

Supporting Information

Palladium(II) Complexes of Bis(diphosphene) with the Different Coordination Behavior

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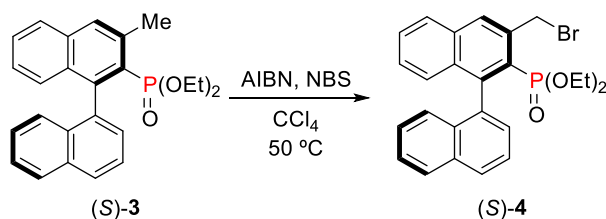
1. Experimental Details

General. All anaerobic and/or moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen atmosphere or with glovebox techniques under argon atmosphere. Analytical thin-layer chromatography (TLC) was performed using Silicagel 70 F₂₅₄ TLC Plate-*Wako*. The developed chromatogram was analyzed by UV lamp (254 nm). The silica gel column chromatography was performed with Wako-gel® 60N (Wako, 150-425 μm, irregular) or Silica Gel 60 (nacalai, spherical, neutral under nitrogen or argon atmosphere). The ¹H (400 or 500 MHz), ¹³C (100 or 125 MHz), and ³¹P NMR (162 MHz) spectra were measured in CDCl₃ or CD₂Cl₂ with a JEOL JNM-ECS400 or JEOL JNM-ECZ500R spectrometers. Signals due to tetramethylsilane (0.0 ppm) for CDCl₃ and CHDCl₂ (5.32 ppm) for CD₂Cl₂ in ¹H NMR and CDCl₃ (77.16 ppm) and CD₂Cl₂ (53.84 ppm) in ¹³C NMR were used as internal references, and chemical shifts are reported in ppm downfield. ³¹P NMR chemical shifts are externally referenced to 85% H₃PO₄ (0 ppm). Low- and high-resolution mass spectra were recorded on a JEOL JMS-700 spectrometer at FAB (3-nitrobenzyl alcohol) mode or Bruker MicroTOF-II time-of-flight mass spectrometer (ESI). All melting points were determined on a Yanaco micro melting point apparatus (MP-J3) and were uncorrected.

Reagents.

THF, Et₂O, dichloromethane, acetonitrile (Wako, Super dehydrated grade), and *n*-pentane (Kanto, dehydrated grade) were purchased and used as received. CDCl₃ and CD₂Cl₂ used in a glovebox was dried over calcium hydride, degassed by freeze-pump-thaw cycles, distilled in a vacuum line, and stored in a glovebox. Azobis(isobutyronitrile) (Wako), *N*-bromosuccinimide (NBS, Oakwood), CCl₄ (Wako), dimethylzinc (Kanto, 1.0 M, *n*-hexane), lithium aluminum hydride, (Aldrich), chlorotrimethylsilane (Aldrich), *n*-BuLi (Mitsuwa or Kanto), allylpalladium(II) chloride dimer (TCI), and sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (NaBAR^F₄, Ark Pharm) were purchased and used as received. and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) was distilled from potassium hydroxide prior to use. (*S*)-Diethyl 3-methyl-(1,1'-binaphthylen)-2-ylphosphonate [(*S*)-**3**],^{S1} chlorotris(triphenylphosphine)-rhodium(I) (Wilkinson's catalyst),^{S2} Mes*PCL₂,^{S3} [Pd(allyl)(cod)](SbF₆),^{S4} and [PdCl₂(cod)]^{S5} were synthesized according to the reported procedures.

Synthesis of (*S*)-Diethyl 3-bromomethyl-(1,1'-binaphthylen)-2-ylphosphonate [(*S*)-**4**]

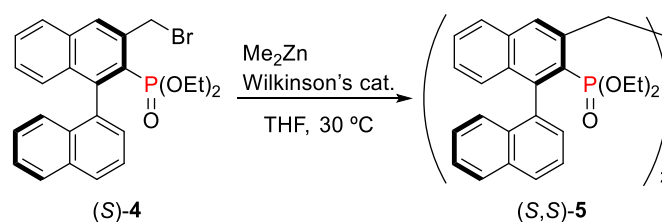


A solution of (*S*)-**3** (404 mg, 1.00 mmol), AIBN (49.3 mg, 0.300 mmol), and NBS (196 mg, 1.10 mmol) in CCl₄ (10 mL) was stirred at 45 °C for 2 h. Saturated aqueous sodium thiosulfate solution and CHCl₃ were added. The organic layer was separated, and then the aqueous layer was extracted with CHCl₃. The combined organic layer was washed with brine, dried over MgSO₄, filtered through a pad of Celite, and

then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 2/1 (R_f = 0.35) to give (*S*)-**4** as colorless solid (406 mg, 0.872 mmol, 87%).

Mp. 93 °C (decomp.); $[\alpha]_D^{24} = +32.2$ ($c = 0.05$ in CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) $\delta = 0.60$ (t, $J = 6.9$ Hz, 3H), 1.12 (t, $J = 6.9$ Hz, 3H), 3.32 (ddq, $J = 9.7, 6.9, 6.9$ Hz, 1H), 3.57 (ddq, $J = 9.7, 6.9, 6.9$ Hz, 1H), 3.80 (ddq, $J = 10.1, 8.2, 6.9$ Hz, 1H), 3.93 (ddq, $J = 10.1, 6.9, 6.9$ Hz, 1H), 5.23 (d, $J = 10.1$ Hz, 1H), 5.70 (d, $J = 10.1$ Hz, 1H), 7.01 (d, $J = 8.7$ Hz, 1H), 7.11 (d, $J = 8.3$ Hz, 1H), 7.20-7.26 (m, 2H), 7.40 (dd, $J = 7.2, 1.2$ Hz, 1H), 7.44 (ddd, $J = 8.3, 6.9, 1.4$ Hz, 1H), 7.52 (ddd, $J = 7.8, 6.9, 0.9$ Hz, 1H), 7.56 (dd, $J = 8.3, 6.9$ Hz, 1H), 7.88 (d, $J = 8.2$ Hz, 1H), 7.93 (d, $J = 9.2$ Hz, 1H), 7.95 (d, $J = 9.6$ Hz, 1H), 8.16 (d, $J = 4.6$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) $\delta = 15.4$ (d, $J = 6.7$ Hz, CH_3), 16.2 (d, $J = 6.7$ Hz, CH_3), 34.6 (CH_2), 61.86 (d, $J = 5.7$ Hz, CH_2), 61.91 (d, $J = 5.8$ Hz, CH_2), 124.96 (CH), 125.02 (d, $J = 185$ Hz), 125.7 (CH), 125.9 (CH), 126.7 (CH), 127.4 (CH), 127.7 (CH), 128.07 (CH), 128.14 (CH), 128.23 (CH), 128.27 (CH), 128.5 (CH), 132.5 (d, $J = 14.5$ Hz, CH), 133.06 (d, $J = 6.8$ Hz), 133.14 (d, $J = 8.6$ Hz), 133.6, 134.4 (d, $J = 2.0$ Hz), 137.3 (d, $J = 4.8$ Hz), 137.6 (d, $J = 11.6$ Hz), 145.5 (d, $J = 9.6$ Hz); ^{31}P $\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) $\delta = 16.9$; HRMS (FAB, NBA): m/z found: 483.0717 $[M+H]^+$; calcd for $\text{C}_{25}\text{H}_{25}\text{BrO}_3\text{P}$: 483.0725.

Synthesis of (*S,S*)-Tetraethyl (ethane-1,2-diylbis([1,1'-binaphthylen]-3,2-diyl))bis(phosphonate) [(*S,S*)-**5**]

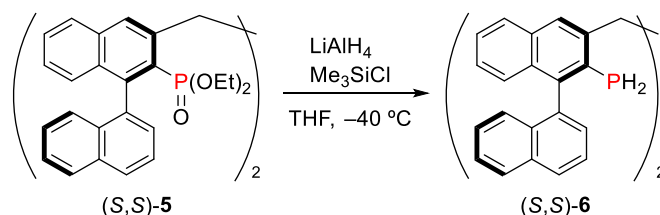


This compound was prepared according to the synthetic procedures reported by Ando and co-worker.^{S6} A solution of (*S*)-**4** (233 mg, 0.482 mmol), Wilkinson's catalyst (23 mg, 0.025 mmol), and ZnMe_2 in *n*-hexane (1.0 M; 500 μL , 0.500 mmol) in THF (10 mL) was stirred at 30 °C for 12 h. Water and ethyl acetate were added. The organic layer was separated, and then the aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine, dried over MgSO_4 , filtered through a pad of Celite, and then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 1/1 (R_f = 0.35) to give (*S,S*)-**5** as colorless solid (148 mg, 0.183 mmol, 76%).

Mp. 105 °C (decomp.); $[\alpha]_D^{24} = +77.0$ ($c = 0.05$ in CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) $\delta = 0.77$ (t, $J = 6.9$ Hz, 6H), 1.01 (t, $J = 6.9$ Hz, 6H), 3.35 (ddq, $J = 10.1, 6.9, 6.9$ Hz, 2H), 3.61 (ddq, $J = 10.1, 8.2, 6.9$ Hz, 2H), 3.71 (ddq, $J = 10.1, 7.4, 6.9$ Hz, 2H), 3.84-3.94 (m, 2H), 3.91 (s, 4H), 6.99 (d, $J = 8.7$ Hz, 2H), 7.13 (ddd, $J = 8.2, 6.4, 1.4$ Hz, 2H), 7.26-7.28 (m, 4H), 7.41-7.48 (m, 6H), 7.59 (dd, $J = 8.2, 6.9$ Hz, 2H), 7.85 (d, $J = 8.2$ Hz, 2H), 7.94 (d, $J = 7.8$ Hz, 2H), 7.96 (d, $J = 7.3$ Hz, 2H), 8.20 (d, $J = 5.0$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) $\delta = 15.7$ (d, $J = 6.7$ Hz, CH_3), 16.1 (d, $J = 5.8$ Hz, CH_3), 38.1 (CH_2), 61.3 (d, $J = 6.7$ Hz, CH_2), 61.7 (d, $J = 5.8$ Hz, CH_2), 125.1 (CH), 125.7 (CH), 125.89 (CH), 125.93 (CH), 126.1 (d, $J = 184$ Hz), 126.9 (CH), 127.5 (CH), 127.65 (CH), 127.74 (CH), 127.9 (CH), 128.0 (CH), 128.1 (CH), 130.3 (d, $J = 14.5$ Hz, CH), 131.9 (d, $J = 16.3$ Hz), 133.2, 133.8, 134.7 (d, $J = 2.9$ Hz), 138.6 (d, $J = 4.9$ Hz), 142.0 (d, $J = 12.5$ Hz), 144.2 (d, $J = 10.6$ Hz); ^{31}P $\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) $\delta = 18.7$; HRMS (FAB, NBA): m/z

found: 807.3004 $[M+H]^+$; calcd for $C_{50}H_{49}O_6P_2$: 807.3004.

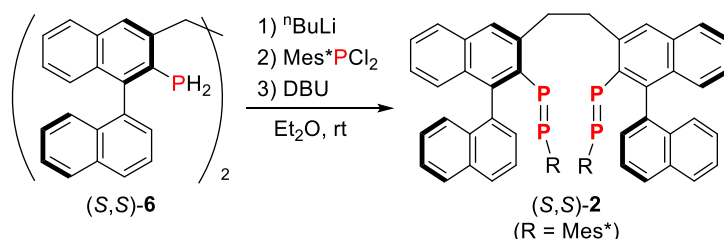
Synthesis of 1,2-bis(2-phosphino-[1,1'-binaphthalen]-3-yl)ethane [(*S,S*)-6]



To a suspension of lithium aluminum hydride (41.7 mg, 1.10 mmol) in THF (2 mL) was added chlorotrimethylsilane (162 μL , 1.28 mmol) at $-40\text{ }^\circ\text{C}$. After the mixture was stirred at $-40\text{ }^\circ\text{C}$ for 5 min and at room temperature for 30 min, (*S,S*)-5 (148 mg, 0.183 mmol) in THF (3 mL) was added. The mixture was stirred at $-40\text{ }^\circ\text{C}$ for 1 h, and then quenched with degassed water (20 μL , 1.1 mmol) at $0\text{ }^\circ\text{C}$ and dried over MgSO_4 . After THF was evaporated under reduced pressure, the residue was chromatographed on silica gel under nitrogen atmosphere with hexane/ $\text{CH}_2\text{Cl}_2 = 3/1$ ($R_f = 0.88$) to give (*S,S*)-6 as colorless solid (77.4 mg, 0.129 mmol, 70%).

Mp. $151\text{ }^\circ\text{C}$ (decomp.); $[\alpha]_D^{24} = +67.7$ ($c = 0.05$ in CHCl_3); $^1\text{H NMR}$ (400 MHz, CDCl_3) $\delta = 3.40\text{-}3.55$ (m, 4H), 3.44 (dd, $J = 214, 12.0$ Hz, 2H), 3.67 (dd, $J = 209, 12.0$ Hz, 2H), 7.05 (d, $J = 8.2$ Hz, 2H), 7.17-7.22 (m, 4H), 7.27 (ddd, $J = 7.8, 6.9, 1.4$ Hz, 2H), 7.37 (dd, $J = 6.9, 0.9$ Hz, 2H), 7.42 (ddd, $J = 8.3, 6.9, 0.9$ Hz, 2H), 7.49 (ddd, $J = 8.3, 6.9, 1.4$ Hz, 2H), 7.62 (dd, $J = 8.3, 6.9$ Hz, 2H), 7.84 (d, $J = 8.3$ Hz, 2H), 7.86 (d, $J = 1.7$ Hz, 2H), 7.97 (d, $J = 8.7$ Hz, 2H), 7.99 (d, $J = 8.7$ Hz, 2H); ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) $\delta = 37.5\text{-}37.6$ (m, CH_2), 125.9 ($\text{CH} \times 2$), 126.0 (CH), 126.23 (CH), 126.26 (CH), 126.63 (CH), 126.66 (CH), 127.4 (CH), 127.6 (CH), 128.1 (CH), 128.3 (CH), 128.5 (CH), 129.5 (d, $J = 12.5$ Hz), 132.2, 132.3, 133.2, 134.0, 138.9, 140.8-140.9 (m), 142.6-142.7 (m). $^{31}\text{P NMR}$ (162 MHz, CDCl_3) $\delta = -142.8$ (t, $^1J_{\text{PH}} = 212$ Hz); HRMS (FAB, NBA): m/z found: 599.2054 $[M+H]^+$; calcd for $\text{C}_{42}\text{H}_{33}\text{P}_2$: 599.2057.

Synthesis of 1,2-bis(2-(2,4,6-tri-*tert*-butylphenyl)diphosphenyl)-[1,1'-binaphthalen]-3-yl)ethane [(*S,S*)-2]

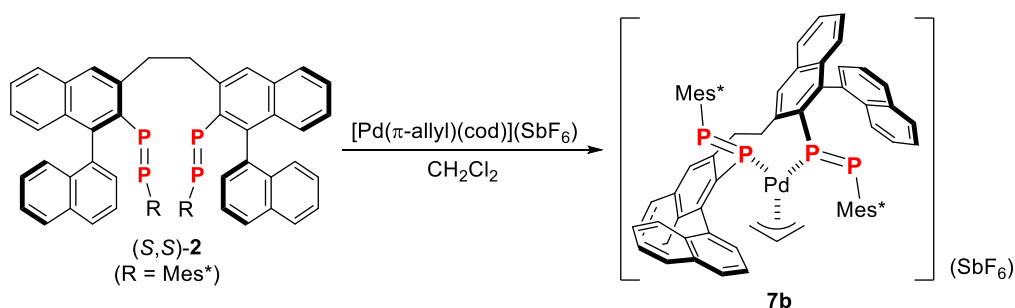


To a solution of phosphine (*S,S*)-6 (45 mg, 75 μmol) in Et_2O (2 mL) was added *n*-BuLi (1.58 M in hexane; 97 μL , 154 μmol) dropwise at room temperature in a glovebox filled with an argon. After the mixture was stirred at room temperature for 10 min, Mes^*PCl_2 (104 mg, 299 μmol) was added in one portion. The mixture was stirred for 30 min. DBU (46 mg, 302 μmol) in Et_2O (2 mL) was added. The reaction mixture was stirred for 30 min, and then the solvent was removed under reduced pressure. The residue was chromatographed on silica gel with hexane/toluene = 3/1 ($R_f = 0.15$) to give (*S,S*)-2 as yellow solid (24 mg,

21 μmol , 28%).

Mp. 153 $^{\circ}\text{C}$ (decomp.); $[\alpha]_{\text{D}}^{24} = +250$ ($c = 0.01$ in CH_2Cl_2); ^1H NMR (400 MHz, CDCl_3) $\delta = 0.90$ (br s, 36H), 1.23 (s, 18H), 3.57 (s, 4H), 6.89 (d, $J = 8.9$ Hz, 2H), 7.13-7.18 (m, 2H), 7.22 (s, 4H), 7.24-7.28 (m, 2H), 7.40-7.47 (m, 8H), 7.50 (dd, $J = 8.0, 6.8$ Hz, 2H), 7.82 (d, $J = 8.0$ Hz, 2H), 7.89 (d, $J = 7.5$ Hz, 2H), 7.905 (s, 2H), 7.906 (d, $J = 7.7$ Hz, 2H). ^{13}C $\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) $\delta = 31.4$ (CH_3), 33.7 (CH_3), 34.8, 37.8 (CH_2), 38.2, 122.3 (CH), 125.8 (CH), 126.0 (CH), 126.3 (CH), 126.5 (CH $\times 2$), 126.7 (CH), 126.9 (CH), 127.2 (CH), 127.5 (CH), 128.3 (CH), 128.4 (CH), 128.6 (CH), 132.5, 133.2, 133.7, 134.3, 137.4 (dd, $J = 48$ Hz), 138.3, 140.8, 141.6, 141.9 (d, $J = 48$ Hz), 149.5, 153.5; ^{31}P $\{^1\text{H}\}$ NMR (162 MHz, CDCl_3) $\delta = 451.1, 528.8$ (d, $^1J_{\text{PP}} = 570$ Hz); HRMS (ESI, positive): m/z found: 1169.5574 [$M+\text{Na}$] $^+$, calcd for $\text{C}_{78}\text{H}_{86}\text{P}_4+\text{Na}$: 1169.5578.

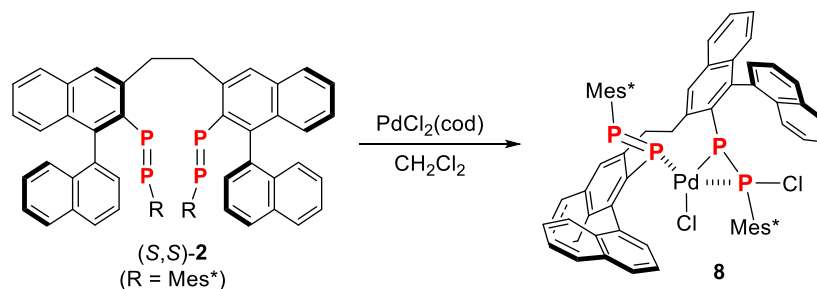
Reaction of (*S,S*)-**2** with $[\text{Pd}(\pi\text{-allyl})(\text{cod})](\text{SbF}_6)$



To a mixture of (*S,S*)-**2** (8.6 mg, 7.5 μmol) and $[\text{Pd}(\pi\text{-allyl})(\text{cod})](\text{SbF}_6)$ (3.6 mg, 7.3 μmol) was added CH_2Cl_2 (1 mL) in a glovebox filled with an argon. After the reaction mixture was stirred at room temperature for 10 min, the volatiles were removed under reduced pressure. The residue was washed with pentane and diethyl ether to give palladium complex **7b** as orange solid (10.5 mg, 6.9 μmol , 91%).

Mp. 193 $^{\circ}\text{C}$ (decomp.). ^1H NMR (500 MHz, CD_2Cl_2) $\delta = 0.44$ (s, 9H), 0.45 (s, 9H), 0.78 (s, 9H), 0.84 (s, 9H), 1.24 (s, 9H), 1.32 (s, 9H), 1.65-1.71 (m, 1H), 2.29-2.34 (m, 1H), 3.38-3.44 (m, 1H), 3.48-3.54 (m, 1H), 3.66-3.85 (m, 4H), 4.48 (tt, $J = 13.6, 7.3$ Hz, 1H), 6.77 (d, $J = 8.6$ Hz, 1H), 6.81 (d, $J = 8.5$ Hz, 1H), 7.04-7.06 (m, 2H), 7.17-7.19 (m, 2H), 7.21-7.31 (m, 8H), 7.36-7.39 (m, 2H), 7.56-7.62 (m, 4H), 7.96 (d, $J = 7.4$ Hz, 1H), 7.98 (d, $J = 8.2$ Hz, 1H), 8.00-8.06 (m, 4H), 8.17 (s, 1H), 8.20 (s, 1H); ^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CD_2Cl_2) $\delta = 31.5$ (CH_3), 31.6 (CH_3), 33.0 (CH_3), 33.1 (CH_3), 34.5 (CH_3), 34.6 (CH_3), 35.1, 35.2, 37.7 ($\times 2$), 39.0 ($\times 2$), 39.3 (CH_2), 75.0 (d, $J = 22$ Hz, CH_2), 78.0 (d, $J = 24$ Hz, CH_2), 118.8 (CH), 121.9 (CH), 122.1 (CH), 123.4 (CH), 123.6 (CH), 124.3 (CH), 124.9 (CH), 126.0 ($\times 2$), 126.5 (CH $\times 2$), 127.0 (CH), 127.1 (CH), 127.22 (CH), 127.25 (CH), 127.4 (CH), 127.5 (CH), 127.77 (CH $\times 3$), 127.85 (CH), 128.1 (CH $\times 2$), 128.7 (CH $\times 2$), 128.8 (CH), 129.0 (CH), 129.1 (CH), 129.2 (CH), 130.60 (CH), 130.65 (CH), 132.8, 132.9, 134.10, 134.14, 135.06, 135.10, 135.21, 135.27, 138.0, 138.4, 141.3 ($\times 2$), 144.3 ($\times 2$), 152.3, 152.4, 158.3, 158.4; Four quaternary carbon signals bound to a phosphorus atom could not be observed due to their low intensity. ^{31}P NMR (162 MHz, CDCl_3) $\delta = 334.2$ ($J_{\text{PP}} = 532, 36$ Hz), 339.0 ($J_{\text{PP}} = 530, 36$ Hz), 470.0 ($J_{\text{PP}} = 532$ Hz), 479.4 ($J_{\text{PP}} = 530$ Hz); HRMS (ESI, positive) m/z found: 1293.5107. (M^+), calcd for $\text{C}_{81}\text{H}_{91}\text{P}_4^{106}\text{Pd}$ 1293.5106. HRMS (ESI, negative) m/z found: 234.8940 ($[\text{SbF}_6]^-$), calcd for SbF_6 234.8942.

Reaction of (*S,S*)-2 with [PdCl₂(cod)]₂



To a mixture of (*S,S*)-2 (19.1 mg, 16.7 μmol) and PdCl₂(cod) (4.8 mg, 16.7 μmol) was added CH₂Cl₂ (1 mL) in a glovebox filled with an argon. After the reaction mixture was stirred at room temperature for 10 min, the volatiles were removed under reduced pressure. Pentane and acetonitrile were added to the residue, and then the pentane layer was collected. The solvent was removed under reduced pressure to give palladium complex **8** as orange solid (12.3 mg, 9.28 μmol , 55%).

Mp. 158 °C (decomp.); ¹H NMR (500 MHz, CD₂Cl₂) δ = 0.41 (s, 9H), 0.8 (br s, 9H), *1) 1.31 (s, 9H), 1.39 (s, 9H), 1.4 (br s, 9H), *1) 1.62 (s, 9H), 3.27-3.36 (m, 2H), 3.90-3.95 (m, 1H), 5.48-5.53 (m, 1H), 5.63 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H), 5.68 (d, J = 8.1 Hz, 1H), 6.28 (d, J = 8.6 Hz, 1H), 6.55 (dd, J = 6.9, 1.2 Hz, 1H), 6.70 (d, J = 9.1 Hz, 1H), 6.90 (dd, J = 8.6, 6.9 Hz, 1H), 6.94 (ddd, J = 8.6, 6.8, 1.2 Hz, 1H), 7.02 (ddd, J = 8.6, 6.8, 1.7 Hz, 1H), 7.16 (d, J = 1.2 Hz, 1H), 7.17 (d, J = 8.0 Hz, 1H), 7.19-7.28 (m, 3H), 7.31 (s, 1H), 7.33-7.39 (m, 3H), 7.38 (d, J = 1.8 Hz, 1H), 7.40-7.43 (m, 1H), 7.45-7.50 (m, 2H), 7.60 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 8.6 Hz, 1H), 7.72 (d, J = 8.6 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.1 Hz, 1H), 7.98 (s, 1H); *1) These signals could not be observed at room temperature likely due to the coalescence, and became sharpened at low temperature (Figures S21 and S22). ¹³C {¹H} NMR (125 MHz, CD₂Cl₂) δ = 31.3 (CH₃), 31.5 (CH₃), 32.6 (br, CH₃), 33.60, 33.65, 34.3 (br, CH₃), 34.9, 35.2, 35.7 (CH₂), 37.5, 39.0, 40.0 (CH₂), 122.9 (CH), 123.1 (CH), 124.9 (CH), 125.73 (CH), 125.78 (CH), 126.1 (CH), 126.2 (CH), 126.32 (CH), 126.36 (CH), 126.5 (CH), 126.64 (CH), 126.67 (CH), 127.0 (CH), 127.1 (CH), 127.2 (CH), 127.49 (CH), 127.52 (CH), 127.6 (CH), 127.8 (CH), 127.9 (CH), 128.0 (CH), 128.18 (CH), 128.21 (CH), 128.6 (CH), 128.9 (CH), 129.0 (d, J = 101 Hz), 129.7 (CH), 131.19 (CH), 131.25, 132.3, 132.6, 134.0 (\times 2), 134.1, 134.2, 134.5, 137.9 (d, J = 6.7 Hz), 138.9 (\times 2), 139.1, 139.7 (d, J = 4.8 Hz), 140.5 (br), 141.8, 145.2 (dd, J = 28.9, 9.6 Hz), 151.7 (d, J = 2.9 Hz), 152.3, 152.5 (d, J = 10.6 Hz), 153.7 (d, J = 8.7 Hz); Several carbon signals could not be observed due to their low intensity and/or superimposition. ³¹P {¹H} NMR (162 MHz, CDCl₃) δ = -39.6 (d, J = 591 Hz), 97.4 (ddd, J = 591, 385, 16 Hz), 338.9 (dd, J = 540, 385 Hz), 463.2 (dd, J = 540, 16 Hz); HRMS (ESI, positive): m/z found: 1287.4396 [M-Cl]⁺; calcd for C₇₈H₈₆ClP₄Pd: 1287.4403.

2. Spectral Data

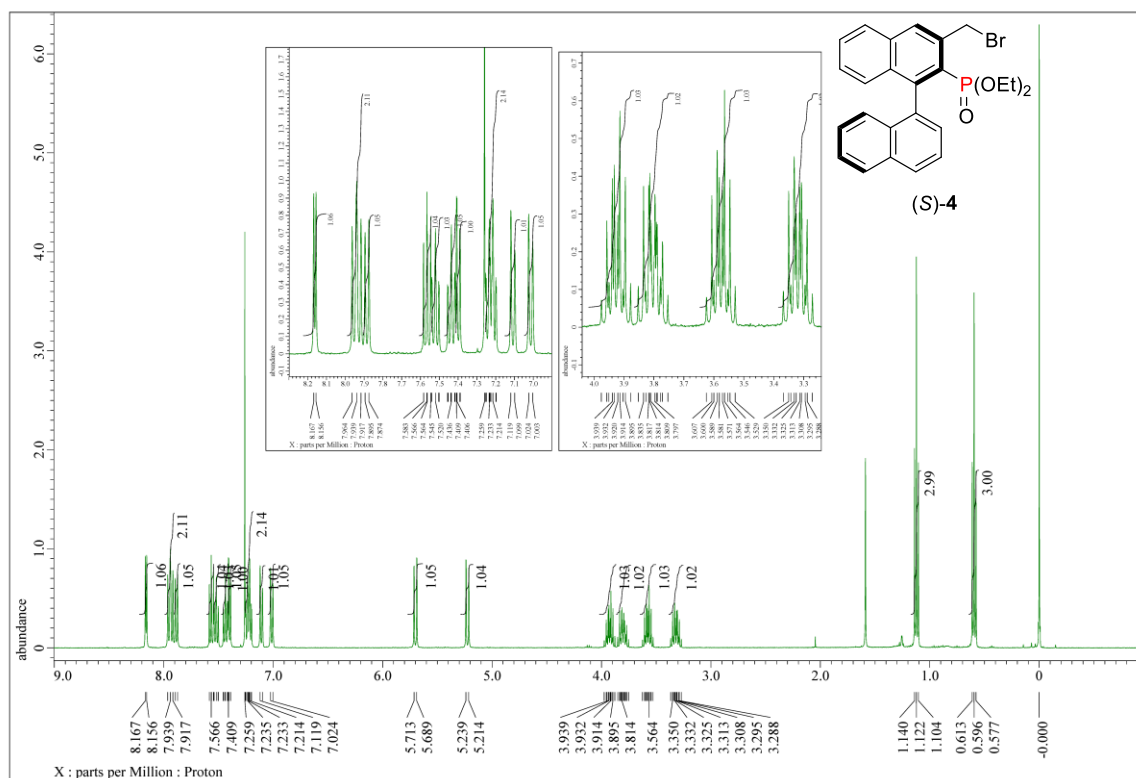


Figure S1. ¹H NMR Spectrum of (S)-4.

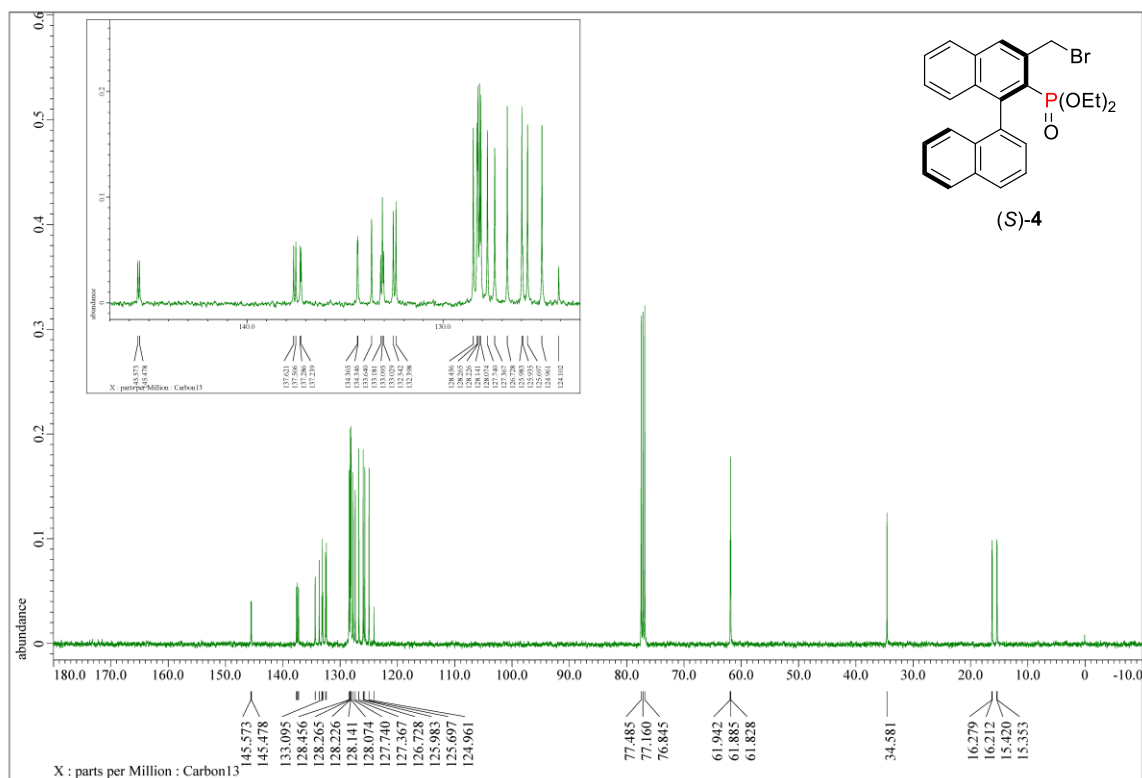


Figure S2. ¹³C NMR Spectrum of (S)-4.

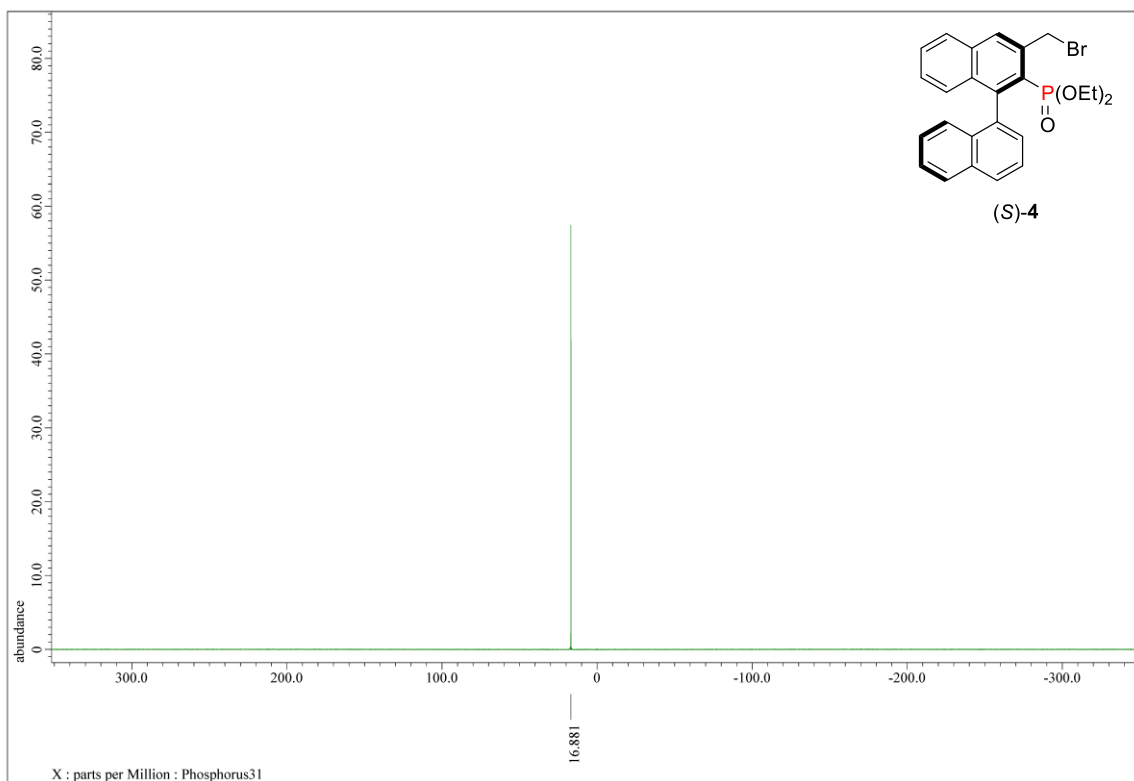


Figure S3. ^{31}P NMR Spectrum of (S)-4.

