25.088792000	9.672840000
C	4.356846000	22.882553000	14.165554000
H	4.110495000	21.934859000	13.690479000
H	3.850444000	22.919742000	15.132681000
H	5.432224000	22.901243000	14.353051000
C	3.039270000	22.913631000	11.139316000

H	3.681262000	22.899048000	10.254505000
H	2.003328000	22.986115000	10.801615000
H	3.159096000	21.960143000	11.650314000
H	3.635316000	25.344883000	19.048239000
Cl	0.071932000	26.867381000	12.616495000
Cl	6.177531000	27.511688000	10.194914000
Ga	1.519631000	28.327271000	13.581293000
Ga	6.763719000	28.513487000	12.149567000
P	3.592665000	28.012462000	12.577660000
P	5.181772000	28.884444000	13.749317000
N	0.675454000	30.075219000	13.259737000
N	0.956760000	28.195867000	15.477955000
N	8.412434000	27.428992000	12.582567000
N	7.818969000	30.097071000	11.570105000
C	-0.469663000	30.339212000	13.885216000
C	-0.912413000	29.650084000	15.019372000
H	-1.871066000	29.957719000	15.405980000
C	-0.202879000	28.750464000	15.823579000
C	-1.355040000	31.444345000	13.368805000
H	-1.787228000	31.142677000	12.412692000
H	-0.794269000	32.358538000	13.185845000
H	-2.161813000	31.651587000	14.067192000
C	-0.815038000	28.427581000	17.163183000
H	-1.332542000	27.468716000	17.111480000
H	-1.538288000	29.189187000	17.444029000
H	-0.059414000	28.346872000	17.941383000
C	1.183278000	31.032770000	12.311782000
C	0.823301000	30.955975000	10.957369000
C	1.258972000	31.965992000	10.102069000
H	0.988582000	31.926457000	9.055074000
C	2.038967000	33.012166000	10.565209000
H	2.366108000	33.788187000	9.884484000
C	2.421742000	33.048960000	11.895376000
H	3.057193000	33.849861000	12.245316000
C	2.006536000	32.066721000	12.791163000
C	0.013418000	29.801796000	10.401456000
H	-0.365863000	29.216007000	11.236739000
C	-1.190576000	30.258936000	9.570874000
H	-0.879844000	30.775525000	8.660571000
H	-1.835196000	30.937639000	10.132683000
C	0.923338000	28.880868000	9.578307000
H	1.285967000	29.392928000	8.683904000
H	0.379688000	27.986294000	9.267841000
H	1.790921000	28.576058000	10.161620000
C	2.403405000	32.167371000	14.253106000
H	2.215154000	31.197832000	14.710334000
C	1.538031000	33.199512000	14.990830000
H	0.481483000	32.931409000	14.975396000
H	1.642491000	34.186089000	14.533313000
H	1.845823000	33.277696000	16.035279000
C	3.889728000	32.479730000	14.430301000
H	4.146145000	33.467319000	14.046374000
H	4.505647000	31.739958000	13.920864000
H	4.147457000	32.465375000	15.491072000
C	1.682347000	27.401272000	16.427109000

