Electronic Supporting Information for:

Stepwise Isolation of Low-Valent, Low-Coordinate Sn and Pb Mono- and Dications in the Coordination Sphere of Platinum

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EXPERIMENTAL DETAILS

General Considerations. All manipulations were performed under an inert atmosphere of argon using standard Schlenk and glove-box techniques. Solvents were distilled over alkali metals, degassed, in the case of dichloromethane P_2O_5 was used, and stored over molecular sieves (4 Å) under argon. Deuterated solvents were degassed by three freeze-pump-thaw cycles and stored under argon over molecular sieves. NMR experiments were performed on a Bruker Avance 500 (^{1}H: 500.1 MHz; ^{11}B{^{1}H}: 160.5 MHz; ^{13}C{^{1}H}: 125.8 MHz; ^{31}P{^{1}H}: 202.5 MHz, ^{195}Pt{^{1}H}: 107.5 MHz) or Bruker Avance 400 (^{1}H: 400.1 MHz, ^{13}C{^{1}H}: 100.6 MHz, ^{27}Al: 104.2 MHz, ^{31}P{^{1}H}: 162.0 MHz, ^{119}Sn{^{1}H}: 149.2 MHz, ^{195}Pt{^{1}H}: 86.0 MHz) spectrometer. ^{1}H NMR and ^{13}C{^{1}H} NMR spectra were calibrated to TMS. External standards were used for ^{31}P{^{1}H} (85% H_3PO_4) and ^{195}Pt{^{1}H} ($Na_2[PtCl_6]$ in D_2O). Elemental analyses were performed on a Elementar Vario Micro Cube elemental analyzer or a Leco Instrumente CHNS 932 elemental analyzer. $[(Cy_3P)_2Pt]$[S1] and $Na[BAr^{Cl}{}_4]$[S2] were prepared according to published methods. Anhydrous $[n Bu_4N]Br$, $AlBr_3$ and $AlCl_3$ were purchased from commercial sources and used after several sublimations. NaI, $PbCl_2$ and $SnBr_2$ were used after drying in vacuum.

Synthesis of $[(Cy_3P)_2Pt(SnBr_2)]$ (4): $SnBr_2$ (74.0 mg, 260 µmol) was added to a solution of $[(Cy_3P)_2Pt]$ (**1**) (200 mg, 260 µmol) in THF at –30 °C, whereupon the color of the solution changed from yellow to green. The solvent was removed under vacuum and the deep pink residue was rinsed with hexane. Single crystals for X-ray diffraction studies were prepared by crystallization from a THF solution at –30 °C (248 mg, 240 µmol, 91%). ^{1}H NMR (400.1 MHz), CD_2Cl_2): δ = 2.36–2.26 (br m, 6H; Cy), 2.08 (br d, $^3J_{H–H}$ = 12 Hz, 12H; Cy), 1.84 (br d, $^3J_{H–H}$ = 12 Hz, 12H; Cy), 1.72 (br d, $^3J_{H–H}$ = 10 Hz, 12H; Cy), 1.66–1.55 (br m, 12H; Cy), 1.37–1.25 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 36.8 (vt, N = $|^1J_{C–P}+^3J_{C–P}|$ = 26 Hz, C1; Cy), 31.6 (s, C3 and C5; Cy), 28.0 (vt, N = $|^2J_{C–P}+^4J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.7 (s, C4; Cy) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 49.7 ($^1J_{P–Pt}$ = 3421 Hz) ppm. ^{195}Pt{^{1}H} NMR (86.0 MHz, $CDCl_2$): δ = 4903 (d, $^1J_{Pt–P}$ = 3421 Hz) ppm. Elemental analysis (%) calcd for $C_{36}H_{66}Br_2P_2PtSn·C_4H_8O$: C 43.42, H 6.74; found: C 43.55, H 6.53.

Synthesis of $[\{(Cy_3P)_2Pt\}_2SnBr_2]$ (5): $[(Cy_3P)_2Pt]$ (**1**) (200 mg, 264 µmol) and $SnBr_2$ (37.0 mg, 132 µmol, 1 equiv.) were stirred at –40 °C in THF. The solvent was removed after 30 min and the resulting purple solid was dried under vacuum (223 mg, 124 µmol, 94%). Single crystals for X-ray diffraction studies were prepared by crystallization from a THF solution at –30 °C. ^{1}H NMR (400.1 MHz), C_6D_6): δ = 2.52–2.36 (br m, 6H, Cy), 2.32 (br d, $^3J_{H–H}$ = 12 Hz, 12H, Cy), 1.89 (br d, $^3J_{H–H}$ = 13 Hz, 12H, Cy), 1.82 (br d, $^3J_{H–H}$ = 12 Hz, 12H, Cy), 1.78–1.68 (br m, 12H, Cy), 1.52–1.30 (br m, 18H, Cy) ppm. ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6): δ = 37.0 (br m, C1, Cy), 31.6 (s, C3 and C5, Cy), 28.1 (vt, N = $|^2J_{C–P}+^4J_{C–P}|$ = 12 Hz C2 and C6, Cy), 27.1 (s, C4, Cy) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, C_6D_6): δ = 51.6 ($^1J_{H–H}$ = 4251 Hz) ppm. ^{195}Pt{^{1}H} NMR (86.0 MHz, $CDCl_2$): δ = –5239 (d, $^1J_{H–H}$ = 4251 Hz) ppm. Elemental analysis (%) calcd for $C_{72}H_{132}Br_2P_4Pt_2Sn$: C 48.30, H 7.43; found: C 48.27, H 7.28.

Synthesis of [(Cy$_3$P)$_2$Pt(SnBr)][AlBr$_4$] (7a): $AlBr_3$ (5.2 mg, 20 µmol) was added to a dichlormethane solution of [(Cy$_3$P)$_2$Pt(SnBr$_2$] (**4**) (20 mg, 20 µmol), whereupon the color of the solution changed from pink to orange. The solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction studies were prepared by dissolving the precipitate in dichloromethane and following crystallization at –30 °C (21 mg, 16 µmol, 83%). ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 2.24–2.14 (br m, 6H; Cy), 2.06 (br d, $^3J_{H–H}$ = 12 Hz, 12H; Cy), 1.90 (br d, $^3J_{H–H}$ = 11 Hz, 12H; Cy), 1.77 (br d, $^3J_{H–H}$ = 8 Hz, 12H; Cy), 1.63–1.51 (br m, 12H; Cy), 1.42–1.28 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 36.5 (vt, N = $|^1J_{C–P}+^3J_{C–P}|$ = 28 Hz, C1; Cy), 31.8 (s, C3 and C5; Cy), 27.7 (vt, N = $|^2J_{C–P}+^4J_{C–P}|$ = 18 Hz, C2 and C6; Cy), 26.4 (s, C4; Cy) ppm. ^{27}Al NMR (104.2 MHz, CD_2Cl_2): δ = 80.1 (s, $[AlCl_4]^-$) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 49.9 ($^1J_{P–Pt}$ = 3130 Hz) ppm. Elemental analysis (%) calcd for $C_{36}H_{66}AlBr_5P_2PtSn$: C 33.23, H 5.11; found: C 33.73, H 5.37.

Synthesis of [(Cy$_3$P)$_2$Pt(SnBr)][BAr$^{Cl}_4$] (7b): [$NaBAr^{Cl}_4$] (5.2 mg, 20 µmol) was added to a dichlormethane solution of [(Cy$_3$P)$_2$Pt(SnBr$_2$] (**4**) (20 mg, 20 µmol) whereupon the color of the solution changed from pink to orange. The solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction were prepared by crystallization from a dichloromethane solution at –30 °C (21 mg, 16 µmol, 83%). ^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 7.05−7.02 (m, 8H, *o*-C*H*; Ar), 7.01−6.99 (m, 4H, *p*-C*H*; Ar), 2.19−2.09 (br m, 6H; Cy), 2.04 (br d, $^3J_{H–H}$ = 11 Hz, 12H; Cy), 1.92 (br d, $^3J_{H–H}$ = 12 Hz, 12H; Cy), 1.78 (br d, $^3J_{H–H}$ = 12 Hz, 6H; Cy), 1.57–1.47 (br m, 12H; Cy), 1.39–1.25 (br m, 18H; Cy) ppm. ^{11}B{^{1}H} NMR (160.5 MHz, CD_2Cl_2): δ = −7.0 ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 165.1 (q, $^1J_{C–B}$ = 49 Hz, *ipso*-C_{ar}; Ar), 133.5 (m, $^2J_{C–B}$ = 2 Hz, *o*-C_{ar}; Ar), 133.3 (q, $^3J_{C–B}$ = 4 Hz, *m*-C_{ar}; Ar), 123.4 (s, *p*-C_{ar}; Ar), 36.3 (vt, *N* = $|^1J_{C–P}+^3J_{C–P}|$ = 26 Hz, C1; Cy), 31.9 (s, C3 and C5; Cy), 27.7 (m, C2 and C6; Cy), 26.4 (s, C4; Cy) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 49.4 ($^1J_{P–Pt}$ = 3104 Hz) ppm.

Synthesis of [(Cy$_3$P)$_2$Pt(PbCl)][AlCl$_4$] (8a): $AlCl_3$ (4.0 mg, 30 µmol) was added to a dichloromethane solution of [(Cy$_3$P)$_2$Pt(PbCl$_2$)] (**2**) (30 mg, 30 µmol) (1.0 mL), whereupon the color of the solution changed from yellow to orange. The solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction were prepared by dissolving the precipitate in toluene and crystallization at −30 °C for 24 h (29 mg, 26 µmol, 86%). ^{1}H NMR (500.1 MHz, CD_2Cl_2): δ=2.40−2.32 (br m, 6H; Cy), 2.07 (br d, $^3J_{H–H}$=11 Hz, 12H; Cy), 1.92 (br d, $^3J_{H–H}$ = 12 Hz, 12H; Cy), 1.78 (br d, $^3J_{H–H}$ = 12 Hz, 6H; Cy), 1.65–1.53 (br m, 12H; Cy), 1.43–1.30 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 36.5 (vt, N = $|^1J_{C–P}+^3J_{C–P}|$ = 26 Hz, C1; Cy), 32.5 (s, C3 and C5; Cy), 27.8 (vt, N = $|^2J_{C–P}+^4J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.5 (s, C4; Cy) ppm. ^{27}Al NMR (130.3 MHz, CD_2Cl_2): δ = 103.6 (br s, $[AlCl_4]^-$) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 46.6 ($^1J_{P–Pt}$ = 3099 Hz) ppm. Elemental analysis (%) calcd for $C_{36}H_{66}AlCl_5P_2PbPt$: C 37.04; H 5.70; found: C 37.32; H 5.69.

Synthesis of [(Cy$_3$P)$_2$Pt(PbCl)][BAr$^{Cl}_4$] (8b): Na[BAr^{Cl}_4] (57 mg, 92 µmol) was added to a dichloromethane solution of [(Cy$_3$P)$_2$Pt(PbCl$_2$)] (**2**) (95 mg, 92 µmol), whereupon the color of the

solution changed to orange and a white solid precipitated. The solution was filtered and the solvent was removed under vacuum. The deep orange residue was washed with hexane. Single crystals for X-ray diffraction analysis were prepared by dissolving the precipitate in dichloromethane at −30 °C over 24 h (120 mg, 75.0 μmol, 82%). ^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 7.05−7.02 (m, 8H, C2+C6; Ar), 7.01−6.99 (m, 4H, C4; Ar), 2.38−2.28 (br m, 6H; Cy), 2.05 (br d, $^{3}J_{H–H}$ = 11 Hz, 12H; Cy), 1.88 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.77 (br d, $^{3}J_{H–H}$ = 12 Hz, 6H; Cy), 1.63–1.50 (br m, 12H; Cy), 1.40–1.22 (br m, 18H; Cy) ppm. ^{11}B{^{1}H} NMR (160.5 MHz, CD_2Cl_2): δ = −7.0 ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 165.1 (q, $^{1}J_{C–B}$ = 49 Hz, C1; Ar), 133.5 (m, $^{2}J_{C–B}$ = 2 Hz, C2 and C6; Ar), 133.3 (q, $^{3}J_{C–B}$ = 4 Hz, C3 and C5; Ar), 123.4 (s, C4; Ar), 36.6 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 26 Hz, C1; Cy), 32.4 (s, C3 and C5; Cy), 27.9 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.5 (s, C4; Cy) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 46.7 ($^{1}J_{P–Pt}$ = 3115 Hz) ppm. Elemental analysis (%) calcd for $C_{60}H_{78}BCl_9P_2PbPt$: C 45.23; H 4.93; found: C 45.75; H 5.43.

Synthesis of $[(Cy_3P)_2Pt(Sn)][AlBr_4]_2$ (10): $AlBr_3$ (10.4 mg, 40.0 μmol) was added to a dichlormethane solution of $[(Cy_3P)_2Pt(SnBr_2]$ (**4**) (20 mg, 20 μmol) whereupon the color of the solution changed from pink to orange. The solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction were prepared by dissolving the precipitate in dichloromethane and crystallization at –30 °C (24 mg, 15 μmol, 79%). ^{1}H NMR (400.1 MHz), CD_2Cl_2): δ = 2.24–2.17 (br m, 6H; Cy), 2.06 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.93 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.79 (br d, $^{3}J_{H–H}$ = 9 Hz, 12H; Cy), 1.62–1.50 (br m, 12H; Cy), 1.41–1.27 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 36.4 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 26 Hz, C1; Cy), 32.0 (s, C3 and C5; Cy), 27.7 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.3 (s, C4; Cy) ppm. ^{27}Al NMR (104.2 MHz, CD_2Cl_2): δ = 80.8 (s, $[AlCl_4]^-$) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 52.1 ($^{1}J_{P–Pt}$ = 3021 Hz) ppm. ^{195}Pt{^{1}H} NMR (86.0 MHz, $CDCl_2$): δ = –3597 (d, $^{1}J_{Pt–P}$ = 3021 Hz) ppm. Elemental analysis (%) calcd for $C_{36}H_{66}Al_2Br_8P_2PtSn$, $C_6H_{12}O_{1.5}$: C 30.09, H 4.72; found: C 30.11, H 4.71.

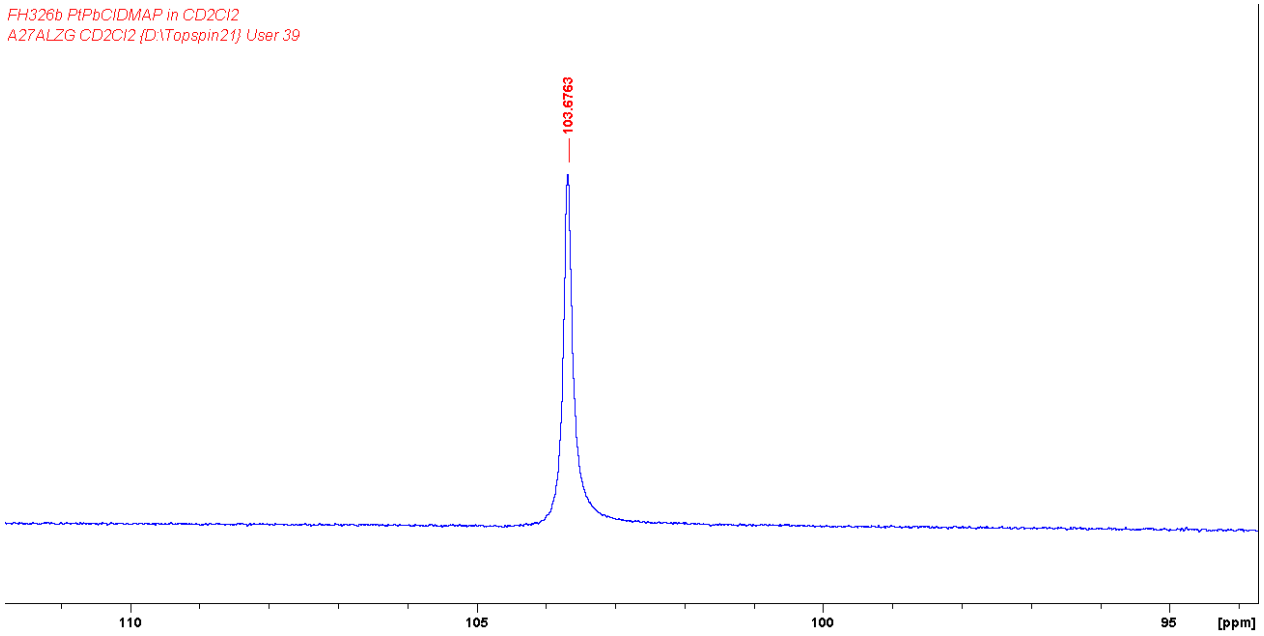
Synthesis of $[(Cy_3P)_2Pt(Pb)][AlCl_4]_2$ (11): $AlCl_3$ (9.0 mg, 68 μmol) was added to a solution of $[(Cy_3P)_2Pt(PbCl_2)]$ (**2**) (35 mg, 34 μmol) in dichloromethane at ambient temperature and kept in a ultrasound bath for 1 h. The solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction were prepared by dissolving the precipitate in dichloromethane and crystallization at room temperature (35 mg, 27 μmol, 80%). ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 2.41−2.29 (br m, 6H; Cy), 2.07 (br d, $^{3}J_{H–H}$ = 11 Hz, 12H; Cy), 1.94 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.80 (br d, $^{3}J_{H–H}$ = 12 Hz, 6H; Cy), 1.67–1.53 (br m, 12H; Cy), 1.45–1.28 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 36.2 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 26 Hz, C1; Cy), 32.6 (s, C3 and C5; Cy), 27.5 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.2 (s, C4; Cy) ppm. ^{27}Al{^{1}H} NMR (130.3 MHz, CD_2Cl_2): δ = 103.6 (br s, $[AlCl_4]^-$) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 47.5 ($^{1}J_{P–Pt}$ = 2950 Hz) ppm. Elemental analysis (%) calcd for $C_{36}H_{66}Al_2Cl_8P_2PbPt$: C 33.24; H 5.11; found: C 32.42; H 5.13.