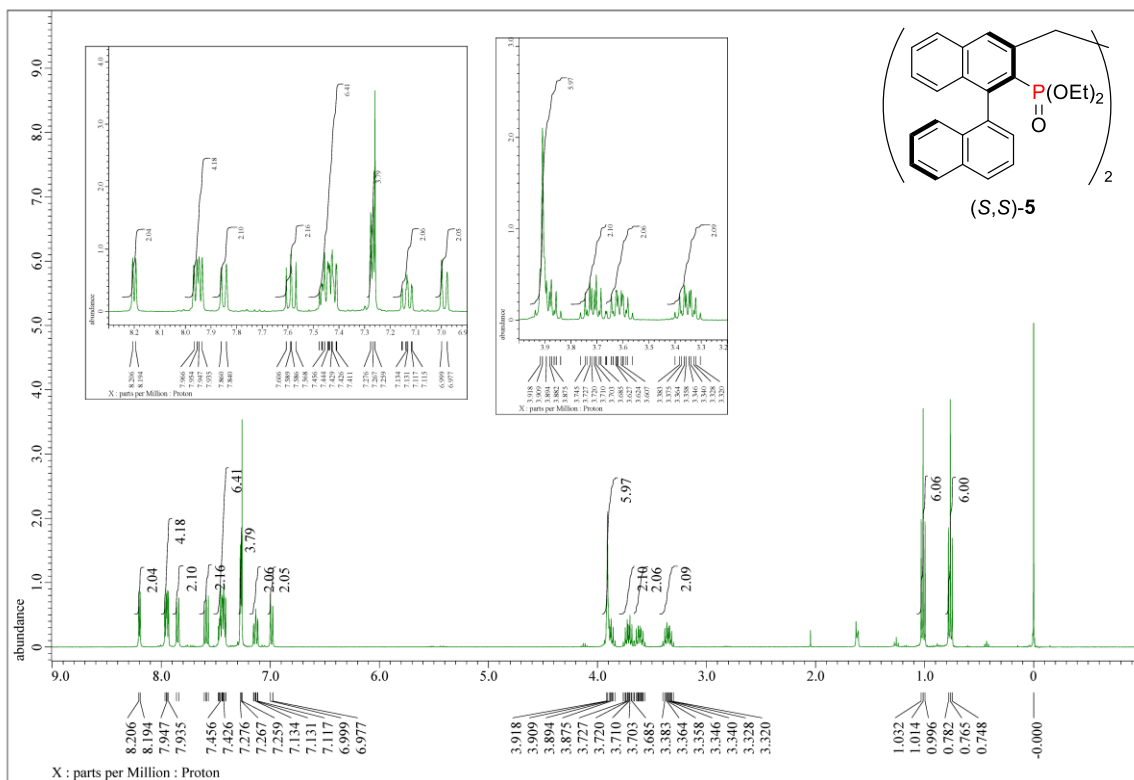


Figure S4. ^1H NMR Spectrum of (S,S)-5.

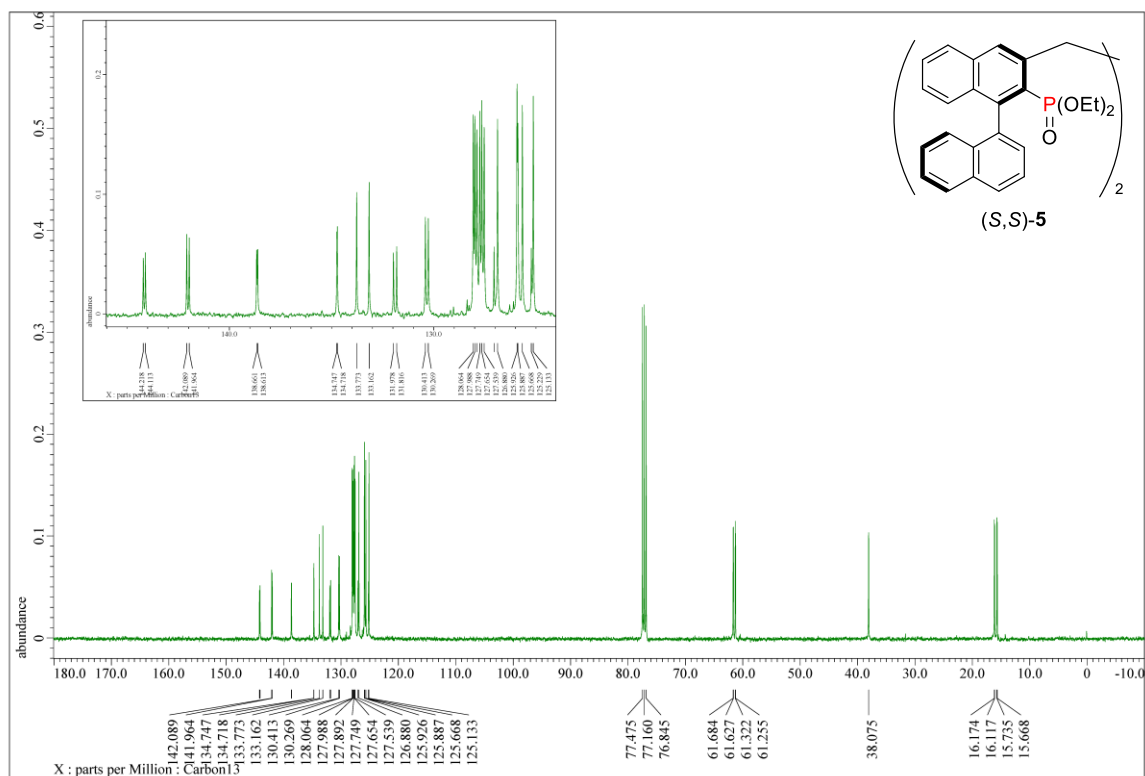


Figure S5. ¹³C NMR Spectrum of (S,S)-5.

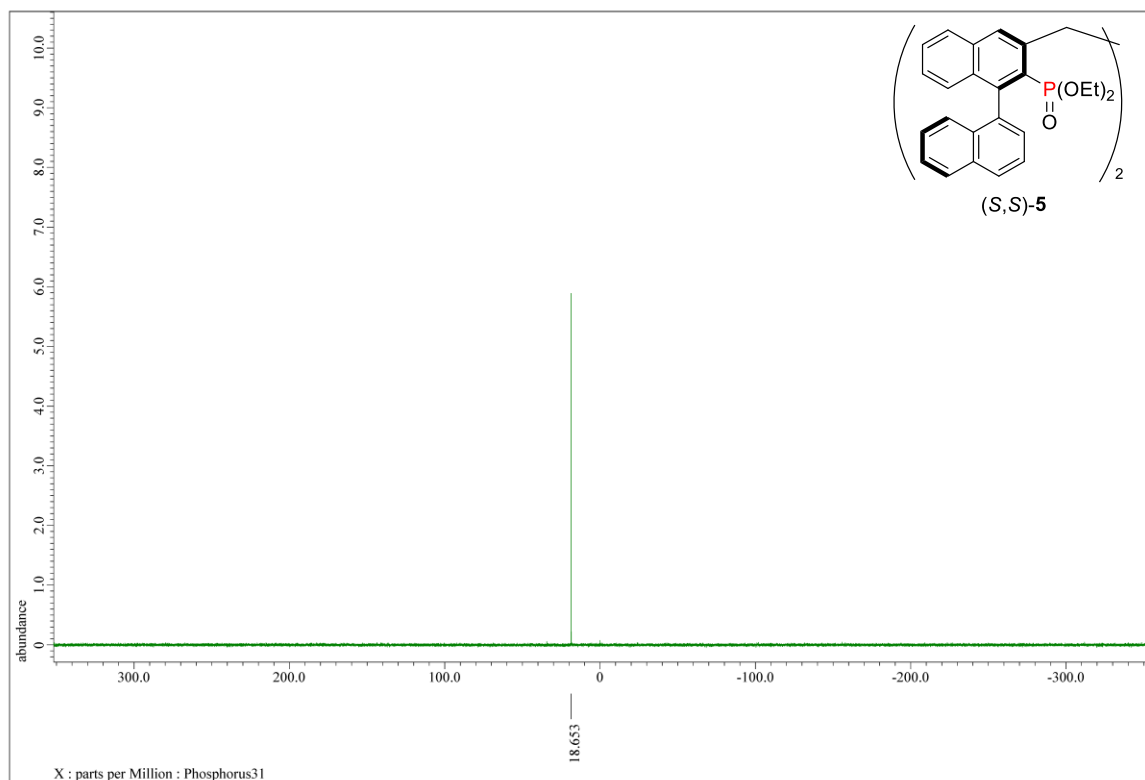


Figure S6. ³¹P NMR Spectrum of (S,S)-5.

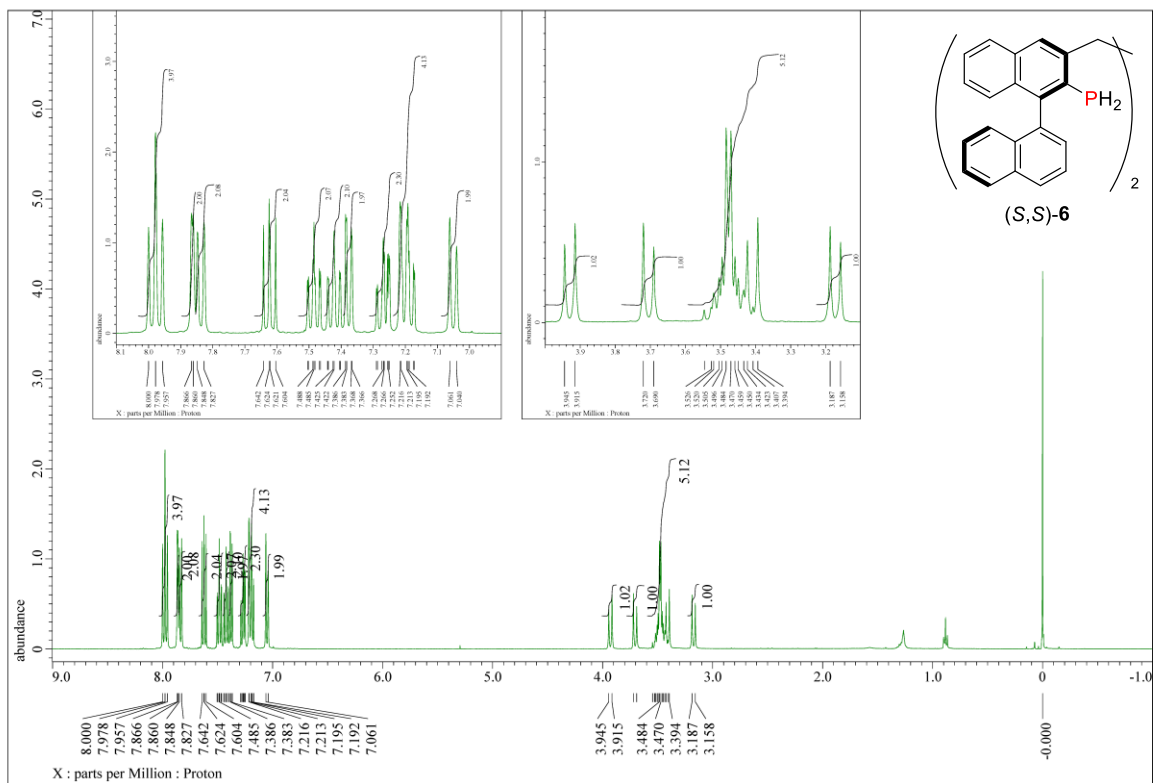


Figure S7. ¹H NMR Spectrum of (S,S)-6.

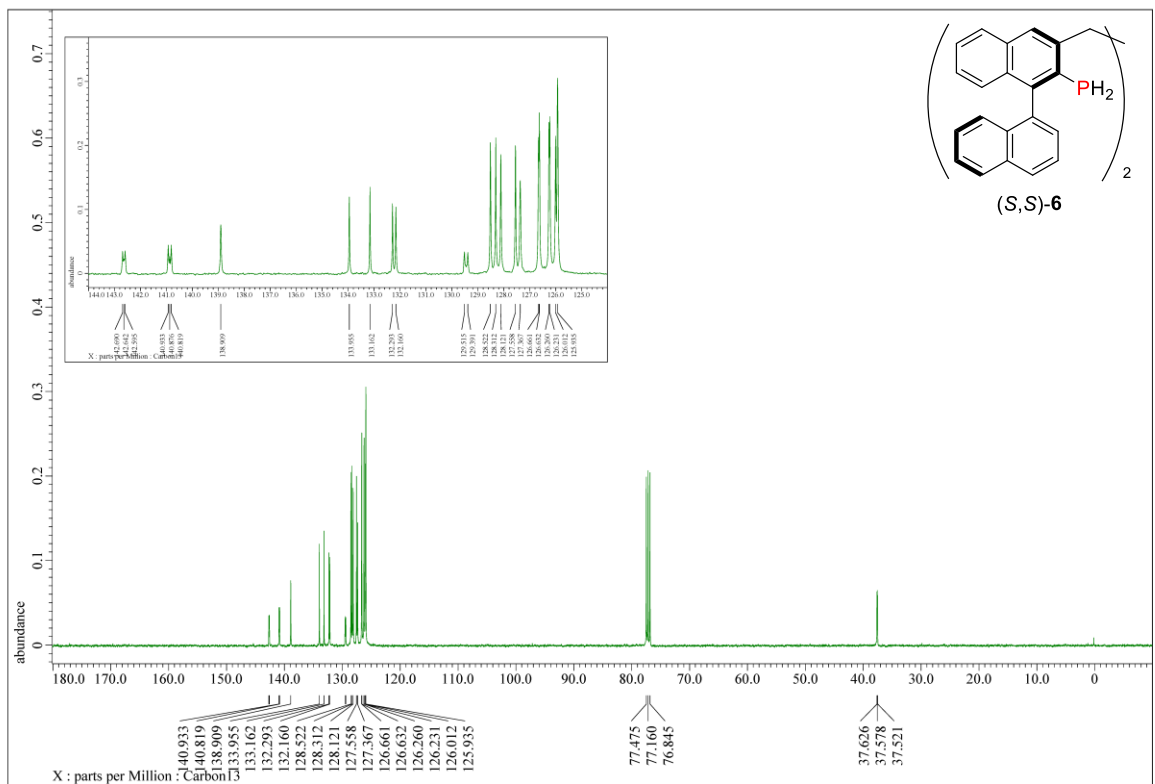


Figure S8. ¹³C NMR Spectrum of (S,S)-6.

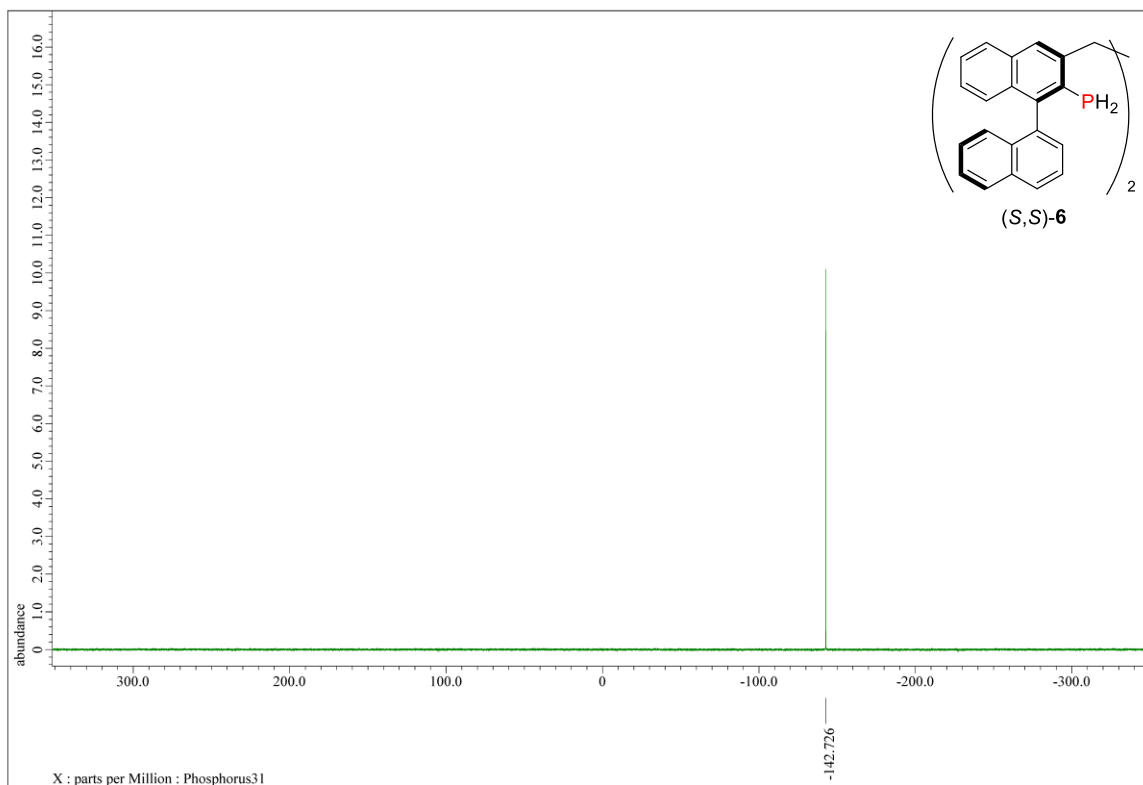


Figure S9. ^{31}P NMR Spectrum of (S,S)-6.

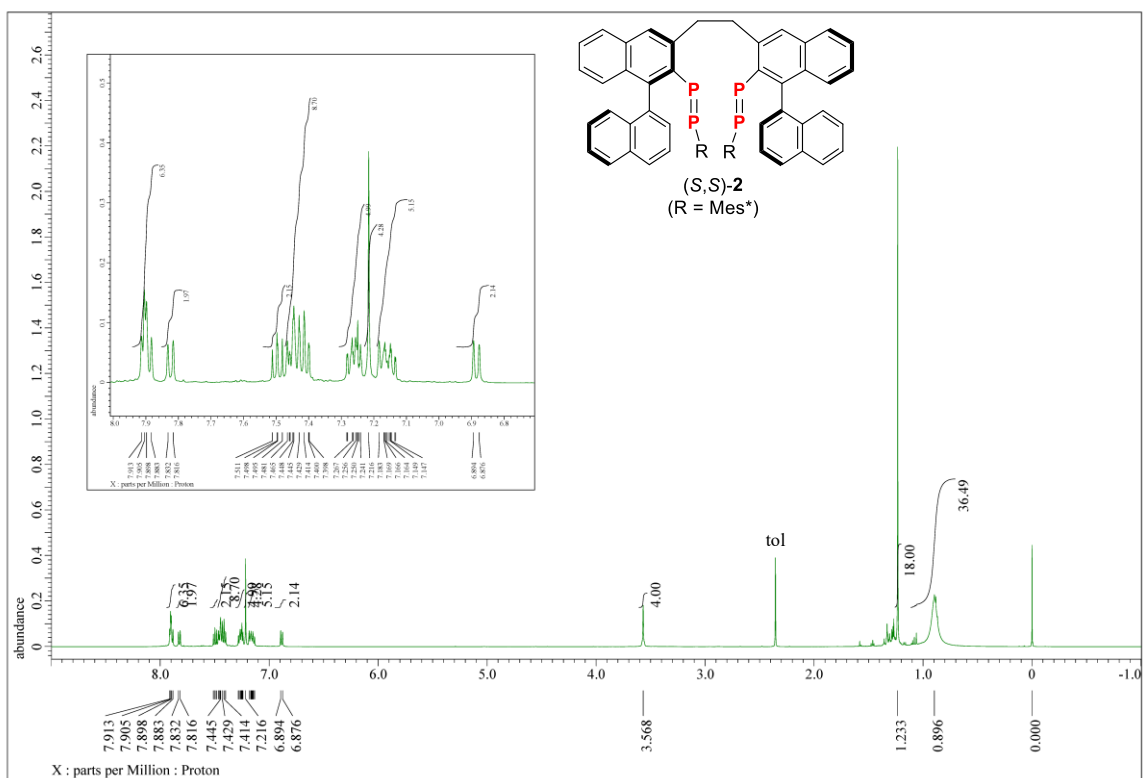


Figure S10. ^1H NMR Spectrum of (S,S)-2.

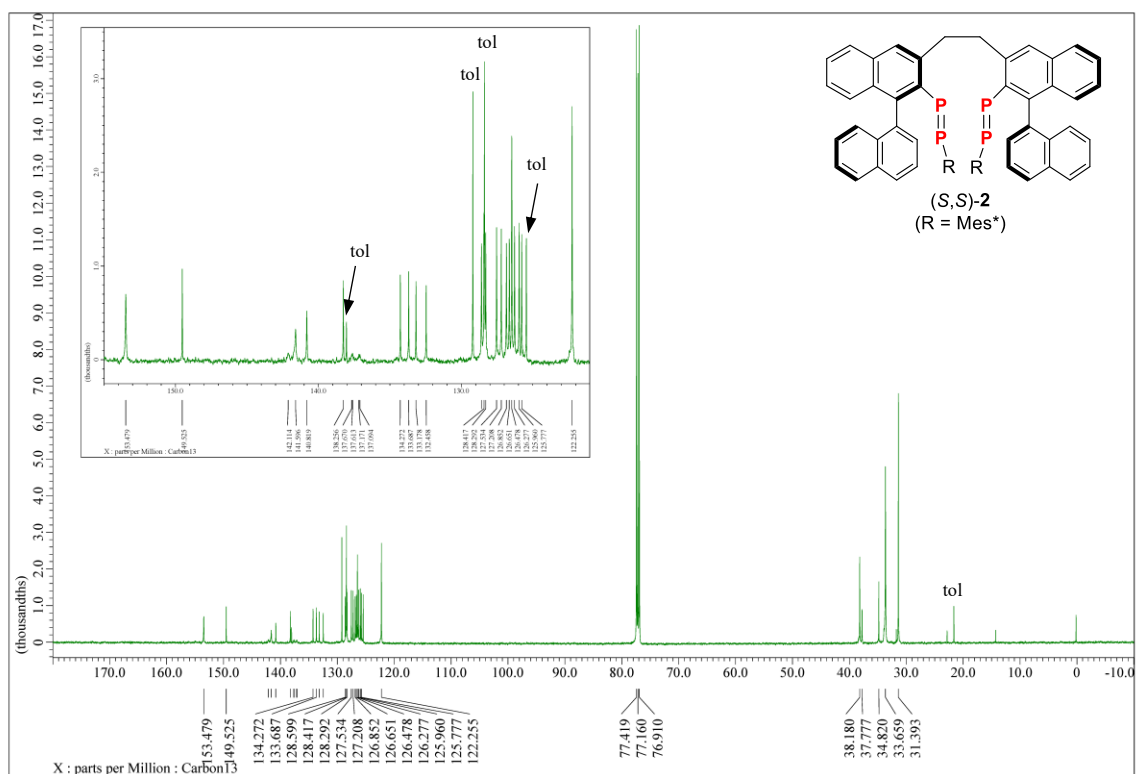


Figure S11. ¹³C NMR Spectrum of (S,S)-2.

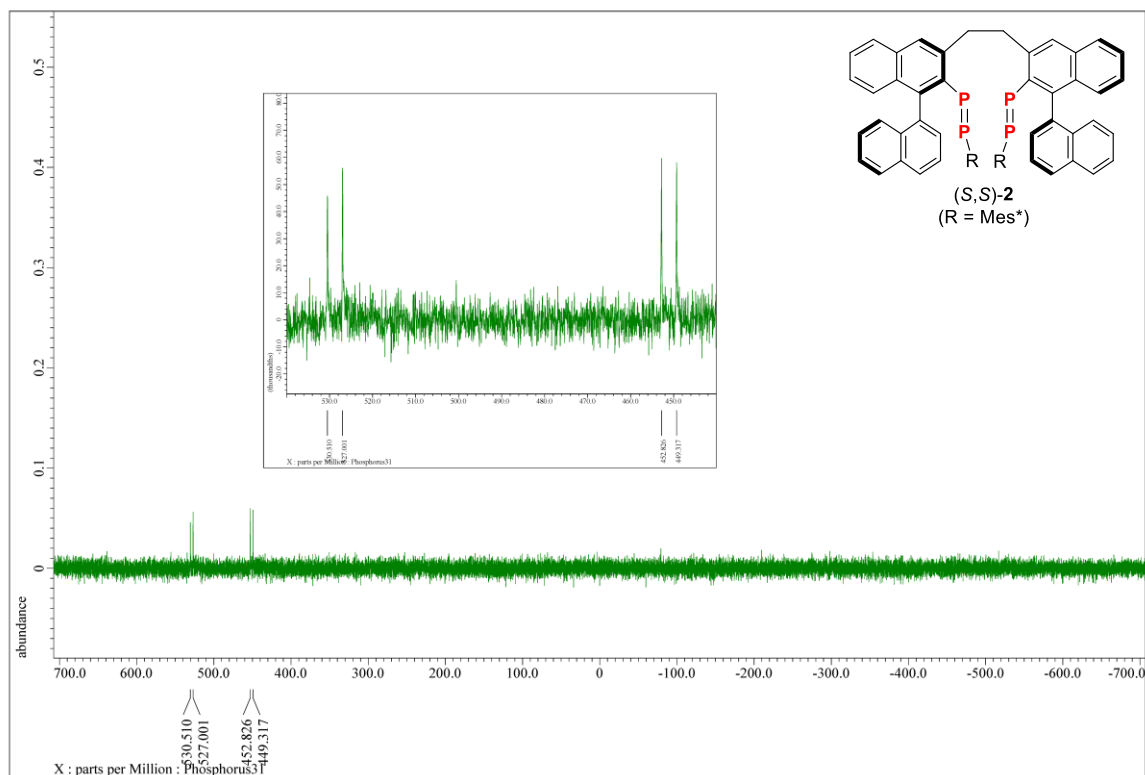


Figure S12. ³¹P NMR Spectrum of (S,S)-2.

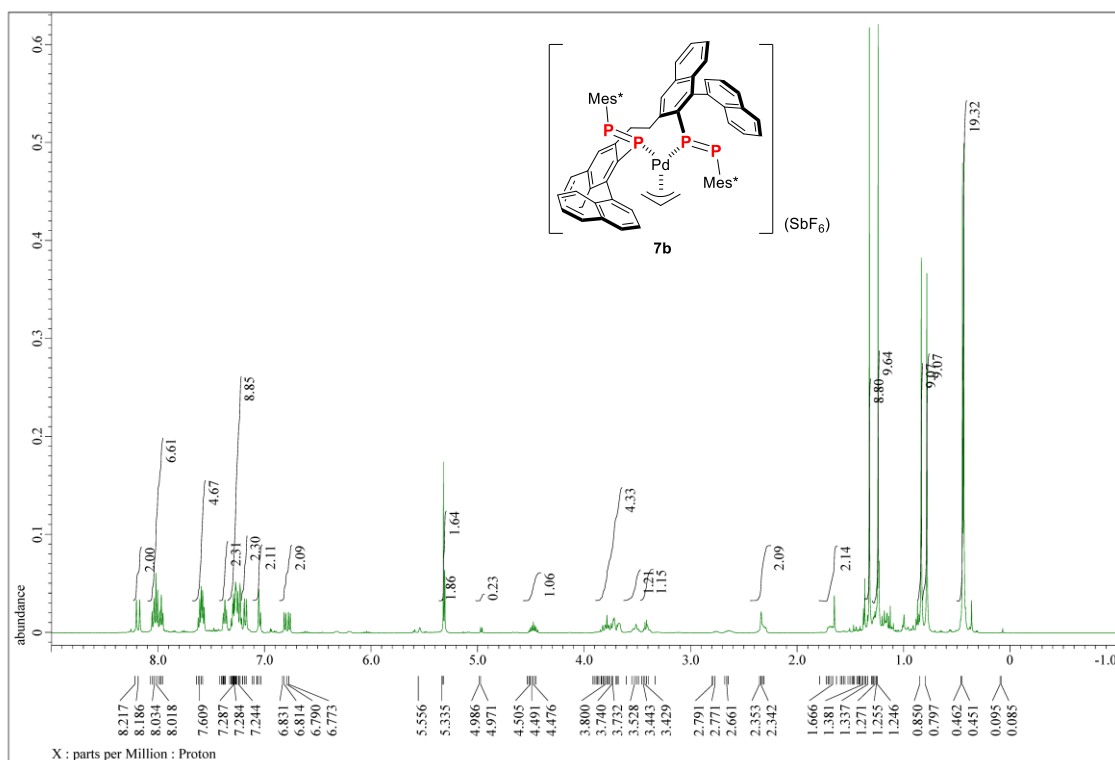


Figure S13. 1H NMR Spectrum of Palladium complex 7b (allyl).

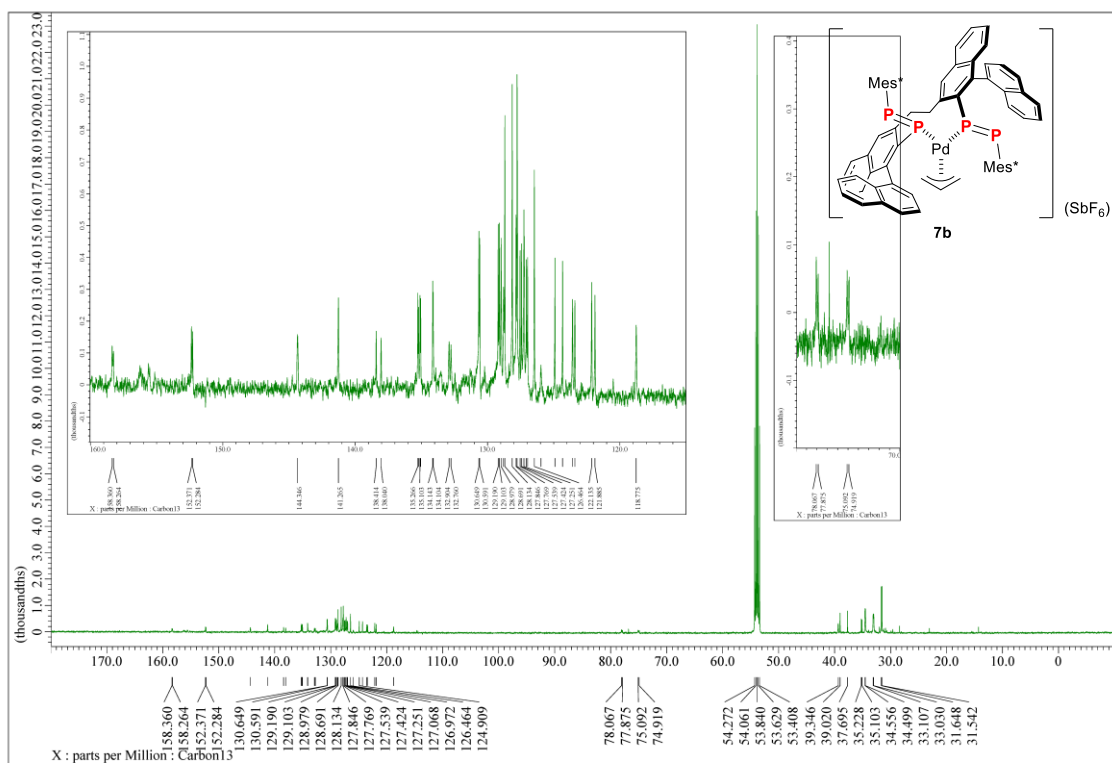


Figure S14. ^{13}C NMR Spectrum of Palladium Complex 7b.

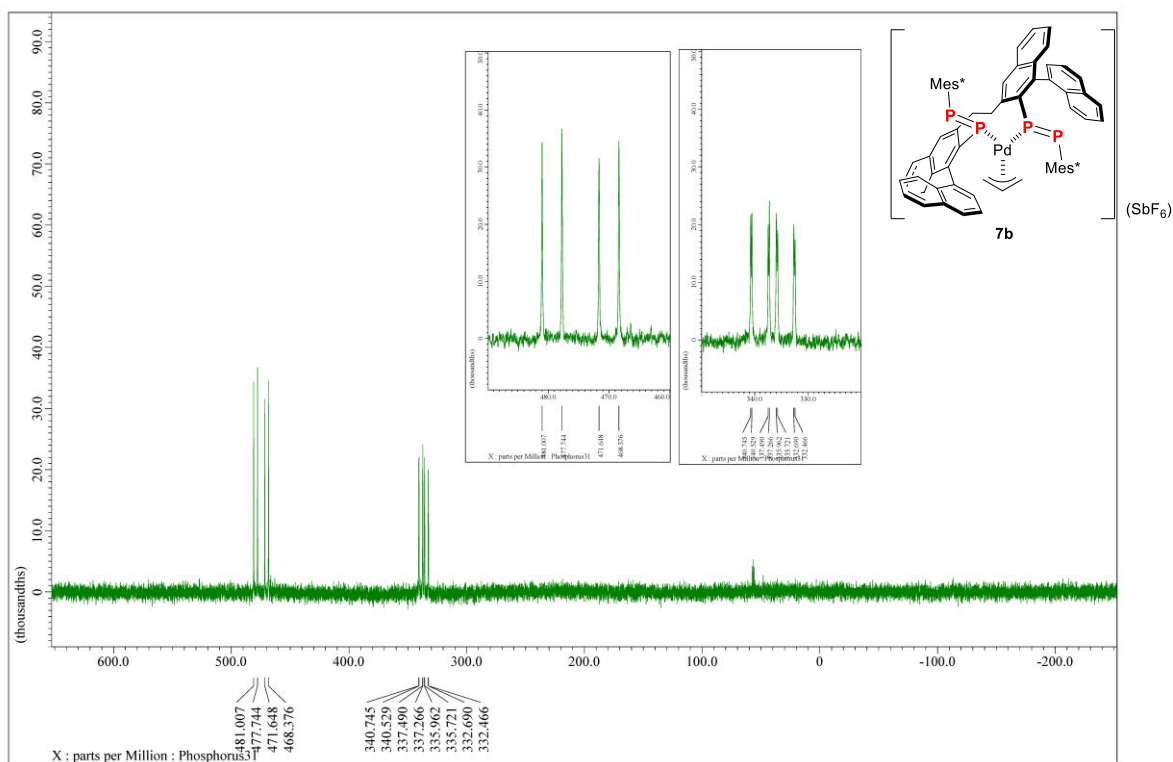


Figure S15. ^{31}P NMR Spectrum of Palladium Complex 7b.

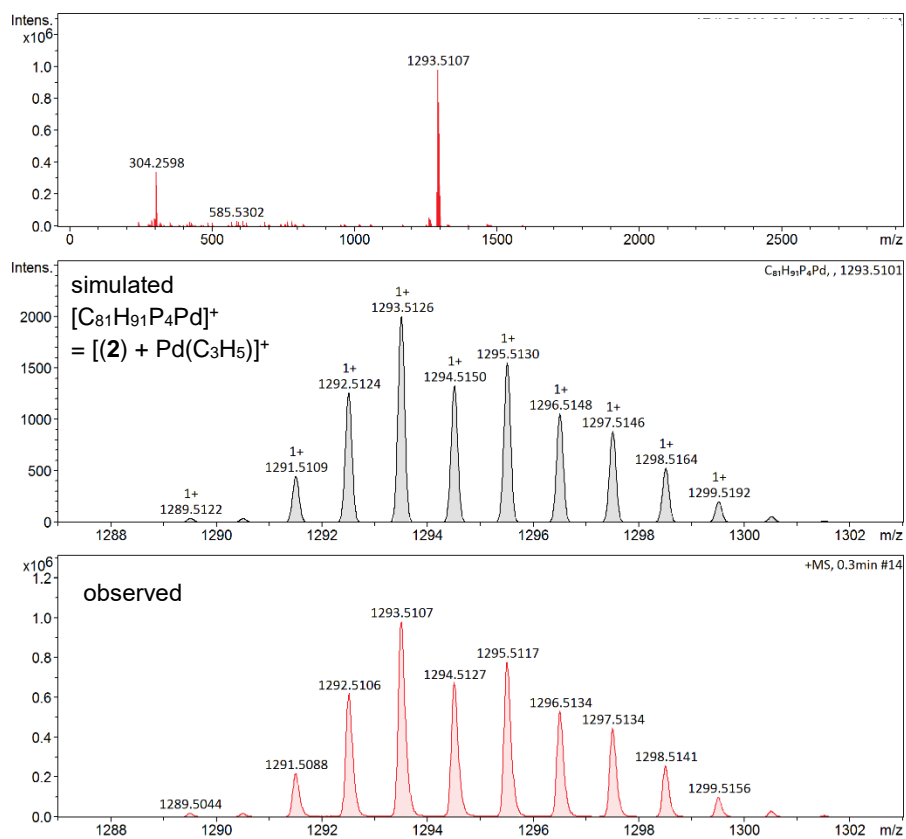


Figure S16. ESI-MS spectra (positive mode) of palladium complex of 7b in THF solution.