C	1.325381000	26.061156000	16.655818000
C	3.446088000	27.235889000	18.053034000
C	2.757662000	28.000309000	17.114162000
H	-0.304102000	26.098941000	15.284081000
C	3.140785000	29.450045000	16.863930000
H	3.061677000	29.620352000	15.788507000
C	4.581670000	29.776859000	17.248421000
H	4.736424000	29.735856000	18.329367000
H	4.821511000	30.787756000	16.920281000
H	5.279311000	29.103592000	16.757817000
C	9.570766000	27.686727000	11.988524000
C	9.818410000	28.818109000	11.199165000
H	10.792947000	28.855428000	10.737499000
C	9.044662000	29.975236000	11.075371000
C	10.737762000	26.743373000	12.158176000
H	11.676894000	27.283013000	12.056526000
H	10.706325000	25.977778000	11.381871000
H	10.717227000	26.238404000	13.120691000
C	9.674590000	31.153861000	10.378206000
H	9.043154000	31.489020000	9.554753000
H	10.657534000	30.895309000	9.991889000
H	9.774288000	32.000097000	11.058316000
C	8.283977000	26.298019000	13.451150000
C	8.211308000	25.419900000	15.692661000
H	8.239237000	25.566722000	16.762638000
C	8.310929000	26.519126000	14.844069000
C	8.473636000	27.919881000	15.410966000
H	7.883698000	28.586103000	14.780616000
C	9.933108000	28.394188000	15.359715000
H	10.314005000	28.435973000	14.341477000
H	10.575627000	27.726500000	15.938958000
H	10.017794000	29.396555000	15.784654000
C	7.930490000	28.055606000	16.833285000
H	6.919007000	27.658125000	16.911436000
H	7.901114000	29.106716000	17.119850000
H	8.561259000	27.537236000	17.559406000
C	7.225449000	31.399149000	11.657035000
C	6.388696000	31.867225000	10.632383000
C	5.853916000	33.148802000	10.751075000
H	5.202643000	33.522110000	9.972054000
C	6.138191000	33.948379000	11.845711000
H	5.719544000	34.944964000	11.915286000
C	6.946385000	33.461451000	12.860582000
H	7.146046000	34.079738000	13.726651000
C	7.492631000	32.182447000	12.793425000
C	6.042261000	31.013663000	9.428143000
H	6.652374000	30.113612000	9.463854000
C	6.341591000	31.723304000	8.102099000
H	6.156488000	31.046096000	7.265657000
H	7.380865000	32.053595000	8.046070000
H	5.706388000	32.600821000	7.963572000
C	4.575530000	30.570945000	9.487927000
H	4.362919000	29.855370000	8.691784000
H	3.909101000	31.425411000	9.372800000
H	4.341300000	30.092592000	10.438252000

C	8.339060000	31.668788000	13.945883000
H	8.662164000	30.659159000	13.698139000
C	9.601396000	32.512938000	14.159533000
H	9.350742000	33.536400000	14.446840000
H	10.210337000	32.560501000	13.255236000
H	10.214517000	32.083704000	14.955154000
C	7.511664000	31.581637000	15.233584000
H	6.654544000	30.923070000	15.096428000
H	7.137690000	32.563486000	15.530960000
H	8.119289000	31.193284000	16.053400000
C	3.607212000	26.167219000	12.735541000
C	4.576328000	25.729736000	15.001931000
H	4.909351000	26.765339000	14.945215000
C	2.721492000	25.828642000	10.431122000
H	3.223341000	26.763801000	10.196075000
H	1.646242000	25.990169000	10.475133000
H	4.275679000	27.673038000	18.588932000
C	2.186103000	30.421914000	17.573624000
H	2.160147000	30.215906000	18.646333000
H	1.170276000	30.367209000	17.188752000
H	2.532650000	31.447387000	17.437495000
H	-1.787221000	29.394836000	9.271441000

3b

N	4.049841000	25.318356000	13.640031000
N	3.211443000	25.358014000	11.654563000
C	2.070017000	25.337609000	17.606602000
H	1.808748000	24.306709000	17.807727000
C	3.122960000	25.919410000	18.290031000
C	0.224063000	25.341782000	15.908825000
C	-0.795311000	24.694887000	16.855561000
H	-1.640903000	24.307801000	16.283594000
H	-1.177944000	25.402074000	17.592472000
H	-0.357477000	23.857249000	17.402564000
C	0.796815000	24.286147000	14.954740000
H	1.487281000	24.732680000	14.243924000
H	-0.005402000	23.818160000	14.381716000
H	1.321587000	23.505358000	15.511145000
C	8.144198000	24.988971000	12.994822000
C	8.036085000	23.944618000	13.915081000
H	7.934649000	22.930722000	13.549069000
C	8.069400000	24.176006000	15.277824000
H	7.993237000	23.350423000	15.974981000
C	8.104329000	24.647567000	11.515837000
H	8.250804000	25.563597000	10.947198000
C	9.198451000	23.644190000	11.122177000
H	9.229034000	23.531281000	10.036394000
H	9.002687000	22.658272000	11.549525000
H	10.186270000	23.955641000	11.461013000
C	6.730714000	24.094460000	11.121500000
H	6.692662000	23.911043000	10.045737000
H	5.947347000	24.806069000	11.362518000
H	6.522829000	23.153320000	11.636567000
C	3.922705000	23.998115000	13.232987000