Synthesis of $[(Cy_3P)_2Pt(SnBr_3)][N\mathit{n}Bu_4]$ (16): $Br[N(\mathit{n}Bu)_4]$ (7.00 mg, 20.0 μmol) was added to a thf solution of $[(Cy_3P)_2Pt(SnBr_2]$ (**4**) (20 mg, 20 μmol), whereupon the color of the solution

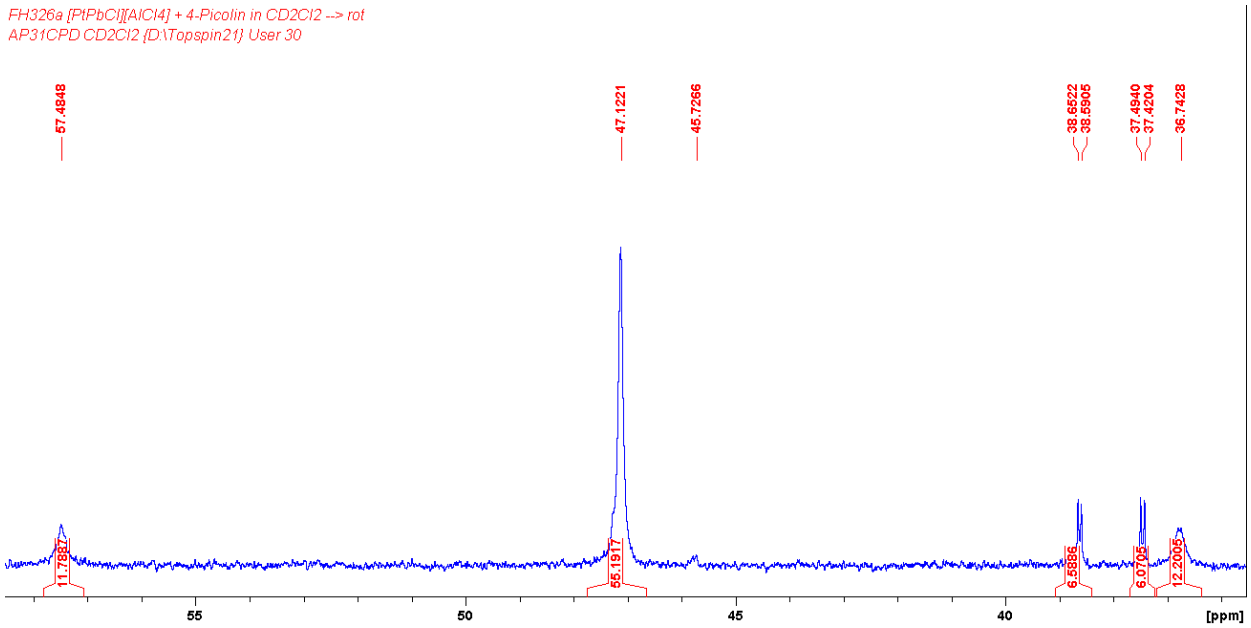
changed from pink to red. The solvent was removed under vacuum and the deep red residue was rinsed with hexane. Single crystals suitable for X-ray diffraction studies were prepared by crystallization from a THF solution at –30 °C (21 mg, 15 µmol, 80%). ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 3.45–3.39 (m, 8H; *n*Bu_4), 2.22–2.12 (br m, 6H; Cy), 2.06 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.78–1.68 (br m, 12H; Cy; 8H; *n*Bu_4), 1.59 (br d, $^{3}J_{H–H}$ = 12 Hz, 18H; Cy), 1.45 (q, $^{3}J_{H–H}$ = 7 Hz, *n*Bu_4), 1.37–1.26 (br m, 18H; Cy) ppm, 0.98 (t, $^{3}J_{H–H}$ = 14 Hz, 12H, *n*Bu_4). ^{13}C{^{1}H} NMR (100.6 MHz, CD_2Cl_2): δ = 59.3 (s, N-*C*H_2; *n*Bu_4) 38.3 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 24 Hz, C1; Cy), 31.9 (s, C3 and C5; Cy), 28.3 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 11 Hz, C2 and C6; Cy), 27.3 (s, C4; Cy), 24.9 (s, -*C*H_2-; *n*Bu_4), 20.5 (s, -*C*H_2-Me; *n*Bu_4), 14.0 (s, *Me*; *n*Bu_4) ppm. ^{31}P{^{1}H} NMR (162.0 MHz, CD_2Cl_2): δ = 56.5 ($^{1}J_{P–Pt}$ = 4634 Hz) ppm. ^{195}Pt{^{1}H} NMR (86.0 MHz, $CDCl_2$): δ = –5226 (d, $^{1}J_{Pt–P}$ = 4634 Hz) ppm. Elemental analysis (%) calcd for $C_{52}H_{102}Al_2Br_3NP_2PtSn$: C 46.03; H 7.58; N 0.98; found: C 46.92, H 7.85, N 1.39.

Synthesis of [$(Cy_3P)_2$Pt(PbCl)(4-Me-C_5H_4N)][$AlCl_4$] (17): 4-picoline was added to a solution of [$(Cy_3P)_2$Pt(PbCl)][$AlCl_4$] (**8a**) (20 mg, 10 µmol) in dichloromethane at ambient temperature, whereupon the color of the solution changed to red. Single crystals suitable for X-ray diffraction or an elemental analysis could not be prepared. ^{1}H NMR (500.1 MHz, CD_2Cl_2): δ = 8.49 (br s, 2H; Ar) 7.27 (br d, $^{3}J_{H–H}$ = 4 Hz, 2H; Ar), 2.37−2.28 (br m, 6H; Cy), 2.35 (br s, 3H, Me), 2.08 (br d, $^{3}J_{H–H}$ = 11 Hz, 12H; Cy), 1.84 (br d, $^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.77 (br d, $^{3}J_{H–H}$ = 12 Hz, 6H; Cy), 1.65–1.55 (br m, 12H; Cy), 1.37–1.26 (br m, 18H; Cy) ppm. ^{13}C{^{1}H} NMR (125.8 MHz, CD_2Cl_2): δ = 151.4 (s, *C*H; Ar), 148.4 (s, C_q; Ar), 125.9 (s, *C*H; Ar), 36.8 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 26 Hz, C1; Cy), 32.1 (s, C3 and C5; Cy), 28.0 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.7 (s, C4; Cy), 21.2 (s, Me) ppm. ^{27}Al{^{1}H} NMR (130.3 MHz, CD_2Cl_2): δ = 103.7 (br s, $[AlCl_4]^-$) ppm. ^{31}P{^{1}H} NMR (202.5 MHz, CD_2Cl_2): δ = 47.1 ($^{1}J_{P–Pt}$ = 3350 Hz) ppm.

^{27}Al{^{1}H} NMR:

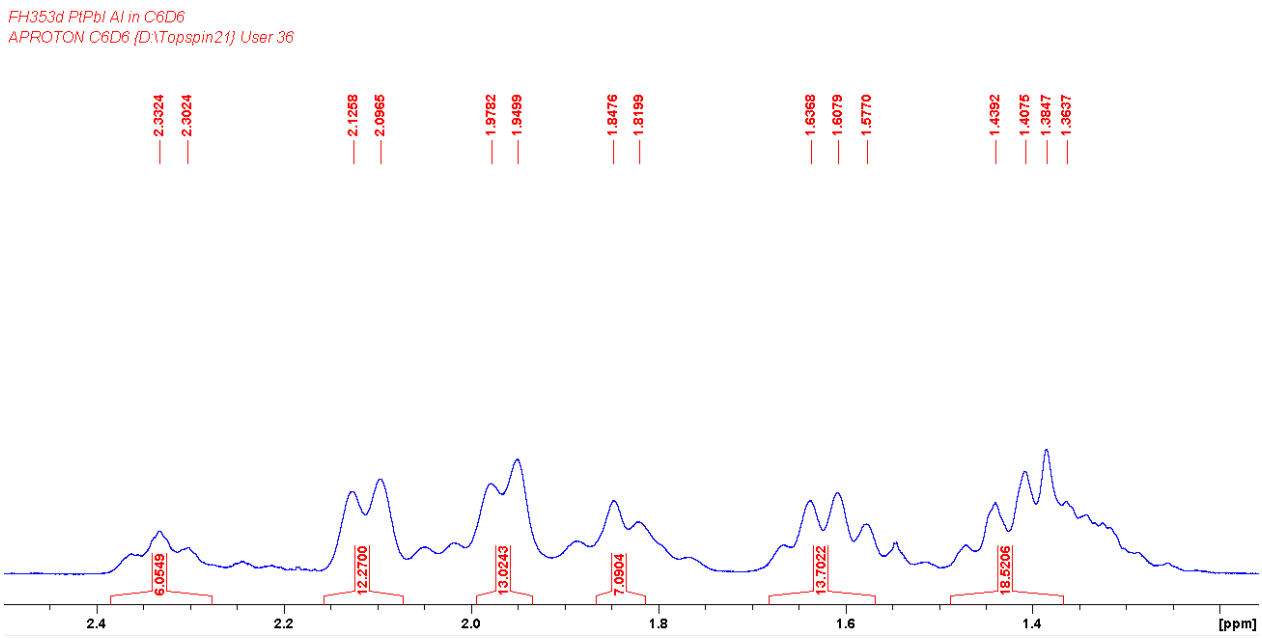


$^{31}P\{^{1}H\}$ NMR:

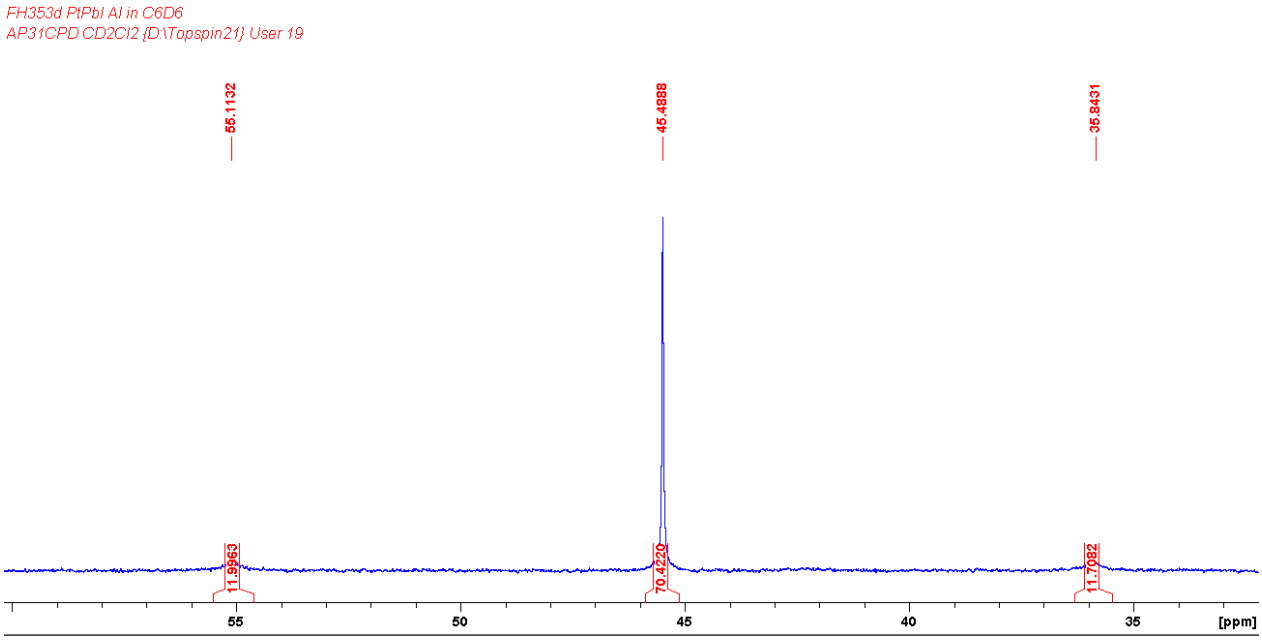


Synthesis of $[(Cy_3P)_2Pt(PbI)][AlCl_4]$ (18): NaI (2.00 mg, 15.0 µmol) was added to a solution of $[(Cy_3P)_2Pt(PbCl)][AlCl_4]$ (**8a**) (15 mg, 15 µmol) in dichloromethane, whereupon the color of the solution changed to red. The white precipitate was filtered off, the solvent was removed under vacuum and the deep orange residue was rinsed with hexane. Single crystals for X-ray diffraction were prepared by dissolving the precipitate in toluene and crystallization at RT over 24 h (10 mg, 12 µmol, 81%). ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 2.38−2.27 (br m, 6H; Cy), 2.11 (br d, $^{3}J_{H-H}$ = 11 Hz, 12H; Cy), 1.96 (br d, $^{3}J_{H-H}$ = 12 Hz, 12H; Cy), 1.84 (br d, $^{3}J_{H-H}$ = 12 Hz, 6H; Cy), 1.68–1.57 (br m, 12H; Cy), 1.48–1.37 (br m, 18H; Cy) ppm. $^{13}C\{^{1}H\}$ NMR (100.6 MHz, CD_2Cl_2): δ = 36.3 (vt, N = $|^{1}J_{C-P}+^{3}J_{C-P}|$ = 26 Hz, C1; Cy), 32.5 (s, C3 and C5; Cy), 27.6 (vt, N = $|^{2}J_{C-P}+^{4}J_{C-P}|$ = 12 Hz, C2 and C6; Cy), 26.3 ppm (s, C4; Cy) ppm. ^{27}Al NMR (130.3 MHz, CD_2Cl_2): δ = 103.4 (br s, $[AlCl_4]^-$) ppm. $^{31}P\{^{1}H\}$ NMR (162.0 MHz, CD_2Cl_2): δ = 45.5 ($^{1}J_{P-Pt}$ = 3130 Hz) ppm.