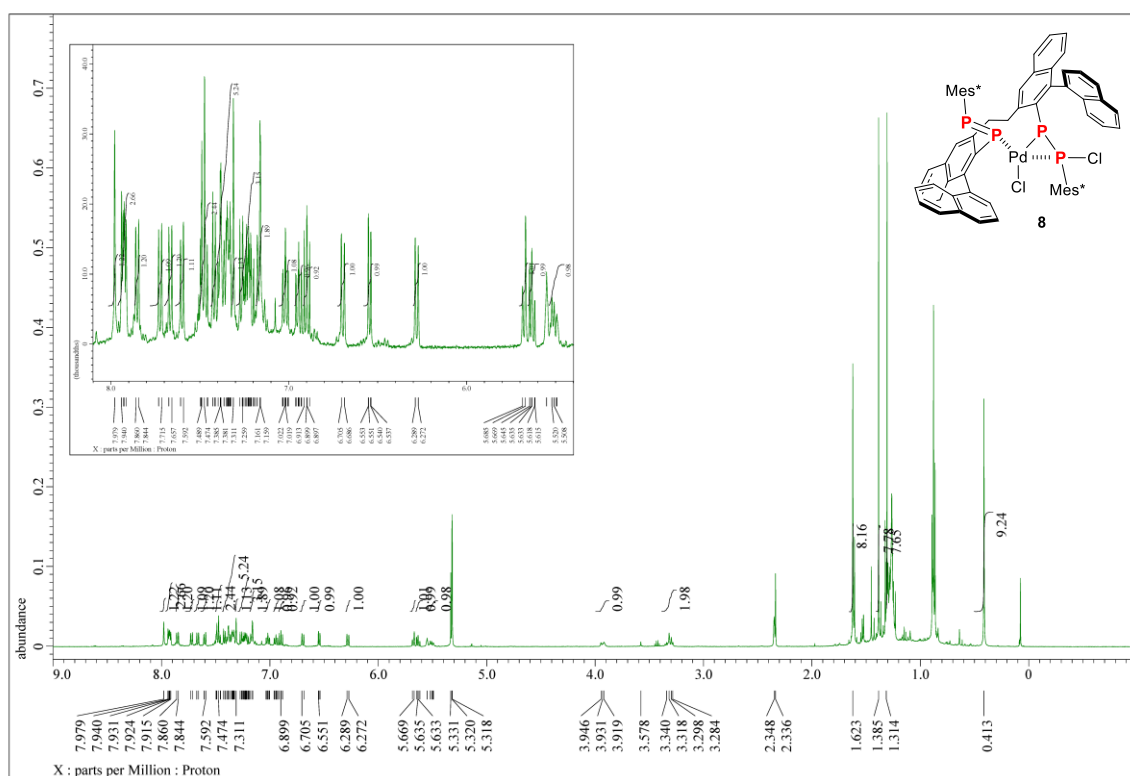


Figure S17. ¹H NMR Spectrum of Palladium Complex 8.

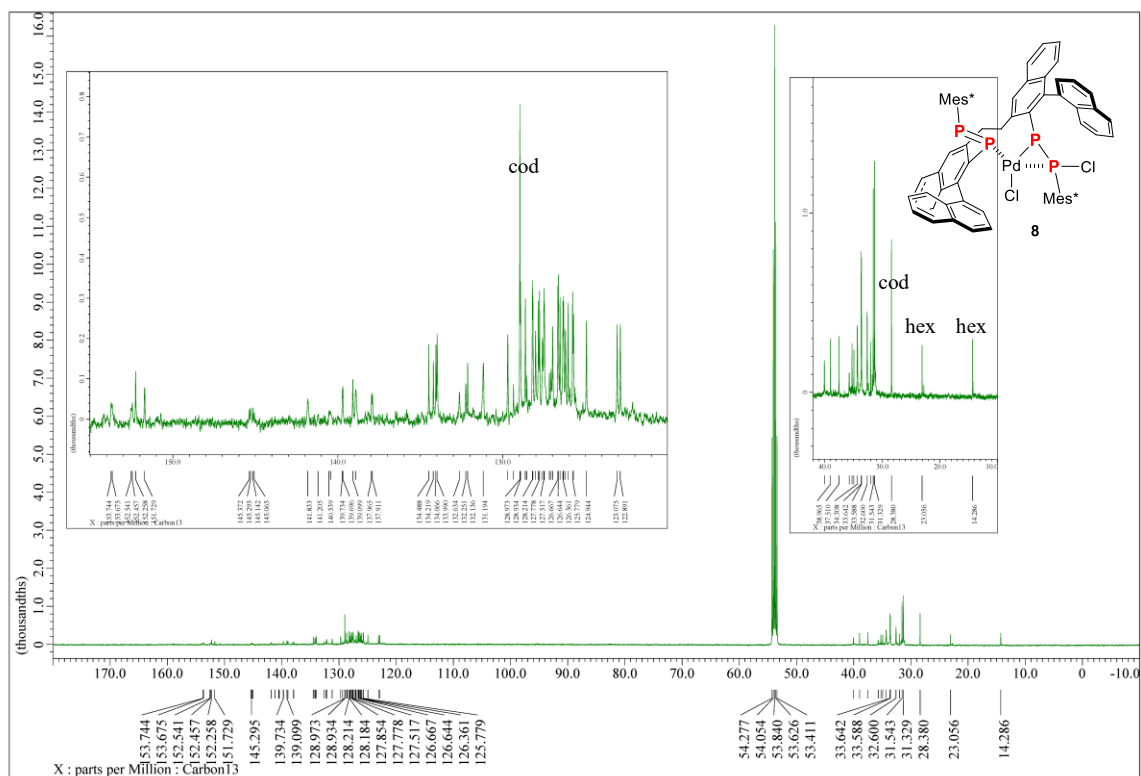


Figure S18. ¹³C NMR Spectrum of Palladium Complex 8.

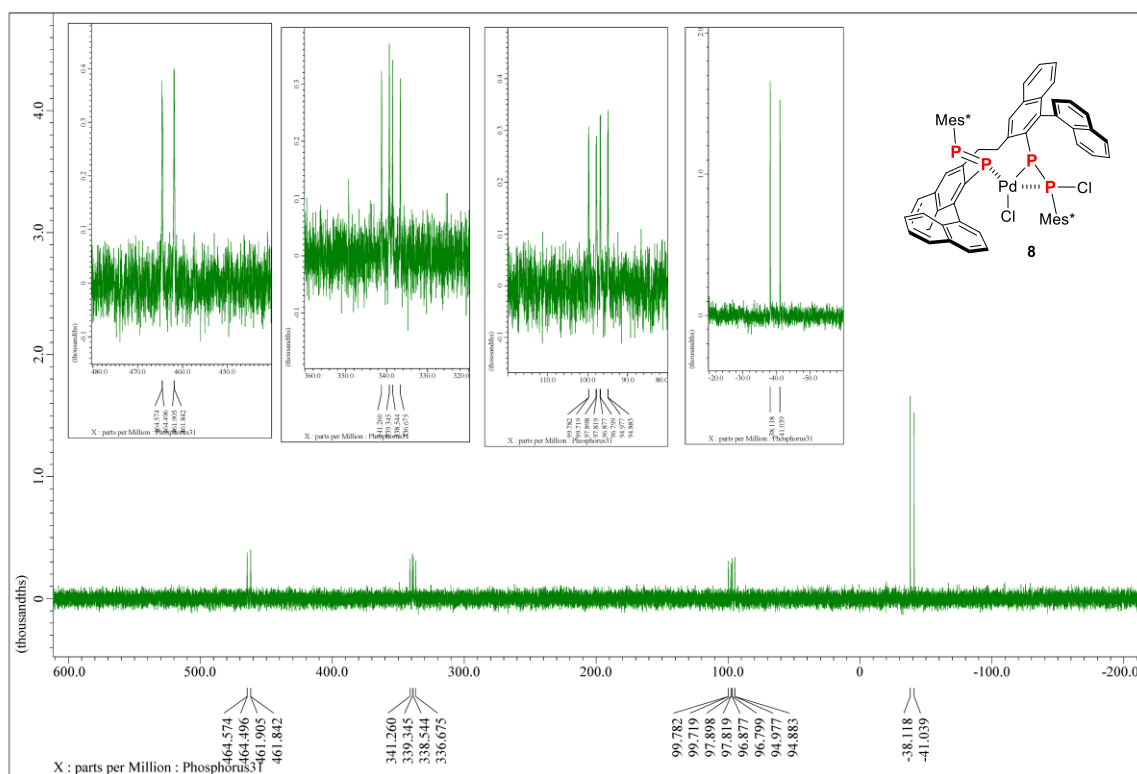


Figure S19. ^{31}P NMR Spectrum of Pd complex 8.

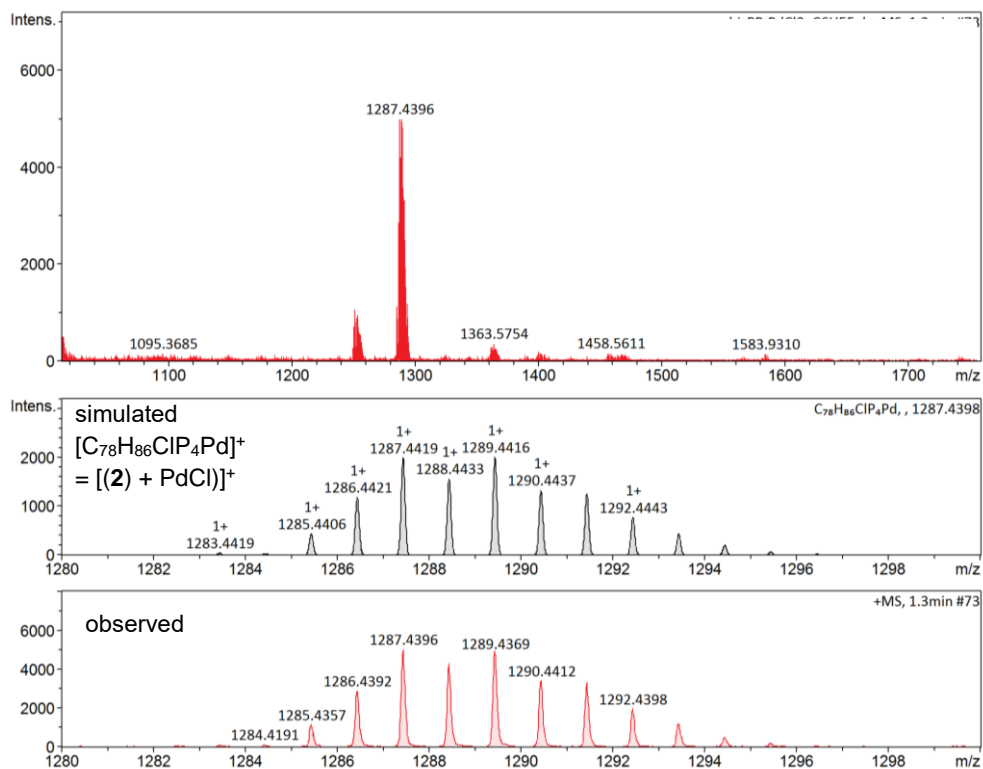


Figure S20. ESI-MS Spectra (positive mode) of Palladium complex of 8 in $\text{C}_6\text{H}_5\text{F}$ solution.

3. Temperature dependent NMR spectra

3-1. Temperature dependent ^1H NMR spectra of **8**.

In the ^1H NMR spectrum of complex **8** in a CD_2Cl_2 solution at room temperature, four of six *t*-butyl signals were observed as the sharp singlet signals whereas two signals assignable to *ortho* position of one of Mes* groups were not observed. We have already confirmed that two *tert*-butyl groups at *ortho*-position of Mes* group were observed as the non-equivalent signals in diphosphene complexes **2** and **7b** whereas those of free diphosphenes **1** and **2** were observed as broad equivalent signals. These results indicate the restricted rotation around P–C(Mes*) bond in both cases. One of P–C(Mes*) bonds in complex **8** should be rotated at a NMR time scale. To confirm the possibility to the frozen rotation at low temperature, the valuable ^1H NMR spectra were measured in a CD_2Cl_2 solution. The result was shown in Figure S21. After cooling a CD_2Cl_2 solution, two *tert*-butyl signals (red squares) were additionally observed along with the others observed initially (blue circles).

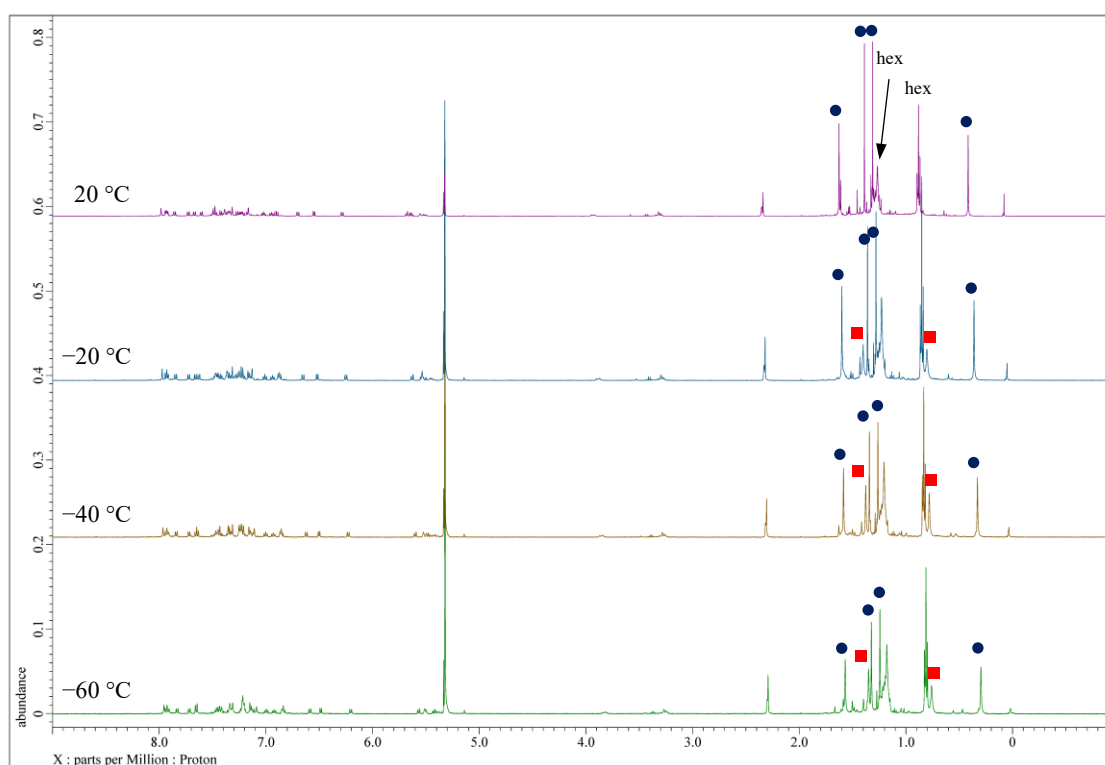


Figure S21. Temperature dependent ^1H NMR spectra (500 MHz) of **8** in CD_2Cl_2 .

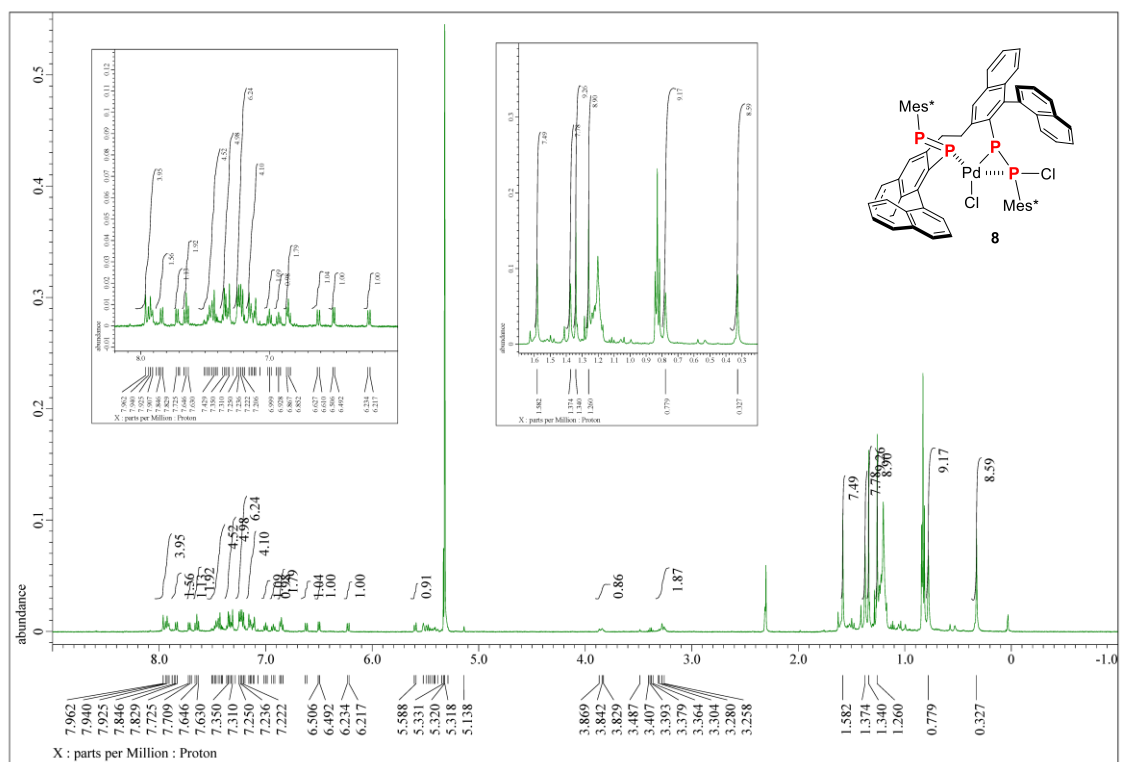


Figure S22. ^1H NMR spectrum (500 MHz) of **8** in CD_2Cl_2 at $-40\text{ }^\circ\text{C}$.

3-2. The monitoring of the reaction of (*S,S*)-**2** and PdCl₂(cod) to form **8** in the ³¹P NMR spectra.

Bis(diphosphene) (*S,S*)-**2** (3.0 mg, 2.6 μmol) and PdCl₂(cod) (0.7 mg, 2.5 μmol) was added to an NMR tube equipped with a J-Young valve in a glovebox filled with an argon, and then CD₂Cl₂ (0.3 mL) dried over CaH₂ was charged via the vacuum transfer at -196 °C. The NMR tube was directly injected to the precooled (-80 °C) JEOL JNM-ECZ500R spectrometer. The measurements were carried out in order at -60 °C, -40 °C, -20 °C, 0 °C, and 20 °C with 1600 scan times (ca. 57 min). The results were shown in Figure S23. The intensity of the signals derived from (*S,S*)-**2** decreased at -20 °C, indicating that the reaction of (*S,S*)-**2** and PdCl₂(cod) occurs around -20 °C. The signals derived from complex **8** became major at 0 °C.

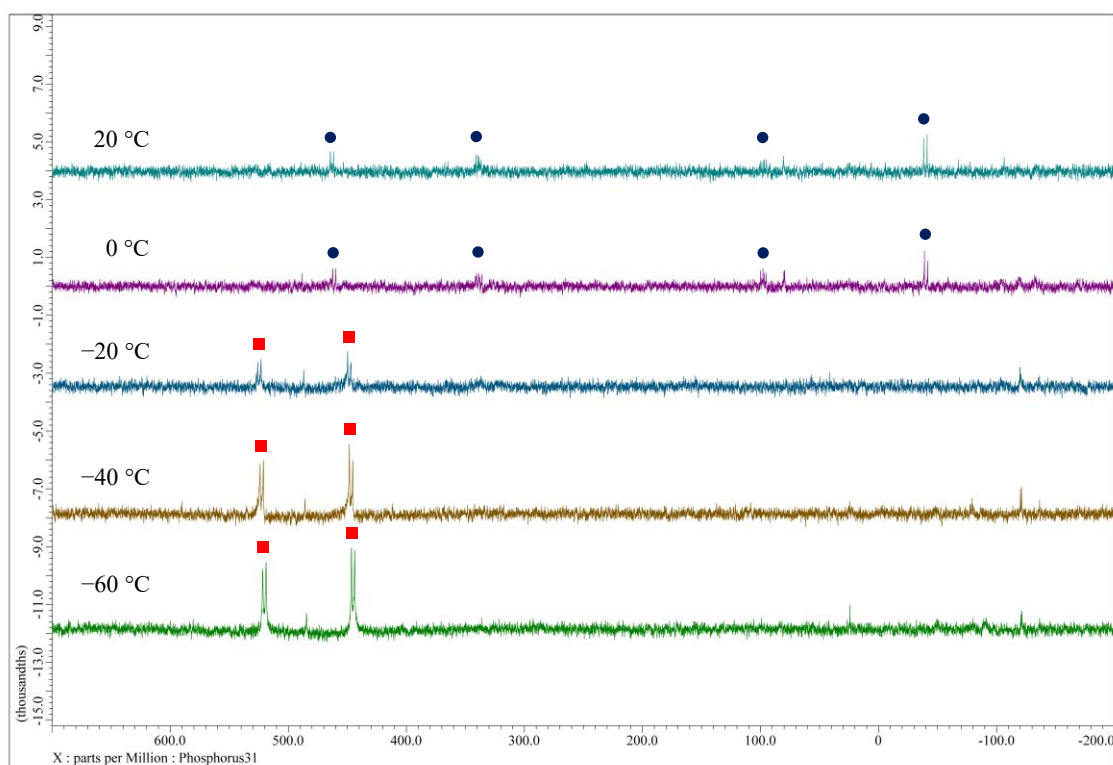


Figure S23. Temperature dependent ³¹P NMR spectra (500 MHz) of the reaction of (*S,S*)-**2** and PdCl₂(cod) in CD₂Cl₂.

4. X-ray Crystallographic Analysis

Single crystals of (*S,S*)-**2** were grown by recrystallization from a toluene/hexane solution at room temperature. X-ray data were collected on a Rigaku Saturn diffractometer with VariMax multi-layer mirror monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) at -170 °C (for (*S,S*)-**2**). The data were corrected for Lorentz and polarization effects. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the REQABS program in CrystalClear software. The structures were solved by direct methods (SIR2014^{S7}) and refined by full-matrix least squares against F^2 using all data. Non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were generated by AFIX instructions. All calculations were performed using Yadokari-XG 2009^{S8} software package except for refinement, which was performed using SHELXL-2013.^{S9}

Crystal data for (*S,S*)-**2** (CCDC-2121271): Crystal Size, $0.27 \times 0.21 \times 0.17$ mm; Molecular formula; $C_{78}H_{86}P_4 \cdot 2(C_8H_7)$; Molecular weight, $M = 1331.61$; $T = -750$ °C; triclinic; $P1$ (#1); $a = 10.603(4)$ Å, $b = 13.870(5)$ Å, $c = 13.974(5)$ Å, $\alpha = 101.884(4)^\circ$, $\beta = 96.491(2)^\circ$, $\gamma = 105.675(2)^\circ$, $V = 1904.9(11)$ Å³, $Z = 1$, $D_{\text{calc}} = 1.161$ g cm⁻³, $\mu = 0.145$ cm⁻¹, $2\theta_{\text{max}} = 55.0^\circ$, 19605 measured reflections, 14949 independent reflections [$R_{\text{int}} = 0.0241$], 885 refined parameters, Completeness to $\theta = 98.1\%$, $R_1 = 0.0373$ [$I > 2\sigma(I)$], $wR_2 = 0.0966$ (all data), GOF = 1.018, largest diff. peak/hole 0.256/ -0.215 e.Å⁻³. Absolute Structural Parameter 0.01(3).

Table S1. Selected Bond Lengths (Å) and Bond Angles (deg) of diphosphenes **1** and **2**.

structural parameter	(<i>S,S</i>)- 2	<i>rac</i> - 1 ^a	(<i>S</i>)- 1 ^a
$d(\text{P-P}) / \text{Å}$	2.0388(12), 2.0355(13)	2.0323(6)	2.0351(7)
$d(\text{P-C}_{\text{Np}}) / \text{Å}$	1.855(3), 1.850(3)	1.8523(13)	1.853(2)
$d(\text{P-C}_{\text{Mes}^*}) / \text{Å}$	1.858(3), 1.863(3)	1.8565(13)	1.8643(19)
$\text{deg}(\text{C}_{\text{Np}}\text{-P-P}) / ^\circ$	99.33(9), 104.66(9)	98.59(4)	102.64(6)
$\text{deg}(\text{P-P-C}_{\text{Mes}^*}) / ^\circ$	98.21(9), 97.03(9)	103.07(4)	97.72(6)
(Naph)-(Naph) / $^\circ$ ^b	79.15(5), 89.93(6)	79.41(3)	82.56(3)
(CPP)-(Naph) / $^\circ$ ^c	75.73(5), 61.46(6)	76.96(3)	86.64(5)
(CPP)-(Mes*) / $^\circ$ ^d	85.79(7), 88.72(8)	89.13(4)	81.39(5)

a) Ref S1. b) Dihedral angles between the two naphthyl rings. c) Dihedral angles between the CPP plane containing the C_{Np} atom and the naphthyl ring. d) Dihedral angles between the CPP plane containing the C_{Mes*} atom and the benzene ring of the Mes* groups.

5. Theoretical Calculations

All theoretical calculations were performed using the Gaussian 09^{S10} and GRRM14^{S11} programs on a NEC LX 110Rh-1 system of the Research Center for Computational Science, Japan. All structures were optimized without any symmetry assumptions, and zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated. Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary). The local minima of palladium complexes **7⁺**, **7b**, and **8** were optimized at an M06 functional^{S12} with the basis set of SDD^{S13} (Pd,Sb) and 6-31G(d) (other atoms) level of theory in conjunction with PCM model (dichloromethane)^{S14} with or without Grimme's D3 dispersion correction.^{S15} NBO calculations^{S16} were carried out at a PBE0 functional^{S17} with the basis set of SDD^{S13} (Pd) and 6-311+G(d) level (other atoms) in conjunction with PCM model (dichloromethane).^{S14}

5-1. Optimization of Local Minima of Palladium Complexes of **7⁺** and **7b**.

The possible structures of palladium complexes **7⁺** are shown in Figures S24 and S25. The anions, NaBAr^F₄ (Ar^F = 3,5-(CF₃)₂C₆H₃) or SbF₆⁻, were not included for the optimization of **7⁺**. Other conformations except for the η^1 coordination of both the P=P moieties were not considered on the basis of the observed ³¹P chemical shifts of **7a** and **7b**. P_{BNp} and P_{Mes*} represent the phosphorus atom of binaphthyl and Mes* groups coordinates to a palladium atom, respectively. The *syn* or *anti* configuration represents the orientation of P atom (pink circle with a white character) and benzene ring **R** (red) in the naphthyl group at 1-position in binaphthyldiphosphene. The *anti* or *gauche* conformation represents the orientation of two binaphthyl groups tethered by the ethylene (C₂H₄) moiety. The optimization of complex **7b** was carried out in the combination of the conformer **7A⁺** and SbF₆⁻, which was located at the proximity of the π -allyl group (**X**), ethylene tether (**Y**), and the P=P moiety (**Z**). The optimized structures of **7b_X** to **7b_Z** were shown in Figure S26.

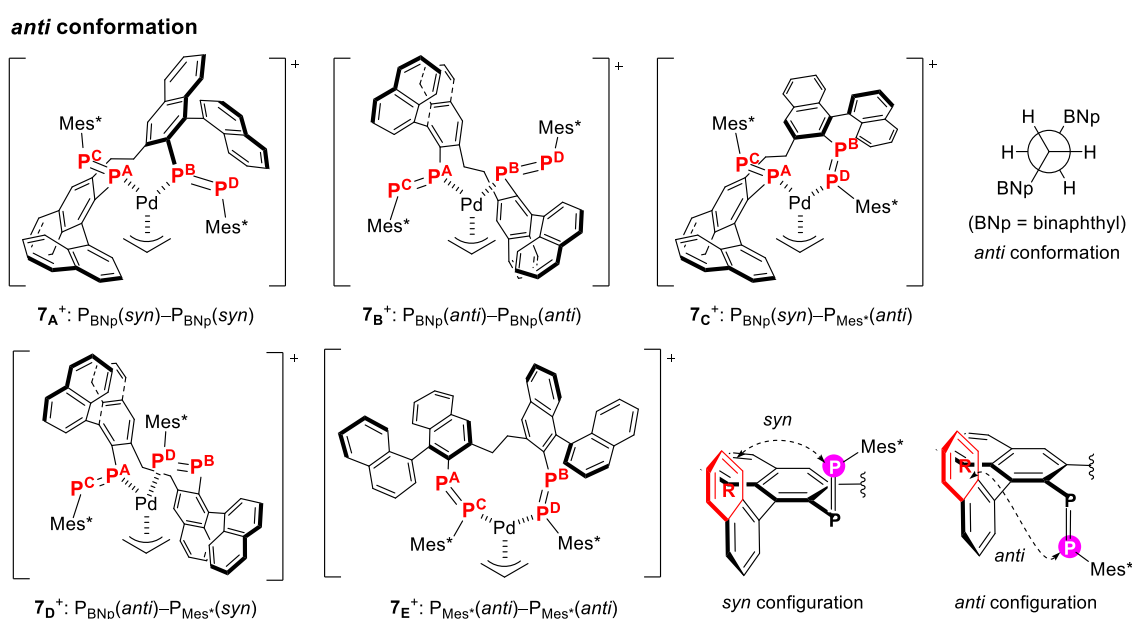


Figure S24. Optimized Structure of **7_A⁺** to **7_E⁺** with the *anti* conformation.

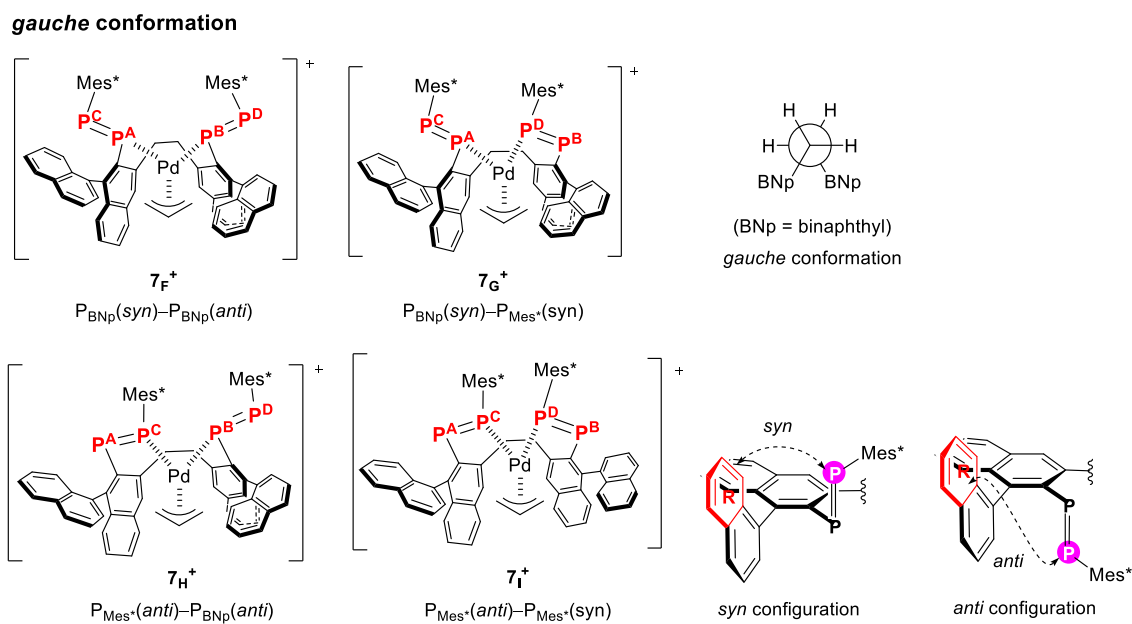


Figure S25. Optimized Structure of 7_F^+ to 7_I^+ with the *gauche* conformation.

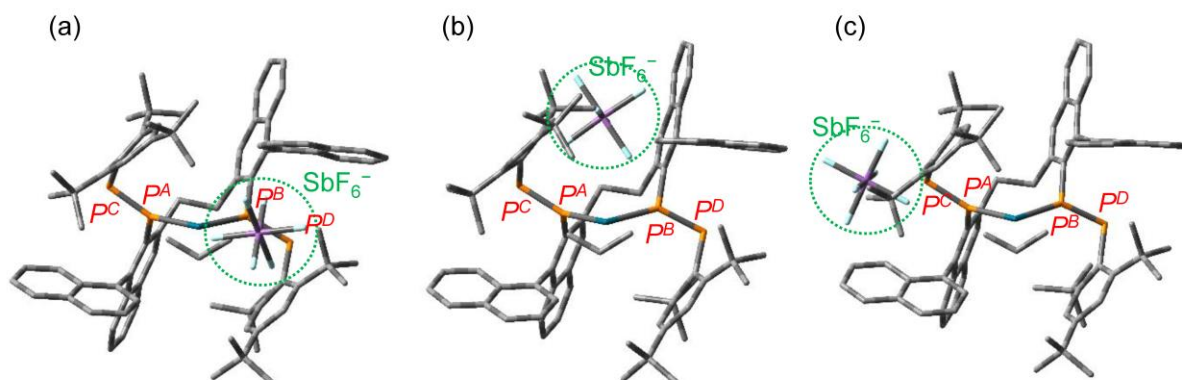


Figure S26. Optimized Structures of (a) $7b_X$, (b) $7b_Y$, and (c) $7b_Z$. Color code: Pd, blue; Sb, purple; P, orange; F, light-blue; and C, gray. Hydrogen atoms were omitted for clarity.

Table S2. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).^a

Structure	E	$E + ZPE$	H	G	ΔG^b
Local minimum optimized at M06/SDD (Pd) and 6-31G(d) (P, C, H) level					
<i>anti</i> conformer					
$7A^+$	-4632.07070813	-4630.567789	-4630.483032	-4630.680611	0.0
$7B^+$	-4632.06569516	-4630.562908	-4630.478063	-4630.675721	3.1
$7C^+$	-4632.05002565	-4630.547100	-4630.462043	-4630.661358	12.1
$7D^+$	-4632.04652534	-4630.542771	-4630.458118	-4630.654531	16.4
$7E^+$	-4632.03286472	-4630.529023	-4630.443972	-4630.645626	22.0
<i>gauche</i> conformer					
$7F^+$	-4632.06042039	-4630.558128	-4630.473350	-4630.672219	5.3
$7G^+$	-4632.05114601	-4630.547100	-4630.462807	-4630.658913	13.6
$7H^+$	-4632.04395729	-4630.540015	-4630.455541	-4630.652569	17.6
$7I^+$	-4632.02393872	-4630.520175	-4630.435100	-4630.635863	28.1
Local minimum optimized at M06/SDD (Pd,Sb) and 6-31G(d) (P, F, C, H) level					
$7b_X$	-5236.65958598	-5235.144362	-5235.048664	-5235.271945	0.0
$7b_Y$	-5236.65305197	-5235.137258	-5235.041571	-5235.265403	4.1
$7b_Z$	-5236.64982625	-5235.131297	-5235.036534	-5235.255643	10.2
Local minimum optimized at M06-D3/SDD (Pd) and 6-31G(d) (P, C, H) level					
<i>anti</i> conformer					
$7A^+$	-4632.15110266	-4630.648152	-4630.563208	-4630.761476	0.0
$7B^+$	-4632.14622479	-4630.642984	-4630.558233	-4630.755231	3.9
$7C^+$	-4632.12463178	-4630.621283	-4630.536340	-4630.735296	16.4
$7D^+$	-4632.12757574	-4630.623333	-4630.538679	-4630.735229	16.5
$7E^+$	-4632.10730671	-4630.603756	-4630.518670	-4630.719825	26.1
<i>gauche</i> conformer					
$7F^+$	-4632.14106127	-4630.637921	-4630.553446	-4630.749734	7.4
$7G^+$	-4632.12974973	-4630.625879	-4630.541373	-4630.738620	14.3
$7H^+$	-4632.12132904	-4630.617823	-4630.533198	-4630.731393	18.9
$7I^+$	-4632.09712449	-4630.592730	-4630.507847	-4630.707661	33.8

a) E : electronic energy; ZPE : zero-point energy; $H (= E + ZPE + E_{vib} + E_{rot} + E_{trans} + RT)$: sum of electronic and thermal enthalpies; $G (= H - TS)$: sum of electronic and thermal free energies. b) kcal mol⁻¹

5-2. Optimization of Local Minima of Palladium Complexes of **8** and Investigation on the Reaction Pathway of the Formation of Palladium complex **8_A** and **8_B**.