C	3.386555000	24.022748000	11.983038000
H	5.400489000	25.080024000	15.204750000
H	3.762831000	25.578609000	15.696473000
H	3.115919000	25.167921000	9.585661000
C	4.331771000	22.863014000	14.095397000
H	4.083802000	21.918665000	13.614332000
H	3.823400000	22.896337000	15.061596000
H	5.406994000	22.877262000	14.285501000
C	3.047709000	22.918553000	11.051380000
H	3.708591000	22.908613000	10.180410000
H	2.020055000	23.002057000	10.691468000
H	3.150060000	21.959508000	11.555914000
H	3.678692000	25.347952000	19.023030000
Br	-0.060549000	26.791875000	12.509252000
Br	6.171449000	27.396289000	10.038402000
Ga	1.509604000	28.327529000	13.563956000
Ga	6.759555000	28.491170000	12.138410000
P	3.575483000	28.004171000	12.543475000
P	5.165262000	28.860652000	13.725255000
N	0.674081000	30.085224000	13.260601000
N	0.959083000	28.181630000	15.465341000
N	8.409557000	27.415024000	12.592161000
N	7.802862000	30.082638000	11.560287000
C	-0.467998000	30.344562000	13.894519000
C	-0.907835000	29.644122000	15.022894000
H	-1.865364000	29.949073000	15.414519000
C	-0.197097000	28.738902000	15.819582000
C	-1.354179000	31.456399000	13.394573000
H	-1.789544000	31.166277000	12.436268000
H	-0.793710000	32.372726000	13.221190000
H	-2.158702000	31.655160000	14.098097000
C	-0.805183000	28.412230000	17.159989000
H	-1.336719000	27.461421000	17.100640000
H	-1.516380000	29.180974000	17.452273000
H	-0.046903000	28.313004000	17.933404000
C	1.178717000	31.055774000	12.322004000
C	0.808707000	31.002548000	10.968744000
C	1.241783000	32.024055000	10.125909000
H	0.962969000	32.000919000	9.080611000
C	2.027823000	33.060979000	10.598905000
H	2.353036000	33.846213000	9.927680000
C	2.416806000	33.077559000	11.927385000
H	3.054053000	33.873230000	12.286192000
C	2.004428000	32.083329000	12.811253000
C	-0.012195000	29.863767000	10.399234000
H	-0.394182000	29.271147000	11.228012000
C	-1.215825000	30.340499000	9.579484000
H	-0.905715000	30.862087000	8.671730000
H	-1.851028000	31.020269000	10.150897000
C	0.886570000	28.945134000	9.561458000
H	1.248064000	29.464603000	8.670794000
H	0.335686000	28.056828000	9.246358000
H	1.754835000	28.628001000	10.137176000
C	2.406261000	32.169018000	14.272458000
H	2.211302000	31.197757000	14.722637000