^{1}H NMR:



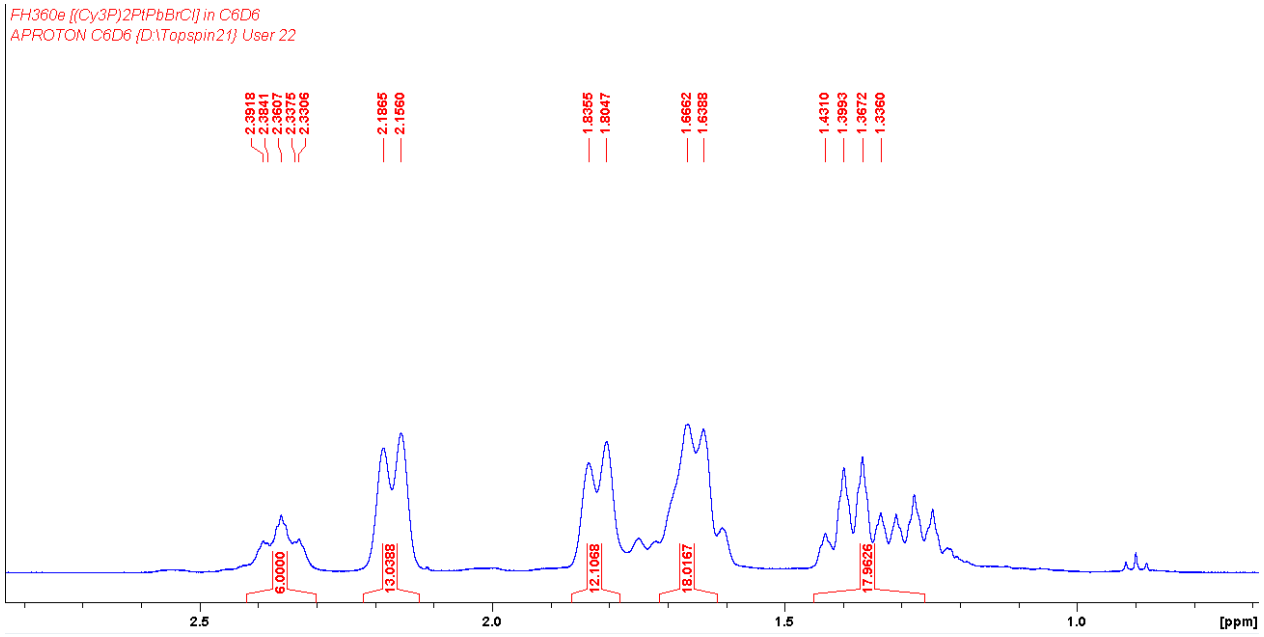
$^{31}P\{^{1}H\}$ NMR:



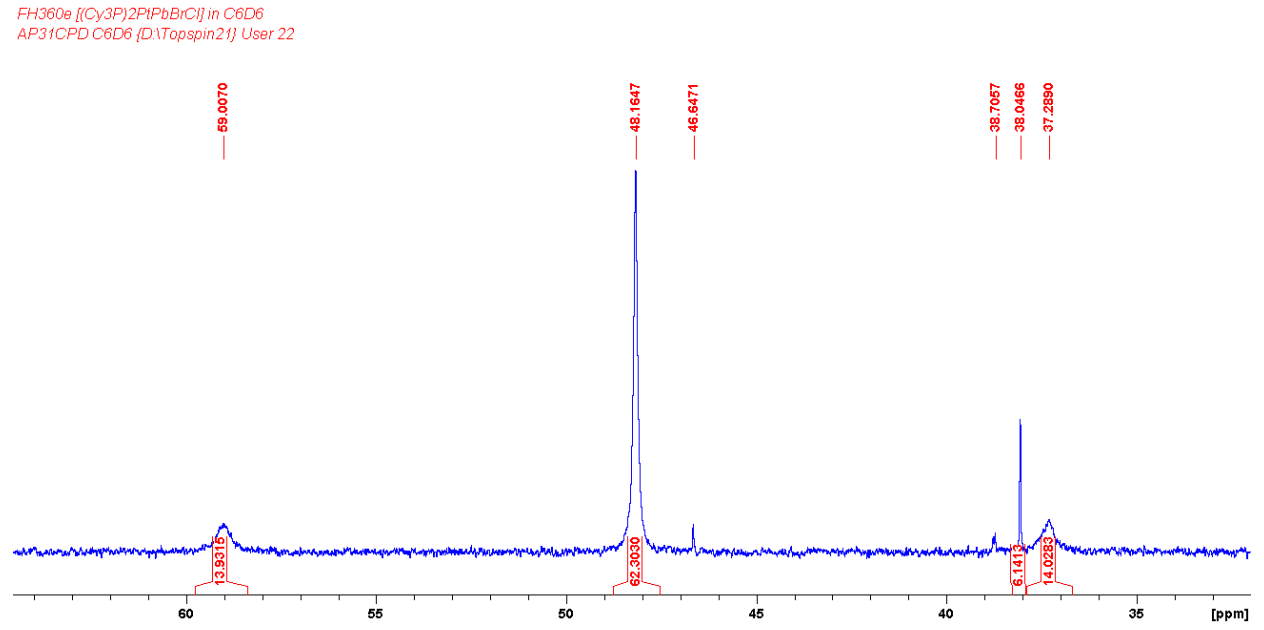
Synthesis of $[(Cy_3P)_2Pt(PbClBr)]$ (19): $[n Bu_4N]Br$ (1 mg, 6 µmol) was added to a solution of $[(Cy_3P)_2Pt(PbCl)][BAr^{Cl}{}_4]$ (**8b**) (10.0 mg, 6.00 µmol) in THF (1.0 mL). After 1 h in an ultrasound bath the color of the solution changed to red and a white solid precipitated. The solution was filtered and the solvent was removed under vacuum. The deep red residue was rinsed with hexane (5 mg, 4 µmol, 76%). Single crystals for X-ray diffraction could not be prepared. ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 2.42−2.30 (br m, 6H; Cy), 2.17 (br d, $^{3}J_{H-H}$ = 11 Hz, 12H; Cy), 1.82 (br d,

$^{3}J_{H–H}$ = 12 Hz, 12H; Cy), 1.71–1.61 (br m, 18H; Cy), 1.45–1.26 (br m, 18H; Cy) ppm. $^{13}C\{^{1}H\}$ NMR (125.8 MHz, CD_2Cl_2): δ = 36.9 (vt, N = $|^{1}J_{C–P}+^{3}J_{C–P}|$ = 26 Hz, C1; Cy), 32.2 (s, C3 and C5; Cy), 27.9 (vt, N = $|^{2}J_{C–P}+^{4}J_{C–P}|$ = 12 Hz, C2 and C6; Cy), 26.7 (s, C4; Cy) ppm. $^{31}P\{^{1}H\}$ NMR (162.0 MHz, CD_2Cl_2): δ = 48.2 ($^{1}J_{P–Pt}$ = 3520 Hz) ppm. $^{195}Pt\{^{1}H\}$ NMR (107.7 MHz, C_6D_6): δ = −3980 ($^{1}J_{Pt–P}$ = 3550 Hz) ppm.

^{1}H NMR:



$^{31}P\{^{1}H\}$ NMR:



CRYSTALLOGRAPHIC DETAILS

Crystal structure determination. The crystal data of **8a**, **8b**, and **11** were collected on a Bruker X8-Apex II diffractometer with a CCD area detector and multi-layer mirror-monochromated $Mo_{K\alpha}$ radiation. The crystal data of **4**, **7a**, **7b**, **10**, **16** and **18** were collected on a Bruker D8-Quest diffractometer with a CCD area detector and multi-layer mirror-monochromated $Mo_{K\alpha}$ radiation. The structures were solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques.[S3] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factor calculations.

Crystal data for **4**: $C_{46\cdot50}H_{78}Br_2P_2PtSn$, M_r = 1172.63, green plate, 0.25×0.19×0.144 mm^3, triclinic space group *P*-1, *a* = 9.682(3) Å, *b* = 10.920(3) Å, *c* = 22.552(8) Å, α = 96.679(13)°, β = 90.154(15)°, γ = 96.092(12)°, *V* = 2354.7(12) Å^3, *Z* = 2, ρ_{calcd} = 1.654 g·cm^{-3}, μ = 5.293 mm^{-1}, *F*(000) = 1170, *T* = 100(2) K, R_1 = 0.0379, wR^2 = 0.0763, 9965 independent reflections [2θ≤53.68°] and 517 parameters.

Crystal data for **5**: $C_{72}H_{132}Br_2P_4Pt_2Sn$, M_r = 1790.35, red block, 0.19×0.17×0.12 mm^3, Triclinic space group *P*-1, *a* = 13.9687(7) Å, *b* = 14.2448(7) Å, *c* = 21.1628(15) Å, α = 96.439(2)°, β = 101.900(2)°, γ = 114.878(2)°, *V* = 3643.1(4) Å^3, *Z* = 2, ρ_{calcd} = 1.632 g·cm^{-3}, μ = 5.394 mm^{-1}, *F*(000) = 1800, *T* = 100(2) K, R_1 = 0.0612, wR^2 = 0.0719, 14914 independent reflections [2θ≤52.74°] and 888 parameters.

Crystal data for **7a**: $C_{36}H_{66}AlBr_5P_2PtSn$, M_r = 1301.13, yellow block, 0.240×0.230×0.180 mm^3, triclinic space group P-1, a = 11.5394(6) Å, b = 12.4690(7) Å, c = 17.7000(10) Å, α = 105.191(2)°, β = 100.053(2)°, γ = 107.994(2)°, V = 2245.2(2) Å^3, Z = 2, ρ_{calcd} = 1.925 g·cm^{-3}, μ = 8.232 mm^{-1}, F(000) = 1256, T = 100(2) K, R_1 = 0.0359, wR^2 = 0.0824, 9176 independent reflections [2θ≤52.744°] and 415 parameters.

Crystal data for **7b**: $C_{60}H_{78}BBrCl_8P_2PtSn$, M_r = 1549.26, orange block, 0.10×0.095×0.085 mm^3, triclinic space group *P*-1, *a* = 13.5049(8) Å, *b* = 15.4437(9) Å, *c* = 15.6528(8) Å, α = 82.203(2)°, β = 78.913(2)°, γ = 85.651(2)°, *V* = 3169.9(3) Å^3, *Z* = 2, ρ_{calcd} = 1.623 g·cm^{-3}, μ = 3.653 mm^{-1}, *F*(000) = 1544, *T* = 100(2) K, R_1 = 0.0477, wR^2 = 0.0876, 12214 independent reflections [2θ≤52.742°] and 667 parameters.

Crystal data for **8a**: $C_{36}H_{66}AlCl_5P_2PbPt$, M_r = 1167.34, orange block, 0.15×0.15×0.10 mm^3, orthorhombic space group *Pca*2$_1$, *a* = 25.2527(4) Å, *b* = 13.9068(2) Å, *c* = 24.7327(5) Å, *V* = 8685.7(3) Å^3, *Z* = 8, ρ_{calcd} = 1.785 g·cm^{-3}, μ = 7.515 mm^{-1}, *F*(000) = 4560, *T* = 100(2) K, R_1 = 0.0444, wR^2 = 0.0821, 13230 independent reflections [2θ≤52.74°] and 866 parameters.

Crystal data for **8b**: $C_{120}H_{156}B_2Cl_{18}P_4Pb_2Pt_2$, M_r = 3186.61, orange block, 0.250×0.120×0.060 mm^3, triclinic space group *P*-1, *a* = 10.5092(6) Å, *b* = 15.3892(10) Å, *c* = 20.0776(12) Å, α = 109.785(2)°, β = 90.439(2)°, γ = 90.796(2)°, *V* = 3054.9(3) Å^3, *Z* = 1,

ρ_{calcd} = 1.732 g·cm^{-3}, μ = 5.523 mm^{-1}, F(000) = 1572, T = 100(2) K, R_1 = 0.0275, wR^2 = 0.0454, 12492 independent reflections [2θ≤52.74°] and 677 parameters.

Crystal data for **10**: $C_{36}H_{66}Al_2Br_8P_2PtSn$, M_r = 1567.84, orange block, 0.390×0.250×0.200 mm^3, monoclinic space group $P2_1/n$, a = 13.2989(18) Å, b = 22.907(3) Å, c = 16.964(4) Å, β = 99.008(7)°, V = 5104.0(14) Å^3, Z = 4, ρ_{calcd} = 2.040 g·cm^{-3}, μ = 9.611 mm^{-1}, F(000) = 2984, T = 100(2) K, R_1 = 0.0367, wR^2 = 0.0693, 10437 independent reflections [2θ≤52.742°] and 649 parameters.

Crystal data for **11**: $C_{36}H_{66}Al_2Cl_8P_2PbPt$, M_r = 1300.67, orange block, 0.139×0.134×0.09 mm^3, monoclinic space group $C2/c$, a = 20.719(2) Å, b = 10.6901(9) Å, c = 23.859(2) Å, β = 111.311(4)°, V = 4923.2(8) Å^3, Z = 4, ρ_{calcd} = 1.755 g·cm^{-3}, μ = 6.813 mm^{-1}, F(000) = 2536, T = 100(2) K, R_1 = 0.0265, wR^2 = 0.0431, 5044 independent reflections [2θ≤52.74°] and 227 parameters.

Crystal data for **16**: $C_{56}H_{110}Br_3NOP_2PtSn$, M_r = 1428.89, orange block, 0.20×0.13×0.09 mm^3, triclinic space group P-1, a = 15.687(3) Å, b = 20.715(4) Å, c = 21.567(3) Å, α = 75.297(9)°, β = 82.231(8)°, γ = 78.538(11)°, V = 6617(2) Å^3, Z = 4, ρ_{calcd} = 1.434 g·cm^{-3}, μ = 4.383 mm^{-1}, F(000) = 2896, T = 100(2) K, R_1 = 0.0307, wR^2 = 0.0568, 27011 independent reflections [2θ≤52.744°] and 1179 parameters.

Crystal data for **18**: $C_{36}H_{66}AlCl_4IP_2PbPt$, M_r = 1258.79, orange block, 0.120×0.089×0.089 mm^3, triclinic space group P-1, a = 13.381(4) Å, b = 13.612(4) Å, c = 13.987(3) Å, α = 92.698(10)°, β = 111.864(13)°, γ = 101.984(10)°, V = 2290.9(10) Å^3, Z = 2, ρ_{calcd} = 1.825 g·cm^{-3}, μ = 7.739 mm^{-1}, F(000) = 1212, T = 100(2) K, R_1 = 0.0575, wR^2 = 0.1442, 9338 independent reflections [2θ≤52.74°] and 461 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication nos. CCDC 1023363 (**4**), CCDC 1023364 (**5**), CCDC 1023365 (**7a**), CCDC 1023366 (**7b**), CCDC 1002025 (**8a**), CCDC 1002026 (**8b**), CCDC 1023367 (**10**), CCDC 1002028 (**11**), CCDC 1023368 (**16**) and CCDC 1002027 (**18**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

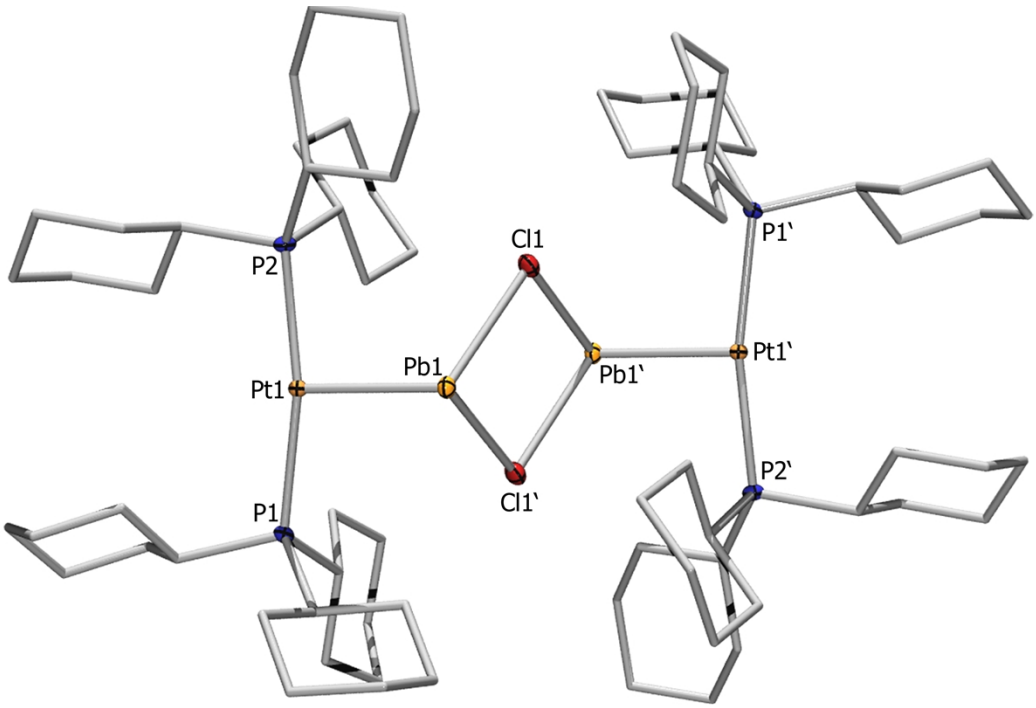


Figure S1. Molecular structure of **8b** and its symmetrical equivalent. Ellipsoids are drawn at the 50% probability level. Hydrogen atoms, counterions (2 $[BAr^{Cl}{}_4]$) and ellipsoids of the cyclohexyl rings are omitted for clarity. Selected bond lengths [Å] and angles [°]: Pt1–Pb1 2.608(2), Pb1–Cl1 2.804(1), Pb1–Cl1’ 2.714(1); P2–Pt1–P1 163.99(3), Cl1–Pb1–Cl1’ 75.85(3), P1–Pt1–Pb1–I1 -37.09(2), P1–Pt1–Pb1–Cl1’ -116.21(2).