The possible structures of palladium complexes **8** are shown in Figure S27. The P=P and the [P–P(Cl)][−] moieties coordinate to a palladium atom in η^1 and η^2 fashions, respectively, in **8_A** to **8_D** and **8_F** to **8_I**, whereas both the P=P moieties coordinate to a palladium atom in η^1 fashions in **8_E** and **8_J**. The transition states were initially searched at B3LYP^{S18} or M06^{S12} functionals with the basis set of LanL2DZ^{S19} (Pd), 6-31G(d) (P, Cl), and 3-21G (C, H) levels. The transition states were verified by IRC calculations at the same level. The obtained structures were reoptimized at M06/SDD (Pd) and 6-31G(d) (P, Cl, C, H) in conjunction with PCM model (dichloromethane). Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary). Single point calculations were carried out at M06/SDD (Pd) and 6-311G(d,p) (P, Cl, C, H) in conjunction with PCM model (dichloromethane).

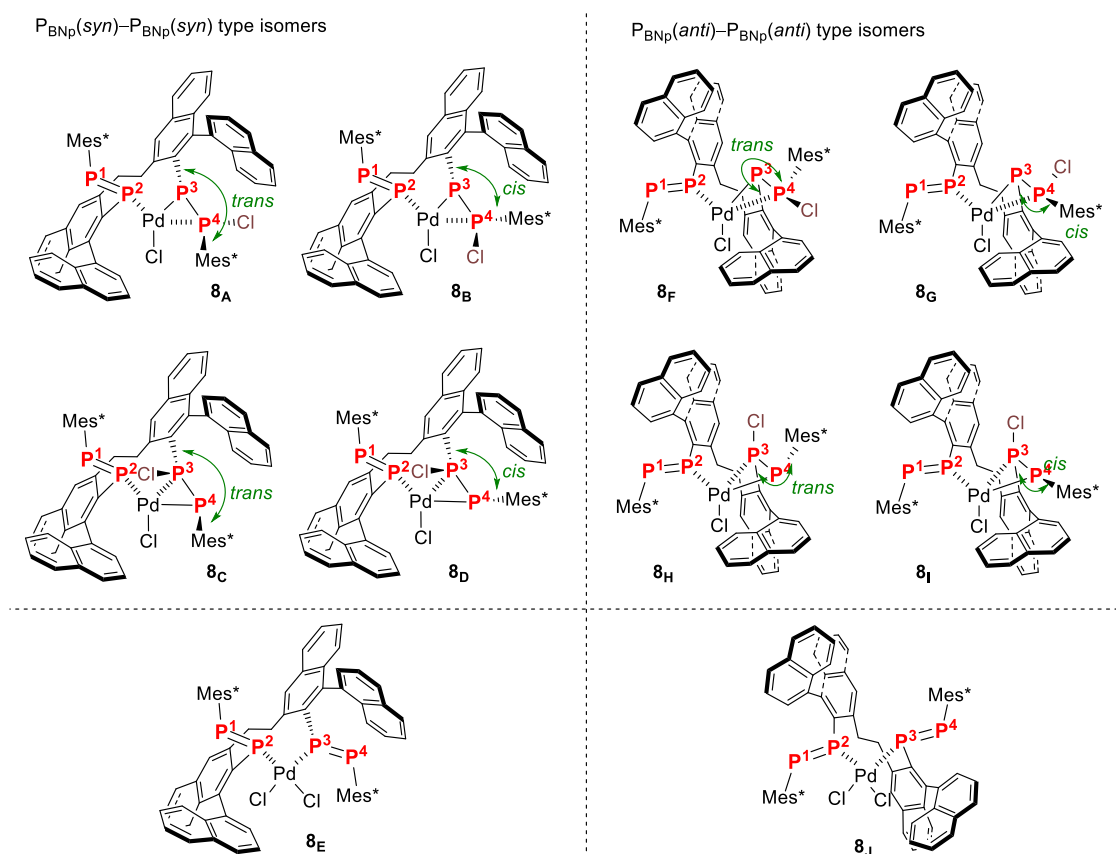


Figure S27. Optimized Structures of **8_A** to **8_J**.

Table S3. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).^a

M06/SDD (Pd) and 6-31G(d) (P, Cl, C, H) level of theory					
Structure	E	$E + ZPE$	H	G	ΔG^b
Local minimum					
8_A	-5435.40021436	-5433.970478	-5433.884494	-5434.087955	0.0
8_B	-5435.39912071	-5433.968891	-5433.883141	-5434.085570	1.5
8_C	-5435.39297301	-5433.962795	-5433.876845	-5434.081827	3.9
8_D	-5435.38268692	-5433.953120	-5433.866971	-5434.072452	9.7
8_E	-5435.39875730	-5433.967041	-5433.881671	-5434.082189	3.6
8_F	-5435.37895628	-5433.948575	-5433.862618	-5434.066358	13.6
8_G	-5435.38366336	-5433.954664	-5433.868150	-5434.074870	8.2
8_H	-5435.38976265	-5433.959249	-5433.873649	-5434.075825	7.6
8_I	-5435.37912346	-5433.948484	-5433.862671	-5434.065761	13.9
8_J	-5435.39303731	-5433.962727	-5433.876677	-5434.079572	5.3

Int-1	-5435.39169337	-5433.962034	-5433.876483	-5434.077020	6.9
Int-2	-5435.37952664	-5433.949774	-5433.863615	-5434.067587	12.9
Int-3_A	-5435.39175510	-5433.961107	-5433.875217	-5434.078038	6.2
Int-3_B	-5435.39066077	-5433.960451	-5433.874253	-5434.078595	5.9
Int-4_B	-5435.39088502	-5433.960106	-5433.874339	-5434.078205	6.1

Transition state					
TS-1	-5435.37549706	-5433.94708604	-5433.86150530	-5434.064174	14.9
TS-2	-5435.38086927	-5433.95166919	-5433.86627347	-5434.067484	12.9
TS-3_A	-5435.37909868	-5433.95030089	-5433.86472663	-5434.067358	12.9
TS-3_B	-5435.37609310	-5433.94530249	-5433.86027236	-5434.061091	16.9
TS-4_B	-5435.38254770	-5433.95304266	-5433.86739215	-5434.070760	10.8

M06-D3/SDD (Pd) and 6-31G(d) (P, Cl, C, H) level of theory					
Local minimum					
8_A	-5435.47534053	-5434.044537	-5433.958910	-5434.160600	0.0
8_B	-5435.47874826	-5434.047562	-5433.962202	-5434.162690	-1.3
8_C	-5435.46520695	-5434.034789	-5433.948925	-5434.153345	4.6
8_D	-5435.45518477	-5434.025304	-5433.939333	-5434.144212	10.3
8_E	-5435.47569606	-5434.044414	-5433.959005	-5434.159285	0.8
8_F	-5435.45297083	-5434.021772	-5433.936057	-5434.138285	14.0
8_G	-5435.46050505	-5434.030518	-5433.944439	-5434.148203	7.8
8_H	-5435.46368701	-5434.032939	-5433.947281	-5434.150653	6.2
8_I	-5435.45405456	-5434.022645	-5433.937173	-5434.138703	13.7
8_J	-5435.47035097	-5434.039934	-5433.953950	-5434.157224	2.1

Int-1	-5435.47069548	-5434.040341	-5433.954990	-5434.154652	3.7

Int-2	-5435.46327202	-5434.033084	-5433.947071	-5434.150504	6.3
Int-3A	-5435.47049090	-5434.039087	-5433.953480	-5434.155071	3.5
Int-3B	-5435.47119185	-5434.040458	-5433.954427	-5434.158166	1.5
Int-4B	-5435.47189015	-5434.039969	-5433.954632	-5434.154901	3.6
Transition state					
TS-1	-5435.45421214	-5434.025718	-5433.940204	-5434.141797	11.8
TS-2	-5435.46036171	-5434.030515	-5433.945267	-5434.146041	9.1
TS-3A	-5435.45527520	-5434.025226	-5433.940092	-5434.140414	12.7
TS-3B	-5435.45696341	-5434.026573	-5433.941284	-5434.144415	10.2
TS-4B	-5435.46255978	-5434.032909	-5433.947254	-5434.150143	6.6

a) E : electronic energy; ZPE : zero-point energy; $H (= E + ZPE + E_{\text{vib}} + E_{\text{rot}} + E_{\text{trans}} + RT)$: sum of electronic and thermal enthalpies; $G (= H - TS)$: sum of electronic and thermal free energies. b) kcal mol⁻¹.

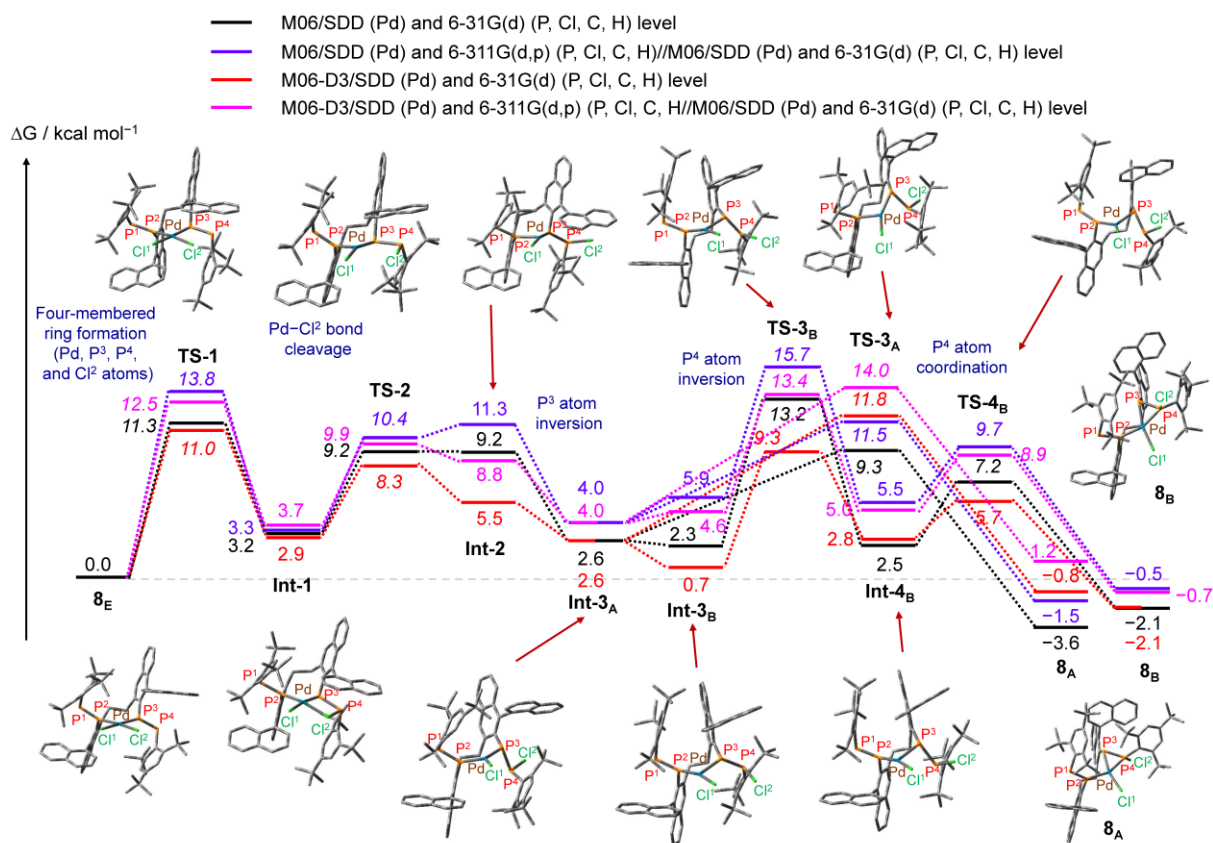
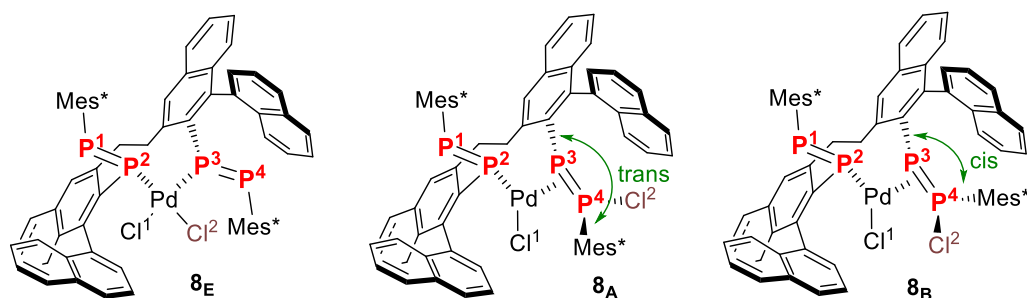


Figure S28. Energy profiles for the formation of palladium complexes 8_A and 8_B from 8_E with η^1 coordination of both P=P moieties. Color code: Pd, blue; Cl, yellow-green; P, orange; and C, gray. Hydrogen atoms were omitted for clarity.

Table S4. Selected Structural Parameters of Palladium Complexes **8_A**, **8_B**, **8_E**, **INT-1** to **Int-4_B**, and **TS-1** to **TS-4_B**.



<Bond Lengths>

Structure	$d(\text{P}^1\text{-P}^2)$ /Å	$d(\text{P}^3\text{-P}^4)$ /Å	$d(\text{Pd-P}^2)$ /Å	$d(\text{Pd-P}^3)$ /Å	$d(\text{Pd-P}^4)$ /Å	$d(\text{Pd-Cl}^1)$ /Å	$d(\text{Pd-Cl}^2)$ /Å	$d(\text{P}^4\text{-Cl}^2)$ /Å
	(WBI) ^a	(WBI) ^a	(WBI) ^a	(WBI) ^a	(WBI) ^a	(WBI) ^a	(WBI) ^a	(WBI) ^a
8_E	2.050 (1.71)	2.050 (1.71)	2.339 (0.42)	2.339 (0.42)	— ^b	2.376 (0.39)	2.376 (0.39)	— ^b
TS-1	2.045 (1.70)	2.132 (1.34)	2.302 (0.45)	2.351 (0.41)	— ^b	2.408 (0.36)	2.409 (0.33)	2.998 (0.21)
Int-1	2.044 (1.69)	2.290 (0.93)	2.284 (0.46)	2.350 (0.52)	— ^b	2.452 (0.29)	2.508 (0.19)	2.206 (0.76)
TS-2	2.052 (1.67)	2.292 (0.90)	2.300 (0.45)	2.340 (0.55)	— ^b	2.433 (0.30)	3.414 (0.04)	2.129 (0.87)
Int-2	2.051 (1.69)	2.157 (1.21)	2.334 (0.42)	2.342 (0.48)	— ^b	2.464 (0.26)	5.522 (0.02)	2.174 (0.74)
Int-3_A	2.050 (1.66)	2.243 (0.95)	2.270 (0.48)	2.277 (0.65)	3.512 (0.06)	2.435 (0.29)	— ^b	2.143 (0.82)
TS-3_A	2.049 (1.70)	2.188 (1.09)	2.343 (0.37)	2.321 (0.59)	2.732 (0.20)	2.430 (0.27)	— ^b	2.126 (0.81)
8_A	2.040 (1.72)	2.216 (1.08)	2.359 (0.33)	2.402 (0.45)	2.338 (0.37)	2.437 (0.30)	— ^b	2.085 (0.87)
Int-3_B	2.051 (1.70)	2.191 (1.12)	2.277 (0.43)	2.336 (0.58)	4.086 (0.12)	2.409 (0.33)	— ^b	2.104 (0.88)
TS-3_B	2.052 (1.68)	2.118 (1.23)	2.286 (0.43)	2.346 (0.52)	3.629 (0.16)	2.441 (0.30)	— ^b	2.065 (0.90)
Int-4_B	2.050 (1.70)	2.298 (0.97)	2.295 (0.42)	2.346 (0.63)	3.418 (0.04)	2.389 (0.34)	— ^b	2.143 (0.84)
TS-4_B	2.054 (1.67)	2.212 (1.09)	2.306 (0.41)	2.304 (0.59)	2.790 (0.15)	2.476 (0.29)	— ^b	2.119 (0.84)
8_B	2.038 (1.72)	2.198 (1.09)	2.356 (0.35)	2.434 (0.47)	2.325 (0.37)	2.448 (0.28)	— ^b	2.104 (0.84)

Structures calculated at M06/SDD (Pd) and 6-31G(d) (P, Cl, C, H) level of theory were used. a) Wiberg's bond index. b) Not analyzed

<Bond Angles>

Structure	Angle (P ² -Pd-Cl ¹) /deg	Angle (P ² -Pd-P ³) /deg	Angle (Pd-P ³ -P ⁴) /deg	Σ Angle (Pd)/deg ^a	Σ Angle (P ³)/deg ^b	Σ Angle (P ⁴)/deg ^c
8_E	85.5	101.6	138.0	359.7	359.9	–
TS-1	91.0	90.2	107.6	358.0	322.9	267.5
Int-1	101.0	86.6	95.6	358.9	304.7	286.2
TS-2	111.3	84.8	103.9	357.4	310.0	309.3
Int-2	98.0	85.3	132.9	354.8	341.5	341.1
Int-3_A	126.1	105.0	102.0	360.0	330.0	319.6
TS-3_A	103.7	111.1	74.5	355.7	307.0	337.2
8_A	99.3	97.0	60.7	358.8	274.0	334.1
Int-3_B	162.5	101.6	129.0	359.9	340.8	339.4
TS-3_B	156.4	105.8	108.7	359.8	324.4	358.2
Int-4_B	164.7	103.6	94.8	359.7	319.6	320.3
TS-4_B	136.9	102.0	76.3	357.0	311.1	332.0
8_B	93.0	103.5	60.0	359.4	273.6	340.9

Structures calculated at M06/SDD (Pd) and 6-31G(d) (P, Cl, C, H) level of theory were used. a) Sum of the bond angles of P²-Pd-P³, P²-Pd-Cl¹, P³-Pd-Cl¹. b) Sum of the bond angles of Pd-P³-P⁴, Pd-P³-C_{Np}, and P⁴-P³-C_{Np}. c) Sum of the bond angles of P³-P⁴-Cl², P³-P⁴-C(Mes*), and Cl²-P⁴-C_{Mes*}.

<NPA charges>

Structure	Pd	P ¹	P ²	P ³	P ⁴	Cl ¹	Cl ²
8_E	+0.379	+0.407	+0.414	+0.409	+0.404	-0.512	-0.512
TS-1	+0.390	+0.403	+0.440	+0.170	+0.686	-0.562	-0.485
Int-1	+0.356	+0.398	+0.434	+0.182	+0.616	-0.659	-0.244
TS-2	+0.391	+0.381	+0.425	+0.232	+0.562	-0.675	-0.278
Int-2	+0.369	+0.407	+0.408	+0.237	+0.550	-0.680	-0.335
Int-3_A	+0.310	+0.374	+0.414	+0.385	+0.505	-0.703	-0.321
TS-3_A	+0.316	+0.358	+0.357	+0.370	+0.517	-0.688	-0.284
8_A	+0.239	+0.358	+0.388	+0.277	+0.642	-0.659	-0.249
Int-3_B	+0.255	+0.369	+0.347	+0.429	+0.518	-0.629	-0.253
TS-3_B	+0.217	+0.354	+0.329	+0.505	+0.494	-0.675	-0.203
Int-4_B	+0.282	+0.378	+0.347	+0.455	+0.499	-0.586	-0.290
TS-4_B	+0.294	+0.361	+0.349	+0.481	+0.517	-0.708	-0.262
8_B	+0.235	+0.384	+0.390	+0.279	+0.610	-0.650	-0.245

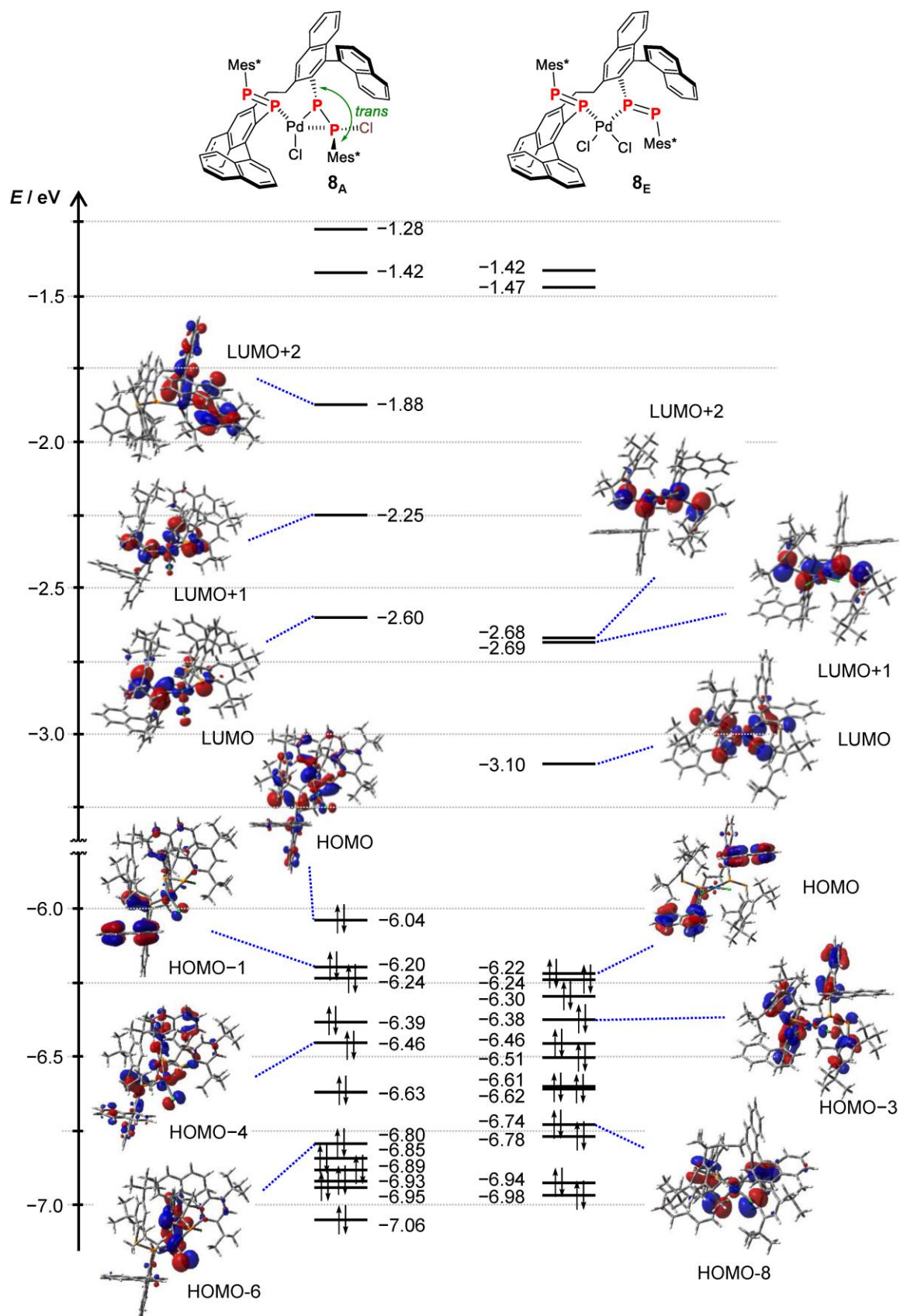


Figure S29. Energy diagram and the selected molecular orbitals of $\mathbf{8}_A$ and $\mathbf{8}_E$ mainly including the central PdP_mCl_n moieties ($m = 2$ or 3 , $n = 1$ or 2 ; isovalue = 0.03).

5-3. GIAO Calculations of Palladium Complexes of 7⁺, 7b, and 8.

5-3-1. Initial Survey of Functionals.

Prior to the GIAO calculations of palladium complexes of 7⁺, 7b, and 8, the suitable functionals were surveyed by the use of binaphthyldiphosphene gold complex [1(AuCl)],^{S20} which was structurally characterized as a *syn* isomer with the η^1 -coordination to a gold atom by the X-ray crystallographic analysis. The GIAO calculations of [1(AuCl)] were carried out at the basis sets of SDD^{S13} (Au) and 6-311G(2d,2p) (P, Cl, C, H) levels in conjunction with PCM model^{S14} (chloroform) after the optimization at an M06 functional^{S12} with the basis set of SDD^{S13} (Au) and 6-31G(d) (P, Cl, C, H) level of theory. The chemical shift of PMe₃ in CDCl₃ (−61.6 ppm)^{S21} was used as the reference for the estimation of chemical shifts. The results were summarized in Table S5. Based on these results, an OLYP functional was selected for the calculations of palladium complexes of 7⁺, 7b, and 8.

Table S5. The calculated ³¹P chemical shifts of gold complex of binaphthyldiphosphene, [1(AuCl)]. The deviation from the experimental values was shown in a bracket with an italic font.

Functional	<i>syn</i> -[1(AuCl)]		<i>anti</i> -[1(AuCl)]	
	<i>P</i> _{BNP}	<i>P</i> _{Mes} *	<i>P</i> _{BNP}	<i>P</i> _{Mes} *
BP86 ^{S18b,22}	308.1 (−7.6)	444.0 (+38.0)	311.8 (−3.9)	471.7 (+65.7)
BLYP ^{S18a,b}	314.9 (−0.8)	449.8 (+43.8)	319.0 (+3.3)	477.0 (+71.0)
B3LYP ^{S18}	352.0 (+36.3)	496.0 (+90.0)	355.4 (+39.7)	522.3 (+116.3)
PBE0 ^{S17}	349.7 (+34.0)	495.2 (+89.2)	352.3 (+36.6)	521.6 (+115.6)
OLYP ^{S23}	296.8 (−18.9)	427.9 (+21.9)	300.1 (−15.6)	450.2 (+44.2)
OPBE ^{S24}	290.8 (−24.9)	423.6 (+17.6)	293.3 (−22.4)	445.1 (+39.1)
BMK ^{S25}	454.0 (+138.3)	613.3 (+207.3)	454.8 (+139.1)	641.4 (+235.4)
B3PW91 ^{S18c}	346.3 (+30.6)	491.8 (+85.8)	349.2 (+33.5)	517.9 (+111.9)
M06 ^{S12}	398.6 (+82.9)	560.9 (+154.9)	401.4 (+85.7)	584.0 (+178.0)
CAM-B3LYP ^{S26}	390.4 (+74.9)	553.5 (+147.5)	391.9 (+76.2)	577.8 (+171.8)
ωB97XD ^{S27}	385.4 (+69.7)	546.3 (+140.3)	386.9 (+71.2)	569.4 (+163.4)
LC-BLYP ^{S28}	446.0 (+130.3)	639.1 (+233.1)	445.6 (+129.9)	663.2 (+257.2)
[1(AuCl)]	315.7	405.9		
(observed) ^{a,b}				
Diphosphene				
(<i>syn,anti</i>)- 2 ^c	473.4 (+22.3)	547.8 (+19.0)	452.4 (+1.3)	556.9 (+28.1)
2 (observed) ^a	451.1	528.8		
<i>syn</i> - 1 ^c	459.8 (+8.3)	534.2 (+8.5)		
1 (observed) ^{a,d}	451.5	525.7		

a) In CDCl₃. b) Ref. S20. c) Calculated at GIAO-OLYP/6-311G(2d,2p)//M06/6-31G(d) level of theory with PCM model (chloroform). d) Ref. 1.

5-3-2. GIAO Calculations of Palladium Complexes 7.

The GIAO calculations of the cation moiety of palladium complexes 7_A^+ to 7_I^+ and the real molecules $7b_X$ to $7b_Z$ were carried out at an OLYP functional^{S24} with the basis set of SDD^{S13} (Pd,Sb) and 6-311G(2d,2p) (P,F,C,H) level of theory in conjunction with PCM model^{S14} (dichloromethane). The optimized structures 7_A^+ to 7_I^+ and $7b_X$ to $7b_Z$ calculated at M06/SDD (Pd,Sb) and 6-31G(d) (P,F,C,H) level were used for calculations. The results are shown in Tables S6 and Figure S30. The chemical shift of PMe_3 in $CDCl_3$ (-61.6 ppm)^{S21} was used as the reference for the estimation of chemical shifts.

Table S6. The calculated ^{31}P chemical shifts of palladium complexes 7_A^+ to 7_I^+ and $7b_X$ to $7b_Z$. The phosphorus atoms coordinated to a palladium atom are shown in brown.

Structure	P^A	P^B	P^C	P^D
	(binaphthyl groups)		(Mes* groups)	
7_A^+	375.4	375.9	469.1	485.8
7_B^+	344.9	373.4	471.8	549.5
7_C^+	386.3	426.9	504.9	407.9
7_D^+	350.6	466.3	525.0	499.2
7_E^+	394.7	496.6	402.9	456.9
7_F^+	370.4	369.6	506.0	512.6
7_G^+	359.6	426.7	460.7	380.1
7_H^+	465.8	380.5	461.2	534.5
7_I^+	497.9	527.1	449.5	419.4
$7b_X$ (= $[7_A(SbF_6)]$)	371.7	374.1	480.7	479.1
$7b_Y$ (= $[7_A(SbF_6)]$)	369.1	381.4	464.2	480.9
$7b_Z$ (= $[7_A(SbF_6)]$)	351.1	383.0	493.9	480.4
$7a$ (observed) ^a	333.8	338.5	469.9	479.3
$7b$ (observed) ^a	334.2	339.0	470.0	479.4

a) In CD_2Cl_2 .

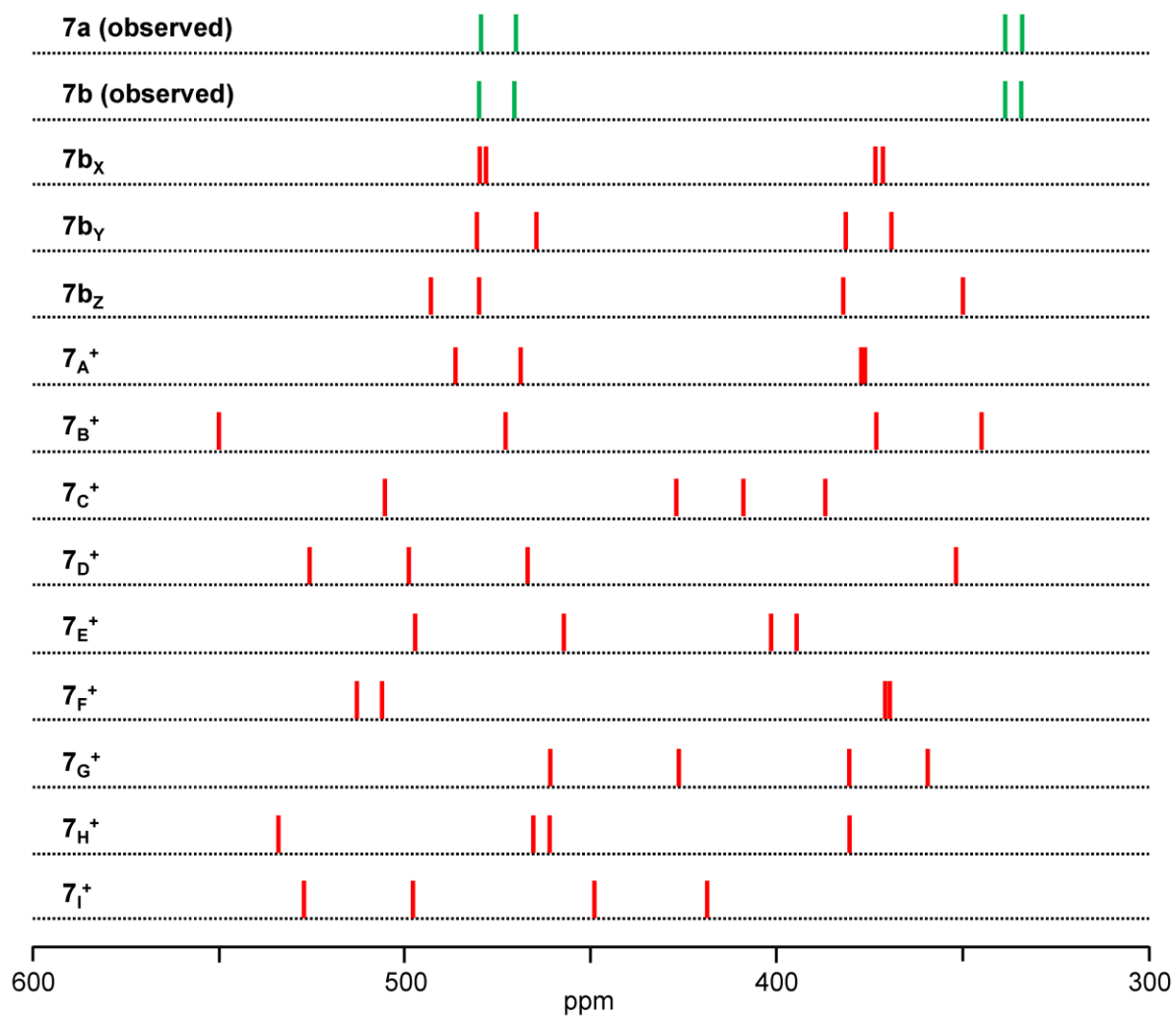


Figure S30. Schematic representation of calculated ^{31}P NMR spectra for the conformationally different palladium complexes .

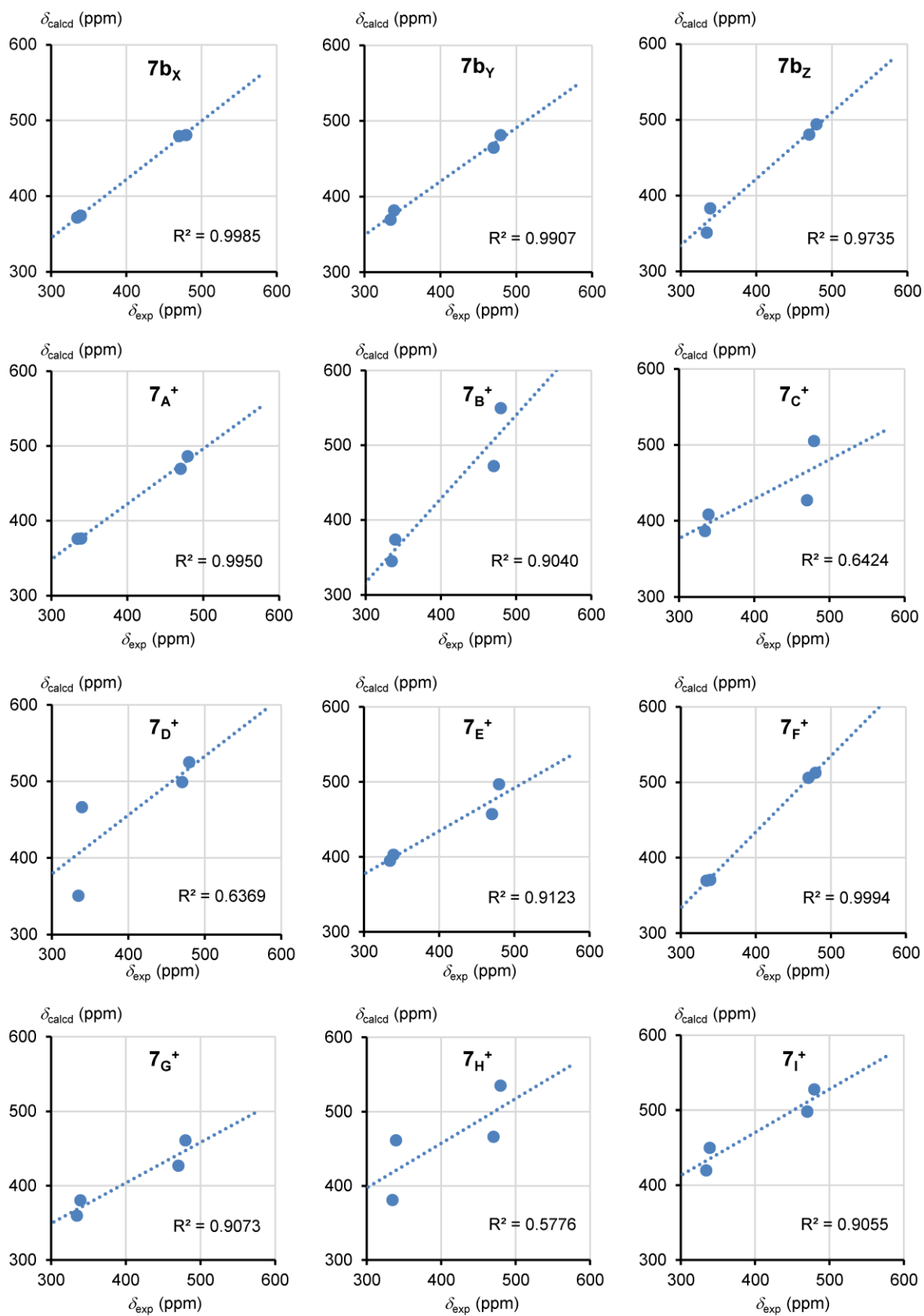


Figure S31. Plots of calculated ^{31}P chemical shifts versus observed ^{31}P chemical shift of **7b**.