C	1.551373000	33.202752000	15.020315000
H	0.492587000	32.943043000	15.006250000
H	1.661961000	34.191844000	14.569594000
H	1.862904000	33.271247000	16.064382000
C	3.895608000	32.468599000	14.446308000
H	4.159208000	33.454937000	14.063967000
H	4.504160000	31.725447000	13.932684000
H	4.156324000	32.450036000	15.506187000
C	1.693746000	27.390357000	16.412219000
C	1.340639000	26.051291000	16.653708000
C	3.474402000	27.234332000	18.021915000
C	2.773390000	27.994216000	17.088781000
H	-0.298013000	26.071610000	15.293305000
C	3.146179000	29.446672000	16.840363000
H	3.054311000	29.622228000	15.767019000
C	4.589010000	29.779275000	17.211412000
H	4.756269000	29.732198000	18.290271000
H	4.820109000	30.793447000	16.887635000
H	5.284075000	29.112605000	16.708418000
C	9.563595000	27.675423000	11.990875000
C	9.799860000	28.799779000	11.186875000
H	10.770769000	28.833849000	10.717050000
C	9.026483000	29.956794000	11.059860000
C	10.740100000	26.745505000	12.166483000
H	11.673560000	27.298255000	12.083275000
H	10.727971000	25.989885000	11.379888000
H	10.713331000	26.229030000	13.122615000
C	9.653019000	31.130980000	10.352729000
H	9.015643000	31.463084000	9.532485000
H	10.632756000	30.869370000	9.960177000
H	9.758691000	31.980151000	11.028403000
C	8.289730000	26.299984000	13.484824000
C	8.200552000	25.474871000	15.747504000
H	8.217952000	25.647882000	16.813619000
C	8.306288000	26.552944000	14.873102000
C	8.468938000	27.964583000	15.411922000
H	7.870211000	28.617489000	14.775958000
C	9.926915000	28.441000000	15.337285000
H	10.296983000	28.468711000	14.314681000
H	10.576571000	27.782553000	15.919196000
H	10.014377000	29.449440000	15.746874000
C	7.943351000	28.123376000	16.838394000
H	6.934134000	27.724788000	16.936965000
H	7.915271000	29.178534000	17.109016000
H	8.585317000	27.618329000	17.564178000
C	7.213269000	31.387526000	11.651677000
C	6.371721000	31.862918000	10.633866000
C	5.844076000	33.146964000	10.757811000
H	5.188547000	33.523390000	9.983830000
C	6.139566000	33.944371000	11.850646000
H	5.726110000	34.942963000	11.924360000
C	6.952605000	33.451835000	12.858495000
H	7.161842000	34.068015000	13.723881000
C	7.491744000	32.170015000	12.786149000
C	6.008820000	31.016521000	9.430517000

H	6.612532000	30.112050000	9.458022000
C	6.302104000	31.725482000	8.103010000
H	6.102888000	31.050545000	7.267901000
H	7.343880000	32.046221000	8.037331000
H	5.673578000	32.608932000	7.971241000
C	4.538992000	30.586534000	9.502913000
H	4.312738000	29.874161000	8.707754000
H	3.878765000	31.446945000	9.395816000
H	4.309415000	30.108886000	10.454901000
C	8.342645000	31.655014000	13.934054000
H	8.657928000	30.642564000	13.688400000
C	9.611042000	32.492847000	14.136301000
H	9.367702000	33.518679000	14.421660000
H	10.214132000	32.534203000	13.227711000
H	10.227550000	32.063338000	14.929210000
C	7.521528000	31.579469000	15.226409000
H	6.663233000	30.920472000	15.098716000
H	7.149318000	32.564028000	15.516851000
H	8.132655000	31.198709000	16.046883000
C	3.590171000	26.156968000	12.682464000
C	4.545348000	25.702129000	14.953554000
H	4.867747000	26.741480000	14.910682000
C	2.730094000	25.823021000	10.362832000
H	3.109818000	26.828001000	10.204802000
H	1.641798000	25.837135000	10.348271000
H	4.308152000	27.675669000	18.547918000
C	2.193422000	30.408216000	17.566535000
H	2.176912000	30.191886000	18.637464000
H	1.174682000	30.352695000	17.189257000
H	2.534750000	31.436337000	17.437407000
H	-1.822186000	29.484494000	9.276132000

4a

N	4.034453000	25.589947000	13.230430000
N	3.310950000	25.927961000	11.225396000
C	2.498624000	25.390436000	17.437983000
H	2.373669000	24.324394000	17.576776000
C	3.527785000	26.045682000	18.091596000
C	0.485947000	25.310499000	15.936266000
C	-0.434130000	24.645685000	16.970197000
H	-1.296001000	24.197331000	16.472903000
H	-0.799381000	25.359579000	17.708175000
H	0.085208000	23.852609000	17.511529000
C	1.024977000	24.260676000	14.958218000
H	1.630219000	24.722011000	14.180630000
H	0.200096000	23.742470000	14.466929000
H	1.625946000	23.513220000	15.481270000
C	8.149712000	24.908326000	13.227224000
C	7.898933000	23.888655000	14.147618000
H	7.841675000	22.866442000	13.796875000
C	7.752639000	24.152949000	15.498211000
H	7.570891000	23.344251000	16.194531000
C	8.356102000	24.538362000	11.767547000
H	8.565250000	25.449235000	11.209381000