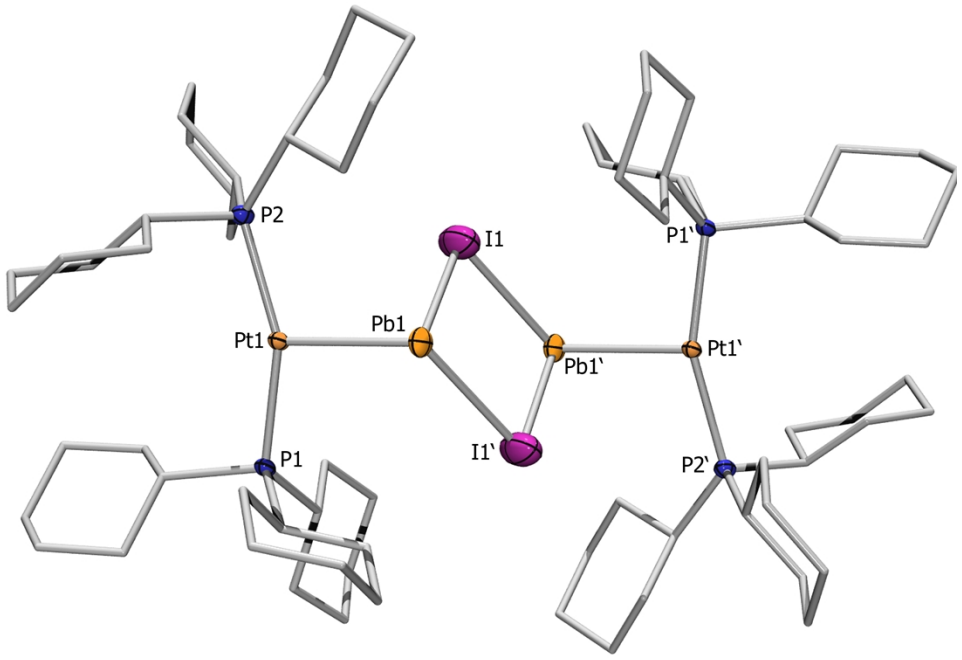


Figure S2. Molecular structure of **18** and its symmetrical equivalent. Ellipsoids are drawn at the 50% probability level. Hydrogen atoms, counterions ($[AlCl_4]^-$) and ellipsoids of the cyclohexyl rings are omitted for clarity. Selected bond lengths [Å] and angles [°]: Pt1–Pb1 2.619(1), Pb1–I1 2.917(2), Pb1–I1' 3.092(2), P2–Pt1–P1 157.96(8), I1–Pb1–I1' 83.11(3), P1–Pt1–Pb1–I1 –58.15(6), P1–Pt1–Pb1–I1' –141.36(6)).

Single crystals of complex **18** for X-ray determination were grown from toluene at room temperature. Because of the small size of the crystal, the collected data are of moderate quality. The data is good enough to provide evidence of connectivity; however bond distances and angles should be discussed with care.

References

S1 T. Yoshida, S. Otsuka and T. Matsuda, In *Inorg. Synth.*; Angelici, R. J., Ed.; John Wiley & Sons: 1990; Vol. **28**, p 113.

S2 R. Anulewiczostrowska, T. Klis, D. Krajewski, B. Lewandowski and J. Serwatowski, *Tetrahedron Lett.,* 2003, **44**, 7329.

S3 G. M. Sheldrick, *Acta Crystallogr., A* 2008, **64**, 112.

DFT Calculations

Table S1. Cartesian coordinates (Å) and energies (a.u) of **2**, **8a**, **11** and all corresponding fragments calculated at RI-D3(BJ)-BP86/def2-TZVP+def2-QZVP.

2

E=-6657.294713365

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C	4.15433652055599	-0.45250571453595	-2.49400497298423
H	4.38616283757219	0.62420572600693	-2.45466493685891
H	4.85623652881413	-0.95542390515146	-1.81147145469665
C	4.33683555337577	-0.96340478953670	-3.92694785449424
H	5.36400625002630	-0.77119603068559	-4.27116824204314
H	4.19839005180500	-2.05952537327214	-3.94451441406694
C	3.33202633708688	-0.30765532605972	-4.87979728624075
H	3.44247044894133	-0.71434893789326	-5.89655624873024
H	3.53989292840597	0.77193751225613	-4.94036188686361
C	1.88840856344724	-0.50856236817185	-4.39809142751892
H	1.64638819943236	-1.58450202976959	-4.42890915805291
H	1.18890218751625	-0.00112355625112	-5.08018154101823
C	-1.09209385356637	0.94518414440378	-3.33068565874332
H	-1.18618319285306	0.44349312593061	-4.30789538699900
C	-0.45820498636799	2.32119070054874	-3.55583002619035
H	-0.13578363605794	2.74727033083185	-2.58442967709062
H	0.46777798060230	2.23952331732247	-4.13910067212924
C	-1.40869353299148	3.32996656350613	-4.19993413891532
H	-0.90502129969470	4.30552880948430	-4.25069396632659
H	-1.61451162783781	3.02008056223782	-5.23912664337926
C	-2.72385542082739	3.42929796575353	-3.42720240680946
H	-2.52624633325409	3.81023765355867	-2.40896611051592
H	-3.39645674082983	4.15760046862388	-3.90279003430162

C	-3.39799892869132	2.05901684727246	-3.33141587233752
H	-3.66712069290565	1.71314574197977	-4.34456406569299
H	-4.33441376145465	2.12675663843981	-2.75848337402782
C	-2.47678407731651	1.03484439954310	-2.66305860720506
H	-2.95302706338210	0.04283327544517	-2.65009213250388
H	-2.33901170080695	1.31421838250130	-1.60487977308426

[$(Cy_3P)_2Pt$-$PbCl_2$]

E=-3328.618324989

Pt	-4.28848247064518	0.13029419959799	-0.20032384381237
Pb	-1.79598822284052	-0.82302602660467	-0.82075300324618
Cl	-1.53194052950532	-3.37938719545569	-0.48681186291376
Cl	-0.68924066892523	-0.12693215001586	1.39619337056836
P	-5.39649948699090	-1.81391101009198	0.24651612923808
P	-3.71149729307039	2.35389598053700	-0.17017693686669
C	-5.00020279266754	-3.32963198669659	-0.72561413510286
H	-3.98482063933701	-3.56226428392593	-0.35460372677738
C	-5.88020986174848	-4.56471886720317	-0.49545447499039
H	-6.88872743302339	-4.38495336525099	-0.90326471229465
H	-5.99964199072597	-4.76734157467903	0.57941239694848
C	-5.26926081966224	-5.78257004327128	-1.20260704990493
H	-5.90578266983157	-6.66684379022040	-1.04372993536149
H	-4.28955988941078	-6.00477525424492	-0.74787794850483
C	-5.08482030821417	-5.51695368028435	-2.70114089092128
H	-6.07800230465868	-5.39275947843211	-3.16957963306957
H	-4.61566675218771	-6.38650905157949	-3.18610847906723
C	-4.24525795816837	-4.25765109225622	-2.94522177634235
H	-3.22180168671647	-4.41588463615191	-2.56875341931510
H	-4.16598614563724	-4.05358407629321	-4.02429135087121
C	-4.83954684791492	-3.04079854447605	-2.22808760468153
H	-4.19903328653917	-2.15572841438467	-2.36928788518410
H	-5.81577843137460	-2.78861097818284	-2.67240551399509
C	-7.20542845864101	-1.39472723917632	0.10951415920129
H	-7.25665735177318	-0.44165409900402	0.66861044607383
C	-8.20712938760580	-2.35602019857626	0.76793158617795
H	-7.91648765706151	-2.57441036992683	1.80532975681313
H	-8.20904484887964	-3.31640777544597	0.23215089742188
C	-9.61802617624030	-1.75269865095452	0.73174943854497
H	-9.63257662820141	-0.83656418536224	1.34810848449077
H	-10.33646824290282	-2.45041180048476	1.18866471811958
C	-10.04524210623996	-1.40752208996633	-0.69968944722732
H	-10.13405267016463	-2.34028376549563	-1.28362634908637

H	-11.04299091491703	-0.94271428314036	-0.69908533816389
C	-9.02738972952736	-0.48544221856429	-1.38070047714703
H	-9.01813506277045	0.49056587106361	-0.86541438824671
H	-9.32297786072563	-0.28877590380185	-2.42262923473092
C	-7.61644085373066	-1.08135306488500	-1.33727965720056
H	-7.59819378602974	-2.01022599836170	-1.92988489035507
H	-6.88379149364770	-0.39789751495454	-1.79428200523997
C	-5.15586269346169	-2.26159646723044	2.02917074850375
H	-5.75151135239327	-3.16650914763362	2.24441035301315
C	-3.67039790517626	-2.55616091058786	2.29593361475959
H	-3.07413283302597	-1.68770783014310	1.96950790111245
H	-3.32097152314285	-3.40470172798875	1.69378508175300
C	-3.38854649605523	-2.80348140836209	3.77921679227141
H	-2.31113733452226	-2.97723525731469	3.91390472036312
H	-3.90543593707403	-3.72125248550961	4.11217683276171
C	-3.85343720022130	-1.61891944160565	4.62934078591631
H	-3.65848720459925	-1.80451072372118	5.69666422079204
H	-3.26752299824236	-0.72686092984581	4.34839309464351
C	-5.34168482304240	-1.34189869928504	4.40019553461848
H	-5.67014139823544	-0.46921648643751	4.98613750711468
H	-5.93152921422732	-2.20337937282804	4.76084706860136
C	-5.64932690187851	-1.10391116838838	2.91782000668243
H	-6.72917617785897	-0.94222696978919	2.78387282325356
H	-5.14918667858712	-0.17982590289964	2.57937612567744
C	-5.29459783656093	3.33010180378207	0.04854548744198
H	-5.37624037093942	3.41617035202245	1.14769088597500
C	-6.52391895106942	2.54317432330560	-0.43686013359308
H	-6.50862627749747	1.53422469400622	0.00815974393533
H	-6.45782766598696	2.39402072278614	-1.52763772929449
C	-7.82482285239629	3.27244197534292	-0.08919324046850
H	-7.93265012823910	3.30824597562868	1.00901721246561
H	-8.68764434211480	2.70558307353453	-0.47115094463829
C	-7.83333988310877	4.69938685385309	-0.64743999956785
H	-7.83776229966522	4.65536782698502	-1.75058393247171
H	-8.75477247688721	5.22288791764801	-0.35040632097802
C	-6.60121083387924	5.48254882352890	-0.18209471971285
H	-6.59529021615543	6.48952909269720	-0.62662378652957
H	-6.64771845922485	5.62139633002467	0.91212815220472
C	-5.30075307348134	4.74916979984506	-0.53824765387546
H	-5.21383513237758	4.68923784242010	-1.63586557728118
H	-4.43507018836446	5.32526593067876	-0.18313659043193
C	-2.86158283111358	3.09917772638383	-1.64319127518523

H	-3.00404358483056	4.19160239303235	-1.59325338356450
C	-3.53230857263359	2.56790157486177	-2.92235555423232
H	-4.60246911254516	2.82631377027862	-2.92494564396865
H	-3.48954199607048	1.46489665857491	-2.90437576927497
C	-2.85262876471666	3.09865379501500	-4.18811500204397
H	-3.00141471586474	4.19087092958078	-4.25317209949318
H	-3.33108240270596	2.66223453247453	-5.07812439780403
C	-1.35177000784728	2.79325149351451	-4.17976570328265
H	-0.87135802805649	3.19986822704615	-5.08238529407578
H	-1.20399663844116	1.69939232773982	-4.20897271752070
C	-0.68562967402297	3.35599818059712	-2.92078409894979
H	0.38647926765886	3.10875042201447	-2.90654644671658
H	-0.75582338662503	4.45785186196336	-2.93289996444451
C	-1.35147074187106	2.82300931401223	-1.64763778982842
H	-1.17293743466545	1.73549030042086	-1.58658852301181
H	-0.87550168957989	3.25844137039527	-0.75857502220436
C	-2.67976215602530	2.79832211550253	1.29582389052805
H	-1.71180553550358	2.31052570631085	1.08483772738935
C	-2.45264120453541	4.29714186912655	1.52774433870648
H	-2.03841331937338	4.77585695210551	0.62674086197882
H	-3.41794378443148	4.79001261925718	1.73516126537260
C	-1.51599583944654	4.52000714178833	2.72316450542591
H	-1.37147559799746	5.59861415179619	2.89064905814306
H	-0.52487225666366	4.09826627499781	2.48472302650507
C	-2.06124433845535	3.84698096711371	3.98779588234811
H	-3.00709451006848	4.33871693275434	4.27821436755289
H	-1.36265738627335	3.99131272053040	4.82598300738926
C	-2.31382387545826	2.35349677629710	3.75636480724800
H	-1.35880283139624	1.83764181785524	3.56499396730590
H	-2.74845825942580	1.89290393939441	4.65687833610116
C	-3.23268821013018	2.11180577068443	2.55566401426636
H	-3.32473492751891	1.03424682778811	2.35587015580113
H	-4.24599012885622	2.49136569745324	2.77963672085723

[$(Cy_3P)_2Pt$] (1)

E=-2214.829297657

Pt	0.00000000000000	0.00000000000000	-0.08488368535305
P	0.37488431293642	-2.21589376178661	0.02370798109694
P	-0.37488431293642	2.21589376178661	0.02370798109694
C	1.93098867270288	-2.74938631296564	-0.84533651561959
H	2.70200770635863	-2.30648889384232	-0.18769467209850
C	2.22209618855311	-4.25068006120457	-0.95732256362679

H	1.48390880055852	-4.71376341114345	-1.63221994917998
H	2.11561194118665	-4.74685545511727	0.01934955681904
C	3.62900843394985	-4.48817840510435	-1.52441225135278
H	3.81894127043369	-5.56826036607228	-1.62535135023472
H	4.37450980050974	-4.10244954685521	-0.80713961067273
C	3.81402970436733	-3.78448452728308	-2.87429082160601
H	3.14091839115454	-4.24894796042784	-3.61651068865705
H	4.83984966429932	-3.93463181792332	-3.24523969042509
C	3.49176651456579	-2.28826114549678	-2.77517084443386
H	4.23064926552757	-1.79942398950395	-2.11595665093511
H	3.58694299792563	-1.81033437201575	-3.76243218215657
C	2.08790456515479	-2.05334759694610	-2.20817408542707
H	1.87251173589137	-0.97967102867837	-2.08776531007950
H	1.33906549310597	-2.44526044143438	-2.91505042511855
C	-1.07371733958844	-3.22329945876727	-0.57381972009906
H	-1.90251943088194	-2.72961955862331	-0.03285530742488
C	-1.12640395705698	-4.71981090305671	-0.23518338200200
H	-0.96208534580641	-4.88378087001033	0.84004378285577
H	-0.31941533392637	-5.25154777266476	-0.76135926330939
C	-2.47798475403354	-5.31563180046238	-0.65482310952217
H	-3.27771887719578	-4.85082319544640	-0.05180259407572
H	-2.50125389025463	-6.39350037953541	-0.43032328274268
C	-2.76168085989814	-5.07367619383386	-2.14213584031705
H	-2.01950236940980	-5.62735329268498	-2.74414692654648
H	-3.74921408827080	-5.47798282101201	-2.41337806764586
C	-2.67794911141639	-3.58340103037779	-2.49260567007528
H	-3.48780746394432	-3.03975775681935	-1.97569424484278
H	-2.83696101744793	-3.43361308599752	-3.57178678546647
C	-1.33141846456227	-2.98658202052498	-2.06999446270955
H	-0.52761863488463	-3.45947129951400	-2.65893482288445
H	-1.29094893800058	-1.90652689414178	-2.28054772147980
C	0.61941216765800	-2.79082490111723	1.77711083258282
H	0.80116066152605	-3.88037891325845	1.78260986875628
C	1.83077979991600	-2.07695090026014	2.40183654352377
H	1.69078435628798	-0.99004730245871	2.26322753509894
H	2.75353639435753	-2.34389973283023	1.86588395346470
C	1.98873778726333	-2.40378541455880	3.89050239287506
H	2.84532107592106	-1.84810961023251	4.30291013576899
H	2.22394116688730	-3.47670147486500	4.00738534799576
C	0.71322330462046	-2.08063913116103	4.67297511042747
H	0.83397138542246	-2.34397450786415	5.73512708964110
H	0.53287575895428	-0.99210756222053	4.63461437277418