5-3-3. GIAO Calculations of Palladium Complexes **8**.

The GIAO calculations of palladium complexes **8** were carried out at an OLYP^{S24} functional with the basis set of SDD^{S13} (Pd) and 6-311G(2d,2p) (P,Cl,C,H) level in conjunction with PCM model^{S14} (dichloromethane). The optimized structures calculated at M06/SDD (Pd) and 6-31G(d) (P,Cl,C,H) level (for **8_A** to **8_D** and **8_F** to **8_I**) and M06-D3/SDD (Pd) and 6-31G(d) (P,Cl,C,H) level (for **8_A** to **8_D**) were used for calculations. An OPBE^{S25} functional instead of OLYP was also used for calculations (for **8_A** to **8_D**). The results were shown in Table S7 and Figure S32. The chemical shift of PMe₃ in CDCl₃ (−61.6 ppm)^{S20} was used as the reference for the estimation of chemical shifts.

Table S7. The calculated ³¹P chemical shifts of palladium complexes **8**. Calculated at GIAO-F1/SDD (Pd) and 6-311G(2d,2p) (P,Cl,C,H) (PCM = CH₂Cl₂)/F2/SDD (Pd) and 6-31G(d) (P,Cl,C,H), (PCM = CH₂Cl₂) level of theory. The deviation from the experimental values was shown in a bracket with an italic font.

Structure	<i>P^A</i> (P ¹)	<i>P^B</i> (P ²)	<i>P^C</i> (P ⁴)	<i>P^D</i> (P ³)
8 (observed)	463.2	338.9	97.4	−39.6
[F1 = OLYP, F2 = M06]				
8_A	457.5 (−5.7)	395.6 (+56.7)	139.2 (+41.8)	15.6 (+55.2)
8_B	475.1 (+11.9)	396.0 (+57.1)	100.6 (+3.2)	39.2 (+78.8)
8_C	482.8 (+19.6)	381.9 (+43.0)	143.0 (+45.6)	92.2 (+131.8)
8_D	485.5 (+22.3)	384.3 (+45.4)	130.7 (+33.3)	93.4 (+133.0)
8_F	516.5 (+53.3)	373.8 (+34.9)	115.7 (+18.3)	67.5 (+107.1)
8_G	509.0 (+45.8)	363.0 (+24.1)	97.7 (+0.3)	56.3 (+95.9)
8_H	512.3 (+49.1)	375.0 (+36.1)	54.3 (−43.1)	133.0 (+172.6)
8_I	483.3 (+20.1)	387.6 (+48.7)	70.2 (−27.2)	76.6 (+116.2)
[F1 = OLYP, F2 = M06-D3]				
8_A	453.8 (−9.4)	395.6 (+56.7)	137.2 (+39.8)	11.0 (+50.6)
8_B	453.9 (−9.3)	396.8 (+57.9)	101.6 (+4.2)	40.9 (+80.5)
8_C	477.9 (+14.7)	381.8 (+42.9)	121.5 (+24.1)	89.2 (+128.8)
8_D	482.7 (+19.5)	382.3 (+43.4)	128.0 (+30.6)	90.2 (+129.8)
[F1 = OPBE, F2 = M06]				
8_A	450.0 (−13.2)	384.8 (+45.9)	133.4 (+36.0)	12.5 (+52.1)
8_B	468.4 (+5.2)	385.0 (+46.1)	95.8 (−1.6)	34.5 (+74.1)
8_C	474.2 (+11.0)	370.0 (+31.1)	136.0 (+38.6)	89.5 (+129.1)
8_D	478.2 (+15.0)	373.0 (+34.1)	126.5 (+29.1)	89.9 (+129.5)
[F1 = OPBE, F2 = M06-D3]				
8_A	445.1 (−18.1)	384.4 (+45.5)	131.5 (+34.1)	8.8 (+48.4)
8_B	446.0 (−17.2)	385.5 (+46.6)	96.8 (−0.6)	38.1 (+77.7)
8_C	468.6 (+5.4)	370.6 (+31.7)	113.3 (+15.9)	86.8 (+126.4)
8_D	474.2 (+11.0)	371.1 (+32.2)	123.4 (+26.0)	87.2 (+126.8)

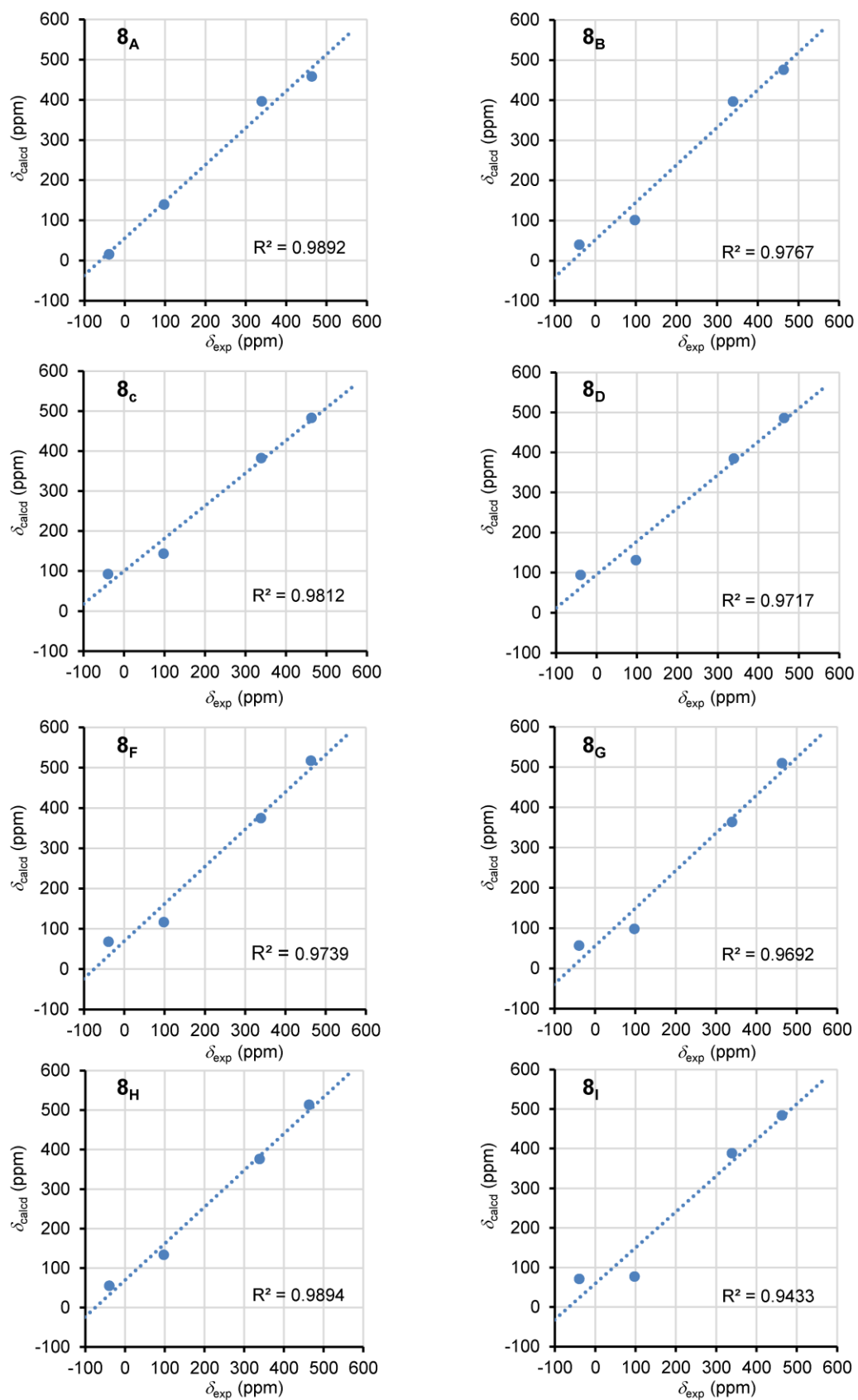


Figure S32. Plots of calculated ^{31}P chemical shifts *versus* observed ^{31}P chemical shift of **8**.

Table S8. Magnet shielding tensors of ^{31}P nuclei of $7_{\text{A}}^+-7_{\text{I}}^+$, $7_{\text{bX}}-7_{\text{bZ}}$, $8_{\text{A}}-8_{\text{D}}$, $8_{\text{F}}-8_{\text{I}}$, and **2** calculated by the GIAO Method [OLYP/SDD (Pd,Sb) and 6-311G(2d,2p) (P,Cl,F,C,H)/M06/SDD (Pd,Sb) and 6-31G(d) (P,Cl,F,C,H) (PCM = CH_2Cl_2)].

SCF GIAO Magnetic shielding tensor (ppm) of 7_{A}^+ :

1 P Isotropic = -60.9116 Anisotropy = 549.9543
 XX= 58.6383 YX= 97.2111 ZX= 303.3392
 XY= 172.3060 YY= -135.5596 ZY= -347.7857
 XZ= 313.4686 YZ= -186.4348 ZZ= -105.8133
 Eigenvalues: -552.0355 63.5762 305.7247

2 P Isotropic = -61.4167 Anisotropy = 542.8649
 XX= 40.3138 YX= 114.8215 ZX= -299.7772
 XY= 216.4369 YY= -161.5917 ZY= 342.8095
 XZ= -306.1988 YZ= 166.0703 ZZ= -62.9720
 Eigenvalues: -552.1031 67.3598 300.4933

3 P Isotropic = -154.6053 Anisotropy = 703.0446
 XX= 11.1063 YX= 182.9026 ZX= 360.6863
 XY= 98.8153 YY= -391.6371 ZY= -332.8134
 XZ= 280.8519 YZ= -350.1097 ZZ= -83.2853
 Eigenvalues: -733.8278 -44.0793 314.0911

4 P Isotropic = -171.3119 Anisotropy = 737.7960
 XX= -13.8327 YX= 218.2050 ZX= -371.6080
 XY= 136.6107 YY= -474.4831 ZY= 335.0383
 XZ= -277.8647 YZ= 303.4237 ZZ= -25.6198
 Eigenvalues: -772.7117 -61.7760 320.5521

SCF GIAO Magnetic shielding tensor (ppm) of 7_{B}^+ :

1 P Isotropic = -30.4115 Anisotropy = 473.3705
 XX= -232.4560 YX= 87.6880 ZX= -389.9696
 XY= -36.7276 YY= 170.3559 ZY= 87.8189
 XZ= -240.6413 YZ= 178.8604 ZZ= -29.1345
 Eigenvalues: -477.5434 101.1399 285.1688

2 P Isotropic = -58.7058 Anisotropy = 577.6078
 XX= -169.2806 YX= 218.0152 ZX= 450.2741
 XY= 78.7150 YY= 60.6744 ZY= -264.0796
 XZ= 248.6724 YZ= -306.4271 ZZ= -67.5114
 Eigenvalues: -608.4265 105.9430 326.3660

3 P Isotropic = -157.3319 Anisotropy = 725.1071
 XX= -551.5277 YX= -191.8395 ZX= -367.8226
 XY= -26.4547 YY= 79.8055 ZY= 206.8452
 XZ= -367.4109 YZ= 102.2433 ZZ= -0.2736
 Eigenvalues: -736.4138 -61.6548 326.0728

4 P Isotropic = -234.9827 Anisotropy = 803.3033
 XX= -561.0428 YX= 14.2978 ZX= 385.1932
 XY= 176.7267 YY= -29.7553 ZY= -311.7798
 XZ= 557.7084 YZ= -240.4538 ZZ= -114.1501
 Eigenvalues: -919.9402 -85.5609 300.5528

SCF GIAO Magnetic shielding tensor (ppm) of 7_{C}^+ :

1 P Isotropic = -71.8657 Anisotropy = 528.7322
 XX= 190.3373 YX= 3.7972 ZX= 139.5132
 XY= -42.1848 YY= -136.6141 ZY= 395.6657
 XZ= 209.4436 YZ= 271.4864 ZZ= -269.3203
 Eigenvalues: -571.9365 75.7170 280.6224

2 P Isotropic = -112.4206 Anisotropy = 639.9216
 XX= -0.6641 YX= 222.3675 ZX= 28.0973
 XY= 101.3470 YY= -306.4842 ZY= -494.7246
 XZ= -86.6052 YZ= -332.1583 ZZ= -30.1135
 Eigenvalues: -625.6441 -25.8115 314.1939

3 P Isotropic = -190.4042 Anisotropy = 786.9472
 XX= 172.5460 YX= 75.6742 ZX= 205.0567
 XY= 102.2010 YY= -408.6670 ZY= 524.3906
 XZ= 146.0962 YZ= 435.1337 ZZ= -335.0915
 Eigenvalues: -855.9978 -49.4421 334.2273

4 P Isotropic = -93.4529 Anisotropy = 643.0132
 XX= 25.6882 YX= 148.7091 ZX= -19.6931
 XY= 355.2112 YY= -325.2381 ZY= -423.2453
 XZ= 184.9171 YZ= -443.0109 ZZ= 19.1913
 Eigenvalues: -708.2784 92.6972 335.2226

SCF GIAO Magnetic shielding tensor (ppm) of 7D^+ :

1 P Isotropic = -36.1244 Anisotropy = 484.0351
 XX= -89.5731 YX= -23.2473 ZX= 410.7023
 XY= -166.5299 YY= 151.1542 ZY= 78.8114
 XZ= 329.8205 YZ= -94.5881 ZZ= -169.9544
 Eigenvalues: -507.2809 112.3420 286.5657

2 P Isotropic = -151.7879 Anisotropy = 659.3069
 XX= -385.7166 YX= -454.5741 ZX= -300.7946
 XY= -251.8844 YY= -133.3391 ZY= 1.9425
 XZ= -389.2220 YZ= -152.5905 ZZ= 63.6920
 Eigenvalues: -765.6729 22.5592 287.7500

3 P Isotropic = -210.5769 Anisotropy = 802.8665
 XX= -316.2050 YX= -403.6355 ZX= 544.5730
 XY= -248.7623 YY= -96.3595 ZY= -9.0058
 XZ= 439.9759 YZ= 99.0222 ZZ= -219.1661
 Eigenvalues: -862.9575 -93.4405 324.6675

4 P Isotropic = -184.7203 Anisotropy = 806.8616
 XX= -500.2899 YX= -445.5676 ZX= -479.2600
 XY= -322.4589 YY= -79.8458 ZY= -55.3905
 XZ= -457.2225 YZ= -95.4042 ZZ= 25.9748
 Eigenvalues: -936.2505 28.9021 353.1874

SCF GIAO Magnetic shielding tensor (ppm) of 7E^+ :

1 P Isotropic = -80.2003 Anisotropy = 606.0633
 XX= -25.3906 YX= -242.1198 ZX= -69.8293
 XY= -126.5619 YY= -173.9630 ZY= -475.9059
 XZ= 57.2869 YZ= -295.3677 ZZ= -41.2472
 Eigenvalues: -540.9789 -23.4638 323.8419

2 P Isotropic = -182.1497 Anisotropy = 776.9079
 XX= 145.6285 YX= -226.9465 ZX= -72.5542
 XY= -355.5210 YY= -650.3520 ZY= 341.0003
 XZ= -61.0468 YZ= 328.9747 ZZ= -41.7257
 Eigenvalues: -857.6357 -24.6023 335.7889

3 P Isotropic = -88.4345 Anisotropy = 650.7189
 XX= -30.1416 YX= -199.5084 ZX= -34.3101
 XY= -383.6880 YY= -197.6437 ZY= -418.4580
 XZ= -215.2670 YZ= -432.8927 ZZ= -37.5182
 Eigenvalues: -692.1415 81.4598 345.3781

4 P Isotropic = -142.4778 Anisotropy = 658.5336
 XX= 62.2466 YX= -251.4026 ZX= -95.4906
 XY= -421.6444 YY= -529.6233 ZY= 170.8382
 XZ= 24.0396 YZ= 313.3921 ZZ= 39.9432
 Eigenvalues: -737.6540 13.6759 296.5446

SCF GIAO Magnetic shielding tensor (ppm) of 7F^+ :

1 P Isotropic = -55.6516 Anisotropy = 562.6102
 XX= -329.3833 YX= -456.8629 ZX= 33.2737
 XY= -280.0465 YY= -108.3294 ZY= 107.6712
 XZ= -98.8850 YZ= 57.7599 ZZ= 270.7578
 Eigenvalues: -604.1460 117.7693 319.4218

2 P Isotropic = -54.8142 Anisotropy = 506.3571
 XX= -149.9062 YX= -210.5249 ZX= 320.8096
 XY= -322.9074 YY= -38.6509 ZY= 168.4620
 XZ= 272.8193 YZ= 11.5991 ZZ= 24.1144
 Eigenvalues: -523.0039 75.8040 282.7571

3 P Isotropic = -191.2727 Anisotropy = 751.4839
 XX= -607.3765 YX= -214.3289 ZX= -143.9985
 XY= -438.9967 YY= -167.2385 ZY= 120.3650
 XZ= -157.7632 YZ= 120.4321 ZZ= 200.7969
 Eigenvalues: -787.3770 -96.1576 309.7166

4 P Isotropic = -197.8465 Anisotropy = 789.0973
 XX= -207.6073 YX= -455.3086 ZX= 389.3730
 XY= -372.5440 YY= -429.0214 ZY= 113.9977
 XZ= 309.4119 YZ= 109.1509 ZZ= 43.0892
 Eigenvalues: -853.4273 -68.3306 328.2184

SCF GIAO Magnetic shielding tensor (ppm) of 7G^+ :

1 P Isotropic = -44.7875 Anisotropy = 508.7776
 XX= -153.4197 YX= -370.3788 ZX= 13.8680
 XY= -256.5603 YY= -215.9519 ZY= 139.3120
 XZ= -78.4287 YZ= 73.1819 ZZ= 235.0090
 Eigenvalues: -504.2091 75.4489 294.3976

2 P Isotropic = -111.9779 Anisotropy = 591.9847
 XX= -3.4962 YX= 55.8229 ZX= 105.4829
 XY= -134.7511 YY= -476.2492 ZY= 336.3103
 XZ= 130.8044 YZ= 217.3636 ZZ= 143.8118
 Eigenvalues: -592.6502 -25.9620 282.6786

3 P Isotropic = -145.9445 Anisotropy = 695.5087
 XX= -423.7509 YX= -342.5856 ZX= -128.1437
 XY= -420.4979 YY= -261.4519 ZY= 72.1407
 XZ= -151.9681 YZ= 43.0192 ZZ= 247.3691
 Eigenvalues: -738.1529 -17.4087 317.7280

4 P Isotropic = -65.3744 Anisotropy = 595.9141
 XX= 116.5146 YX= -116.7600 ZX= 120.5129
 XY= 223.1172 YY= -526.7791 ZY= 254.6035
 XZ= -33.7491 YZ= 331.2116 ZZ= 214.1413
 Eigenvalues: -630.3279 102.3031 331.9017

SCF GIAO Magnetic shielding tensor (ppm) of 7H^+ :

1 P Isotropic = -151.0655 Anisotropy = 719.1117
 XX= -195.3708 YX= 450.3989 ZX= -249.1794
 XY= 402.5750 YY= -329.4874 ZY= 12.1693
 XZ= -283.4709 YZ= 33.5286 ZZ= 71.6618
 Eigenvalues: -741.0133 -40.5253 328.3423

2 P Isotropic = -65.7873 Anisotropy = 572.7067
 XX= -382.0819 YX= 292.1648 ZX= -417.7608
 XY= 135.7412 YY= 111.4521 ZY= 224.0884
 XZ= -175.1339 YZ= 212.5187 ZZ= 73.2678
 Eigenvalues: -640.5888 127.2096 316.0171

3 P Isotropic = -146.3960 Anisotropy = 640.2008
 XX= -141.3223 YX= 495.2018 ZX= -188.8805
 XY= 317.2593 YY= -432.7406 ZY= -5.4014
 XZ= -184.9325 YZ= 81.3836 ZZ= 134.8749
 Eigenvalues: -741.0413 21.4487 280.4045

4 P Isotropic = -219.7323 Anisotropy = 758.1170
 XX= -728.4497 YX= 45.7956 ZX= -102.3688
 XY= 219.5452 YY= 9.1863 ZY= 239.2779
 XZ= -355.3997 YZ= 245.2396 ZZ= 60.0666
 Eigenvalues: -835.5365 -109.3395 285.6791

SCF GIAO Magnetic shielding tensor (ppm) of 7I^+ :

1 P Isotropic = -183.1363 Anisotropy = 784.0616
 XX= -85.7860 YX= -241.2365 ZX= -135.6361
 XY= -277.4510 YY= -735.4109 ZY= 96.7555
 XZ= -66.9967 YZ= 179.8051 ZZ= 271.7881
 Eigenvalues: -834.9365 -54.0438 339.5715

2 P Isotropic = -212.3188 Anisotropy = 773.1862
 XX= 24.9543 YX= 245.5929 ZX= 77.7605
 XY= 214.8701 YY= -708.9421 ZY= 353.1323
 XZ= 46.5667 YZ= 436.1358 ZZ= 47.0315
 Eigenvalues: -915.5051 -24.5898 303.1387

3 P Isotropic = -134.6952 Anisotropy = 617.3087
 XX= -77.7569 YX= -250.1546 ZX= -114.9827
 XY= -363.2379 YY= -546.5741 ZY= -15.0007
 XZ= -76.1705 YZ= 112.0614 ZZ= 220.2453
 Eigenvalues: -698.1850 17.2555 276.8439

4 P Isotropic = -104.6072 Anisotropy = 586.0903
 XX= 59.5345 YX= 164.7779 ZX= 56.7650
 XY= 386.6812 YY= -532.9208 ZY= 175.6460
 XZ= -74.9578 YZ= 340.5117 ZZ= 159.5647
 Eigenvalues: -710.2200 110.2787 286.1197

SCF GIAO Magnetic shielding tensor (ppm) of 7b_x :

1 P Isotropic = -56.9576 Anisotropy = 553.6938
 XX= -169.2200 YX= 72.7193 ZX= -278.6511
 XY= 37.8253 YY= 271.8161 ZY= -107.0691
 XZ= -382.6654 YZ= -37.8432 ZZ= -273.4688
 Eigenvalues: -556.5358 73.4915 312.1716

2 P Isotropic = -59.3571 Anisotropy = 537.9462
 XX= 261.1880 YX= -5.0230 ZX= 71.6712
 XY= -37.3757 YY= -533.1554 ZY= 13.5461
 XZ= 95.0540 YZ= -194.9893 ZZ= 93.8963
 Eigenvalues: -546.1255 68.7806 299.2738

3 P Isotropic = -165.9426 Anisotropy = 727.9035
 XX= -215.9652 YX= 48.3759 ZX= -393.1666
 XY= 19.8532 YY= 268.1032 ZY= -176.6162
 XZ= -307.3517 YZ= -133.1207 ZZ= -549.9659
 Eigenvalues: -783.2783 -33.8759 319.3264

4 P Isotropic = -164.3508 Anisotropy = 742.3270
 XX= 222.0589 YX= -81.9208 ZX= 168.5057
 XY= 33.6222 YY= -666.7996 ZY= -235.9003
 XZ= 190.6468 YZ= -253.0289 ZZ= -48.3118
 Eigenvalues: -753.1533 -70.4330 330.5338

SCF GIAO Magnetic shielding tensor (ppm) of 7b_y :

1 P Isotropic = -54.3283 Anisotropy = 547.5532
 XX= 153.3808 YX= -162.8847 ZX= 8.9018
 XY= -196.9677 YY= 50.8778 ZY= -235.0906
 XZ= -157.6023 YZ= -307.7900 ZZ= -367.2434
 Eigenvalues: -532.9991 59.3071 310.7072

2 P Isotropic = -66.6305 Anisotropy = 552.9113
 XX= -365.7631 YX= 341.2340 ZX= 69.6214
 XY= 276.7384 YY= 66.4901 ZY= 85.5821
 XZ= 247.8341 YZ= 14.5133 ZZ= 99.3816
 Eigenvalues: -548.6737 46.8052 301.9771

3 P Isotropic = -149.8562 Anisotropy = 695.1049
 XX= 162.5490 YX= -173.7356 ZX= 18.3891
 XY= -184.5090 YY= -3.7143 ZY= -329.5972
 XZ= 36.4363 YZ= -225.2934 ZZ= -608.4032
 Eigenvalues: -718.2551 -44.8605 313.5471

4 P Isotropic = -166.1315 Anisotropy = 735.7482
 XX= -491.2208 YX= 274.6574 ZX= 322.2726
 XY= 383.0901 YY= 14.7270 ZY= 46.0202
 XZ= 361.5477 YZ= 57.3149 ZZ= -21.9008
 Eigenvalues: -767.5914 -55.1705 324.3673

SCF GIAO Magnetic shielding tensor (ppm) of **7bz**:

1 P Isotropic = -36.3576 Anisotropy = 506.2136
 XX= 16.1262 YX= -40.3198 ZX= 170.2991
 XY= -146.1773 YY= -27.5708 ZY= 375.8873
 XZ= 269.8003 YZ= 290.5492 ZZ= -97.6281
 Eigenvalues: -498.3992 88.2083 301.1181

2 P Isotropic = -68.2751 Anisotropy = 558.6646
 XX= 194.9444 YX= 119.5987 ZX= -53.6200
 XY= 58.7126 YY= -383.8356 ZY= -406.8744
 XZ= -127.2793 YZ= -222.2611 ZZ= -15.9340
 Eigenvalues: -565.7017 56.7085 304.1680

3 P Isotropic = -179.1225 Anisotropy = 748.8653
 XX= -41.7746 YX= -72.9893 ZX= 220.2221
 XY= -7.7399 YY= -305.4607 ZY= 565.0425
 XZ= 123.4316 YZ= 505.2535 ZZ= -190.1324
 Eigenvalues: -813.5528 -43.9358 320.1210

4 P Isotropic = -165.6694 Anisotropy = 737.9023
 XX= 109.7705 YX= 130.7039 ZX= -161.6482
 XY= 227.8496 YY= -632.4053 ZY= -327.5653
 XZ= -113.8824 YZ= -275.0622 ZZ= 25.6265
 Eigenvalues: -765.9832 -57.2905 326.2654

SCF GIAO Magnetic shielding tensor (ppm) of **8A**:

1 P Isotropic = -143.0670 Anisotropy = 747.1206
 XX= -165.7632 YX= 369.7507 ZX= -107.6036
 XY= 398.1725 YY= -499.1895 ZY= -142.1719
 XZ= -160.5733 YZ= -100.0789 ZZ= 235.7518
 Eigenvalues: -751.8787 -32.3356 355.0134

2 P Isotropic = -81.1037 Anisotropy = 575.5504
 XX= -145.7642 YX= 285.9960 ZX= -143.3326
 XY= 436.0517 YY= -335.5349 ZY= 8.0215
 XZ= -66.2681 YZ= -75.3537 ZZ= 237.9880
 Eigenvalues: -615.5954 69.6876 302.5965

3 P Isotropic = 298.8445 Anisotropy = 281.1025
 XX= 260.6029 YX= -47.3733 ZX= 55.8776
 XY= -78.0330 YY= 436.7583 ZY= -155.0248
 XZ= 37.1921 YZ= -7.7590 ZZ= 199.1722
 Eigenvalues: 165.2578 245.0295 486.2461

4 P Isotropic = 175.3038 Anisotropy = 99.0679
 XX= 150.4942 YX= 28.1040 ZX= -7.5564
 XY= -75.3849 YY= 234.5519 ZY= -4.8795
 XZ= 9.7930 YZ= 21.5729 ZZ= 140.8653
 Eigenvalues: 138.5078 146.0546 241.3491

SCF GIAO Magnetic shielding tensor (ppm) of **8B**:

1 P Isotropic = -160.5968 Anisotropy = 763.8506
 XX= 45.4868 YX= 204.4706 ZX= -211.9865
 XY= 250.7422 YY= -695.9931 ZY= 116.3428
 XZ= -251.2812 YZ= 130.2527 ZZ= 168.7159
 Eigenvalues: -795.9435 -34.4837 348.6369

2 P Isotropic = -81.5221 Anisotropy = 542.1071
 XX= 47.2141 YX= 173.4693 ZX= -188.6233
 XY= 245.6704 YY= -437.3876 ZY= 196.5533
 XZ= -164.8757 YZ= 125.2631 ZZ= 145.6071
 Eigenvalues: -579.2289 54.7799 279.8826

3 P Isotropic = 275.3131 Anisotropy = 289.9077
 XX= 218.3535 YX= -26.0364 ZX= 49.9453
 XY= 14.2335 YY= 419.3805 ZY= -208.7540
 XZ= 66.4876 YZ= -17.3435 ZZ= 188.2051
 Eigenvalues: 115.5715 241.7828 468.5849

4 P Isotropic = 213.9008 Anisotropy = 180.5778
 XX= 126.4778 YX= -51.3031 ZX= -20.3274
 XY= -139.3626 YY= 196.2368 ZY= -64.5876
 XZ= 127.2039 YZ= 89.3862 ZZ= 318.9879
 Eigenvalues: 50.1354 257.2811 334.2860

SCF GIAO Magnetic shielding tensor (ppm) of **8C**:

1 P Isotropic = -168.3042 Anisotropy = 761.9712
 XX= -72.2827 YX= 243.2343 ZX= 284.8402
 XY= 279.2342 YY= 172.3864 ZY= -232.9140
 XZ= 234.5289 YZ= -167.8956 ZZ= -605.0161
 Eigenvalues: -796.8768 -47.7124 339.6767

2 P Isotropic = -67.4131 Anisotropy = 615.6858
 XX= -17.4022 YX= 237.7966 ZX= 188.7043
 XY= 226.5999 YY= 189.0787 ZY= -149.7593
 XZ= 329.9070 YZ= -280.7730 ZZ= -373.9157
 Eigenvalues: -622.2916 77.0083 343.0441

3 P Isotropic = 222.2816 Anisotropy = 138.1731
 XX= 235.2599 YX= 16.4129 ZX= -6.0571
 XY= -26.6657 YY= 149.4195 ZY= -109.2715
 XZ= -27.3279 YZ= -30.3988 ZZ= 282.1652
 Eigenvalues: 118.3480 234.0998 314.3969

4 P Isotropic = 171.4495 Anisotropy = 199.9409
 XX= 92.4747 YX= 83.5393 ZX= -62.2379
 XY= 104.2631 YY= 166.2264 ZY= -8.0075
 XZ= -116.6774 YZ= 153.6400 ZZ= 255.6475
 Eigenvalues: -19.5906 229.1958 304.7435

SCF GIAO Magnetic shielding tensor (ppm) of δ_D :

1 P Isotropic = -171.0692 Anisotropy = 754.4179
 XX= -27.8555 YX= -12.6498 ZX= 339.6181
 XY= -17.4482 YY= -15.8474 ZY= -396.1723
 XZ= 348.9727 YZ= -384.4146 ZZ= -469.5048
 Eigenvalues: -807.5266 -37.5571 331.8760

2 P Isotropic = -69.8524 Anisotropy = 607.1623
 XX= 18.6267 YX= -59.8306 ZX= 274.5838
 XY= 43.0140 YY= 134.5027 ZY= -330.7850
 XZ= 375.5551 YZ= -191.4718 ZZ= -362.6868
 Eigenvalues: -616.7942 72.3144 334.9224

3 P Isotropic = 221.0956 Anisotropy = 71.9994
 XX= 200.2721 YX= -28.6634 ZX= -72.2734
 XY= -22.7864 YY= 259.3148 ZY= -116.6293
 XZ= 0.3443 YZ= 84.2002 ZZ= 203.6999
 Eigenvalues: 157.2382 236.9534 269.0952

4 P Isotropic = 183.7899 Anisotropy = 267.0243
 XX= 86.3936 YX= -81.0954 ZX= 34.2066
 XY= -50.0788 YY= 241.9601 ZY= 20.1087
 XZ= 121.5793 YZ= 237.6219 ZZ= 223.0161
 Eigenvalues: -7.2582 196.8218 361.8061

SCF GIAO Magnetic shielding tensor (ppm) of δ_F :

1 P Isotropic = -201.9815 Anisotropy = 771.3722
 XX= -402.4096 YX= -116.9259 ZX= 426.0680
 XY= 45.9956 YY= -63.2532 ZY= -222.7321
 XZ= 592.4922 YZ= -92.7916 ZZ= -140.2817
 Eigenvalues: -803.7596 -114.4516 312.2666

2 P Isotropic = -59.3690 Anisotropy = 533.8178
 XX= -174.3099 YX= 155.5170 ZX= 458.4052
 XY= 31.5297 YY= 108.8254 ZY= -160.0280
 XZ= 311.3146 YZ= -245.7478 ZZ= -112.6225
 Eigenvalues: -591.1564 116.5398 296.5095

3 P Isotropic = 246.9993 Anisotropy = 187.8381
 XX= 367.1235 YX= 2.2961 ZX= 70.9275
 XY= 17.8327 YY= 226.8782 ZY= 22.0074
 XZ= -16.0218 YZ= 66.8816 ZZ= 146.9960
 Eigenvalues: 125.3367 243.4364 372.2246

4 P Isotropic = 198.7662 Anisotropy = 153.2161
 XX= 72.0511 YX= -48.3251 ZX= -55.5549
 XY= -0.8711 YY= 279.6321 ZY= 52.1939
 XZ= -75.3281 YZ= -13.3344 ZZ= 244.6152
 Eigenvalues: 48.7538 246.6345 300.9102

SCF GIAO Magnetic shielding tensor (ppm) of δ_G :

1 P Isotropic = -194.5743 Anisotropy = 725.7792
 XX= 3.2119 YX= -30.6732 ZX= 169.9870
 XY= 237.1601 YY= -631.9848 ZY= 347.4984
 XZ= 26.9588 YZ= 443.8217 ZZ= 45.0500
 Eigenvalues: -817.6193 -55.3821 289.2785

2 P Isotropic = -48.5092 Anisotropy = 543.2884
 XX= 181.1420 YX= 78.1120 ZX= 43.2829
 XY= -58.9144 YY= -370.5980 ZY= 450.4711
 XZ= 149.3096 YZ= 274.7016 ZZ= 43.9285
 Eigenvalues: -583.1012 123.8906 313.6831