C	9.543125000	23.577341000	11.597221000
H	9.757613000	23.429709000	10.537331000
H	9.319457000	22.599283000	12.027402000
H	10.445961000	23.947609000	12.080397000
C	7.097717000	23.916492000	11.152897000
H	7.254991000	23.728216000	10.089414000
H	6.245054000	24.582184000	11.252101000
H	6.859426000	22.962510000	11.628181000
C	3.926636000	24.345822000	12.630665000
C	3.462875000	24.561538000	11.363944000
H	5.595619000	25.913143000	14.593166000
H	4.240193000	24.940798000	15.195604000
H	3.451311000	26.217054000	9.167665000
C	4.278536000	23.085946000	13.330200000
H	4.238762000	22.250545000	12.634850000
H	3.583996000	22.877219000	14.146469000
H	5.285933000	23.134819000	13.744579000
C	3.172297000	23.612352000	10.261630000
H	3.827358000	23.786091000	9.404765000
H	2.139558000	23.702893000	9.918994000
H	3.325317000	22.589405000	10.597475000
H	4.205589000	25.492888000	18.729428000
Cl	0.310508000	26.809858000	12.613974000
Cl	6.262774000	27.242514000	10.355616000
Ga	1.411897000	28.421551000	13.695770000
Ga	6.914986000	28.358542000	12.177115000
P	3.519173000	28.345638000	12.640549000
P	5.239296000	29.052071000	13.678637000
N	0.495884000	30.100311000	13.371416000
N	0.945363000	28.219527000	15.571943000
N	8.462947000	27.320710000	12.810283000
N	7.912892000	29.920481000	11.582442000
C	-0.572490000	30.396689000	14.107765000
C	-0.948257000	29.681138000	15.253832000
H	-1.876139000	29.993040000	15.707185000
C	-0.216955000	28.739195000	15.980453000
C	-1.443137000	31.559555000	13.717772000
H	-2.156286000	31.236245000	12.957057000
H	-0.861680000	32.372970000	13.290715000
H	-2.004180000	31.924685000	14.574233000
C	-0.808253000	28.291714000	17.290414000
H	-1.450879000	27.428375000	17.103463000
H	-1.421250000	29.076403000	17.727221000
H	-0.049236000	27.986569000	18.005182000
C	0.936238000	30.967629000	12.309705000
C	0.349782000	30.888889000	11.038156000
C	0.818705000	31.751662000	10.046326000
H	0.376497000	31.713185000	9.059582000
C	1.836216000	32.652705000	10.301534000
H	2.182658000	33.315717000	9.519041000
C	2.421485000	32.698817000	11.558096000
H	3.232589000	33.387761000	11.737499000
C	1.989573000	31.862107000	12.582906000
C	-0.748996000	29.899366000	10.695615000
H	-1.031052000	29.369229000	11.604548000