C	-0.49212367725299	-2.80891376822924	4.07247252361940
H	-1.41313351645489	-2.54117852361807	4.61353664982355
H	-0.35826452186071	-3.89807402989619	4.19919228156903
C	-0.65575472960529	-2.48542009519692	2.58399935588473
H	-1.51297581321871	-3.03966350188606	2.17393091080917
H	-0.88577320456850	-1.41281610954686	2.45148443005559
C	1.07371733958844	3.22329945876727	-0.57381972009906
H	1.90251943088194	2.72961955862331	-0.03285530742488
C	1.12640395705698	4.71981090305671	-0.23518338200200
H	0.96208534580641	4.88378087001033	0.84004378285577
H	0.31941533392637	5.25154777266476	-0.76135926330939
C	2.47798475403354	5.31563180046238	-0.65482310952217
H	3.27771887719578	4.85082319544640	-0.05180259407572
H	2.50125389025463	6.39350037953541	-0.43032328274268
C	2.76168085989814	5.07367619383386	-2.14213584031705
H	2.01950236940980	5.62735329268498	-2.74414692654648
H	3.74921408827080	5.47798282101201	-2.41337806764586
C	2.67794911141639	3.58340103037779	-2.49260567007528
H	2.83696101744793	3.43361308599752	-3.57178678546647
H	3.48780746394432	3.03975775681935	-1.97569424484278
C	1.33141846456227	2.98658202052498	-2.06999446270955
H	0.52761863488463	3.45947129951400	-2.65893482288445
H	1.29094893800058	1.90652689414178	-2.28054772147980
C	-0.61941216765800	2.79082490111723	1.77711083258282
H	-0.80116066152605	3.88037891325845	1.78260986875628
C	0.65575472960529	2.48542009519692	2.58399935588473
H	1.51297581321871	3.03966350188606	2.17393091080917
H	0.88577320456850	1.41281610954686	2.45148443005559
C	0.49212367725299	2.80891376822924	4.07247252361940
H	0.35826452186071	3.89807402989619	4.19919228156903
H	1.41313351645489	2.54117852361807	4.61353664982355
C	-0.71322330462046	2.08063913116103	4.67297511042747
H	-0.83397138542246	2.34397450786415	5.73512708964110
H	-0.53287575895428	0.99210756222053	4.63461437277418
C	-1.98873778726333	2.40378541455880	3.89050239287506
H	-2.84532107592106	1.84810961023251	4.30291013576899
H	-2.22394116688730	3.47670147486500	4.00738534799576
C	-1.83077979991600	2.07695090026014	2.40183654352377
H	-1.69078435628798	0.99004730245871	2.26322753509894
H	-2.75353639435753	2.34389973283023	1.86588395346470
C	-1.93098867270288	2.74938631296564	-0.84533651561959
H	-2.70200770635863	2.30648889384232	-0.18769467209850

C	-2.22209618855311	4.25068006120457	-0.95732256362679
H	-2.11561194118665	4.74685545511727	0.01934955681904
H	-1.48390880055852	4.71376341114345	-1.63221994917998
C	-3.62900843394985	4.48817840510435	-1.52441225135278
H	-3.81894127043369	5.56826036607228	-1.62535135023472
H	-4.37450980050974	4.10244954685521	-0.80713961067273
C	-3.81402970436733	3.78448452728308	-2.87429082160601
H	-3.14091839115454	4.24894796042784	-3.61651068865705
H	-4.83984966429932	3.93463181792332	-3.24523969042509
C	-3.49176651456579	2.28826114549678	-2.77517084443386
H	-4.23064926552757	1.79942398950395	-2.11595665093511
H	-3.58694299792563	1.81033437201575	-3.76243218215657
C	-2.08790456515479	2.05334759694610	-2.20817408542707
H	-1.87251173589137	0.97967102867837	-2.08776531007950
H	-1.33906549310597	2.44526044143438	-2.91505042511855

[$PbCl_2$-$PbCl_2$-Pt(PCy_3)]

E= -4442.378344592

Pb	-1.68986996411980	-0.50338128426403	-0.68603003275818
Cl	-1.24162030705854	-3.00266952287515	-0.85193016135974
Cl	-1.10900865380497	-0.17883138520131	1.82216320557554
Pt	4.28006993827181	-0.15805855447515	0.17939609736487
Pb	1.89619197203035	0.82176721618870	1.07848040615655
Cl	1.48800488209707	3.32080670825383	0.57114157158539
Cl	0.80267918711326	0.19057732508671	-1.42342440225723
P	5.39320017013620	1.79347035204322	-0.23334701418120
P	3.71522663338371	-2.39643995191922	0.15593431349394
C	4.99521238676641	3.30128308851034	0.75310910418313
H	3.96620531310119	3.51310057791192	0.40764125073469
C	5.83842521695656	4.55715946984144	0.49615496285674
H	6.85964732795139	4.40624361835619	0.88308146258196
H	5.92996105716158	4.75539180316695	-0.58213342365962
C	5.20772149652202	5.76307690549230	1.20686988623101
H	5.81676403445255	6.66314544926500	1.03082005704685
H	4.21473056203126	5.95560299554985	0.76744654782465
C	5.05587664660825	5.50521302599788	2.71049897564488
H	6.05936588041181	5.41602805014261	3.16405590864222
H	4.56770770416123	6.36403618678791	3.19545300575868
C	4.26014436307946	4.22284007113347	2.98092216522705
H	3.22536301391580	4.34770564088160	2.62317636377447
H	4.20780148608041	4.02540671819472	4.06269307635017
C	4.88152794923140	3.02134630026459	2.26099809412804

H	4.28279038790757	2.11118225867527	2.43089674875834
H	5.87674074684109	2.81057940365509	2.68369233291767
C	7.20062489228444	1.37084896687621	-0.10519050363373
H	7.24967234022920	0.42858547946462	-0.68249272258432
C	8.20363770520883	2.34282332439862	-0.74483493140877
H	7.91390108307716	2.58142490292496	-1.77814988954073
H	8.20663740168940	3.29289356239043	-0.19043454656108
C	9.61360333601488	1.73623943340247	-0.71956312567494
H	9.62624806366891	0.83259113041352	-1.35404823994997
H	10.33352908684525	2.44148206962018	-1.16227875528471
C	10.03952776253816	1.36159612401298	0.70489562737806
H	10.12945886721358	2.28219442167342	1.30772378667815
H	11.03644771494828	0.89529846463621	0.69510897758612
C	9.02001304142905	0.42761804409560	1.36685432066125
H	9.00846162706553	-0.53790846165296	0.83262737448683
H	9.31440960707944	0.20957914995380	2.40476521312980
C	7.61080506353659	1.02800640507971	1.33532894246869
H	7.59674946122400	1.94551468442064	1.94526681910333
H	6.87595299051862	0.33850900383411	1.77915904934666
C	5.14566519637362	2.26793030408804	-2.00861192160061
H	5.75750996684540	3.16149402317582	-2.22393295624034
C	3.66342339141148	2.59652839770879	-2.25193978005936
H	3.05674287514461	1.74476734474292	-1.90317700380522
H	3.34654887908905	3.45745512372151	-1.64903684817814
C	3.35752762568435	2.84116341608792	-3.73093281418719
H	2.28101879797881	3.03462328964173	-3.84702622153189
H	3.88349904704950	3.74849603432038	-4.07717579264530
C	3.78699380511527	1.64692783321120	-4.58595506652960
H	3.57230755434425	1.83262454845078	-5.64932582526063
H	3.19554236870471	0.76303066657040	-4.29064181716111
C	5.27543700243084	1.35035215486911	-4.38599314961980
H	5.58066850577370	0.47415832003672	-4.97871666732043
H	5.86887640401088	2.20441781586597	-4.75771522032004
C	5.60597849918820	1.10617873734554	-2.90996901258955
H	6.68574454688375	0.93010197022372	-2.79423840756796
H	5.09905992701097	0.18765303469551	-2.56558177081680
C	5.30557047808148	-3.35835470383916	-0.07216053389972
H	5.36426318337316	-3.47930361626939	-1.16952452359489
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H	6.51365650591729	-1.55773601818191	-0.11288911082751
H	6.49558953933160	-2.36948816336009	1.45003574576579
C	7.83678854037555	-3.28798961187825	0.01088975520159

H	7.92022373710545	-3.35962848413058	-1.08772969741595
H	8.70569472342503	-2.70599758637307	0.35437965436476
C	7.86403968105086	-4.69578826461992	0.61506127648019
H	7.89205335610033	-4.61555098477195	1.71579120673841
H	8.78136268005568	-5.22476445350690	0.31491814893652
C	6.62566813494108	-5.49769908830492	0.20155623099715
H	6.63248836031097	-6.48959393539127	0.67847225837769
H	6.64996357476250	-5.67213972472044	-0.88824242755845
C	5.33020651325431	-4.75774043001639	0.56041380853950
H	5.26460588908490	-4.66083497316187	1.65681834765938
H	4.45960117384190	-5.34727868532277	0.24209587920018
C	2.88091471744389	-3.10929597660367	1.65005076767272
H	3.04648223866937	-4.19900168559156	1.64244367898829
C	3.52926729370764	-2.51514655935702	2.91364529382526
H	4.59498021070147	-2.78992060167567	2.95967526755512
H	3.50987420346057	-1.41370241065095	2.83116831858338
C	2.80572950864126	-2.94806692754256	4.19217100708352
H	2.93127140936339	-4.03599283530570	4.33382476869402
H	3.27234432834382	-2.46147124429461	5.06257367902108
C	1.31172977902982	-2.61819028949064	4.12007317552641
H	0.80306574567050	-2.93558510086376	5.04270282336919
H	1.17888195702242	-1.52392015744996	4.04896549768697
C	0.66837418464537	-3.27574013383851	2.89800343490734
H	-0.39443766175031	-3.00635300631197	2.82393608903555
H	0.71896608124648	-4.37386173692014	3.00245205251708
C	1.36953590789792	-2.85749774876800	1.60506166589794
H	1.16637897090930	-1.78552157283782	1.44428557989093
H	0.91006397548652	-3.36858976578074	0.75058238827591
C	2.67867335240916	-2.86252928859708	-1.30120036172061
H	1.68767295640228	-2.43535642058349	-1.07304697394644
C	2.51731323416102	-4.37007960742527	-1.53832709473281
H	2.10351243273922	-4.85911774675589	-0.64330642232221
H	3.50676677419702	-4.82178076095703	-1.72565399683025
C	1.60858605481605	-4.63786666111819	-2.74588026254075
H	1.53265813942542	-5.72250717388611	-2.91880810736658
H	0.59476155625713	-4.27715779492941	-2.51035311668890
C	2.12284979710912	-3.92890647087717	-4.00295803457328
H	3.09835665500001	-4.35825310639948	-4.29516809716101
H	1.43672320346648	-4.10644960666713	-4.84513463761384
C	2.28571071123119	-2.42509878369546	-3.75845623058175
H	1.29941814119095	-1.97586202658515	-3.55647495036923
H	2.68658813661897	-1.92695025698057	-4.65495895246673

C	3.19654655125570	-2.14773249293143	-2.55967053041005
H	3.25498049637410	-1.06776175174937	-2.35773318459644
H	4.22263927182380	-2.48701225293248	-2.79066393193948

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P	-4.58555044603985	2.32228322177597	0.26109250373555
C	-1.94650839462697	-2.99790266768181	-3.61203593207064
H	-2.29246292819235	-2.75016606196851	-4.62633188891019
H	-1.00985434080995	-2.43710495973328	-3.45229706457285
C	-2.54615235917637	-2.91654343065788	-1.15796839372114
H	-1.59719417601363	-2.38458388063114	-0.95924472115106
C	-2.98610848043697	-2.53781997271630	-2.58350619717290
H	-3.95079163768172	-3.02156890212410	-2.80918247695842
H	-3.14809214405960	-1.45013083463832	-2.65001775056727
C	-1.66956724280525	-4.50024866171599	-3.49038082148436
H	-0.89648742766190	-4.80367934389299	-4.21088029600498
H	-2.58245138693880	-5.06101506517652	-3.75635526848374
C	-4.37142360724171	3.36173314928975	-1.24581219380507
H	-5.14777679490659	2.98934247233467	-1.93769152763869
C	-6.31321307350143	2.56206797773222	0.86615708469535
H	-6.41400537652497	3.60591422882548	1.20874957283267
C	-3.49615614407238	-2.59503919576114	4.26215873359309
H	-4.15375099771419	-2.14883947222421	5.02275100514387
H	-3.54320682611661	-3.68752353331453	4.40934683753852
C	-3.40561003768986	2.96936103609058	1.53988864918060
H	-2.57378711630309	3.37954854852289	0.93874749157654
C	-4.59130033769626	4.86565618691419	-1.02366731986235
H	-3.84421239049388	5.23745112134447	-0.30278517391926
H	-5.58180002108961	5.05371681993928	-0.58226901679073
C	-4.02403465180878	-2.24964422560059	2.86553782720542
H	-5.04842187096731	-2.63315944646346	2.75131628834222
H	-4.08599579747891	-1.15209871323339	2.75200656715512
C	-4.44085423850895	5.63656442688524	-2.34224173944558
H	-5.24879348774476	5.33407912025137	-3.03026388061020
H	-4.57092537333393	6.71327338267459	-2.15959343076769
C	-2.28117799770437	-4.42567591788061	-1.02987031139639
H	-1.93169905652641	-4.67380536845956	-0.01695745223795
H	-3.21896733475401	-4.98007193027498	-1.18654936527189
C	-3.11349798829480	-2.80423379073870	1.75362888272218

H	-3.16326650392847	-3.90662186401374	1.75898898522075
C	-5.43403290614018	-2.73749092330437	-0.14919568430719
H	-5.87055895920547	-2.57724026685493	0.85337409527752
C	-1.14413909820630	-2.70722102099831	3.36651241506615
H	-0.11342512608403	-2.34157666605439	3.48323797152223
H	-1.10273370115772	-3.80399538064916	3.47788429764971
C	-6.08922059343541	-1.70141794395968	-1.07848296567482
H	-5.68115012149710	-1.77798210035271	-2.09666971564208
H	-5.79949926315324	-0.64907897894114	-0.72422523955632
C	-2.05291570431948	-2.12139501896528	4.44935094492899
H	-1.68574240481786	-2.39718622285091	5.44826006324589
C	-7.31054651206952	-4.33077326005309	-0.62485038831529
H	-7.56714567610893	-5.33960515322455	-0.97908134864859
H	-7.70657791883252	-4.24870265525127	0.40171766117186
C	-2.84814716104625	1.77941292521921	2.34242446628097
H	-2.49366576625288	0.98879579483427	1.63352591643781
H	-3.65887081312769	1.31555120941410	2.92720404726267
C	-5.78346145007073	-4.16349993693896	-0.58522454626529
H	-5.33490371324196	-4.89894191443263	0.09860539354019
H	-5.36633051641131	-4.35927700332314	-1.58581803629049
C	-1.71816454987214	2.21098226682218	3.27824209973516
H	-1.35477020691766	1.34993689682485	3.85867687068294
H	-0.86703721569290	2.57517781343279	2.67898007571672
C	-7.60723111338825	-1.84257392795345	-1.09199195974750
H	-8.00289551654254	-1.63752897445975	-0.08324286228440
H	-8.06080781285036	-1.10939409600264	-1.77427993977396
C	-6.57618399750142	1.61254777772734	2.05118101149330
H	-5.88516455357180	1.83045375801072	2.87853016190381
H	-6.34951003023648	0.58050694292607	1.72524534709908
C	-1.65191833795405	-2.36149105714634	1.96281253201522
H	-0.99958299196739	-2.81887124340118	1.20498093650385
H	-1.59067832862766	-1.26851369582136	1.81260575471101
C	-2.20639441662337	3.32546207381497	4.21548034216077
H	-1.38161360359287	3.65978882443872	4.86138818431831
H	-2.98409973835503	2.91877006170686	4.88449822108648
C	-7.98050594612334	-3.27600745423290	-1.51434209139534
H	-7.67323754856560	-3.43177261009958	-2.56217661082952
H	-9.07368328724382	-3.39320439920018	-1.48771164276023
C	-9.01042610084090	1.42755877604212	1.39575559135966
H	-10.04637421094044	1.51725701951437	1.75301094863461
H	-8.88678164957659	0.38720385611602	1.04643917024628
C	-3.00471093367715	3.08235095067195	-1.89675209622904