3 P Isotropic = 258.2090 Anisotropy = 280.3469
 XX= 213.9466 YX= 52.5432 ZX= 33.1040
 XY= -13.7775 YY= 437.0310 ZY= 23.7008
 XZ= 9.4634 YZ= -118.0666 ZZ= 123.6495
 Eigenvalues: 111.1118 218.4083 445.1070

4 P Isotropic = 216.7314 Anisotropy = 88.6366
 XX= 121.8989 YX= 60.2986 ZX= -0.7586
 XY= -108.6366 YY= 264.7216 ZY= 57.7394
 XZ= -47.7671 YZ= -81.0491 ZZ= 263.5737
 Eigenvalues: 113.4629 260.9089 275.8225

SCF GIAO Magnetic shielding tensor (ppm) of δ_H :

1 P Isotropic = -197.8781 Anisotropy = 769.5475
 XX= -200.4592 YX= 63.6139 ZX= 125.4961
 XY= 207.9783 YY= -171.6208 ZY= -521.1423
 XZ= 284.3087 YZ= -493.0677 ZZ= -221.5544
 Eigenvalues: -801.9689 -106.8191 315.1535

2 P Isotropic = -60.5065 Anisotropy = 579.3606
 XX= 94.9106 YX= 139.6322 ZX= 182.6550
 XY= 23.8675 YY= -79.4746 ZY= -494.1445
 XZ= -25.7842 YZ= -425.4426 ZZ= -196.9556
 Eigenvalues: -619.5849 112.3314 325.7338

3 P Isotropic = 181.4274 Anisotropy = 94.1671
 XX= 179.2632 YX= 57.0595 ZX= -35.9818
 XY= 58.7406 YY= 158.6242 ZY= 28.1513
 XZ= -25.6838 YZ= 82.9317 ZZ= 206.3947
 Eigenvalues: 79.2843 220.7924 244.2055

4 P Isotropic = 260.1761 Anisotropy = 313.9210
 XX= 218.0328 YX= -9.1466 ZX= -29.3512
 XY= -119.2502 YY= 438.1163 ZY= -143.5998
 XZ= -81.1534 YZ= -25.7085 ZZ= 124.3792
 Eigenvalues: 69.3293 241.7423 469.4568

SCF GIAO Magnetic shielding tensor (ppm) of **8₁**:

1 P Isotropic = -168.8547 Anisotropy = 736.8264
 XX= -11.8217 YX= -303.8990 ZX= 143.9955
 XY= -138.2512 YY= -655.5614 ZY= -194.6958
 XZ= 141.1813 YZ= -195.4543 ZZ= 160.8191
 Eigenvalues: -748.2338 -80.6931 322.3630
 2 P Isotropic = -73.1320 Anisotropy = 606.6993
 XX= 56.6854 YX= -218.2304 ZX= 129.0635
 XY= -383.2621 YY= -501.3761 ZY= 16.3705
 XZ= 74.5014 YZ= -164.3604 ZZ= 225.2948
 Eigenvalues: -633.4720 82.7419 331.3343

3 P Isotropic = 237.8458 Anisotropy = 82.5189
 XX= 195.8515 YX= 45.1910 ZX= -103.0502
 XY= 14.3433 YY= 261.4139 ZY= -41.6967
 XZ= 9.8029 YZ= 105.8807 ZZ= 256.2721
 Eigenvalues: 154.2217 266.4573 292.8585
 4 P Isotropic = 244.2787 Anisotropy = 331.7821
 XX= 170.1971 YX= -35.6105 ZX= 9.9586
 XY= -23.9621 YY= 232.6443 ZY= 83.9367
 XZ= 164.5087 YZ= 251.2228 ZZ= 329.9946
 Eigenvalues: 53.8591 213.5102 465.4668

SCF GIAO Magnetic shielding tensor (ppm) of *syn*-[**1**(AuCl)]:

1 P Isotropic = 17.6210 Anisotropy = 421.3286
 XX= -315.3101 YX= 140.9516 ZX= -138.9675
 XY= 167.4091 YY= 228.7602 ZY= -22.8288
 XZ= -93.1153 YZ= -49.3283 ZZ= 139.4128
 Eigenvalues: -376.7792 131.1354 298.5067

2 P Isotropic = -113.4495 Anisotropy = 692.9322
 XX= -525.8946 YX= 324.7324 ZX= -2.1870
 XY= 244.2542 YY= 143.1606 ZY= -180.9703
 XZ= -65.7643 YZ= -167.7368 ZZ= 42.3857
 Eigenvalues: -631.7602 -57.0936 348.5054

SCF GIAO Magnetic shielding tensor (ppm) of *anti*-[**1**(AuCl)]:

1 P Isotropic = 14.3982 Anisotropy = 413.7721
 XX= -303.5011 YX= -230.4804 ZX= -44.2684
 XY= -179.9422 YY= 204.0588 ZY= -62.7342
 XZ= -12.1002 YZ= -51.2450 ZZ= 142.6369
 Eigenvalues: -380.0855 133.0338 290.2463

2 P Isotropic = -135.7075 Anisotropy = 723.1981
 XX= -611.3188 YX= -195.0824 ZX= 168.7439
 XY= -264.3457 YY= 221.2657 ZY= -114.1681
 XZ= 121.0099 YZ= -125.7324 ZZ= -17.0694
 Eigenvalues: -689.2842 -64.2629 346.4246

SCF GIAO Magnetic shielding tensor (ppm) of **2**:

1 P Isotropic = -158.9408 Anisotropy = 787.5404
 XX= -226.0544 YX= -595.6506 ZX= -12.4108
 XY= -597.3358 YY= -271.6427 ZY= -120.4618
 XZ= 68.5706 YZ= -48.1085 ZZ= 20.8748
 Eigenvalues: -847.7481 4.8397 366.0862
 2 P Isotropic = -137.8821 Anisotropy = 752.7701
 XX= -120.7784 YX= -520.1573 ZX= 1.1854
 XY= -557.4170 YY= -332.0914 ZY= -168.4450
 XZ= 53.5660 YZ= -125.1812 ZZ= 39.2234
 Eigenvalues: -786.7949 9.1839 363.9646

3 P Isotropic = -233.3531 Anisotropy = 860.2944
 XX= -315.8077 YX= -664.8014 ZX= 60.5062
 XY= -668.7644 YY= -365.6881 ZY= -32.6611
 XZ= 62.5236 YZ= -41.4850 ZZ= -18.5636
 Eigenvalues: -1008.2559 -31.9799 340.1765
 4 P Isotropic = -242.4649 Anisotropy = 871.0814
 XX= -243.8035 YX= -679.3387 ZX= 52.4307
 XY= -632.6067 YY= -491.4750 ZY= -108.5773
 XZ= 60.6357 YZ= -106.8599 ZZ= 7.8838
 Eigenvalues: -1037.3182 -28.3325 338.2560

SCF GIAO Magnetic shielding tensor (ppm) of PMe₃:

1 P Isotropic = 376.0647 Anisotropy = 15.8424
 XX= 386.4302 YX= 0.0000 ZX= 0.0000
 XY= 0.0000 YY= 386.6234 ZY= -0.2031
 XZ= 0.0000 YZ= -0.4020 ZZ= 355.1404
 Eigenvalues: 355.1375 386.4302 386.6263

5-4. Estimation of the Dissociation Energies of the Pd–Cl bond in **8_E** and P–Cl bond in **8_A**.

The bond dissociation energies of the Pd–Cl bond in **8_E** and the P⁴–Cl bond in **8_A** were estimated by changing the Pd–Cl bond and P⁴–Cl bond distances from the values of the optimized structure to 5.0 Å (M06/SDD (Pd) and 6-31G(d) (P,Cl,C,H) level). The molecular structures were optimized with the fixation of the Pd–Cl bond (for **8_E**) and the P⁴–Cl bond (for **8_A**). The results were shown in Figure S33 and Table S9.

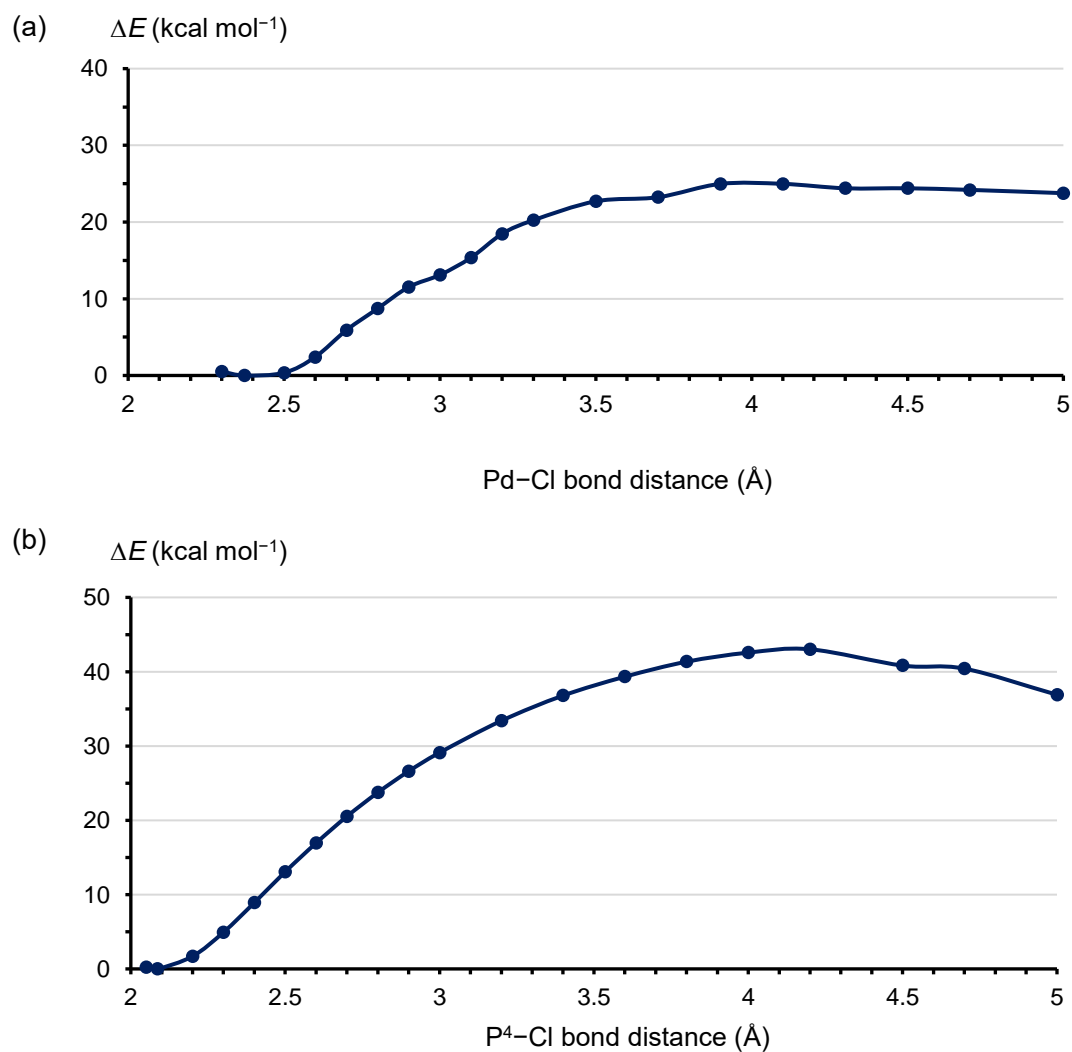


Figure S33. The bond dissociation energies of (a) the Pd–Cl bond in **8_E** and (b) the P⁴–Cl bond in **8_A**.

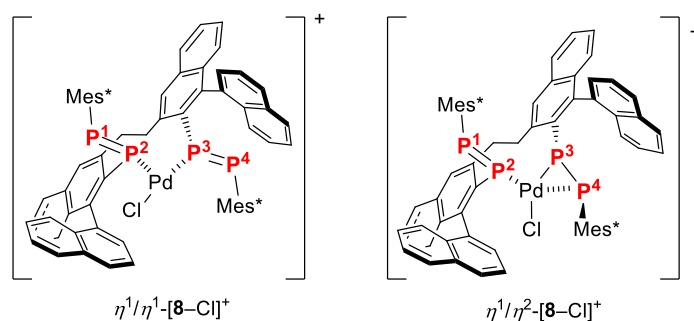
Table S9. Uncorrected energies of stationary points (Hartree).^a

Compound 8E			Compound 8A		
Pd–Cl bond distance	<i>E</i>	ΔE	P ⁴ –Cl bond distance	<i>E</i>	ΔE
2.3	-5435.39783889	0.5	2.05	-5435.39995068	0.2
2.373 ^{*a}	-5435.39866264	0.0	2.086 ^{*a}	-5435.40029569	0.0
2.5	-5435.39809834	0.4	2.2	-5435.39758780	1.7
2.6	-5435.39482384	2.4	2.3	-5435.39244067	4.9
2.7	-5435.38925810	5.9	2.4	-5435.38609185	8.9
2.8	-5435.38476805	8.7	2.5	-5435.37947070	13.1
2.9	-5435.38028529	11.5	2.6	-5435.37330307	16.9
3.0	-5435.37777747	13.1	2.7	-5435.36758281	20.5
3.1	-5435.37416942	15.4	2.8	-5435.36246777	23.7
3.2	-5435.36922050	18.5	2.9	-5435.35790445	26.6
3.3	-5435.36640794	20.2	3.0	-5435.35391562	29.1
3.5	-5435.36247805	22.7	3.2	-5435.34708321	33.4
3.7	-5435.36162834	23.2	3.4	-5435.34167404	36.8
3.9	-5435.35885944	25.0	3.6	-5435.33762978	39.3
4.1	-5435.35885283	25.0	3.8	-5435.33441002	41.3
4.3	-5435.35977248	24.4	4.0	-5435.33246260	42.6
4.5	-5435.35977260	24.4	4.2	-5435.33173764	43.0
4.7	-5435.36010915	24.2	4.5	-5435.33523778	40.8
5.0	-5435.36079031	23.8	4.7	-5435.33589309	40.4
			5.0	-5435.34149062	36.9

a) Optimized structure.

Table S10. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).^a

Structure	<i>E</i>	<i>E</i> + ZPE	<i>H</i>	<i>G</i>	ΔG^b
η^1/η^1 -[8 -Cl] ⁺	-4975.02875099	-4973.599356	-4973.515317	-4973.714562	0.0
η^1/η^2 -[8 -Cl] ⁺	-4975.00061517	-4973.574223	-4973.489490	-4973.692544	13.8



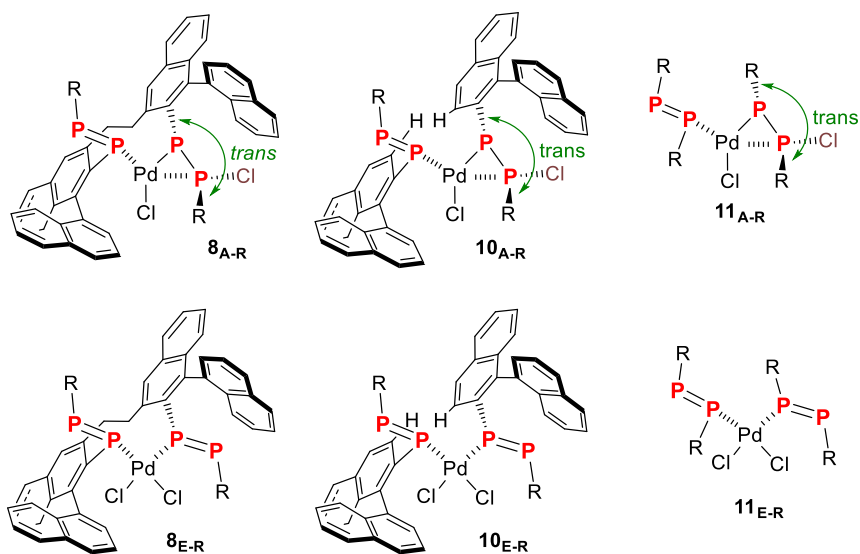
5-5. Optimization of Local Minima of Model Palladium Complexes.

The model palladium complexes **8_{A-R}**, **8_{E-R}**, **10_{A-R}**, **10_{E-R}**, **11_{A-R}**, and **11_{E-R}** were optimized at M06/SDD (Pd) and 6-31G(d) (P,Cl,C,H) level of theory. The symbol R represents the substituent on the phosphorus atom instead of the Mes* group for **8** and **10** and both substituents on phosphorus atoms for **11**. Compounds **10_R** were derivatives of **8** replaced the ethylene linker with the two hydrogens without ethylene linker.

Table S11. Relative energies (kcal mol⁻¹) of palladium complexes **8**, **10**, and **11**.

	(R = H)	(R = Me)	(R = Ph)	(R = Mes)	(R = Mes*)
8_{A-R}	0.0	0.0	0.0	0.0	0.0
8_{E-R}	4.5	11.4	11.7	4.0	3.6
Compounds without ethylene linker					
10_{A-R}	0.0	0.0	0.0	0.0	0.0
10_{E-R}	0.6	2.1	7.1	4.6	1.8
Compounds with same substituents on phosphorus atoms					
11_{A-R}	0.0	0.0	0.0	0.0	— ^a
11_{E-R}	11.0	9.4	11.5	1.9	— ^a

a) Not calculated.



R = H, Me, Ph, Mes, Mes*

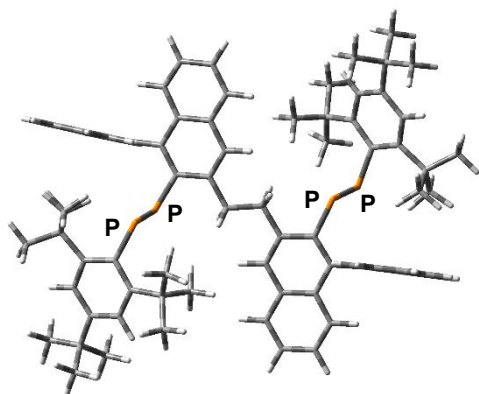
Table S12. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).^a

Structure	E	$E + ZPE$	H	G
Compound 8				
8_{A-H}	-4030.94958315	-4030.357114	-4030.312966	-4030.436720
8_{E-H}	-4030.94357170	-4030.351667	-4030.307382	-4030.429504
8_{A-Me}	-4109.53449380	-4108.884750	-4108.836887	-4108.968538
8_{E-Me}	-4109.51785073	-4108.867873	-4108.820022	-4108.950451
8_{A-Ph}	-4492.70809157	-4491.950017	-4491.896621	-4492.038977
8_{E-Ph}	-4492.68691300	-4491.929518	-4491.875499	-4492.020316
8_{A-Mes}	-4728.41486929	-4727.489690	-4727.427527	-4727.585365
8_{E-Mes}	-4728.40825335	-4727.483596	-4727.420825	-4727.578980
Compound 10				
10_{A-H}	-3953.58215459	-3953.026309	-3952.982956	-3953.107866
10_{E-H}	-3953.58726742	-3953.030606	-3952.987796	-3953.106939
10_{A-Me}	-4032.16439481	-4031.549905	-4031.503367	-4031.632767
10_{E-Me}	-4032.15984624	-4031.546343	-4031.499543	-4031.629360
10_{A-Ph}	-4415.34048159	-4414.619760	-4414.567080	-4414.709088
10_{E-Ph}	-4415.32586660	-4414.605762	-4414.552433	-4414.697704
10_{A-Mes}	-4651.05356080	-4650.163318	-4650.102404	-4650.258373
10_{E-Mes}	-4651.04211587	-4650.154173	-4650.092365	-4650.251049
10_{A-Mes*}	-5358.03327652	-5356.640456	-5356.554932	-5356.760573
10_{E-Mes*}	-5358.03399372	-5356.640102	-5356.555240	-5356.757641
Compound 11				
11_{A-H}	-2416.00350452	-2415.960571	-2415.947145	-2416.003314
11_{E-H}	-2415.98617348	-2415.943421	-2415.929853	-2415.985835
11_{A-Me}	-2573.16332906	-2573.004786	-2572.984109	-2573.056349
11_{E-Me}	-2573.14866026	-2572.989943	-2572.969286	-2573.041433
11_{A-Ph}	-3339.50484278	-3339.132039	-3339.099335	-3339.199596
11_{E-Ph}	-3339.48583628	-3339.112840	-3339.079882	-3339.181238
11_{A-Mes}	-3810.91848547	-3810.211473	-3810.160726	-3810.294704
11_{E-Mes}	-3810.90529616	-3810.202376	-3810.149733	-3810.291674

a) E : electronic energy; ZPE : zero-point energy; H ($= E + ZPE + E_{\text{vib}} + E_{\text{rot}} + E_{\text{trans}} + RT$): sum of electronic and thermal enthalpies; G ($= H - TS$): sum of electronic and thermal free energies. b) kcal mol⁻¹.

Table S13. Atomic coordinates of the optimized structures.

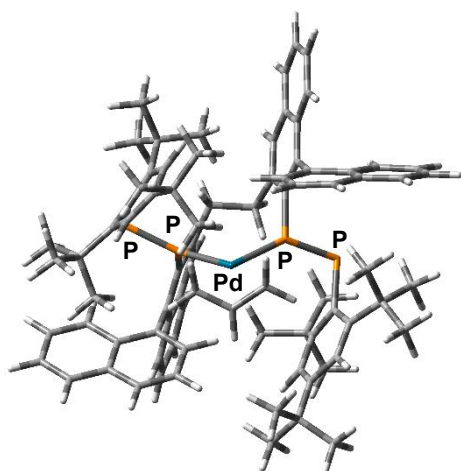
2



P	-3.72687400	0.43860700	-0.74887500	C	6.98820200	1.09081400	-0.31560900
P	-4.53422100	0.18586600	1.11893800	C	-7.01552000	-0.97279300	0.24158900
P	3.79958500	-0.56783400	0.16669900	C	2.60117800	-5.71624900	-0.76571800
P	4.84552600	-0.35115700	-1.57957600	H	3.64499500	-5.97805800	-0.60635800
C	-5.71977500	-1.22120500	0.76806800	C	-7.24499600	-3.34626900	-0.32530900
C	-2.48938500	1.76784100	-0.31607900	C	5.72560700	3.54686600	-0.62505100
C	2.68120600	-1.98377400	-0.30007700	H	5.25065600	4.51608200	-0.76034700
C	5.80375800	1.18093900	-1.09284200	C	0.80749400	-0.26406800	-0.26134700
C	-1.91248400	4.12349900	0.02433200	H	1.22242000	0.36050100	-1.07177800
C	-2.86315200	3.10380300	-0.29955100	H	1.26396700	0.13098800	0.66075700
C	2.20812700	-4.35527200	-0.68737500	C	0.01550700	6.05459600	0.72903400
C	5.23509900	2.46009800	-1.34805400	H	0.74938500	6.80859300	1.00854500
C	-0.23035900	2.37276300	0.29083100	C	0.35805300	4.72672600	0.71883400
H	0.80565900	2.12157200	0.51622200	H	1.36543600	4.40671000	0.98872300
C	-4.88654700	3.98651200	1.68155300	C	1.28092000	-1.68588400	-0.43770700
H	-3.93328500	3.58241800	2.01968300	C	-5.16490800	4.01270000	0.29190200
C	-2.23046400	5.50554700	0.02473500	C	1.68494300	-6.70259900	-1.03438900
H	-3.23452300	5.82069000	-0.25249300	H	2.00923900	-7.74052900	-1.08719600
C	3.13027400	-3.29240000	-0.42079800	C	-4.23568700	3.53885900	-0.68277400
C	0.83368800	-4.04265400	-0.86852800	C	-7.03913900	4.97432700	2.16017800
C	-1.12620200	1.39445500	-0.06212200	H	-7.75518100	5.34483500	2.89175200
C	-6.41928200	4.53467700	-0.14346400	C	-5.80075400	4.45452800	2.59250000
C	-0.58721400	3.73769700	0.35757600	H	-5.57019200	4.42358700	3.65580100
C	-7.71862800	-2.04450200	-0.31998700	C	-0.08605300	-5.07797600	-1.15699100
H	-8.68136500	-1.84366100	-0.77700500	H	-1.13329300	-4.81308900	-1.30678100
C	6.77805800	3.45844200	0.27835500	C	-7.74710300	0.38822500	0.23844100
C	-0.69766000	-0.04855800	-0.19778000	C	7.41867500	2.23204200	0.36922600
H	-1.11608600	-0.64480100	0.63152500	H	8.28853900	2.14747300	1.01237300
H	-1.16513600	-0.45928300	-1.10845700	C	7.87029900	-0.16677100	-0.15743600
C	-6.05158800	-3.57822100	0.34901600	C	8.35572700	4.39260600	2.03123900
H	-5.70133800	-4.60438100	0.41943100	H	8.09213100	3.61128200	2.75741900
C	-1.29077600	6.44535400	0.36861800	H	8.60857900	5.29978200	2.59676800
H	-1.55626500	7.50113800	0.36388600	H	9.26186900	4.07506600	1.49698200
C	-4.57771200	3.57651800	-2.01799100	C	-5.82202700	4.08524500	-2.44490800
H	-3.85633000	3.22313500	-2.75495000	H	-6.05716300	4.10483000	-3.50743100
C	0.40957600	-2.70147200	-0.73707400	C	-7.33937600	5.01002800	0.82175500
H	-0.65235200	-2.49733300	-0.87030800	H	-8.29434500	5.40786900	0.47655900
C	-5.28288400	-2.56947400	0.92713200	C	-6.71911700	4.56449000	-1.52684200
C	0.32769300	-6.38275700	-1.24195600	H	-7.67995900	4.97099900	-1.84425300
H	-0.38857100	-7.17232700	-1.46271500	C	5.30179500	-4.00186500	-1.38182900

H	4.83667000	-3.91197600	-2.36392200	C	-2.85166300	-3.15173500	0.68017900
C	4.56327400	-3.67047900	-0.26572400	H	-2.66334900	-2.19497300	0.17615000
C	5.15300300	-3.79911600	1.02670000	H	-3.08142700	-3.89589500	-0.09628600
C	7.20359700	4.68881600	1.07382900	H	-1.92725800	-3.46337700	1.19113500
C	-7.99308600	-4.50693100	-0.97403600	C	9.35615300	0.23223200	-0.08139400
C	7.52004700	-0.91032800	1.13644600	H	9.61967700	0.75372600	0.84631800
H	6.49106900	-1.29382300	1.12971800	H	9.64581000	0.87041000	-0.92746900
H	7.62630500	-0.24957200	2.00790600	H	9.97413800	-0.67498300	-0.11313600
H	8.19326800	-1.76992800	1.27556700	C	-9.26585400	-4.05342500	-1.68569500
C	6.50163100	-4.25602700	1.13081000	H	-9.98871800	-3.60648300	-0.98921700
C	6.01595200	5.19018900	1.90363700	H	-9.75386300	-4.91798300	-2.15590800
H	5.16004200	5.46743800	1.27434200	H	-9.05216900	-3.32171500	-2.47706400
H	6.30396800	6.07867200	2.48396500	C	-8.38704100	-5.52693000	0.10047600
H	5.67700400	4.41765200	2.60730900	H	-7.51168600	-5.93652300	0.62125400
C	4.09918000	2.79382700	-2.34418600	H	-8.93000500	-6.36887900	-0.35298100
C	-4.01103900	-3.03634600	1.67425400	H	-9.03992300	-5.06670800	0.85488700
C	-4.22269200	-4.42269500	2.30981600	C	2.80303400	3.03591700	-1.56421200
H	-3.35218300	-4.66983900	2.93137600	H	1.96200900	3.23238500	-2.24627900
H	-4.31330100	-5.23077300	1.57470900	H	2.89366800	3.89743400	-0.88820200
H	-5.11432700	-4.44014500	2.95139500	H	2.54959100	2.15806100	-0.95310900
C	7.77864000	-1.12118600	-1.34991000	C	-3.60579500	-2.12902200	2.84184400
H	8.54744400	-1.90117000	-1.25572100	H	-3.17591000	-1.16987500	2.53069300
H	7.94165300	-0.59274300	-2.30009300	H	-2.83291000	-2.62918800	3.44129900
H	6.82476300	-1.65952300	-1.41419900	H	-4.45927500	-1.91535500	3.50046800
C	3.83232000	1.73971700	-3.42365200	C	-9.26905200	0.18856000	0.36654500
H	3.19191300	2.18027900	-4.20068800	H	-9.52431700	-0.44616500	1.22620900
H	3.29572500	0.85763500	-3.05456600	H	-9.72836300	-0.24550900	-0.52980200
H	4.75787000	1.40214100	-3.91030400	H	-9.74539100	1.16667600	0.51456400
C	7.65688100	5.79196900	0.11083900	C	-7.36714800	1.27584900	1.42612500
H	8.51038700	5.45589000	-0.49391100	H	-7.46607900	0.73385800	2.37754100
H	7.96692500	6.68548400	0.67191100	H	-8.03039000	2.15151800	1.46101900
H	6.85700500	6.09234800	-0.57870000	H	-6.35005600	1.68278800	1.37294400
C	-7.49215200	1.12726000	-1.07924300	C	5.05996500	-3.59247100	3.44385700
H	-8.05787800	2.07103400	-1.10004900	H	4.50674900	-3.34050300	4.34680400
H	-7.81350600	0.51644100	-1.93463400	C	7.21831200	-4.58575900	-0.04338900
H	-6.43215400	1.37272800	-1.22143200	H	8.24637800	-4.93689400	0.05282300
C	4.45864300	4.06982300	-3.12867300	C	-7.08637100	-5.18069700	-2.01018400
H	5.39736500	3.93668300	-3.68386500	H	-6.79456100	-4.47028100	-2.79568100
H	4.56340100	4.96112600	-2.50083400	H	-7.61133900	-6.02086300	-2.48727400
H	3.66320900	4.28757900	-3.85418200	H	-6.16708200	-5.57640000	-1.55947200
C	4.45140500	-3.48679800	2.21856600	C	7.09592200	-4.36326800	2.41105100
H	3.41567500	-3.15793400	2.14778100	H	8.12781800	-4.71042800	2.47600300
C	6.63073300	-4.46013500	-1.27553700	C	6.39730200	-4.03140500	3.54327000
H	7.18605500	-4.70762200	-2.17875600	H	6.86901600	-4.11131200	4.52109100

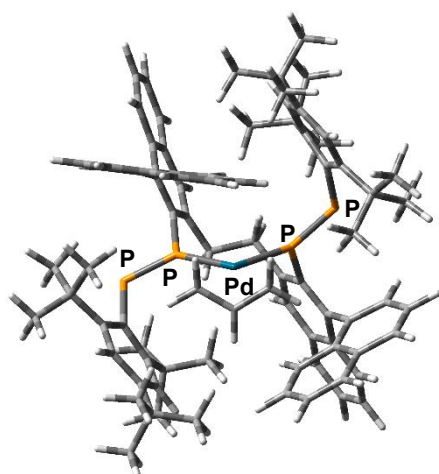
7A⁺



C	5.99250300	-3.27054600	3.10549800	C	1.93020200	-0.24531700	3.30168400
C	6.93462800	1.66502000	0.59195100	H	3.64887900	-2.12319300	-2.89909200
C	4.25342800	-1.67880900	2.52709700	C	-1.19389800	5.08956300	-3.33558700
C	5.26977600	0.02771100	-0.07402100	H	2.65938300	-2.11839000	-0.61206300
C	4.11286200	-0.76645400	0.19671400	C	-1.84560300	-0.04610300	3.36652300
C	3.57740400	-0.84466900	1.58451700	C	-2.48228600	0.69517000	4.33199300
C	4.11100900	-1.52478600	-2.11432400	C	-2.39830100	-0.07190700	2.04735800
C	5.24943500	-0.80804700	-2.38143400	C	-3.63008100	1.46819000	4.04660600
C	5.85267800	-0.01522000	-1.37570700	H	-2.07659900	0.71857800	5.34597400
C	6.99807400	0.77192800	-1.64745200	C	-3.51706800	0.68103000	1.72128800
C	7.52566500	1.60092700	-0.68882400	C	-4.14984100	1.48208000	2.71923600
H	8.39769400	2.21216000	-0.91343000	C	-4.24101100	2.27330600	5.03896800
H	7.43912900	0.72011400	-2.64314200	C	-4.03241100	0.72325300	0.32422000
H	5.69982200	-0.82836100	-3.37374500	P	-2.46877700	-2.92034500	1.00363600
C	5.51338400	-3.32636100	4.43285500	C	-5.25761500	2.32091300	2.43286500
C	4.42371400	-2.57909600	4.80280200	C	-5.31067300	3.07514600	4.72992800
C	3.76515900	-1.74737500	3.86426000	H	-3.83378200	2.25161300	6.04962900
H	6.00880500	-3.96792900	5.15903700	C	-5.21194200	0.01056300	-0.04998800
H	4.03892200	-2.62049100	5.82159900	C	-3.38348700	1.50241600	-0.61324500
C	2.60745900	-1.01693200	4.21394100	C	-1.52979100	-3.89564200	-0.26511700
H	2.22964700	-1.09424800	5.23593500	C	-5.82030200	3.10062600	3.41256700
C	5.84228300	0.88837000	0.89652000	H	-5.65333900	2.35037500	1.41894800
H	5.40046700	0.93712000	1.89122500	H	-5.76768800	3.69717400	5.49718500
C	5.38097200	-2.46595200	2.17657500	C	-5.71829900	0.15757300	-1.37675100
H	5.75608100	-2.43549500	1.15509000	C	-5.88047900	-0.86892100	0.83857200
H	7.35191800	2.33154000	1.34455100	C	-3.87326800	1.62110600	-1.93163700
H	6.85308000	-3.87177400	2.81834700	H	-2.47684800	2.04071300	-0.32852200
C	2.44592500	-0.14136400	1.97095400	C	-2.06876700	-4.07322400	-1.57322300
C	3.54776100	-1.51444200	-0.81792900	C	-0.19630700	-4.29060800	0.00010300
P	2.41525600	2.75872600	1.06857200	H	-6.66538300	3.74357700	3.17411400
C	1.44862200	3.79275100	-0.13221900	C	-5.02494500	0.97550900	-2.30246400
C	1.97132000	4.04213200	-1.43896900	C	-6.88770900	-0.54803300	-1.75135200
C	0.13459500	4.21360700	0.18902000	C	-6.99605400	-1.56258500	0.43486600
C	1.07188200	4.43046900	-2.42746700	H	-5.49158200	-0.99711300	1.84852700
C	-0.71164800	4.58171600	-0.86922400	H	-3.33897200	2.24693500	-2.64722600
C	-0.28786400	4.65328100	-2.18775100	C	-1.17245600	-4.32957900	-2.60898500
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H	-1.73649900	4.85683600	-0.63192000	C	0.64464800	-4.52791300	-1.09540800
C	-0.43100000	4.49496600	1.60174500	C	0.40619300	-4.63231700	1.38073700
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H	-7.27169200	-0.41865700	-2.76342700	H	-1.58570300	6.25095100	0.90306700
H	-7.49030500	-2.24263100	1.12619000	H	0.06689700	6.61917400	1.43444000
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H	1.68402200	-4.77532900	-0.89468500	H	3.01151100	-4.24512100	-2.51672600
H	-8.40364300	-1.94039500	-1.17033700	H	3.20473800	-5.07850400	-4.06751800
C	1.14317600	-4.63602500	-3.60274400	C	0.64464700	-5.72806700	-4.55537000
C	-0.52151300	-0.68596100	3.67835200	H	-0.33829100	-5.49687200	-4.98480800
H	-0.55238800	-1.19875600	4.65050200	H	0.57103300	-6.69520500	-4.03929300
H	-0.27603900	-1.45928600	2.93625600	H	1.34853200	-5.84244400	-5.39149500
P	-1.59921200	-1.08847000	0.74367100	C	1.18818600	-3.29353200	-4.34429200
P	1.59149700	0.91758100	0.73527700	H	1.52950400	-2.49063600	-3.67065000
C	0.61258000	0.36602000	3.68560200	H	0.20136100	-3.00858200	-4.73556300
H	0.34578000	1.17282300	2.98891300	H	1.88643800	-3.34336100	-5.19213200
H	0.67293800	0.83261400	4.67943800	C	-3.88101700	-4.93958400	-3.11931000
C	3.95215000	2.58195700	-2.13526900	H	-3.49945100	-5.96063900	-2.98240800
H	3.45869900	2.19928300	-3.04120200	H	-3.47207900	-4.54014400	-4.05552800
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H	5.03547400	2.58973600	-2.32661200	C	-4.41989100	-4.62195000	-0.75354300
C	4.32799700	4.58123100	-0.66754900	H	-5.45733600	-4.75464100	-1.08970800
H	5.36787600	4.68655500	-1.00577100	H	-4.47064400	-3.95908100	0.12049400
H	4.36108100	3.94386300	0.22586900	H	-4.03866500	-5.59807300	-0.42307600
H	3.96317200	5.57313300	-0.36709200	C	-4.05607600	-2.63714100	-2.23366100
C	3.77167300	4.86771300	-3.03233600	H	-3.57275800	-2.26497700	-3.14924900
H	3.40669600	5.89647100	-2.90699100	H	-3.84893300	-1.92983900	-1.41903300
H	3.34682500	4.45766100	-3.95729600	H	-5.14315700	-2.63066300	-2.40261800
H	4.85876700	4.91093000	-3.17941200	C	-0.56293800	-4.59710900	2.56437500
C	-0.63530300	6.37880600	-3.95501700	H	-0.07601400	-5.06719600	3.43028700
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H	0.35584200	6.23058000	-4.40333500	H	-0.83426200	-3.58360500	2.88498100
H	-0.54961900	7.17044300	-3.19786100	C	1.59472800	-3.72371200	1.69910300
C	-1.23973700	3.99670400	-4.40924300	H	1.29200000	-2.66559100	1.72592400
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H	-0.23696500	3.69500400	-4.74132800	H	2.01926600	-3.97992800	2.68132300
H	-1.79414200	4.35138000	-5.28953400	C	0.89330700	-6.09389100	1.30953300
C	-2.62185300	5.37458100	-2.87505500	H	1.32491000	-6.38550800	2.27697000
H	-2.66264400	6.21946500	-2.17324900	H	1.66260800	-6.25443500	0.54595900
H	-3.08212800	4.50431200	-2.38495600	H	0.05576300	-6.77160200	1.09300400
H	-3.24293300	5.63387700	-3.74281800	Pd	-0.05394900	-0.00690900	-0.69108000
C	-1.67989600	3.65803500	1.88744000	C	0.94007100	0.70611200	-2.53802900
H	-1.45334800	2.58106200	1.88608700	C	-1.04903000	-0.69446000	-2.54558700
H	-2.47913400	3.83439700	1.15417800	C	-0.42821200	0.53820800	-2.79639300
H	-2.08633300	3.91032000	2.87861900	H	-0.50955100	-1.63925400	-2.66066300
C	0.54170100	4.31074000	2.76748700	H	-2.13572500	-0.75488700	-2.56539300
H	0.08575200	4.73304100	3.67414300	H	-1.05078900	1.42926700	-2.90495800
H	1.48873600	4.84591300	2.60768900	H	1.36190000	1.71031000	-2.54877700
H	0.75891900	3.26068400	3.00062800	H	1.64557400	-0.12205400	-2.64969100
C	-0.81185500	5.99014100	1.63401300				