C	-2.000894000	30.590723000	10.139660000
H	-1.804589000	31.046598000	9.167728000
H	-2.360554000	31.378569000	10.802321000
C	-0.232956000	28.850318000	9.702673000
H	0.035180000	29.311811000	8.750098000
H	-0.996652000	28.093896000	9.513137000
H	0.646185000	28.349323000	10.100451000
C	2.630844000	31.933450000	13.958943000
H	2.708879000	30.909730000	14.334500000
C	1.774440000	32.723695000	14.959178000
H	0.807599000	32.260364000	15.143794000
H	1.601995000	33.737376000	14.591995000
H	2.291138000	32.798034000	15.917675000
C	4.045431000	32.503723000	13.932067000
H	4.044789000	33.571516000	13.708719000
H	4.669548000	32.004732000	13.194884000
H	4.513974000	32.377464000	14.907291000
C	1.787748000	27.462474000	16.457146000
C	1.611399000	26.077586000	16.607989000
C	3.676878000	27.417592000	17.944593000
C	2.811123000	28.153436000	17.139282000
H	-0.107027000	26.014066000	15.354845000
C	2.917684000	29.668471000	17.075090000
H	2.512726000	29.985000000	16.114767000
C	4.350374000	30.191803000	17.167277000
H	4.787665000	30.014058000	18.151143000
H	4.358890000	31.269884000	17.003027000
H	4.989796000	29.733754000	16.416462000
C	9.669382000	27.579086000	12.311694000
C	9.954716000	28.654186000	11.457770000
H	10.962198000	28.675782000	11.071951000
C	9.178060000	29.778818000	11.178627000
C	10.842813000	26.700778000	12.661801000
H	11.728321000	27.312111000	12.826059000
H	11.057462000	26.033940000	11.825215000
H	10.660999000	26.092031000	13.542151000
C	9.823261000	30.895338000	10.403198000
H	9.290752000	31.042767000	9.461949000
H	10.863552000	30.667991000	10.186993000
H	9.770177000	31.839727000	10.942200000
C	8.242329000	26.225772000	13.712071000
C	7.851846000	25.457488000	15.959460000
H	7.741038000	25.653846000	17.015910000
C	8.092904000	26.513955000	15.084262000
C	8.242817000	27.931669000	15.610616000
H	7.845830000	28.607509000	14.851932000
C	9.721624000	28.296233000	15.806147000
H	10.278663000	28.235331000	14.873240000
H	10.190556000	27.622865000	16.526421000
H	9.814335000	29.315915000	16.184176000
C	7.454179000	28.184717000	16.894902000
H	6.417392000	27.862950000	16.797286000
H	7.456127000	29.249425000	17.126556000
H	7.893067000	27.665899000	17.749167000
C	7.323871000	31.232899000	11.589678000

C	6.525094000	31.662584000	10.519410000
C	6.032397000	32.967133000	10.550461000
H	5.420254000	33.320082000	9.731061000
C	6.328946000	33.822428000	11.598339000
H	5.953543000	34.837866000	11.593984000
C	7.095563000	33.370815000	12.661434000
H	7.303828000	34.037761000	13.487817000
C	7.592952000	32.070979000	12.688582000
C	6.197047000	30.764281000	9.341807000
H	6.769869000	29.844986000	9.448410000
C	6.591295000	31.397443000	8.001645000
H	6.430386000	30.686741000	7.188990000
H	7.641874000	31.692182000	7.990063000
H	5.996886000	32.287020000	7.785037000
C	4.711708000	30.382666000	9.345413000
H	4.502909000	29.671464000	8.543792000
H	4.078974000	31.258865000	9.198296000
H	4.420172000	29.925285000	10.290619000
C	8.412769000	31.606556000	13.882666000
H	8.632903000	30.548507000	13.747063000
C	9.756804000	32.341369000	13.973176000
H	9.611007000	33.415964000	14.098384000
H	10.358496000	32.187794000	13.077409000
H	10.331464000	31.979550000	14.828040000
C	7.630010000	31.746065000	15.193261000
H	6.695188000	31.187952000	15.155270000
H	7.388610000	32.788593000	15.406461000
H	8.222185000	31.367837000	16.028650000
C	3.652653000	26.555011000	12.366348000
C	4.515188000	25.796806000	14.590642000
H	4.054116000	26.682884000	15.011659000
C	2.857371000	26.575317000	10.005168000
H	3.001153000	27.646028000	10.106594000
H	1.802718000	26.359803000	9.845820000
H	4.467612000	27.924303000	18.479138000
C	2.053998000	30.319166000	18.167194000
H	2.377625000	29.990256000	19.156905000
H	0.999796000	30.072608000	18.059178000
H	2.146923000	31.405590000	18.123374000
H	-2.804636000	29.864467000	10.006447000

4b

N	4.013120000	25.555661000	13.182982000
N	3.258340000	25.871841000	11.185080000
C	2.570124000	25.423357000	17.444617000
H	2.461721000	24.357391000	17.596911000
C	3.598002000	26.099457000	18.077785000
C	0.534662000	25.295119000	15.983031000
C	-0.360651000	24.643134000	17.046608000
H	-1.225133000	24.173861000	16.573684000
H	-0.722235000	25.369426000	17.774128000
H	0.176602000	23.868487000	17.597050000
C	1.069198000	24.229249000	15.020227000
H	1.656599000	24.679253000	14.222393000