H	-2.19814927070960	3.38289924604096	-1.20616206767074
H	-2.88784917240153	1.99957787496213	-2.06552333648973
C	-3.08292437584322	5.36295395386044	-2.99735422987821
H	-2.28159574868920	5.76400888003694	-2.35274013772216
H	-3.00885227794480	5.89720485659074	-3.95548396005351
C	-2.78183151566300	4.51130597455159	3.43200977477079
H	-3.15944149139414	5.27755486343053	4.12441003373766
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H	-8.18153526687710	0.98270174652036	3.35991608871636
H	-8.21360337883184	2.70059264179920	2.95338087463488
C	-2.85650664054720	3.86193497446313	-3.20894140126207
H	-1.86083277867208	3.67943490952704	-3.63915160087775
H	-3.59055542414191	3.47961815799888	-3.93871820843236
C	-3.90507622267121	4.07513293170572	2.47960369856475
H	-4.27468231622113	4.93707038654880	1.90643431604333
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C	-1.24322147623254	-4.87552917506842	-2.06729636408700
H	-0.27500819685811	-4.39846080174941	-1.83731937709499
H	-1.08517910659143	-5.96078778138963	-1.98521776217519
H	-2.02076602735350	-1.01866640081415	4.39485110385296
C	-7.31839456464082	2.31153064754322	-0.27245748543070
H	-7.13059099142993	1.31177830102518	-0.70262152728200
H	-7.16784554712584	3.03716932021453	-1.08434047076033
C	-8.76627760146882	2.38476679213906	0.22635387160243
H	-8.98468555190150	3.41695147211928	0.54870128333803
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Cl	-1.28705509114652	-3.34730502589025	-0.87431752114559
Cl	-1.60228003315991	-0.59117581240770	1.87023590722663
Pt	4.16811125873588	-0.08649596525195	0.25894625275959
Pb	1.78793513103331	0.93426835465065	1.18897593740738
Cl	1.51112167580138	3.49150940937994	0.52156152861636
Cl	0.56660356845013	0.10736353053687	-1.20609228137094
P	5.41230904892694	1.73929230157233	-0.22782634637232
P	3.74397699750599	-2.31533549584789	0.20492127536163
C	5.03090762624580	3.28762185572982	0.71877519498875
H	3.97729077058958	3.44394463177978	0.41658645847085

C	5.79080588510175	4.58077803691868	0.40267791048208
H	6.83153287229092	4.50666021244994	0.76097724742124
H	5.83756607488023	4.75450680959151	-0.68317207956568
C	5.10813429407787	5.76741392622917	1.09960762784543
H	5.64879999569015	6.70246937494312	0.87793944478540
H	4.08871457176306	5.87593921158345	0.69355411501126
C	5.02434923734448	5.54577012901179	2.61536232690745
H	6.04840592020822	5.53108353435248	3.03294330818046
H	4.50070702229261	6.38865215972742	3.09434199303065
C	4.32019340415872	4.22448815129455	2.94873486110311
H	3.26927591666357	4.27711223627250	2.62075142883424
H	4.31613246934005	4.05755789463232	4.03813060787435
C	4.98845775103908	3.04402374537045	2.23577397504883
H	4.44924739929466	2.10384083699672	2.43724949498839
H	6.01113808429087	2.90657090691437	2.62678137497975
C	7.24949444164845	1.39288742512361	-0.14517219055797
H	7.31058724962291	0.48420691157032	-0.77273994658856
C	8.22715234727122	2.42260739483420	-0.72730876399420
H	7.92009623737179	2.72478152400660	-1.73989751495248
H	8.21764673487516	3.33425459314449	-0.11078065577161
C	9.65189253123138	1.85016835709915	-0.75523107733741
H	9.67773299960446	0.98956560653166	-1.44687747211226
H	10.35661303921505	2.59781193524123	-1.15477526966886
C	10.09788577111753	1.39000585753389	0.63870173962193
H	10.17340553757953	2.27266184916900	1.29890404976436
H	11.10535807361776	0.94596877880873	0.59106760057497
C	9.10090544231224	0.39601448490178	1.24814993750075
H	9.10107946468346	-0.53275617930627	0.65137068464953
H	9.41367938649120	0.11568821909611	2.26680566991483
C	7.68062487831854	0.96993909069479	1.26551576840061
H	7.65139441507776	1.84411393583587	1.93668137172541
H	6.95794122799649	0.23847431866498	1.66031291904669
C	5.15144565887779	2.22445250861568	-2.00669390924948
H	5.70403866979761	3.16058824347305	-2.20903103634067
C	3.65067070150377	2.46143281499671	-2.24709224661359
H	3.10605454193690	1.55752850593866	-1.92539151095570
H	3.26826171427654	3.26927691123573	-1.60887871377477
C	3.33561866498962	2.74557406099055	-3.71647498702860
H	2.24906299205520	2.87464222533245	-3.83406187400748
H	3.80593236343867	3.69782839194945	-4.02453583925171
C	3.84398072024592	1.61561886606521	-4.61580230323243
H	3.62898133790233	1.83039180910930	-5.67520561215160

H	3.30351875453895	0.68784971184351	-4.36196295394952
C	5.34581002430499	1.39535882273387	-4.41033626894090
H	5.70325301415408	0.55877148065072	-5.03262342166082
H	5.89198046220628	2.29547101188879	-4.74763324197809
C	5.68158613551287	1.12106963237726	-2.93965408729259
H	6.77032228649801	1.00669726421571	-2.82552996408597
H	5.23168211406875	0.16449579483435	-2.62400228066460
C	5.30141385207267	-3.37023720120670	0.00016549326882
H	5.39557971987849	-3.44233534628958	-1.10028260851300
C	6.55121851361610	-2.64068352736073	0.51168607975363
H	6.55610557555746	-1.61905073277176	0.10022252382065
H	6.47958425928451	-2.51996855878052	1.60684888879627
C	7.83030370516375	-3.40474368430734	0.15922253890836
H	7.94446905866259	-3.42335253147537	-0.93963969017036
H	8.71115664429112	-2.87586850904680	0.55792885096819
C	7.79075375464755	-4.84393912993531	0.68642639285596
H	7.79238276567038	-4.82071139212019	1.79076975261680
H	8.69501449393148	-5.39552895573746	0.38131402199131
C	6.53132840982548	-5.57420694985988	0.20686406369486
H	6.48964438642901	-6.58917580310704	0.63509058993136
H	6.57706091164774	-5.69645626943443	-0.88997251717376
C	5.25713990819620	-4.79611286079725	0.56735693345059
H	5.16983266975435	-4.74428629443226	1.66586147860028
H	4.37274229129368	-5.33893751154943	0.20683087820058
C	2.86811750577289	-3.07598757979650	1.66132662376898
H	3.00208360212434	-4.17022023369704	1.62196441781441
C	3.51720131890221	-2.53859839439606	2.94928464709110
H	4.58093665067255	-2.82388388820341	2.98831631452717
H	3.50573201882966	-1.43504356798821	2.89978722141012
C	2.78972353594743	-3.01264520005832	4.21158594271021
H	2.91021011097335	-4.10673752175093	4.31470222515339
H	3.25647302015760	-2.55908381130601	5.10123872670592
C	1.29612528620253	-2.67616597497142	4.15062719016851
H	0.78280973613132	-3.03538893961520	5.05707041717339
H	1.16779446383431	-1.57947957271074	4.12635168739950
C	0.65529801404905	-3.27060456706578	2.89491429024227
H	-0.40619916406567	-2.99401453048721	2.83159975656580
H	0.70646584164056	-4.37384831400424	2.94182467458559
C	1.36397351367691	-2.78378137608096	1.62983715557437
H	1.19243089045486	-1.69683929702783	1.54167268090558
H	0.88957705376789	-3.23144994573051	0.74731197839374
C	2.71596967312829	-2.77813259857259	-1.27067587250076

H	1.71901885833205	-2.37698917536523	-1.02449990520430
C	2.57759667365008	-4.27543569885832	-1.56996246846392
H	2.16570968987428	-4.80358082503053	-0.69598763984859
H	3.57441023618261	-4.70644316315705	-1.77001071520453
C	1.67581118127385	-4.51535803528615	-2.78918324673629
H	1.62431229330048	-5.59459065895588	-3.00845670662101
H	0.65417968717667	-4.18879086175012	-2.53800612441673
C	2.17028111060833	-3.74265620480606	-4.01649248951617
H	3.15788211613439	-4.13313968501430	-4.32566636561441
H	1.48728588866944	-3.90378432807334	-4.86626804075376
C	2.29636142376498	-2.24708995163050	-3.70709323487191
H	1.30063661253411	-1.83228386957523	-3.47829967160017
H	2.67754360318740	-1.70034368166380	-4.58494720177379
C	3.20705818297047	-2.00224259094091	-2.50192086560517
H	3.24273996794182	-0.93230864525437	-2.24529913154255
H	4.24129442528652	-2.30468664433241	-2.74998331624587

$[(Cy_3P)_2Pt\text{-}PbCl]^+$

E=-2868.101362902

Pt	0.36034364323222	0.07340880121620	-0.44149884824453
Pb	2.81061816147034	0.23803880958363	-1.38153563521932
Cl	3.96295161501073	1.43230421152447	0.50391445629850
P	0.42476819221909	-2.22733216115803	-0.31339421051209
P	-0.07818422977061	2.32143962965437	-0.13086106702342
C	1.60692168347743	-2.99378183837880	-4.25731587981867
H	1.24499224439878	-2.60071506759259	-5.21859235753949
H	2.62795273377904	-2.59487286342481	-4.11810363627707
C	1.19792373258847	-3.06185181204099	-1.77326415097415
H	2.25602970867647	-2.74490919316111	-1.65804124304035
C	0.71516797033935	-2.49110063973418	-3.11718266392066
H	-0.32369801291814	-2.80719130548196	-3.29720951406308
H	0.69462273565598	-1.38914703010875	-3.07960474608576
C	1.65841470360341	-4.52588847039877	-4.28980073038547
H	2.34057542996215	-4.86688980570449	-5.08176842127225
H	0.65875781586685	-4.91365705021882	-4.55060498667895
C	0.35965545424525	3.54449229737601	-1.45895982233585
H	-0.26582885394216	3.23210877162183	-2.31290161775245
C	-1.92239456869706	2.40762040166445	0.03213951782807
H	-2.18906594778055	3.39451700271591	0.44554182278189
C	1.59391350283183	-2.50572994332308	3.68564267997870
H	1.13567744579461	-2.01691995305914	4.55797228233559
H	1.55220753931934	-3.59168732865260	3.87721822368857

C	0.66770213744802	2.93174269785326	1.45808464285079
H	1.62581477411165	3.37840122878926	1.13413611017400
C	0.00300650160209	4.99845994381792	-1.09867166056399
H	0.60153558436757	5.31026837027193	-0.22833281801411
H	-1.05437431360651	5.07137049188065	-0.80488713074367
C	0.77302623909275	-2.18024101157944	2.43332489666721
H	-0.25849356832013	-2.53924234664950	2.55990786343394
H	0.71375028670496	-1.08588522882047	2.30321978499337
C	0.29946268620289	5.94893752382051	-2.26468215805769
H	-0.34977170514928	5.69396844449595	-3.11954742009648
H	0.04547189629440	6.97816810638316	-1.97234722020787
C	1.19574832322343	-4.59610175253264	-1.79565416625670
H	1.53479058562983	-5.00629731805773	-0.83312228190145
H	0.16547498568312	-4.95279921893156	-1.95139839396724
C	1.39806173226312	-2.78201457366891	1.16022176182098
H	1.33848251350343	-3.88283513966849	1.20933127010203
C	-1.30866395587857	-2.80278095019018	-0.00498532717635
H	-1.61002407282027	-2.15369046597244	0.83939450679017
C	3.68227741933061	-2.71478265655555	2.29097749838590
H	4.71911522557359	-2.37316026393766	2.16046552785490
H	3.72047079551437	-3.81013321644503	2.41661339652830
C	-2.24813037006871	-2.47263800832087	-1.17672336945348
H	-1.98398561187049	-3.09615707337842	-2.04553774990691
H	-2.11306847521171	-1.42380665704821	-1.48768121319095
C	3.05357676205103	-2.07283595123657	3.52982498847988
H	3.62888576240587	-2.33596892937540	4.42883338121680
C	-2.93780263657610	-4.52928043482503	0.83659161470658
H	-3.05306444791915	-5.58044181298051	1.13838246414981
H	-3.19593812473585	-3.91875901149647	1.71912649676829
C	1.01163484293330	1.76952806535352	2.40925715669475
H	1.59649551382104	1.01213744002265	1.86989217271206
H	0.07979058223927	1.28181844745492	2.74136793633092
C	-1.47620711626010	-4.26053692247052	0.45280699397012
H	-0.81693409809824	-4.48247179895127	1.30400648594928
H	-1.18296686972240	-4.93949004318094	-0.36148726356699
C	1.78945840968564	2.27593611513404	3.62585156274740
H	2.00903829171981	1.43538994584794	4.30134854188326
H	2.76299123648495	2.66396264683380	3.28179498651810
C	-3.70439050199580	-2.74688635175043	-0.78633260160951
H	-3.99426564000607	-2.05749082955804	0.02541376222770
H	-4.36693387337505	-2.52875541830277	-1.63680398614974
C	-2.38360366684264	1.31191165157022	1.01404356796466

H	-1.92184945011767	1.45714162627619	2.00054100833600
H	-2.01036669658386	0.33397516532125	0.64291183055101
C	2.87549146647272	-2.37655449187171	1.03255879145298
H	3.33791348840362	-2.84924098215326	0.15241503221309
H	2.92554426875314	-1.27899508871789	0.89803312753881
C	1.02225678862121	3.37446912637138	4.36817729008210
H	1.62203247261683	3.76316124783387	5.20388300972582
H	0.10791275740565	2.94345805485653	4.81206540213648
C	-3.89279590886639	-4.19205373823833	-0.31312263972446
H	-3.70327894449387	-4.87792388119869	-1.15670536429401
H	-4.93471263969881	-4.35841042473460	-0.00379315540633
C	-4.57583004864461	1.08741389380706	-0.22773844846116
H	-5.67011592806629	1.08912746779628	-0.12130458477759
H	-4.30229456333536	0.10374984496278	-0.64585746331135
C	1.82270720136943	3.44879390892919	-1.90587302807523
H	2.50344050325416	3.61960097145781	-1.05688899531417
H	2.01764232351926	2.41879445836353	-2.27353677780639
C	1.76702586918334	5.85701677673210	-2.68764846585366
H	2.40884878723628	6.20490649161390	-1.86044642389198
H	1.96560216015314	6.52170863099464	-3.54048103118297
C	0.63079126859031	4.51451415007821	3.42287294645332
H	0.02926584283860	5.26654922458293	3.95434747931401
H	1.54089347693824	5.03009959126551	3.07126632842702
C	-3.90800593030587	1.25859035118245	1.13872729692384
H	-4.19465898531572	0.44206675821670	1.81816000319150
H	-4.26220784583659	2.19303024968323	1.60678776678246
C	2.14085941865909	4.41640917395940	-3.05142563683398
H	3.20771477984335	4.34484553317767	-3.30813836942519
H	1.57486626267105	4.10916865338685	-3.94705860124954
C	-0.15106793471886	3.99803022861722	2.20681883379860
H	-0.42133234554730	4.83518327092910	1.55093241446840
H	-1.09707164208864	3.54879112065722	2.55226079087937
C	2.08634666578449	-5.10675188421563	-2.93734137639430
H	3.13262334696038	-4.82333962743927	-2.72903872704521
H	2.06055580689432	-6.20564893396700	-2.96612592093286
H	3.10356209967761	-0.97469784474081	3.43064994851428
C	-2.60612562426500	2.23457382670722	-1.33506934015199
H	-2.24244642416811	1.29881891275113	-1.79804697752877
H	-2.32558217450147	3.05255113365496	-2.01338543459694
C	-4.13201009752799	2.18494741347233	-1.19722721585598
H	-4.49331116634965	3.16238315515577	-0.83480281845777
H	-4.58516648587210	2.03217010097500	-2.18767404687681