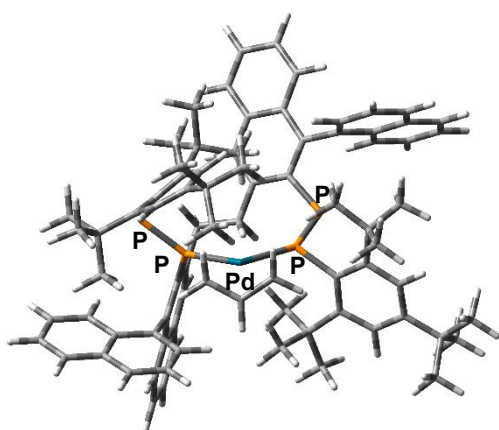
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C	1.79838400	-1.68609500	4.32819900	C	-3.87008600	5.31706400	4.46986800
C	0.85323600	-2.03280200	2.13531100	H	3.82201300	-2.35693400	5.94855100
P	-1.81346400	-3.21122400	1.61416600	H	4.14640600	-4.38993800	1.42092700
C	0.82493400	-1.38190600	3.40809700	H	-2.96799100	3.86016500	5.76014200
C	-0.40623800	2.19716900	3.09162400	H	-4.52965200	5.71262300	5.23992400
C	-1.24004600	2.72261600	4.04895200	H	-4.58321100	6.68787100	2.94860900
C	-0.47001500	2.71598100	1.75605100	H	-3.10422400	5.81833400	1.18858600
P	2.21800900	3.10748100	0.54651800	C	-1.36810900	4.37585100	0.08367700
C	0.53641900	1.08939200	3.47640700	C	-0.49975600	5.39325500	-0.24936500
H	1.08703500	1.36683700	4.38827800	C	-2.36105300	3.97001400	-0.85644600
H	1.30392900	0.96018400	2.70167500	C	-0.55024500	6.01633200	-1.51467800
P	0.56184700	1.90257500	0.45659400	H	0.23547800	5.72559400	0.48457800
P	-0.54041500	-1.74829800	0.96638600	C	-2.40707600	4.59539900	-2.13909500
Pd	-0.51704900	0.03718300	-0.62504700	C	-1.47927400	5.62081200	-2.44374700
C	-0.15060600	-0.27444400	3.70230200	H	0.15457500	6.81351500	-1.74530100
H	-1.03607200	-0.33984800	3.05444600	C	-4.31222900	3.21385000	-2.74330000
H	-0.52164300	-0.34046700	4.73508900	C	-3.39506100	4.18213400	-3.06950400
H	1.77586000	-1.21125500	5.31167400	C	-4.28192700	2.61636300	-1.46277000
C	-2.14783500	3.76520300	3.76385800	C	-3.32499400	2.97926800	-0.54826000
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C	-1.32216000	3.76930400	1.44477100	H	-5.07085600	2.90994000	-3.46284000
H	-1.19219800	2.33784300	5.07029800	H	-3.41827100	4.65974400	-4.04905400
C	4.97324100	-3.59331900	4.62654100	H	-1.52562200	6.09519800	-3.42400400
H	5.76535900	-3.77187400	5.35124400	H	-3.30159400	2.52093700	0.43936400
C	5.06154200	-4.15925700	3.33570900	C	2.23140600	-1.51514900	-0.82881800
H	5.92716500	-4.76314700	3.07006300	C	1.95323600	-2.94837900	-3.21143700
C	4.06537100	-3.95176500	2.41365400	C	2.25890800	-0.86419100	-2.04023400
C	3.89609500	-2.81222300	4.96102300	C	2.09982600	-1.58247600	-3.24562600
C	1.88863000	-3.61752200	0.48505400	H	1.86341600	-3.52170700	-4.13422400
C	1.74012700	-4.99066800	0.46783800	H	2.11640400	-1.05096100	-4.19739000
C	2.02105700	-2.91627700	-0.75404000	H	2.42570300	0.21264500	-2.06765200
C	1.70199000	-5.71613900	-0.74054400	H	2.39082600	-0.94755700	0.08740200
H	1.63768900	-5.52081600	1.41543100	C	-3.28313300	-3.02194700	0.50484300
C	1.92028300	-3.64811800	-1.97740000	C	-3.41829600	-3.86842200	-0.62830000
C	1.78014300	-5.05610700	-1.94005300	C	-4.20475400	-1.95078600	0.69859800
H	1.58279600	-6.79771200	-0.71196000	C	-4.30325800	-3.46825100	-1.63708400
H	1.71880300	-5.60076000	-2.88239200	C	-5.03096400	-1.60424300	-0.37084500

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C	3.52697400	2.33292500	-0.51019400	H	-2.78226400	-1.79379500	3.36880200
C	3.62589700	2.60419900	-1.90736600	C	1.48650200	3.38684700	-3.00914000
C	4.43667300	1.41769200	0.09197700	H	1.49431700	2.48926500	-3.64624900
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C	5.18990900	0.60633900	-0.76024500	H	1.00542600	4.20075700	-3.57204900
C	5.17257700	0.71453000	-2.14405900	C	3.64346400	4.14211000	-3.93505300
H	4.48936000	1.94316700	-3.74859100	H	3.19569900	5.05729600	-4.34400700
H	5.83003100	-0.15045600	-0.31350400	H	4.71227800	4.33487500	-3.77002300
C	-4.40689300	-1.14584100	2.00309800	H	3.54465000	3.37182300	-4.71016400
C	-2.68174400	-5.19642000	-0.91449000	C	2.92426700	5.05414500	-1.78798600
C	-5.98795100	-1.87917600	-2.70981300	H	3.94371300	5.31407100	-1.47064600
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C	6.01463900	-0.22445500	-3.00388100	H	2.29200000	5.00024500	-0.89074400
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H	-0.91822500	-4.25561300	-1.79684400	H	4.57019700	-0.28027700	3.13847700
H	-1.18533800	-5.93242800	-2.30808000	C	4.21657800	2.31140700	2.54501800
C	-1.91807300	-5.80919300	0.26021100	H	4.67984400	2.17346000	3.53219100
H	-2.53909800	-5.89775600	1.16283500	H	4.46321000	3.32940100	2.21199200
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H	-0.99476200	-5.26854700	0.50755400	C	6.29423700	1.31932600	1.76800800
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H	-4.45289300	-6.41330100	-0.50886200	H	6.83580700	0.52098300	1.24939400
H	-4.27197700	-6.01668200	-2.22855700	H	6.67835300	2.28172500	1.40234600
H	-3.21221200	-7.21832500	-1.49327900	C	5.88633800	-1.67277800	-2.51558400
C	-5.87162900	-0.37248300	-2.95832700	H	6.23682900	-1.80413900	-1.48370400
H	-6.18126400	0.22188300	-2.08847200	H	4.84396000	-2.02087600	-2.56931000
H	-4.83972200	-0.09415500	-3.22179100	H	6.49673100	-2.32995200	-3.15066400
H	-6.52017300	-0.08046700	-3.79585000	C	7.48114000	0.21546700	-2.90479300
C	-5.64996800	-2.58875300	-4.02093400	H	8.11856200	-0.43761800	-3.51836900
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H	-6.28054200	-2.19086300	-4.82710600	H	7.84663500	0.17134900	-1.86935400
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C	-7.43295000	-2.21826600	-2.32288100	H	4.52913100	-0.44072800	-4.59191500
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H	-7.54855200	-3.29744900	-2.15058100	H	6.17686300	-0.93200900	-5.03781300
H	-7.73948300	-1.69436900	-1.40712600	C	-1.52938300	-1.21381700	-2.15748000
C	-5.91469800	-0.96647100	2.26566000	H	-0.62606300	-1.58181100	-2.65419200
H	-6.05423000	-0.43112900	3.21414700	H	-2.24712700	-1.96522100	-1.83239200
H	-6.42864300	-0.38154100	1.49522300	C	-0.95883000	1.10450300	-2.53000600
H	-6.41786200	-1.93972300	2.34827300	H	-1.22411100	2.16098500	-2.48592000
C	-3.77328700	0.24205000	1.85310700	H	-0.05121500	0.85329600	-3.08186100
H	-3.83982800	0.81203200	2.79307900	C	-1.93550400	0.12083200	-2.30979200
H	-2.71359700	0.17568200	1.56158300	H	-2.93731800	0.41648500	-1.98658900
H	-4.29534100	0.81308800	1.07265400				

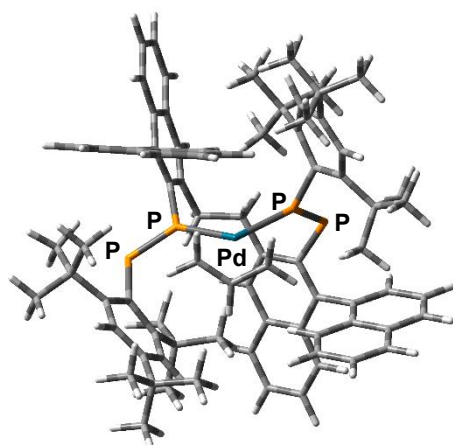
7c⁺



C	4.50597400	5.03680200	-3.74404000	H	4.37167000	3.50852800	2.34345800
C	7.41531600	0.41603300	-1.97056200	C	1.83142900	-3.49813000	4.73704700
C	3.53751900	2.96380900	-2.93143600	H	2.83545200	3.10259600	0.42556600
C	5.62279200	1.57942400	-0.81751600	C	-1.48075700	-1.22026200	-2.89936100
C	4.27453100	2.04882500	-0.73748200	C	-1.35698200	-2.29617900	-3.73964400
C	3.39528000	1.94630100	-1.93592400	C	-2.58791800	-1.17348300	-1.98925600
C	4.73151500	2.96557700	1.47064800	C	-2.29037900	-3.36031700	-3.74687600
C	6.03591100	2.54582100	1.40388100	H	-0.51816100	-2.35510100	-4.43396000
C	6.51263000	1.85191100	0.26450500	C	-3.53640100	-2.18972700	-1.98671500
C	7.85561600	1.40877600	0.18290700	C	-3.40597000	-3.30914600	-2.86577300
C	8.29949800	0.70371200	-0.90811000	C	-2.13662800	-4.46952200	-4.61121500
H	9.33192700	0.36299100	-0.95714700	C	-4.69480100	-2.17321500	-1.04901200
H	8.52713600	1.63202400	1.01217200	P	-1.47720600	0.81816900	0.31540200
H	6.72793100	2.74321200	2.22241800	C	-4.34038600	-4.37595300	-2.89115800
C	3.74490100	4.93873900	-4.92949300	C	-3.05801500	-5.48782800	-4.61373000
C	2.89921100	3.87502800	-5.11771900	H	-1.27264200	-4.49629400	-5.27533200
C	2.77726300	2.86746200	-4.13072200	C	-5.94745800	-1.61592700	-1.44922800
H	3.83507600	5.70859400	-5.69349800	C	-4.58357200	-2.79336700	0.17827300
H	2.30967100	3.78569300	-6.02993700	C	-2.36153400	2.22602000	1.12587800
C	1.93234400	1.75151500	-4.31688900	C	-4.17135400	-5.43650100	-3.74780100
H	1.38101700	1.66943100	-5.25565900	H	-5.19837600	-4.34973200	-2.22185200
C	6.11296400	0.85342000	-1.93289300	H	-2.93312100	-6.33667800	-5.28323900
H	5.44503100	0.64138000	-2.76707900	C	-7.05400200	-1.69251500	-0.55098300
C	4.40838600	4.07356700	-2.77035500	C	-6.13205000	-0.99138800	-2.70806200
H	4.99968200	4.15873000	-1.86021800	C	-5.68287400	-2.87597400	1.05887500
H	7.77187100	-0.14684900	-2.83121800	H	-3.63051600	-3.24433400	0.45996600
H	5.17652000	5.88216200	-3.60282200	C	-2.14896600	3.56309600	0.64360000
C	2.51206500	0.89056700	-2.13407300	C	-3.34942200	1.96690700	2.11181800
C	3.85718800	2.72635000	0.38808900	H	-4.89827200	-6.24637500	-3.75678600
P	3.28508700	-1.95317600	-1.01945700	C	-6.89170200	-2.33529300	0.70144000
C	2.93237900	-2.84285800	0.57764600	C	-8.29609100	-1.13392300	-0.94154300
C	3.94231700	-2.86444900	1.59124000	C	-7.35046000	-0.46242000	-3.05784500
C	1.64312500	-3.34824300	0.88072600	H	-5.29192300	-0.93797700	-3.40041000
C	3.53597100	-3.10543600	2.90208600	H	-5.56180300	-3.36888800	2.02264400
C	1.30444400	-3.52471100	2.23057000	C	-3.01956900	4.55005200	1.09175200
C	2.20889800	-3.35052800	3.26636500	C	-0.96395800	4.03639800	-0.23951800
H	4.28443700	-3.08468900	3.68961700	C	-4.15863900	3.04283400	2.51705000
H	0.28954800	-3.83625000	2.46460400	C	-3.68701900	0.65362700	2.87655100
C	0.59518500	-3.87484000	-0.12106900	H	-7.74743900	-2.39096300	1.37440100
C	5.45165800	-2.64929000	1.34181600	C	-8.44312900	-0.53103200	-2.16591600
C	1.78681000	0.77241700	-3.36569300	H	-9.13470400	-1.19507200	-0.24780900

H	-7.47740500	0.01171600	-4.02941800	H	-5.54313600	4.66700500	4.37659700
C	-4.04445900	4.32204400	2.01050500	H	-6.63452300	5.89707600	3.71662300
H	-2.90807700	5.55887400	0.71107700	C	-0.70796500	-3.07960100	-0.01578100
H	-4.92832700	2.85411700	3.25839700	H	-1.13650500	-3.11307700	0.99654500
H	-9.40283500	-0.10705300	-2.45533200	H	-0.54706400	-2.02311000	-0.27535000
C	-4.96146000	5.46894200	2.42430600	H	-1.45416200	-3.48620900	-0.71416100
C	-0.49000100	-0.09504500	-2.92368100	C	1.03476800	-3.90754700	-1.58465600
H	-0.95460200	0.80599100	-3.36199300	H	2.00012900	-4.41867100	-1.71327300
H	-0.26039400	0.18664800	-1.88803100	H	0.28886700	-4.46360000	-2.17095600
P	-3.02162300	0.27317300	-0.93361500	H	1.09521900	-2.91422800	-2.04067700
P	2.20948600	-0.24172500	-0.70951100	C	0.31439300	-5.34692900	0.24476900
Pd	0.80084800	0.40527400	1.09739300	H	-0.10350900	-5.46879700	1.25025500
C	0.83234700	-0.35537600	-3.63392100	H	-0.41058200	-5.76829100	-0.46528800
H	1.25786700	-1.31335800	-3.30123800	H	1.23456800	-5.94456200	0.18567500
H	0.67735500	-0.44581900	-4.71771700	C	0.33062800	-3.70567900	4.93400600
C	-0.74892800	3.24633700	-1.53833400	H	-0.25802000	-2.87902500	4.50808300
H	-1.68343200	3.12141200	-2.10370700	H	-0.01948900	-4.64470700	4.48359000
H	-0.02991700	3.78060600	-2.17677500	H	0.10627700	-3.75342400	6.00799200
C	0.31303200	3.96384600	0.60478900	C	2.23668400	-2.23253100	5.50270600
H	0.21515200	4.55190300	1.52889900	H	3.31025900	-2.01840000	5.41972700
H	0.55524800	2.92731600	0.88275200	H	1.68638400	-1.35344500	5.13427700
H	1.16053700	4.36591200	0.02848200	H	2.00160200	-2.34806300	6.57017400
C	-1.11034300	5.50316900	-0.67362200	C	2.56552300	-4.70780500	5.32897000
H	-1.11882500	6.19907900	0.17473400	H	2.28742200	-4.83938200	6.38422500
H	-0.24593500	5.77148600	-1.29405400	H	2.30025800	-5.62773700	4.78968000
H	-2.01472400	5.66997000	-1.27460200	H	3.65609500	-4.59091700	5.28353000
C	-2.90109400	-0.62746300	2.56874000	C	5.78735300	-1.15731600	1.32905300
H	-3.18253700	-1.08118500	1.61416600	H	5.26815000	-0.61330200	0.52834300
H	-1.81123900	-0.49915600	2.57821900	H	5.52272800	-0.68747800	2.28871000
H	-3.13886200	-1.36382000	3.35090600	H	6.86593400	-1.01317100	1.17117300
C	-5.16190800	0.29872600	2.62417300	C	5.92187800	-3.30509800	0.03687300
H	-5.34438300	0.16294300	1.54788900	H	7.01660300	-3.24286000	-0.02997600
H	-5.40782300	-0.64853300	3.12480100	H	5.63722700	-4.36578500	0.00049200
H	-5.85930700	1.05883800	2.99537400	H	5.53392700	-2.81652700	-0.86553300
C	-3.46590200	0.91697500	4.37945800	C	6.29663700	-3.29551100	2.45098700
H	-2.40160200	1.09288200	4.59478400	H	6.19862900	-2.78642800	3.41783500
H	-4.02599200	1.77886500	4.75786500	H	6.04777600	-4.35660900	2.58985800
H	-3.78202100	0.03867700	4.95888800	H	7.35612300	-3.23233000	2.17095200
C	-5.69730700	5.99844500	1.18757800	H	-0.31997400	2.25153900	-1.37306500
H	-6.36807800	6.82122400	1.47297500	C	0.29036200	0.91033700	3.20171900
H	-5.00525400	6.38244900	0.42669500	H	0.03554400	-0.09600300	3.54496200
H	-6.30522700	5.20877800	0.72462100	C	2.49838200	0.24599100	2.50122100
C	-4.12498300	6.59500200	3.04474000	H	2.34595900	-0.79942900	2.78608100
H	-3.58491400	6.23818100	3.93292900	H	3.49465100	0.51103700	2.14802700
H	-3.38736300	7.00243300	2.34102000	C	1.63166200	1.24578100	2.97379200
H	-4.77834100	7.42280400	3.35500800	H	1.92367200	2.29482200	2.89755900
C	-6.00620300	5.03647900	3.45077400	H	-0.44938600	1.69019800	3.38546000
H	-6.66868100	4.25210400	3.05844200				

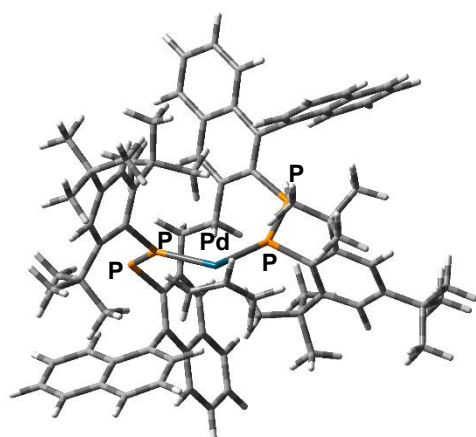
7d⁺



C	-3.94392400	1.83672700	2.98714800	C	5.70757700	-2.35487700	2.30153200
C	-2.90776500	2.07805600	2.02943700	C	6.76351100	-1.68771200	2.87311400
C	-3.59695800	1.31499700	4.26610600	C	6.53522000	-0.63392100	3.78477900
C	-2.23950600	1.05900800	4.55796000	H	-4.33186000	0.64836500	6.18456600
C	-1.59060000	1.73567500	2.32993300	H	-5.59944400	2.45477300	1.72624200
P	0.56539300	3.63740100	1.38448400	H	5.06459500	0.53849900	4.81752300
C	-1.24513600	1.23138500	3.62707800	H	7.38048500	-0.11526700	4.23322500
C	1.73295800	-1.12273000	3.20961300	H	7.78398300	-1.97299900	2.62465100
C	2.81626700	-0.52621100	3.80371500	H	5.89132700	-3.17028900	1.60368100
C	1.95791700	-2.21118000	2.30202100	C	3.46410800	-3.77003100	1.06489200
P	-0.40044600	-2.15871000	0.30433600	C	3.37256400	-5.07165500	1.51601600
C	0.33218100	-0.66063500	3.48400100	C	3.79081100	-3.52154100	-0.30296400
H	-0.16802600	-1.34270400	4.19425200	C	3.58298900	-6.16382900	0.64765900
H	-0.23777200	-0.76328200	2.55667500	H	3.13401700	-5.25450000	2.56409000
P	0.58847300	-3.29133300	1.69181000	C	4.03522500	-4.62749400	-1.16949700
P	-0.34146000	1.84252600	0.97287600	C	3.91519300	-5.94582000	-0.66566800
Pd	0.01613800	0.05716600	-0.62484400	H	3.49230000	-7.17763100	1.03231400
C	0.14912600	0.77980600	3.96677700	C	4.45050300	-3.10077800	-3.01120100
H	0.89835000	1.42662300	3.49388500	C	4.36969700	-4.38174100	-2.52449700
H	0.31216400	0.85824900	5.05022200	C	4.20418800	-2.00430800	-2.15472600
H	-1.98234100	0.67770100	5.54857400	C	3.88262900	-2.21051300	-0.83440100
C	4.14346000	-0.92922500	3.52532100	H	4.28314300	-0.98871100	-2.54428900
C	4.37084700	-1.99186400	2.60486900	H	4.70728400	-2.92508400	-4.05409000
C	3.24561200	-2.63809900	2.01045400	H	4.55532700	-5.23570900	-3.17623600
H	2.67022900	0.29514600	4.50742800	H	4.09262100	-6.78207400	-1.34200500
C	-5.93460000	1.27537100	4.90319200	H	3.69691800	-1.36207500	-0.17767800
H	-6.71228300	1.06273900	5.63429000	C	-3.21205500	0.78672600	-0.70986400
C	-6.28524900	1.78904900	3.63535900	C	-3.92239500	2.37395800	-2.89610900
H	-7.33245500	1.96339600	3.39565500	C	-3.31712000	0.23506200	-1.96628200
C	-5.31598400	2.06739800	2.70317700	C	-3.65896100	1.03891800	-3.07529100
C	-4.61710400	1.04561100	5.21053300	H	-4.21348700	3.00050200	-3.73925600
C	-3.28929600	2.80104600	0.77961900	H	-3.73002600	0.59452600	-4.06718500
C	-3.58313500	4.14546700	0.90382600	H	-3.14282900	-0.83283000	-2.10300400
C	-3.43607700	2.17174800	-0.49418100	H	-2.96108000	0.15004400	0.13960700
C	-4.02022800	4.91659600	-0.19117400	C	1.71065500	3.95973400	-0.04175100
H	-3.48385900	4.61475400	1.88358000	C	1.28652300	4.83974700	-1.07801500
C	-3.83589500	2.96921900	-1.61249300	C	2.95280700	3.27347800	-0.18255400
C	-4.14198900	4.33827700	-1.42763500	C	1.98541100	4.80787900	-2.29285600
H	-4.24417300	5.97225200	-0.04805700	C	3.56210800	3.27250300	-1.43634600
H	-4.45862300	4.92365900	-2.29100300	C	3.08312000	3.99341200	-2.52683300
C	5.25144300	-0.26971100	4.10969900	H	1.63314700	5.44164800	-3.10064600

H	4.47330100	2.69149100	-1.56463200	H	-5.43115400	-2.68697300	-5.27783100
C	-1.86943200	-3.07268800	-0.39799100	H	-4.35203900	-1.65708700	-4.31047600
C	-3.19199100	-2.73572000	0.02434100	H	-3.77071600	-3.21188300	-4.94595900
C	-1.71026100	-3.84140700	-1.60541300	C	-5.53968600	-4.83029800	-3.55212200
C	-4.23232200	-2.89410700	-0.90264400	H	-6.33388100	-4.85450300	-4.31176500
C	-2.79358400	-3.90455500	-2.47725100	H	-4.68981000	-5.40966400	-3.93710700
C	-4.04683700	-3.36519300	-2.19049900	H	-5.91391300	-5.33579300	-2.65102200
H	-5.23263900	-2.60704800	-0.60116000	C	-6.39823700	-2.63004700	-2.77599700
H	-2.67155300	-4.42017100	-3.42423700	H	-6.87803600	-3.11313600	-1.91362700
C	3.75379700	2.55631900	0.92344000	H	-6.16599300	-1.58935900	-2.50472200
C	0.11651700	5.85081500	-1.06081400	H	-7.13620000	-2.60806900	-3.58901000
C	3.80568700	3.92357800	-3.86880500	C	3.73470400	1.04680900	0.66828200
C	-3.67262100	-2.44287600	1.46933600	H	2.71184000	0.63642800	0.73179900
C	-5.15093800	-3.38046500	-3.24030100	H	4.13603000	0.81244200	-0.32888600
C	-0.51061400	-4.77156200	-1.91236600	H	4.35706300	0.52291800	1.40857600
C	0.20481700	1.60077700	-2.22610600	C	3.28967400	2.84133600	2.35127400
H	-0.81847500	1.50689600	-2.60186900	H	4.03913500	2.45650700	3.05751200
H	0.53943600	2.60330900	-1.96555000	H	3.18609500	3.91944400	2.54177000
C	0.71538200	-0.74349800	-2.56962300	H	2.34924600	2.34254800	2.60766300
H	1.46007000	-1.53775000	-2.55449500	C	5.21392600	3.04994400	0.88192900
H	-0.24961100	-0.98021900	-3.02593800	H	5.78216500	2.56390100	1.68721900
C	1.14632100	0.58779800	-2.44556400	H	5.73077500	2.82038000	-0.05644200
H	2.19898400	0.80162600	-2.24307400	H	5.26327400	4.13633800	1.03869000
C	-0.35101600	-5.74145200	-0.73073800	C	-0.96560900	5.37014700	-2.03445500
H	0.48438800	-6.43035700	-0.92549500	H	-0.58029900	5.24989700	-3.05555200
H	-0.14567800	-5.23358400	0.21721200	H	-1.38044000	4.40442700	-1.70876200
H	-1.26455900	-6.33830700	-0.59783000	H	-1.79494100	6.09110100	-2.06859600
C	-0.76290600	-5.65972100	-3.13935600	C	-0.54566800	6.10929900	0.29236400
H	-1.67106400	-6.26870500	-3.03846300	H	0.18002100	6.38520800	1.07028500
H	-0.82628300	-5.08412900	-4.07283900	H	-1.24444300	6.95222400	0.18673800
H	0.08406400	-6.35045800	-3.24447200	H	-1.15574400	5.26675900	0.64329100
C	0.80650200	-4.05661700	-2.20174900	C	0.64555700	7.22539800	-1.51355200
H	0.71882600	-3.45202700	-3.11489300	H	-0.17417500	7.95595300	-1.49055000
H	1.15742400	-3.41883400	-1.38298200	H	1.43477800	7.58112600	-0.83686900
H	1.59243500	-4.80463600	-2.37595900	H	1.04793800	7.22838400	-2.53217400
C	-2.69694300	-1.72308900	2.38902400	C	3.84966700	2.46942700	-4.35247500
H	-1.84158800	-2.34819300	2.64947500	H	4.35752800	1.80600400	-3.63855800
H	-2.33111400	-0.77489300	1.96929800	H	2.83410000	2.08154700	-4.51875600
H	-3.20589700	-1.47554500	3.33086500	H	4.39364200	2.40684200	-5.30539000
C	-4.98663100	-1.64187300	1.51804800	C	5.23608000	4.45046400	-3.69827300
H	-5.19412100	-1.36223700	2.55992200	H	5.76430900	4.42225500	-4.66176300
H	-4.93050200	-0.71454900	0.92965300	H	5.22945800	5.49033500	-3.34347000
H	-5.85611900	-2.21342500	1.17205900	H	5.81615800	3.85251800	-2.98285700
C	-3.93434900	-3.82889900	2.08669000	C	3.11428200	4.75770100	-4.94517200
H	-4.68964200	-4.38648900	1.51679200	H	3.11207200	5.82846300	-4.69849200
H	-3.01173500	-4.42781100	2.10958000	H	3.64829900	4.64142100	-5.89769500
H	-4.29741800	-3.71687700	3.11893400	H	2.07489500	4.43764600	-5.10560400
C	-4.64017100	-2.69892600	-4.51500500				

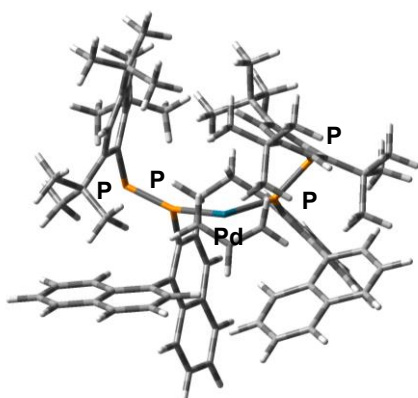
7E⁺



C	2.63001200	-6.35871400	2.33184700	H	4.07575700	-3.56992600	-2.62951300
C	7.20315800	-2.01455300	2.39793800	C	3.65743500	5.76477100	-3.19614300
C	2.56748700	-3.92844900	2.31573200	H	2.46044700	-3.17902800	-0.77823800
C	5.34960100	-2.54722000	0.92248000	C	-1.36118000	1.03953300	2.91649700
C	3.95412500	-2.69646500	0.66526400	C	-1.11322000	2.02979600	3.82976500
C	2.96189100	-2.66165700	1.77499400	C	-2.44296700	1.20272600	1.99035600
C	4.44587300	-3.27989700	-1.64684000	C	-1.88181200	3.21875500	3.87554800
C	5.79321600	-3.16874500	-1.41453500	H	-0.29087800	1.93086200	4.53987900
C	6.27518600	-2.78540100	-0.13869800	C	-3.22824400	2.34663200	2.01823300
C	7.66006400	-2.61174400	0.10431200	C	-2.95654200	3.38856700	2.95835800
C	8.11583100	-2.22833100	1.34137700	C	-1.58577400	4.25125400	4.79608300
H	9.18205100	-2.09438700	1.51393500	C	-4.31207800	2.56336700	1.01842600
H	8.35819600	-2.78710900	-0.71439200	P	-1.53127500	-0.70137700	-0.44767200
H	6.51467800	-3.35709200	-2.20976400	C	-3.70484400	4.59222200	3.00195600
C	1.63940900	-6.39129800	3.33764000	C	-2.32688400	5.40771200	4.81368200
C	1.13997700	-5.21766300	3.84380600	H	-0.75638100	4.11008800	5.48939500
C	1.59208000	-3.96880300	3.35279700	C	-5.66634900	2.21585100	1.30859900
H	1.28090500	-7.34735700	3.71427800	C	-4.00927000	3.20052700	-0.16790400
H	0.38279100	-5.22434700	4.62796800	C	-2.54231500	-1.97653400	-1.33473500
C	1.06151300	-2.75579200	3.83972500	C	-3.39785300	5.57668100	3.91009800
H	0.29673800	-2.79576800	4.61882500	H	-4.52741200	4.73114200	2.30197300
C	5.85440300	-2.17734700	2.19569300	H	-2.09075400	6.19756700	5.52420300
H	5.15541300	-2.02193900	3.01735400	C	-6.67733100	2.52289200	0.34785900
C	3.08596100	-5.16142200	1.83662800	C	-6.04592600	1.58342400	2.51892600
H	3.84882800	-5.15687900	1.06063300	C	-5.01119400	3.50268200	-1.11374700
H	7.57330300	-1.72176600	3.37862600	H	-2.97656300	3.49500200	-0.36466600
H	3.03549500	-7.29188900	1.94538800	C	-2.51332800	-3.33779600	-0.88824400
C	2.40481000	-1.48783600	2.27149100	C	-3.44062300	-1.58048300	-2.36312000
C	3.52877000	-3.04367100	-0.60042500	H	-3.98137900	6.49506700	3.93113300
P	2.30147500	0.76388600	0.08453400	C	-6.31749300	3.17091000	-0.85975900
C	2.99755300	2.40368800	-0.48962200	C	-8.02237400	2.18107900	0.63193200
C	2.12751300	3.54513300	-0.46708500	C	-7.36007300	1.26807900	2.76502200
C	4.22417600	2.48590600	-1.22525000	H	-5.27906400	1.35178500	3.25807500
C	2.39720800	4.59576300	-1.34122500	H	-4.73841200	4.00147300	-2.04244600
C	4.39517200	3.58073800	-2.08205400	C	-3.45992800	-4.21041400	-1.41785900
C	3.48096100	4.61408300	-2.21215700	C	-1.56887900	-3.95212400	0.17693500
H	1.72869400	5.44997800	-1.34776900	C	-4.33960400	-2.54447600	-2.84558500
H	5.29584200	3.62360300	-2.67962800	C	-3.61334300	-0.20352900	-3.06972200
C	5.44214400	1.53911100	-1.09259000	H	-7.10051700	3.39918400	-1.58304400
C	0.95823800	3.75224200	0.51954900	C	-8.35907700	1.56798200	1.81266500
C	1.44208600	-1.53966700	3.33231400	H	-8.78622800	2.41745700	-0.10892400