H	0.242689000	23.691265000	14.553736000
H	1.687378000	23.500624000	15.549727000
C	8.142207000	24.899664000	13.252229000
C	7.887863000	23.893676000	14.186832000
H	7.841989000	22.865667000	13.851797000
C	7.724307000	24.177996000	15.530975000
H	7.539312000	23.379384000	16.237981000
C	8.369499000	24.501232000	11.803452000
H	8.561928000	25.403550000	11.225655000
C	9.577681000	23.561035000	11.664968000
H	9.805156000	23.395496000	10.610441000
H	9.367726000	22.588143000	12.113371000
H	10.468766000	23.957201000	12.148745000
C	7.132214000	23.833263000	11.193589000
H	7.299742000	23.633052000	10.133991000
H	6.258837000	24.474026000	11.277393000
H	6.918970000	22.880390000	11.682717000
C	3.911264000	24.306433000	12.592852000
C	3.428741000	24.508475000	11.330576000
H	5.583233000	25.932617000	14.522554000
H	4.273711000	24.911855000	15.143659000
H	3.346387000	26.133198000	9.120846000
C	4.281773000	23.054118000	13.296777000
H	4.254030000	22.216101000	12.604034000
H	3.590429000	22.838172000	14.113964000
H	5.288457000	23.118561000	13.710336000
C	3.134873000	23.548193000	10.238777000
H	3.777767000	23.723064000	9.372978000
H	2.097063000	23.624970000	9.908457000
H	3.303308000	22.529443000	10.579975000
H	4.292758000	25.563394000	18.711627000
Br	0.108126000	26.711345000	12.560495000
Br	6.279969000	27.178385000	10.155645000
Ga	1.385649000	28.397794000	13.668229000
Ga	6.897531000	28.347275000	12.142613000
P	3.473995000	28.303880000	12.574722000
P	5.189056000	29.023222000	13.618838000
N	0.494275000	30.094498000	13.355485000
N	0.959165000	28.210743000	15.558109000
N	8.440777000	27.311625000	12.801551000
N	7.900507000	29.922818000	11.586940000
C	-0.569007000	30.388817000	14.100037000
C	-0.939824000	29.667037000	15.244710000
H	-1.867314000	29.975709000	15.701089000
C	-0.202481000	28.729666000	15.971189000
C	-1.440275000	31.555355000	13.723069000
H	-2.160521000	31.235579000	12.967600000
H	-0.861147000	32.369329000	13.294041000
H	-1.993130000	31.918027000	14.585853000
C	-0.785869000	28.284755000	17.285351000
H	-1.425012000	27.417578000	17.103642000
H	-1.400690000	29.067777000	17.722490000
H	-0.022250000	27.985570000	17.997748000
C	0.931747000	30.969812000	12.297724000
C	0.337541000	30.907753000	11.028353000