[PbCl-PbCl-Pt(PCy_3)$_2$]$^{2+}$

E=-3521.257515884

C	2.32094745509886	-6.25812901779674	-0.71582721703738
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H	1.33304025587273	-6.12452014427155	-0.24412699894899
C	2.64395482341958	2.71014903369673	-4.77466496365704
H	1.64217328972176	2.80887947994445	-5.21578808022108
H	3.17145427784492	3.65511644119265	-4.98583721426533
C	6.46194529127046	-3.55476931176074	0.39478679507708
H	6.00598912121015	-4.54527011877512	0.52638782826597
H	6.61582340647997	-3.13558808626381	1.40221171605509
C	2.77659693117216	-3.68958069153881	-2.07107697174719
H	3.77971316620618	-3.85658536579101	-2.49671072838304
H	2.50088918639900	-2.66516449106660	-2.39214324070756
C	3.40728852473153	1.54388132285912	-5.40502811580803
H	3.51004907871954	1.69575830070613	-6.48794780976968
H	2.82448475684020	0.61243083481171	-5.27831428397136
C	7.56434799718364	-1.38266945433811	-1.31329111713791
H	8.02571732851928	-0.38908949764002	-1.41794743233430
H	7.41696100707144	-1.77320709231242	-2.33402810228021
C	2.53866869221848	-3.36517373687335	4.14428199309548
H	1.52730497376056	-3.54383345791445	4.53550453335651
H	3.10435843223439	-4.29771922258004	4.30579758563561
C	4.78329551674615	1.37396835176586	-4.75788852368433
H	5.31389496023833	0.51255129590102	-5.18771481094989
H	5.40285910235364	2.26022745338541	-4.97291994577320
C	8.48315325205922	-2.32405261493276	-0.52610340562297
H	9.43935140252347	-2.44460803559259	-1.05342986949833
H	8.71989442688628	-1.86907680797047	0.45098505469988
C	7.82325092908841	-3.68897879696250	-0.30387943066258
H	8.47707571011543	-4.33781273887568	0.29525552723896
H	7.68418701860410	-4.19487555438680	-1.27397933464776
C	2.18862936719758	-6.13444083517738	-2.23638125701377
H	1.44874476835326	-6.85345818587845	-2.61366743104036
H	3.14916142641091	-6.39762838453351	-2.71045911086058
C	1.79544449816963	-4.71226194431525	-2.65344916076113
H	0.77914130898562	-4.48608369619042	-2.28822162525053
H	1.77054872050883	-4.62571537962128	-3.74913595812522
C	7.02337836488192	1.63456554249158	1.80821981521654
H	7.54825679085562	0.87781929632646	1.19964211507182
H	7.06855052381559	1.28951099173120	2.85126251381671

C	7.73314135238159	2.98561569234066	1.65582205958998
H	7.28794208323126	3.71077754146033	2.35754941521189
H	8.79026628962119	2.88860037730781	1.93891473054618
C	7.61398014491754	3.52487285700753	0.22647827713887
H	8.15593723924333	2.86096788306294	-0.46851889186761
H	8.08860360597307	4.51285399847674	0.14855214092659
Pt	3.32307654878967	-0.16583507641026	-0.25124261522918
Pb	1.22832695512814	0.16693782288619	1.52711166842946
P	3.75041534002396	2.10963661471024	-0.75733187243406
P	3.80525174465535	-2.43833414694249	0.23454311068739
Cl	-0.03239263922126	-1.86302248459365	0.15568507488551
C	6.14671170749602	3.62653442461411	-0.21525716564404
H	5.62564081296686	4.34795338768677	0.43219396699844
H	6.08254437566846	4.01036689221829	-1.24359974907638
C	5.56397413443968	1.72223774558244	1.35217686013561
H	5.00525144854778	2.38602732873105	2.02882165330654
H	5.07429909689800	0.73290227763768	1.42281205651038
C	6.20387457636653	-1.25510918411923	-0.62326713852780
H	5.53447769020661	-0.60743004627789	-1.22689775508116
H	6.33513797433169	-0.76056091432784	0.35203430974262
C	5.47333321755205	2.25107556483347	-0.09120163103135
H	6.03752423860707	1.54796159192244	-0.73043506079376
C	4.60718033515307	-1.92699677163892	4.31894608492942
H	5.26645735204047	-2.79416880593309	4.48908444813772
H	5.07302861001213	-1.07553794914595	4.83506087351934
C	1.41303438592930	4.46048341283361	1.80513483993982
H	1.34076050657852	4.49871784427035	2.90148147823374
H	0.45729335035147	4.05476433449235	1.43198704541849
C	2.46187672569159	-3.08828369820858	2.63962493748934
H	1.98047281659207	-3.92378294762809	2.11463358517426
H	1.78984229268609	-2.22067300838375	2.48134493968967
C	4.53481861079579	-1.63970407305790	2.81667878733120
H	5.53906377515023	-1.44733648439958	2.41089813799824
H	3.95887119624615	-0.70780543840394	2.65642128541625
C	2.55070250102900	3.52252065153634	1.38911543009025
H	3.49995585855202	3.87124098301143	1.82498511785763
H	2.39316909972896	2.51100256262788	1.81630537382016
C	2.82911348887286	-3.79912987036185	-0.54102046747397
H	1.80859795341562	-3.64554138920196	-0.15403519472678
C	3.21875841063567	-2.21726659099019	4.89359972363611
H	2.59376803243987	-1.30781760829480	4.81583234276206
H	3.28830962662252	-2.44905512357207	5.96491304409664

C	4.67156459207067	1.20023658481020	-3.23996475883157
H	5.67396153683997	1.11159836033082	-2.79653777084684
H	4.14921683537235	0.24738300128272	-3.01953426199763
C	3.88814855670576	2.35402531738324	-2.58758844352513
H	4.46313601401752	3.28733616987114	-2.71801093041615
H	1.96911094474046	3.38551252310616	-2.81812305752321
H	1.89176493324499	1.64946489435703	-3.06363531538296
H	3.35689441830254	-5.31970150825129	0.94768800458126
H	4.30191885746312	-5.39694286991671	-0.54616957323401
C	1.83378086673568	5.83174402134135	-0.28528282526965
H	2.05034070950892	6.84000312438609	-0.66511057552074
H	0.90141772379703	5.50396458872416	-0.77562570993346
C	2.97252806815641	4.88152464005648	-0.68486584775477
H	3.08906535516827	4.87310947315199	-1.77682945107094
H	3.92010560360220	5.24951730268657	-0.26799820740123
C	1.63413984410952	5.86594488451779	1.23299463884728
H	0.78440378003648	6.51275461801515	1.49069692371088
H	2.52274562464000	6.31450552243342	1.70807511214641
C	2.66925971625475	3.47006651944478	-0.13994162054529
H	1.68317390637388	3.17006059829721	-0.53319825573107
C	5.54133724680199	-2.62565365522879	-0.41266467732399
H	5.38762824478737	-3.07636285469067	-1.40916225598137
C	3.84621953346326	-2.78297545666273	2.05246064201978
H	4.46414208812994	-3.69072131868950	2.15491849460725
C	2.51941491388186	2.54393727084908	-3.25748956101789
C	3.29245559784835	-5.21471907130585	-0.14421400830335
Pb	1.12533602486306	-0.52723604952846	-1.92260327718971
Cl	-0.12179882355787	1.44594076851782	-0.48977970986885

[PbCl-PbCl-Pt(PCy_3)$_2$]$^+$

E= -3521.537701385

C	2.20746779558821	-6.08303630728168	-0.81109889776182
H	2.46943491831674	-7.12215939770053	-0.56444654481027
H	1.22802043397248	-5.88430711216640	-0.34427528280682
C	2.57799627728071	2.59485599381567	-4.74046102140990
H	1.56553893797882	2.63302306528674	-5.16811877138594
H	3.04441596672674	3.57246614385137	-4.94957792540438
C	6.45631283447783	-3.67899651877318	0.49687717561653
H	5.90492796894191	-4.62244268916116	0.61036471239765
H	6.60839343438356	-3.27413708913447	1.51092770150260
C	2.86608118026545	-3.51884444116060	-2.09431873689952
H	3.85982015755865	-3.75710730451841	-2.50934555630006

H	2.67800890053441	-2.46830393234148	-2.38072964483503
C	3.40183241950532	1.48273491857012	-5.39422643230570
H	3.48387840125019	1.65310490516139	-6.47709613345682
H	2.87518881183138	0.51963466178200	-5.26826937692070
C	7.82622210200544	-1.62266713280364	-1.13359529623312
H	8.38383592016286	-0.67702548178839	-1.21419076052167
H	7.68826957603101	-1.99451795000439	-2.16365001825711
C	2.48054445056487	-3.29063258586652	4.09961497425238
H	1.45086241742698	-3.45936237062468	4.44683592277354
H	3.03799281839813	-4.21986243498031	4.30652830985552
C	4.79278011162744	1.38393754427901	-4.76187827744302
H	5.36213986332691	0.55426882207938	-5.20607203704240
H	5.35987722040519	2.30475460995091	-4.98008360630211
C	8.62371694245706	-2.64970217712341	-0.32363067252138
H	9.58641647887069	-2.85932602041468	-0.81176526271440
H	8.86002644371015	-2.22556369819809	0.66772727802730
C	7.82768096103003	-3.94543477987695	-0.13998872728727
H	8.38953921979557	-4.65807500924018	0.48147440058448
H	7.68233922125783	-4.42994938773085	-1.12073715161011
C	2.09543682175887	-5.90918848439572	-2.32974418808094
H	1.30681495370661	-6.56208844251876	-2.73025282724818
H	3.03905888484449	-6.23164483534553	-2.80251135880732
C	1.81898669385502	-4.45041520616665	-2.71297126520186
H	0.81825643314735	-4.15740243468438	-2.35087369765048
H	1.80973078778794	-4.33562544634908	-3.80692064468427
C	7.19599835775386	1.81676387870316	1.66984178561605
H	7.72311022666429	1.08360316488624	1.03470722854329
H	7.32344857878566	1.48208613340244	2.71020106407610
C	7.82231168524185	3.20194483760155	1.47074018201116
H	7.37363734764239	3.90857640585799	2.19000253056158
H	8.89821903163631	3.16957953519436	1.69530933868619
C	7.59291014129866	3.72107576129598	0.04707786111929
H	8.13473226769310	3.08111926107488	-0.67056045016080
H	8.00509923452355	4.73469351135343	-0.06309394877614
Pt	3.23433298485604	-0.16351114062664	-0.21304597763229
Pb	1.04190303442020	0.12575623500878	1.45670005350903
P	3.77943051891951	2.03994708745647	-0.74435657081059
P	3.90335961522683	-2.35352647535995	0.24125982686875
Cl	-0.35228101934757	-1.96683863404702	0.26269507199843
C	6.10075872787656	3.72539196428150	-0.31461924333360
H	5.57226211100202	4.42456950788656	0.35204011662572
H	5.95928746780355	4.09333578981753	-1.34152588293263

C	5.71011310459953	1.81757602544277	1.29860284584212
H	5.15767792153922	2.46453508817968	1.99763874353297
H	5.27901002527511	0.80786143138886	1.39624704678183
C	6.45313231390661	-1.36313961130087	-0.50865140107887
H	5.87029394171976	-0.65386737800776	-1.11651921567890
H	6.58101961992698	-0.88691115381847	0.47759971924304
C	5.51387956488935	2.31782627407177	-0.14189150377052
H	6.08775209620371	1.63197000962713	-0.79216729582421
C	4.54431230848298	-1.86058405788738	4.34890221991566
H	5.18498370953278	-2.73133520794899	4.56868268740891
H	4.99060017501137	-1.00310700775463	4.87368556624172
C	1.40274124953520	4.30033873023046	1.85154888599107
H	1.36135782998888	4.34276261644399	2.94998758631004
H	0.46223634412873	3.83487424921368	1.51109320230500
C	2.47442429065922	-3.03822449200397	2.58891191911949
H	2.01939236317395	-3.88521237847775	2.05917009879728
H	1.80939842259025	-2.17906310429754	2.38307537045594
C	4.54648956047322	-1.59888914897295	2.84071135046447
H	5.57224942306241	-1.43044546077294	2.47982550647721
H	3.99531849343992	-0.66433946864996	2.62830259297711
C	2.57903695785924	3.42742838911868	1.40322006257606
H	3.51927002981564	3.83752578663182	1.80549095556273
H	2.49601331938919	2.41066014584026	1.82995820668276
C	2.89193685513851	-3.67520463524366	-0.56608305432713
H	1.87368876300144	-3.46453631365345	-0.19203192175829
C	3.12671757653293	-2.13014668871291	4.86030519995883
H	2.51256068678731	-1.22067692293839	4.72694489534553
H	3.13985187728834	-2.33952200302950	5.93930653645323
C	4.70749035838434	1.19428627548645	-3.24386618274247
H	5.71837675707912	1.15555615404343	-2.81283088265306
H	4.23614146160666	0.22076974656982	-3.01333978863891
C	3.87585119151404	2.30447416166574	-2.57748157762491
H	4.38929076924946	3.27068275444535	-2.72517093297508
H	1.88281532933681	3.19473362454312	-2.76710024409031
H	1.94058055118882	1.45656155470725	-3.03488465786727
H	3.29933246872357	-5.26586790871315	0.88167067451817
H	4.24378438298598	-5.37073834129799	-0.60958446579853
C	1.66897661543433	5.67852912733128	-0.25996156579730
H	1.80520584626371	6.69667428858362	-0.65292164637801
H	0.74326255365873	5.28492653050340	-0.71305782714609
C	2.84926014401932	4.79447556485975	-0.68882644891283
H	2.93178172190696	4.78417213886872	-1.78439055988098

H	3.78586631929845	5.22550927981159	-0.30660526760785
C	1.51715183598860	5.71231913103013	1.26484904472012
H	0.63938704508079	6.31108973135919	1.54718944446403
H	2.39516469059144	6.21590532574594	1.70485515092897
C	2.65504113980421	3.37412618200450	-0.12956532217837
H	1.67363515448279	3.01059969587205	-0.48468311980574
C	5.65688530925590	-2.66613118776409	-0.33895994862527
H	5.50990710976945	-3.09580603050925	-1.34648180073846
C	3.88150250271647	-2.74279609185304	2.05561567394128
H	4.48602652513392	-3.65565971138758	2.18316579815152
C	2.48725297480005	2.40081965409927	-3.22415787847042
C	3.24681212322863	-5.12686501347339	-0.20756614244582
Pb	0.92544335220095	-0.53279786416367	-1.70392384903481
Cl	-0.43433070823737	1.50112225686336	-0.44632387403929

Cl_4Al-Pb-$AlCl_4^-$

E= -4360.878589632

Pb	-6.50355479479057	11.44755400031835	16.67109898390564
Al	-9.69840434832977	12.22280605519711	18.53697062809975
Cl	-9.03537560396577	10.22472386011569	17.91589698408315
Cl	-9.54276594112149	12.41881403037142	20.65764362928221
Cl	-11.65475262745576	12.61719648415623	17.77688376419365
Cl	-8.25505064386736	13.59587805246908	17.57326450023012
Al	-3.30824285236967	12.22334810063435	14.80421340559786
Cl	-3.97200740150942	10.22573126966950	15.42623453032342
Cl	-3.46330967256866	12.41971390378169	12.68347960014483
Cl	-1.35124918359436	12.61612805410209	15.56360143537402
Cl	-4.75167749057340	13.59620288874696	15.76792411319831

Cl_4Al-Pb-$AlCl_4$

E=-4360.777728334

Pb	-6.50531865529820	11.29589617685437	16.66774682947221
Al	-9.17769605574168	12.27023371374937	18.22521434742480
Cl	-9.24090266920195	12.12217411347535	16.02506271552810
Cl	-8.57314872984688	10.26241346748645	18.79978973609017
Cl	-10.82654439131140	13.14492688725588	19.15946452331160
Cl	-7.24896775862074	13.35581423554338	18.44455327788263
Al	-3.82834820116608	12.27062522581068	15.11698425174703
Cl	-3.77445538006333	12.12481059792859	17.31780584816963
Cl	-4.42558668717056	10.26084071433798	14.54321697864522
Cl	-2.17725039292413	13.14755438387678	14.18870768288292