C	0.798376000	31.784442000	10.044932000
H	0.349099000	31.757560000	9.061061000
C	1.815722000	32.683914000	10.304096000
H	2.155097000	33.358152000	9.528144000
C	2.410034000	32.712933000	11.556651000
H	3.221370000	33.400630000	11.739502000
C	1.986901000	31.861856000	12.573328000
C	-0.760525000	29.922277000	10.674009000
H	-1.031403000	29.369509000	11.572638000
C	-2.020952000	30.619253000	10.145156000
H	-1.835276000	31.099773000	9.183054000
H	-2.380032000	31.388537000	10.829394000
C	-0.248392000	28.900400000	9.650778000
H	-0.002690000	29.384222000	8.703333000
H	-1.005069000	28.137655000	9.459293000
H	0.644976000	28.403469000	10.021763000
C	2.640061000	31.918225000	13.944161000
H	2.724505000	30.890205000	14.305770000
C	1.790380000	32.694548000	14.960716000
H	0.825826000	32.227260000	15.147212000
H	1.613237000	33.712228000	14.607123000
H	2.314107000	32.758359000	15.916034000
C	4.052577000	32.493302000	13.910284000
H	4.046737000	33.562233000	13.693096000
H	4.672733000	32.000780000	13.165392000
H	4.529388000	32.364363000	14.880790000
C	1.817505000	27.473711000	16.446422000
C	1.661510000	26.088565000	16.619747000
C	3.721082000	27.472164000	17.917894000
C	2.835875000	28.186236000	17.114452000
H	-0.076526000	25.979406000	15.397703000
C	2.916629000	29.702161000	17.043995000
H	2.492935000	30.010001000	16.089464000
C	4.341954000	30.248012000	17.114911000
H	4.795632000	30.082025000	18.093354000
H	4.331240000	31.325238000	16.946283000
H	4.978207000	29.795529000	16.358033000
C	9.648195000	27.571322000	12.306045000
C	9.933960000	28.644399000	11.449164000
H	10.940777000	28.662416000	11.061359000
C	9.164739000	29.776289000	11.180244000
C	10.824625000	26.700757000	12.664923000
H	11.703762000	27.318499000	12.839237000
H	11.052160000	26.038595000	11.828117000
H	10.639445000	26.088578000	13.542070000
C	9.816688000	30.895170000	10.414132000
H	9.283807000	31.053925000	9.474921000
H	10.855139000	30.662685000	10.194604000
H	9.770605000	31.835136000	10.961499000
C	8.220676000	26.226157000	13.715951000
C	7.812492000	25.490035000	15.972028000
H	7.690062000	25.702595000	17.023914000
C	8.058500000	26.533513000	15.082867000
C	8.203878000	27.958097000	15.591373000
H	7.799676000	28.623969000	14.827474000

C	9.682434000	28.329748000	15.775808000
H	10.235191000	28.264543000	14.840807000
H	10.157149000	27.662813000	16.498235000
H	9.773790000	29.351952000	16.146670000
C	7.421864000	28.221464000	16.877373000
H	6.387452000	27.889966000	16.790352000
H	7.416796000	29.288696000	17.095398000
H	7.870611000	27.716786000	17.735004000
C	7.325996000	31.241962000	11.613942000
C	6.541647000	31.703828000	10.546204000
C	6.068612000	33.015027000	10.597533000
H	5.467841000	33.391502000	9.780223000
C	6.372413000	33.847935000	11.661073000
H	6.012760000	34.868975000	11.672067000
C	7.126637000	33.366291000	12.719608000
H	7.342291000	34.016293000	13.557465000
C	7.603012000	32.058338000	12.727078000
C	6.208485000	30.834330000	9.349466000
H	6.778323000	29.911028000	9.434252000
C	6.603093000	31.493842000	8.022193000
H	6.444770000	30.797736000	7.196564000
H	7.653017000	31.791166000	8.017435000
H	6.006747000	32.385644000	7.820914000
C	4.721629000	30.458903000	9.347229000
H	4.508548000	29.764769000	8.532059000
H	4.093411000	31.341219000	9.218743000
H	4.428036000	29.982613000	10.282395000
C	8.412127000	31.563241000	13.915541000
H	8.607863000	30.502014000	13.768847000
C	9.773112000	32.265285000	14.012654000
H	9.652851000	33.341296000	14.152016000
H	10.369224000	32.109069000	13.113606000
H	10.340540000	31.878415000	14.861364000
C	7.632128000	31.707759000	15.226677000
H	6.691152000	31.160220000	15.186978000
H	7.402416000	32.751995000	15.443687000
H	8.219933000	31.320618000	16.060770000
C	3.609975000	26.510784000	12.317149000
C	4.507849000	25.778020000	14.536165000
H	4.021753000	26.646308000	14.966191000
C	2.774700000	26.504104000	9.968038000
H	2.923177000	27.575889000	10.050992000
H	1.715547000	26.289417000	9.839824000
H	4.507216000	27.997144000	18.441162000
C	2.059057000	30.340689000	18.147990000
H	2.403025000	30.019133000	19.133247000
H	1.007653000	30.076312000	18.056314000
H	2.133286000	31.428387000	18.100990000
H	-2.821287000	29.891326000	10.001067000

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