Cl	-5.75817168715432	13.35280727356652	14.88866550727303

$[(Cy_3P)_2Pt\text{-}Pb]^{2+}$

E=-2407.456946787

Pb	-6.50335568428134	10.64531353350062	16.67067580307432
Pt	-6.50330986300866	8.11261227615317	16.67066216738904
P	-6.52828837031023	7.81614017264008	18.99274188753802
C	-5.85511425385967	6.10316556753705	19.21924207090205
H	-6.76364967617936	5.47464210606589	19.16899532567804
C	-5.15770178596997	5.83615342953127	20.56287167834826
H	-4.25543931941310	6.46537279931008	20.63720579412133
H	-5.80880419599854	6.10680811513753	21.40544289582552
C	-4.74862453777946	4.35890829570249	20.66065881482170
H	-4.23126716390147	4.18667293488560	21.61463318519946
H	-5.65716672983968	3.73382946846335	20.67982317920105
C	-3.85887330900773	3.93979053045683	19.48572789639941
H	-2.90135105515992	4.48509842634820	19.53904517635712
H	-3.61270390757505	2.87136534980967	19.55804668459624
C	-4.53255853257495	4.23159328829030	18.13943224115361
H	-5.42983249275216	3.59963398813086	18.02903114871272
H	-3.86034276429802	3.97667755808618	17.30759172248959
C	-4.94384178330544	5.70366696091811	18.04196727513636
H	-5.45912198965159	5.88821269943688	17.07577347505631
H	-4.04706375022256	6.34392373094188	18.03375382403251
C	-8.24189664553681	7.85286404875421	19.66425911963337
H	-8.53179259369734	8.91798974227904	19.60678405067851
C	-9.19618013599345	7.06902348883339	18.74377340746954
H	-9.11181363763152	7.44970201389942	17.71176980034667
H	-8.89585868651963	6.00759668300468	18.71704992477982
C	-10.64217090664033	7.17498350139628	19.24418367223671
H	-10.97751995852964	8.22223875746393	19.15152714868336
H	-11.30025100452965	6.57623556085927	18.59843048128809
C	-10.76616560457869	6.72674214991798	20.70400501705443
H	-11.80190607340965	6.84991626903635	21.04925877258998
H	-10.53918574861951	5.64955468111537	20.77694419833878
C	-9.81091515623060	7.50874113546762	21.61027082040105
H	-9.88037428499930	7.15003333367719	22.64665576443465
H	-10.10253526297623	8.57269590124230	21.62632970382419
C	-8.35879122053853	7.39046547105410	21.12610750118122
H	-8.04017701378242	6.33791342395910	21.19914544294388
H	-7.68990224577648	7.97255466386275	21.77828454060875
C	-5.49764677123959	9.00173568149116	19.97231878930914

H	-5.34687095366719	8.52417562579828	20.95504794504889
C	-6.22256048198930	10.33164909234928	20.20464991576732
H	-6.55084029220917	10.75815752693907	19.22208690000791
H	-7.15125720277584	10.18049723783398	20.77120189577976
C	-5.33794767481637	11.38020000795164	20.88551549886424
H	-5.88805439149217	12.32820637487780	20.96497598923747
H	-5.13867424912960	11.04936963661679	21.91813552447740
C	-4.01301967012516	11.57021672953132	20.14720478038055
H	-4.20909279995466	11.98573761856946	19.13813850177431
H	-3.39135931820263	12.31374369998526	20.66367599878758
C	-3.26705985786935	10.24252674824795	20.01193614355300
H	-2.99716059205189	9.86939720759854	21.01373961412983
H	-2.32268132911752	10.37583107968804	19.46586985105973
C	-4.12776382196147	9.19858184621850	19.29863782512142
H	-3.59720682855234	8.23879006846009	19.22029118416547
H	-4.29244815164780	9.52393046403793	18.24838792463160
P	-6.47825225421945	7.81613216985075	14.34853820097977
C	-7.15150138496319	6.10316523270697	14.12209492305027
H	-6.24294977347344	5.47466826494993	14.17233094743271
C	-7.84889663919302	5.83616261108046	12.77845528151908
H	-8.75116405455901	6.46538939723309	12.70412524163471
H	-7.19779328647048	6.10681406964394	11.93588290242520
C	-8.25794620889638	4.35891332245799	12.68066077936543
H	-8.77531567130641	4.18668363290651	11.72670299674674
H	-7.34940073583534	3.73381803442860	12.66148875884018
C	-9.14770893253827	3.93979905163739	13.85557968729698
H	-10.10525567464516	4.48508000158641	13.80227720035109
H	-9.39387710614908	2.87138223730884	13.78327189974150
C	-8.47403277962177	4.23156879008485	15.20188600468791
H	-7.57673446662040	3.59962271712599	15.31229009698452
H	-9.14624580450864	3.97667693444936	16.03372369935968
C	-8.06276445502769	5.70364981859181	15.29937846708844
H	-7.54746105097224	5.88820588650864	16.26556228257003
H	-8.95953510546097	6.34392542775179	15.30756175165111
C	-4.76462326112713	7.85283640185533	13.67706893033134
H	-4.47483379173794	8.91797920705620	13.73455387941205
C	-3.81035939026438	7.06903246506946	14.59757998315388
H	-3.89479948564103	7.44972832743804	15.62959053313940
H	-4.11075568502842	6.00763022465820	14.62425631382092
C	-2.36443581937452	7.17499944250894	14.09710230900593
H	-2.02908960487115	8.22222843569074	14.18981794289599
H	-1.70639971372456	6.57630330550635	14.74287190666891

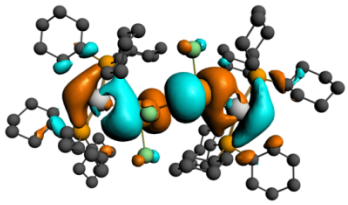
C	-2.24045832208067	6.72679598417473	12.63730761538396
H	-1.20471391468997	6.84993181313742	12.29208493795942
H	-2.46737868252233	5.64961482513194	12.56438127958264
C	-3.19571270263346	7.50877370857244	11.73108992813334
H	-3.12622664617671	7.15010033159538	10.69474504084452
H	-2.90406618418348	8.57270207844985	11.71498940203681
C	-4.64780795022744	7.39049373792558	12.21521405095260
H	-4.96642179588310	6.33794490335827	12.14219637677719
H	-5.31670990734553	7.97258280149523	11.56302486908972
C	-7.50896079509310	9.00176127973533	13.36901338655601
H	-7.65972140167399	8.52415756207171	12.38630140773842
C	-6.78405713731478	10.33168362731139	13.13670319477172
H	-6.45576855851926	10.75816594083146	14.11929296522446
H	-5.85536802107870	10.18050897562705	12.57012990359409
C	-7.66868918782836	11.38019818269806	12.45582263847571
H	-7.11859032873165	12.32818572203934	12.37638481143238
H	-7.86794471228474	11.04939745489314	11.42317720656692
C	-8.99359338964053	11.57020273177957	13.19416391959294
H	-8.79754238866686	11.98575381240405	14.20323018287722
H	-9.61525365481034	12.31373051102253	12.67769711145252
C	-9.73956443044091	10.24251503254674	13.32938127856739
H	-10.00947076225590	9.86938461851972	12.32756045239034
H	-10.68391908892172	10.37581429598758	13.87545916636664
C	-8.87886081480442	9.19857533191556	14.04271455123554
H	-9.40941685402335	8.23876239244870	14.12101919614556
H	-8.71415780108449	9.52393160079123	15.09297486743299

$AlCl_4^-$

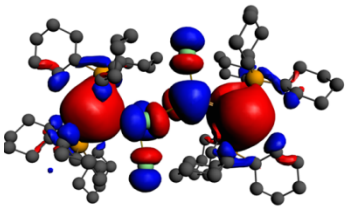
E=-2083.932615698

Al	-9.65300183129583	12.29202776511151	18.67062164401518
Cl	-9.44528614610726	10.60441140110014	17.32021401770709
Cl	-10.03836220217950	11.56834443980142	20.68119375905132
Cl	-11.30688520665761	13.53732442320297	18.01653820363833
Cl	-7.81987244401425	13.45620840276917	18.66428424334171

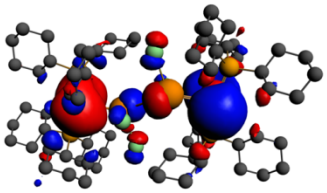
Table S2. Plot of the frontier molecular orbitals of **2** (eV) at D3(BJ)+BP86/TZ2P//RI-D3(BJ)-BP86/def2-TZVP+def2-QZVP.



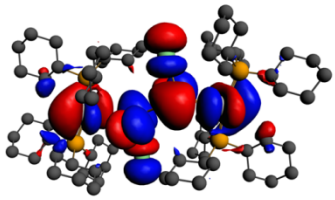
LUMO -1.958



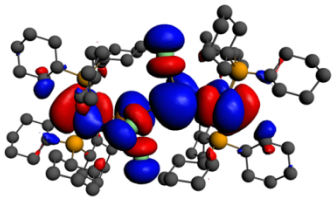
HOMO -4.562



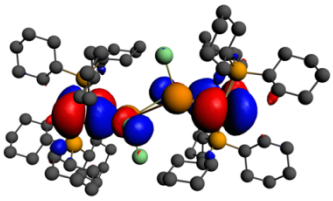
HOMO-1 -4.668



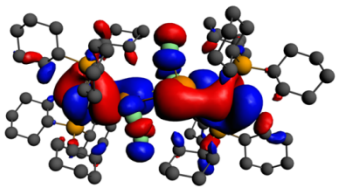
HOMO-2 -4.824



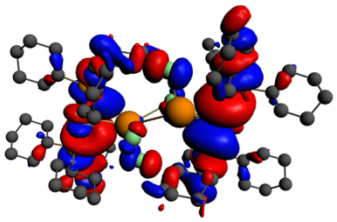
HOMO-3 -4.856



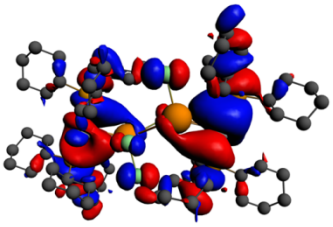
HOMO-4 -5.025



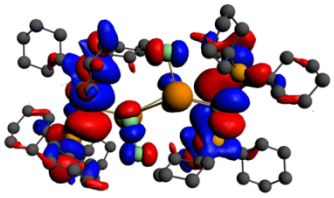
HOMO-5 -5.081



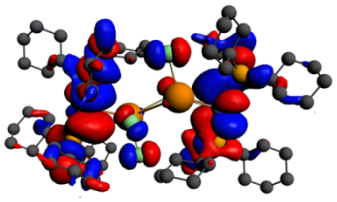
HOMO-6 -5.306



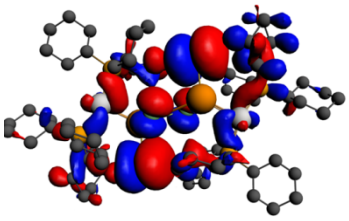
HOMO-7 -5.318



HOMO-8 -5.451

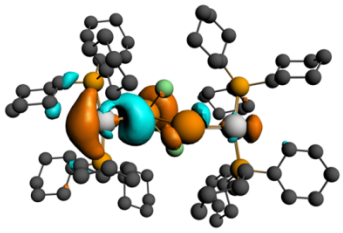


HOMO-9 -5.464

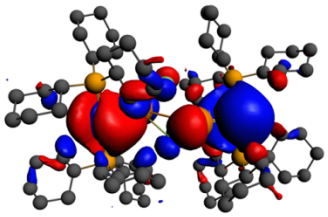


HOMO-10 -5.743

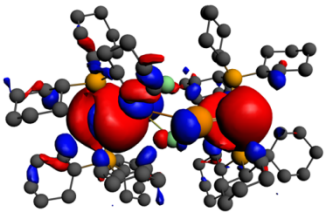
Table S3. Plot of the frontier molecular orbitals of **8** (eV) at D3(BJ)+BP86/TZ2P//RI-D3(BJ)-BP86/def2-TZVP +def2-QZVP.



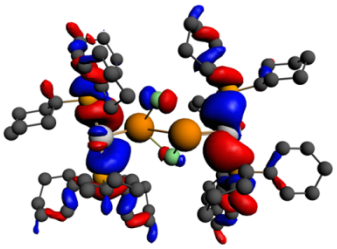
LUMO -6.894



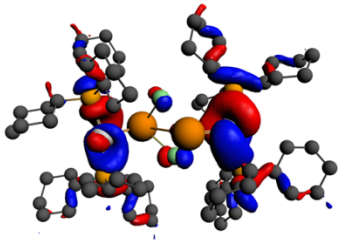
HOMO -9.417



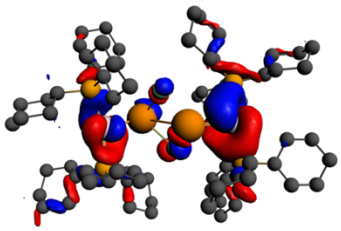
HOMO-1 -9.444



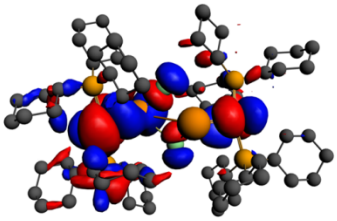
HOMO-2 -9.886



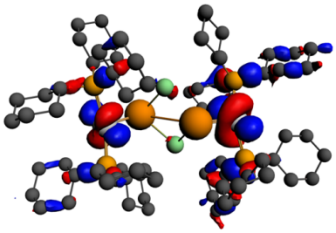
HOMO-3 -9.939



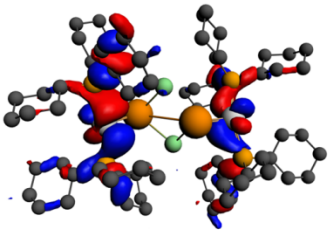
HOMO-4 -9.992



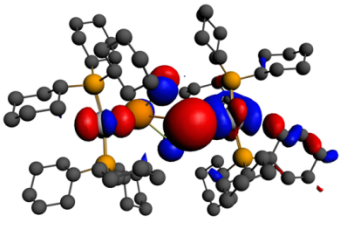
HOMO-5 -10.018



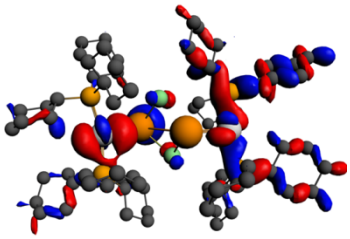
HOMO-6 -10.076



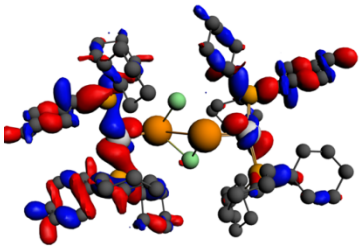
HOMO-7 -10.110



HOMO-8 -10.185

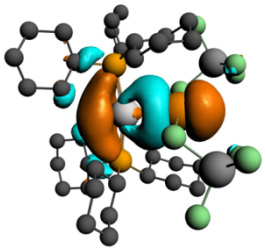


HOMO-9 -10.334

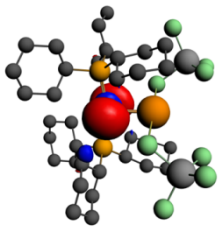


HOMO-10 -10.388

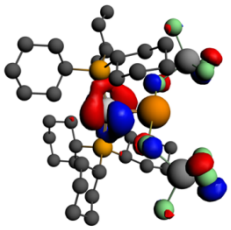
Table S4. Plot of the frontier molecular orbitals of **11** (eV) at D3(BJ)+BP86/TZ2P//RI-D3(BJ)-BP86/def2-TZVP +def2-QZVP.



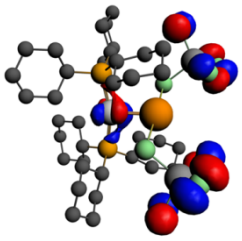
LUMO -3.239



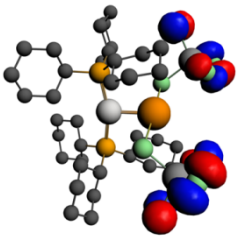
HOMO -5.967



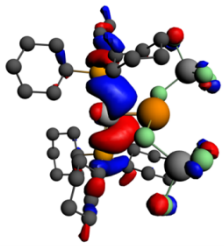
HOMO-1 -6.561



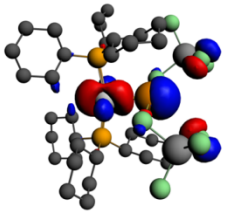
HOMO-2 -6.606



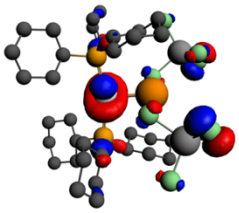
HOMO-3 -6.613



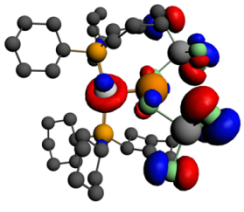
HOMO-4 -6.650



HOMO-5 -6.656

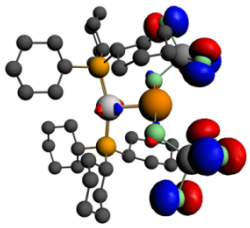


HOMO-6 -6.703

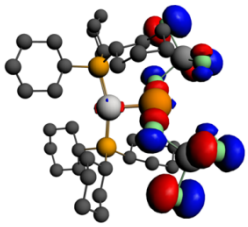


HOMO-7 -6.758

HOMO-8 -6.767



HOMO-9 -6.894



HOMO-10 -6.927