H	-7.63565300	0.78389700	3.70010100	H	6.42653600	1.95231000	-3.02551000
C	-4.39690500	-3.84601500	-2.38184100	H	6.99949500	2.98683500	-1.68710100
H	-3.48112500	-5.23365500	-1.05620700	H	7.46660300	1.28452100	-1.76300800
H	-5.04531000	-2.24188900	-3.61188800	C	5.15962800	0.10690400	-1.53924400
H	-9.39646700	1.31250800	2.02050500	H	4.36040700	-0.39443600	-0.98379200
C	-5.41272100	-4.86896200	-2.88149100	H	4.91290900	0.07719600	-2.61000300
C	-0.50794000	-0.18657100	2.82359900	H	6.06422200	-0.49750800	-1.39562400
H	-1.13527600	-1.08754600	2.94208200	C	5.95506900	1.58263200	0.35505600
H	-0.11658500	-0.25684900	1.79543900	H	5.20699200	1.28664600	1.09599800
P	-3.02279400	-0.11919000	0.84601000	H	6.81440500	0.90335200	0.46487900
P	3.12196700	0.16427700	1.86027900	H	6.28761200	2.59911800	0.60860000
C	0.68553700	-0.31469300	3.76332800	C	-2.66339500	0.94708800	-2.71479300
H	1.31401000	0.58961700	3.71612000	H	-2.85717400	1.38305700	-1.72951400
H	0.35297100	-0.41579300	4.80600600	H	-1.60030900	0.67675800	-2.77385000
Pd	0.72356700	-0.28666800	-1.41264100	H	-2.82338500	1.75262400	-3.44675700
C	2.20339600	-0.18208900	-3.01056500	C	-5.03324200	0.31212500	-2.78022800
C	0.18267400	-1.46402200	-3.24651800	H	-5.19279600	0.42069800	-1.69721700
C	0.93776000	-0.34825900	-3.61211200	H	-5.17583600	1.30136300	-3.23874900
H	0.68044600	-2.38864900	-2.94371700	H	-5.81332200	-0.35165700	-3.17221400
H	-0.86107000	-1.56214100	-3.53927400	C	-3.44564300	-0.40594800	-4.58921200
H	0.46057800	0.48906100	-4.12428000	H	-2.41265600	-0.68768900	-4.84327700
H	2.73493300	0.76294800	-3.12391500	H	-4.10841000	-1.17119600	-5.00656500
H	2.81546300	-1.05788800	-2.77991600	H	-3.66548000	0.53629700	-5.10950200
C	0.32328500	5.14740100	0.41594300	C	-6.35844800	-4.28806200	-3.93049900
H	-0.45223600	5.22794500	1.19190800	H	-6.94086300	-3.44386700	-3.53553700
H	1.04675200	5.95525700	0.58885300	H	-5.81920500	-3.94729600	-4.82562400
H	-0.17016400	5.31539700	-0.55166100	H	-7.07006200	-5.06141700	-4.24896400
C	1.48117200	3.64571000	1.95921800	C	-6.25668500	-5.36054200	-1.69908000
H	0.66620900	3.84140600	2.67060300	H	-6.99503500	-6.09783200	-2.04499700
H	1.89479000	2.65990800	2.19661300	H	-5.64575000	-5.84114000	-0.92391300
H	2.27005400	4.39147400	2.13075800	H	-6.80024300	-4.52717500	-1.23249800
C	-0.18875200	2.77737600	0.26434500	C	-4.67409000	-6.05601300	-3.51220000
H	-0.48937700	2.79229400	-0.79605900	H	-4.06236000	-5.72971600	-4.36498200
H	0.04748100	1.74223900	0.53028800	H	-4.01340100	-6.56200500	-2.79630300
H	-1.05267100	3.06670500	0.87433200	H	-5.39822000	-6.79760600	-3.87840100
C	2.41298200	5.86372700	-4.08699700	C	-0.17798100	-3.31693500	0.23004100
H	1.50236500	6.06749800	-3.50863400	H	0.25094100	-3.18816600	-0.77470500
H	2.53418900	6.67968300	-4.81343800	H	-0.14330300	-2.35103500	0.75045400
H	2.25714200	4.93123500	-4.64779100	H	0.49566700	-3.97438000	0.79668600
C	3.83767500	7.07619100	-2.42121700	C	-1.30546500	-5.44410700	-0.10655800
H	3.96995600	7.91150800	-3.12349700	H	-2.18709400	-6.07896300	0.03752400
H	2.97012600	7.30707600	-1.78932800	H	-0.92845400	-5.60238000	-1.12666900
H	4.72563100	7.03130300	-1.77543000	H	-0.54466900	-5.80939700	0.59721500
C	4.87404900	5.57513500	-4.10054200	C	-2.21656200	-3.85735300	1.56522300
H	5.81362600	5.56236600	-3.53078600	H	-1.54876600	-4.30104100	2.32037400
H	4.81033000	4.64476800	-4.68218900	H	-2.41519900	-2.81681500	1.85581700
H	4.93335900	6.40951200	-4.81198700	H	-3.17099100	-4.40092500	1.59006200
C	6.63999500	1.98298500	-1.94838500				

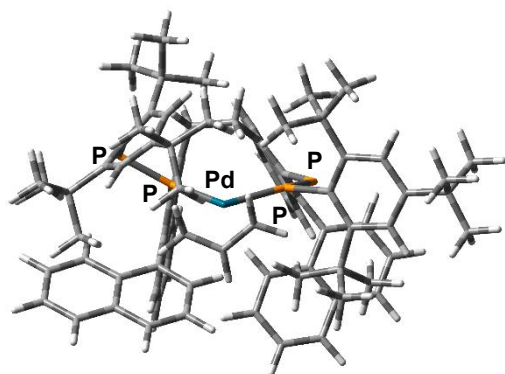
7F⁺



C	-7.60497000	-0.53127000	2.57953300	P	2.28897200	-2.70251900	1.30581800
C	-3.67976600	-1.37019600	-2.52942700	C	-2.77173700	-4.85925700	-1.72563200
C	-5.27243800	-0.02009400	2.13466400	C	-4.88941400	-5.25596200	-0.62481400
C	-4.40359700	0.53553800	-1.20889200	H	-5.10694900	-4.46957300	1.36038300
C	-4.62404400	1.19018200	0.04115300	C	0.74237700	-4.67846300	-1.86680900
C	-4.23885000	0.53280000	1.31754100	C	-0.32099500	-2.73318500	-2.84962900
C	-5.69287600	3.04165800	-1.11932200	C	-4.03109100	-5.40694200	-1.73662600
C	-5.44935300	2.45420600	-2.33511100	H	-2.11906000	-4.97157400	-2.59035300
C	-4.80026000	1.19825600	-2.41133700	H	-5.88868400	-5.68602700	-0.65346000
C	-4.56908000	0.56487800	-3.65923500	C	1.49378300	-4.85132000	-3.06791700
C	-4.01979900	-0.69109500	-3.72086900	C	0.92809500	-5.60581700	-0.81011400
H	-3.86660000	-1.17665500	-4.68313400	C	0.43156200	-2.89935000	-4.03253800
H	-4.86161500	1.08948900	-4.56896100	H	-1.04715600	-1.92218900	-2.77601800
H	-5.75461800	2.94223200	-3.26093400	H	-4.37237400	-5.96109400	-2.60888700
C	-7.25675400	-1.07746800	3.83482400	C	1.31825500	-3.94014600	-4.13890100
C	-5.94343400	-1.11106800	4.22919900	C	2.40117400	-5.93451900	-3.16458500
C	-4.92363900	-0.59839600	3.39005500	C	1.81370900	-6.64894200	-0.93667800
H	-8.03298900	-1.47794400	4.48413900	H	0.36222600	-5.47906700	0.11244300
H	-5.65928300	-1.54270700	5.18875600	H	0.29122600	-2.20631900	-4.86140200
C	-3.56150800	-0.69905600	3.74341700	H	1.89824800	-4.08729700	-5.05018800
H	-3.30498700	-1.19857200	4.68074100	C	2.55803200	-6.81726700	-2.12460200
C	-3.84961400	-0.76813200	-1.30601600	H	2.97075500	-6.05314400	-4.08668800
H	-3.57921500	-1.30577400	-0.39543600	H	1.94299200	-7.35305000	-0.11679900
C	-6.63969200	-0.01560700	1.75108400	H	3.25616500	-7.64761600	-2.21199000
H	-6.92024400	0.40160400	0.78620200	C	-0.98095600	-2.18099300	3.05526800
H	-3.29337100	-2.38805900	-2.57762100	H	-1.55626500	-2.67077200	3.85252200
H	-8.64743600	-0.52172200	2.26722200	H	0.06629200	-2.45788300	3.23581600
C	-2.90972400	0.43099400	1.71590800	P	0.80555100	-1.62790900	0.37801700
C	-5.27214600	2.40806000	0.06708200	P	-1.59932200	1.28373100	0.73683900
P	-1.64302700	3.15263600	1.56827400	C	-1.14270100	-0.65813300	3.22624900
C	-2.55802800	-0.25775800	2.91523800	H	-0.87941800	-0.39787200	4.26252200
H	-6.19573600	4.00583000	-1.06233600	H	-0.42565100	-0.12597700	2.58404000
H	-5.46544300	2.88195600	1.03073000	Pd	-0.03826900	0.33059900	-0.78946600
C	-1.44802400	-2.75314500	1.73964800	C	-0.60617600	1.83801400	-2.27878600
C	-2.68107200	-3.36185700	1.69041300	C	1.29543700	0.36943600	-2.59085700
C	-0.65061800	-2.74726100	0.54765900	C	0.00882900	0.77108300	-2.96089900
C	-3.16410600	-4.01163100	0.53309800	H	2.00977800	1.08462400	-2.16906900
H	-3.31140000	-3.36675700	2.58161300	H	1.70538100	-0.55489100	-2.99130400
C	-1.04936200	-3.45858900	-0.57770800	H	-0.60408000	0.10877500	-3.57552800
C	-2.31283500	-4.12260900	-0.60188300	H	-1.67034100	2.02750500	-2.42630400
C	-4.46037500	-4.58024400	0.48974400	H	-0.00939900	2.67800500	-1.91391800
C	-0.17492600	-3.58661600	-1.77702400	C	-0.37927200	4.05060100	0.54716400

C	-0.80541100	4.88800900	-0.52526400	H	3.86858200	-1.16626400	-2.59548100
C	1.00646400	3.78688900	0.70944200	H	3.73617200	-2.88886200	-3.03187700
C	0.12723000	5.19836900	-1.51555300	C	4.35235800	-3.95721700	-0.59387000
C	1.86836900	4.10803400	-0.34614400	H	3.30743500	-4.14124500	-0.30761600
C	1.45037500	4.76483400	-1.49530100	H	4.55960300	-4.66943200	-1.40459300
H	-0.20578100	5.78227500	-2.37084600	H	4.99274900	-4.21494500	0.26174300
H	2.91647900	3.83749300	-0.25237900	C	6.03441800	-2.57334800	-1.69315900
C	3.81092300	-1.63812700	1.26538000	H	6.29043600	-1.66815700	-2.25699800
C	4.20518300	-0.91619000	2.42958600	H	6.80355200	-2.72986700	-0.92445900
C	4.57144700	-1.49905800	0.06782200	H	6.08868400	-3.40921300	-2.40301600
C	5.13859800	0.11167500	2.26730500	C	-2.86248500	4.86229200	-1.96018800
C	5.43098000	-0.40494600	-0.02570800	H	-2.24422300	4.94970800	-2.86400600
C	5.68753200	0.45548200	1.03772300	H	-3.05501500	3.79531000	-1.77574600
H	5.42376800	0.69321600	3.13664900	H	-3.83232500	5.33825300	-2.16642500
H	5.95394600	-0.23841900	-0.96458500	C	-2.03160200	7.02364600	-0.99102600
C	-2.20054300	5.51296900	-0.74110400	H	-3.02088400	7.48409200	-1.11728400
C	1.70847600	3.26577700	1.98024300	H	-1.53946300	7.50766700	-0.13607800
C	2.36708700	5.05382200	-2.67915800	H	-1.45220000	7.25820700	-1.89053200
C	4.62135000	-2.53018800	-1.08238200	C	-3.16718100	5.40998000	0.43771500
C	3.73898400	-1.24505500	3.86846200	H	-2.73069100	5.79418400	1.37057100
C	6.58800200	1.67089100	0.84086700	H	-4.05979200	6.01373600	0.21891200
C	2.29396300	-0.81660000	4.13592700	H	-3.53065900	4.38801500	0.60799400
H	2.18836900	0.27685100	4.10022900	C	1.78369700	4.39028300	-3.93344000
H	1.59486300	-1.23712100	3.40810500	H	0.76415400	4.73767400	-4.14979300
H	1.98005400	-1.15348400	5.13489000	H	2.40848300	4.61821400	-4.80856800
C	4.59569100	-0.53842700	4.92703900	H	1.74907000	3.29645500	-3.81936600
H	4.27358000	-0.87777700	5.92034400	C	3.77795500	4.51043900	-2.46566200
H	5.66341100	-0.77405500	4.82360000	H	3.77752100	3.42181100	-2.30625900
H	4.47437500	0.55333600	4.90847600	H	4.38894500	4.71652000	-3.35456300
C	3.90378000	-2.74932900	4.13389600	H	4.27489400	4.98263300	-1.60571300
H	4.93488700	-3.06874600	3.92871700	C	2.46247300	6.56879900	-2.89696200
H	3.68118500	-2.96980400	5.18699700	H	1.48549100	7.01890500	-3.11687000
H	3.23167200	-3.37345700	3.53114400	H	2.87113800	7.06667400	-2.00673700
C	6.00673500	2.54380700	-0.27784100	H	3.12738100	6.78706100	-3.74447300
H	6.62935100	3.43762700	-0.42746100	C	2.34480500	1.90061400	1.71938800
H	5.94957700	2.01254300	-1.23728700	H	1.57726400	1.12751500	1.55549600
H	4.99051200	2.88090000	-0.01991500	H	3.00699700	1.90001700	0.84025100
C	7.99928600	1.21443000	0.45300700	H	2.95250200	1.59686300	2.58331600
H	8.65250600	2.08664800	0.30753900	C	0.83958700	3.15887000	3.23651100
H	8.43811400	0.58916200	1.24289000	H	1.49319300	2.98880100	4.10431700
H	8.00456600	0.63406000	-0.47925300	H	0.27906400	4.08429200	3.43376800
C	6.68829800	2.52804500	2.10088900	H	0.13785800	2.31644900	3.21731900
H	7.16924400	1.99043500	2.92959400	C	2.81332200	4.27737500	2.34974500
H	7.29620100	3.41829400	1.89056500	H	3.32069200	3.94672800	3.26689900
H	5.69909700	2.87015000	2.43968600	H	3.58065600	4.38889300	1.57412500
C	3.64842400	-2.17019200	-2.20343500	H	2.38305100	5.27048000	2.54014800
H	2.60718200	-2.19121000	-1.85656600				

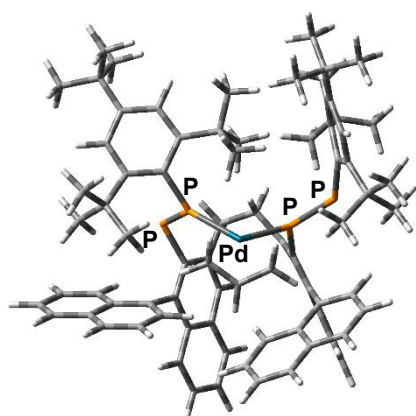
7G⁺



C	-6.40208200	-4.07763200	2.58452600	C	-1.19336900	-5.10787700	-1.50390200
C	-3.34728400	-2.56736400	-2.59769100	C	-2.83507400	-6.31773000	-0.19976400
C	-4.75626300	-2.33711000	2.20077800	H	-2.99590800	-5.78842400	1.87757800
C	-4.68082900	-1.25211100	-1.05537000	C	1.91978600	-3.66748900	-2.16432600
C	-4.99869100	-0.78821400	0.25746600	C	0.19325100	-1.99681700	-2.51965800
C	-4.22400900	-1.25587200	1.43998400	C	-2.16805500	-6.07186500	-1.42146700
C	-6.88404200	0.46280500	-0.63490400	H	-0.69022800	-4.91982900	-2.45210700
C	-6.59086600	0.03894900	-1.90680300	H	-3.61805500	-7.07218400	-0.15531200
C	-5.49474500	-0.82397100	-2.14784600	C	2.46553600	-3.35206700	-3.44578900
C	-5.19072200	-1.27365300	-3.45671100	C	2.54134100	-4.68074400	-1.39095800
C	-4.13791500	-2.12395100	-3.68062700	C	0.73701600	-1.68658600	-3.78494500
H	-3.91397600	-2.46756100	-4.68876700	H	-0.70676700	-1.47963800	-2.17823000
H	-5.81633100	-0.93116800	-4.28147700	H	-2.43541600	-6.64836100	-2.30502100
H	-7.19742200	0.35854600	-2.75453400	C	1.85312600	-2.34635800	-4.23547200
C	-5.78418600	-4.40147100	3.81302700	C	3.59940500	-4.06563900	-3.90704400
C	-4.66905700	-3.71507300	4.22649300	C	3.64102300	-5.35289400	-1.86677700
C	-4.12594000	-2.67833200	3.43025200	H	2.13309000	-4.92353800	-0.40990300
H	-6.19201800	-5.20186800	4.42743000	H	0.25286300	-0.93373000	-4.40636900
H	-4.17628000	-3.96446500	5.16634800	H	2.27556200	-2.12221800	-5.21497300
C	-2.92434900	-2.02665500	3.78206800	C	4.17479400	-5.04611600	-3.13797900
H	-2.41779700	-2.35212600	4.69340300	H	4.00550800	-3.81846500	-4.88804800
C	-3.60844400	-2.14475700	-1.31619500	H	4.10630000	-6.12839800	-1.26069400
H	-2.99365400	-2.50191400	-0.48576500	H	5.04448700	-5.58911400	-3.50322200
C	-5.90300100	-3.06908200	1.79760200	C	0.00427200	-2.03048500	3.22738100
H	-6.38391400	-2.82776600	0.85142400	H	-0.23979900	-2.63878300	4.10790500
H	-2.52896800	-3.26250500	-2.77934000	H	1.05075400	-1.72756300	3.35520900
H	-7.27879700	-4.63521900	2.26074500	P	1.70055100	-1.25662000	0.59051800
C	-3.02455800	-0.64403100	1.80775000	P	-2.82879100	1.02212400	1.04795500
C	-6.08988400	0.03693500	0.44826400	C	-0.87751300	-0.75968900	3.23641600
P	-0.96981500	1.51088700	0.31746900	H	-0.75845300	-0.26240600	4.21159900
C	-2.31418600	-1.10781600	2.96320600	H	-0.50683500	-0.05642800	-2.47844900
H	-7.73002800	1.12259300	-0.45381300	Pd	1.15753800	0.74119700	-0.54000400
H	-6.33368500	0.36269600	1.45988500	C	1.50641400	2.56256600	-1.79748200
C	-0.19314000	-2.86872200	1.99071400	C	2.86465100	0.57416100	-1.90619300
C	-1.11237000	-3.89215000	2.02322800	C	1.92370200	1.43513200	-2.50658000
C	0.44650600	-2.58320900	0.74302200	H	3.65602100	0.96754900	-1.26072600
C	-1.47778700	-4.62506200	0.87495800	H	3.04869200	-0.40176800	-2.35671800
H	-1.60447300	-4.14416800	2.96293300	H	1.34242800	1.08378700	-3.36163800
C	0.12853800	-3.29353100	-0.40861600	H	0.65929500	3.16378800	-2.12541400
C	-0.83765100	-4.34008500	-0.36458300	H	2.18968300	3.04410500	-1.09400500
C	-2.49037500	-5.61400000	0.92656600	C	-1.44266300	3.23826600	-0.16591200
C	0.76501500	-2.96084800	-1.71336300	C	-2.20521300	3.46376600	-1.34205500
P	3.37674000	-2.03718300	1.46578700	C	-1.15829700	4.32376400	0.73246400

C	-2.75244200	4.74609700	-1.52478200	H	-3.45398300	7.06980200	-2.99646200
C	-1.76067300	5.54856200	0.46723300	C	-4.13677400	7.45416400	0.37324200
C	-2.58088300	5.78823500	-0.63578500	H	-3.58754300	7.46084000	1.32397600
H	-3.35682100	4.92058700	-2.40875700	H	-4.60750500	8.44041800	0.25372400
H	-1.59666100	6.37331700	1.15106500	H	-4.93545700	6.70314700	0.44977600
C	4.52198500	-0.58406300	1.30288700	C	-2.12532800	8.23086100	-0.90257800
C	4.32049500	0.56844500	2.11336000	H	-1.51454500	8.27167900	0.00864200
C	5.46254000	-0.53278500	0.23968700	H	-1.45416200	8.03988700	-1.75158600
C	4.77570400	1.79650300	1.62545100	H	-2.57790700	9.22273700	-1.04296900
C	5.91676000	0.72740200	-0.15697700	C	5.32275000	4.43893600	0.58971700
C	5.52067000	1.91459700	0.45444100	H	4.22799500	4.39020000	0.49059300
H	4.54793300	2.69294700	2.19688400	H	5.56930600	4.50049700	1.65833700
H	6.59332200	0.78920900	-1.00707000	H	5.65917300	5.37468100	0.12354600
C	-0.17737300	4.27616100	1.93648700	C	5.71136900	3.34692600	-1.59642400
C	-2.53327000	2.51143700	-2.53052700	H	6.08672800	4.30090300	-1.99235500
C	-3.22086000	7.16070100	-0.82166400	H	6.18931600	2.54115900	-2.16877400
C	3.72815100	0.55753200	3.54133400	H	4.63014900	3.30581700	-1.79553700
C	6.00299500	3.25441500	-0.09414300	C	7.51627000	3.36236800	0.13512600
C	6.07257600	-1.73605600	-0.51071100	H	7.89212500	4.32308500	-0.24502500
C	-4.05959100	2.37241100	-2.65072200	H	7.75441600	3.30285400	1.20638900
H	-4.56509400	3.32745600	-2.83644200	H	8.06295000	2.55933800	-0.37758400
H	-4.30355100	1.69962200	-3.48551700	C	5.54052700	-1.79565600	-1.94500100
H	-4.48418900	1.93375200	-1.73543500	H	4.46211900	-2.01231600	-1.95785300
C	-1.98262100	1.08066700	-2.52890600	H	5.71120500	-0.85292600	-2.48420100
H	-2.48932400	0.41526100	-1.82121800	H	6.03868600	-2.60211500	-2.50221600
H	-2.14979000	0.65399000	-3.52963200	C	5.83712300	-3.09390600	0.15003200
H	-0.90112200	1.02704500	-2.33938700	H	6.45704500	-3.84974000	-0.35303900
C	-1.97427500	3.15093200	-3.81838000	H	6.11511300	-3.09081400	1.21387700
H	-2.32165000	4.17580200	-3.98678800	H	4.80324000	-3.44918200	0.05068200
H	-0.87429100	3.17211300	-3.80365100	C	7.60276900	-1.56065400	-0.54968900
H	-2.28020300	2.55325100	-4.68801200	H	7.92641700	-0.68201500	-1.11904000
C	-0.59029600	3.29441200	3.04533200	H	8.01403300	-1.47707500	0.46576600
H	-1.65254000	3.41107800	3.30352700	H	8.05738500	-2.43811900	-1.02898000
H	-0.42087500	2.24407600	2.78725300	C	2.28204200	1.05692900	3.55012300
H	0.00214500	3.49601400	3.94912000	H	2.22296600	2.09420600	3.19451400
C	1.23091800	3.94437300	1.42645100	H	1.63945300	0.44882400	2.89982600
H	1.30448700	2.92391800	1.02505600	H	1.86735900	1.02503600	4.56943900
H	1.52724500	4.65093100	0.63668800	C	4.55965400	1.49266900	4.43932900
H	1.96422800	4.02856200	2.24303500	H	4.19396200	1.41836300	5.47216000
C	-0.05065800	5.64180100	2.62958000	H	5.62126200	1.21003000	4.43339900
H	0.69498800	5.55601000	3.43016000	H	4.48504900	2.54793000	4.15326000
H	0.29505700	6.43009500	1.94787100	C	3.81030700	-0.81438300	4.21877300
H	-0.99132500	5.96510500	3.09535200	H	4.82022100	-1.24153700	4.14260600
C	-4.05869600	7.24493600	-2.09551100	H	3.56803000	-0.70870400	5.28482400
H	-4.88778100	6.52346300	-2.09070400	H	3.10100600	-1.55185900	3.82131800
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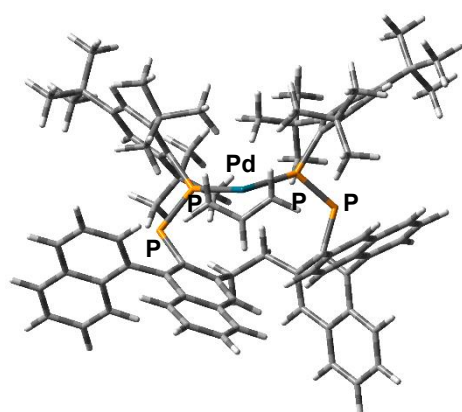
7H⁺



C	3.46725100	-6.27663600	2.20737300	P	0.28943400	1.90633800	-0.17311700
C	4.13568200	-2.63724000	-2.15139000	C	5.92517300	-0.67936600	0.18162900
C	1.93667100	-4.46039700	1.70559300	C	6.46077300	-2.60810900	1.54747900
C	2.08516400	-3.79706500	-1.55839900	H	5.13077100	-3.01746600	3.18541100
C	1.06749200	-4.16123800	-0.62336900	C	4.91570200	2.71240900	-0.27281800
C	1.13509000	-3.70593900	0.79260200	C	3.97829900	1.05623400	-1.77338100
C	-0.01689700	-5.51459200	-2.33143500	C	6.75029500	-1.73879600	0.47218700
C	0.94571400	-5.17615400	-3.24789900	H	6.16717500	-0.02638100	-0.65481800
C	2.01668200	-4.32096800	-2.88672200	H	7.11455900	-3.45372400	1.75173300
C	3.02014900	-3.96914300	-3.82347100	C	5.38653400	3.44268100	-1.40726200
C	4.06050800	-3.14858500	-3.46611500	C	5.21531300	3.20521200	1.02359500
H	4.83157500	-2.89277700	-4.19021400	C	4.44918000	1.77492400	-2.89228500
H	2.95069100	-4.37306100	-4.83349000	H	3.47741600	0.09678800	-1.91261000
H	0.90719400	-5.56276700	-4.26614700	H	7.63560100	-1.91364400	-0.13650200
C	3.43397600	-5.93913900	3.57795200	C	5.13790500	2.94736300	-2.71096400
C	2.66228400	-4.88856700	4.00905100	C	6.11368400	4.64162900	-1.20211700
C	1.90169600	-4.12664600	3.08912100	C	5.92285900	4.37056900	1.18766300
H	4.02083300	-6.51606900	4.29012200	H	4.88214400	2.64192700	1.89507600
H	2.62987500	-4.61566800	5.06401200	H	4.27349600	1.38439500	-3.89425500
C	1.17137800	-2.99075700	3.50345900	H	5.51364100	3.51126400	-3.56474800
H	1.21694500	-2.70577600	4.55747700	C	6.37366200	5.09999500	0.06497400
C	3.17155300	-2.94723500	-1.22086200	H	6.46445400	5.19178200	-2.07550100
H	3.24368500	-2.54267900	-0.20802200	H	6.14379000	4.73393000	2.18959300
C	2.73299600	-5.55988200	1.29433400	H	6.93274800	6.02244800	0.20985100
H	2.75923400	-5.83493400	0.24135400	C	1.27064000	0.08260900	3.49156800
H	4.96989100	-1.99683900	-1.86755200	H	1.56726200	-0.20983400	4.50830900
H	4.07757700	-7.11389900	1.87428400	H	0.90772600	1.11890900	3.56750900
C	0.41648100	-2.60917000	1.24648700	P	1.65749300	2.33005200	1.28659000
C	0.05477000	-5.01047900	-1.01565600	P	-0.85343900	-1.79092100	0.17442200
P	-2.43407400	-2.89326500	0.90717700	C	0.08038000	-0.80533400	3.04791100
C	0.51635800	-2.17973800	2.61130700	H	-0.62863800	-0.85794300	3.88674400
H	-0.83470400	-6.17793100	-2.60783600	H	-0.44666000	-0.29906800	2.22873400
H	-0.69801100	-5.30561100	-0.28373600	Pd	0.01490300	-0.15611400	-1.39253000
C	2.48040200	-0.02287900	2.60152800	C	-0.04716800	-1.51760100	-3.16317400
C	3.39664100	-1.00676800	2.88908900	C	0.84694500	0.71357800	-3.25094900
C	2.69417300	0.80392500	1.45022400	C	1.06153800	-0.67409700	-3.27961600
C	4.50730500	-1.27701600	2.06877000	H	-0.07842800	1.13469100	-3.65330800
H	3.26363800	-1.62249000	3.77790700	H	1.69488300	1.39134700	-3.18080500
C	3.82945700	0.62073700	0.66022800	H	2.06586900	-1.07993500	-3.13281500
C	4.75407400	-0.43424800	0.94973900	H	0.08598800	-2.59055900	-3.03307400
C	5.36710900	-2.36997600	2.33953000	H	-1.01779800	-1.18448500	-3.53563500
C	4.18765300	1.50262700	-0.48584600	C	-0.65788300	3.50505900	-0.24410200

C	-2.01531100	3.54464600	0.21201300	H	-8.49031900	0.45289800	0.81361000
C	0.03663200	4.73296800	-0.42695700	H	-7.33086700	1.75229100	0.43944800
C	-2.50016300	4.74419500	0.71824400	C	-8.51393900	-0.76122000	-1.62183800
C	-0.50338400	5.88366500	0.16347300	H	-8.15948500	-1.38429200	-2.45353600
C	-1.73612500	5.91126300	0.79257200	H	-8.88720200	-1.43009800	-0.83380200
H	-3.51763600	4.77494200	1.09586600	H	-9.36052200	-0.16485500	-1.99054700
H	0.07241900	6.80286700	0.09860300	C	-6.91053700	1.07221100	-2.20358900
C	-4.04151100	-2.19172600	0.32819200	H	-6.14581300	1.77185700	-1.83649500
C	-4.53946400	-2.36451400	-0.99456400	H	-6.47253000	0.49816600	-3.03084400
C	-4.81846000	-1.46416400	1.28187800	H	-7.74167000	1.66404000	-2.61235100
C	-5.60032300	-1.55678800	-1.40040000	C	-2.60947600	1.34376300	1.26807400
C	-5.89366800	-0.71042700	0.79459200	H	-3.35301100	0.53560600	1.28681400
C	-6.26500900	-0.68239200	-0.54505400	H	-1.62925900	0.88209500	1.11116200
H	-5.95146700	-1.63675700	-2.42530000	H	-2.59699100	1.83494500	2.25337300
H	-6.47052300	-0.11653100	1.49303000	C	-2.96898200	1.69105500	-1.21847000
C	-4.07535000	-3.46732700	-1.97115900	H	-3.41803600	2.37039200	-1.95764400
C	-4.70696800	-1.62131900	2.82458800	H	-1.96475800	1.43476900	-1.58475600
C	-7.41863000	0.16483200	-1.07612500	H	-3.56090700	0.76088800	-1.20573600
C	1.24827000	4.99460300	-1.34694400	C	-4.42927000	2.74083000	0.43733800
C	-2.97174400	2.34463800	0.17290200	H	-4.78298000	3.52346700	-0.24848000
C	-2.30098300	7.15172800	1.47473600	H	-5.05132500	1.84887700	0.28240400
C	-3.34244500	-1.33179600	3.46384300	H	-4.59824800	3.07364200	1.47059600
H	-2.55324700	-2.02302100	3.14641500	C	1.62169100	3.81723000	-2.23980700
H	-3.00300000	-0.30800000	3.26600100	H	2.36395800	4.14477100	-2.98142900
H	-3.43311100	-1.44783000	4.55311400	H	2.08084500	2.98442800	-1.69701800
C	-5.69155900	-0.70546500	3.56416300	H	0.74209900	3.45047400	-2.78970500
H	-6.73998400	-0.92360200	3.32478800	C	0.84262200	6.11782400	-2.32612200
H	-5.57167700	-0.85602100	4.64464300	H	-0.06261100	5.84264600	-2.88546300
H	-5.49521900	0.35710800	3.35412500	H	0.65577000	7.07796000	-1.83241300
C	-5.10424600	-3.07236400	3.14428300	H	1.65317500	6.27772100	-3.05038000
H	-6.10025400	-3.30110100	2.74087700	C	2.47829000	5.45615800	-0.56014400
H	-4.39457200	-3.79944400	2.72479200	H	2.85304500	4.66990500	0.11037600
H	-5.13186100	-3.22415300	4.23267200	H	3.28849700	5.71687200	-1.25632300
C	-2.84200800	-3.02829400	-2.75528000	H	2.26354300	6.34479500	0.04788200
H	-3.03327200	-2.06696600	-3.25617400	C	-1.30287300	8.30743700	1.49693300
H	-1.97285500	-2.91206600	-2.10034100	H	-0.37145800	8.03276300	2.01135000
H	-2.58368300	-3.77183700	-3.52490400	H	-1.05070100	8.65356200	0.48488500
C	-5.17118400	-3.80063300	-2.99559200	H	-1.74180700	9.15835800	2.03477800
H	-4.86451300	-4.68684900	-3.56665800	C	-2.66331800	6.80793200	2.92491100
H	-6.13200300	-4.02607200	-2.51288000	H	-3.06937500	7.69560700	3.43022000
H	-5.33085300	-2.99679800	-3.72577500	H	-3.41965300	6.01473100	2.98692200
C	-3.79625000	-4.77865800	-1.22764800	H	-1.77681500	6.47547000	3.48283600
H	-4.67306700	-5.09799600	-0.64706700	C	-3.55773600	7.61705400	0.72909000
H	-3.55436700	-5.57128800	-1.94891000	H	-3.32394800	7.86473100	-0.31575400
H	-2.94403000	-4.71954400	-0.53546900	H	-4.34554800	6.85243700	0.72799100
C	-8.05039100	1.04674800	0.00039600	H	-3.96864800	8.51724600	1.20798400
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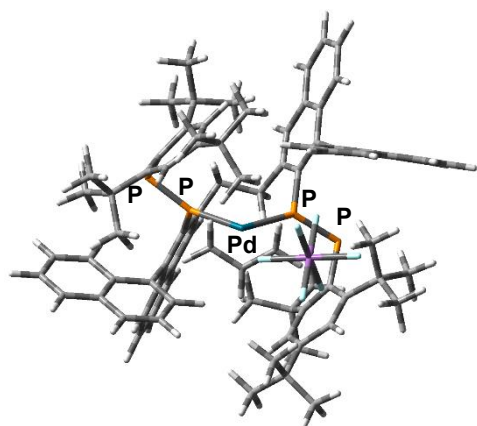
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C	-3.74570500	-3.72828200	2.30051400	C	0.55214400	-6.41173700	-1.56701300
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C	-4.69224800	-2.35152400	0.43688600	C	5.45004400	-3.18237900	-0.10848400
C	-3.70987800	-2.52612200	1.54108900	C	4.51123000	-2.41168300	-2.20833200
C	-6.81227000	-1.56113600	-0.45023900	C	1.79681600	-6.18241000	-2.19559200
C	-6.51684100	-2.07725700	-1.68614600	H	3.55621800	-4.96986800	-2.28702200
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C	-4.99195400	-3.33417600	-3.17280300	C	6.75547900	-2.90084700	-0.61492400
C	-3.83371700	-4.04675800	-3.36505400	C	5.34046900	-3.75005500	1.18705600
H	-3.61398700	-4.48170800	-4.33810900	C	5.80271000	-2.14104000	-2.70515500
H	-5.70244000	-3.19818800	-3.98827600	H	3.66040000	-2.23581700	-2.86563900
H	-7.21631600	-1.97018500	-2.51519100	H	2.12235400	-6.84020900	-2.99908500
C	-3.80159600	-6.01917000	3.93184400	C	6.90153500	-2.36742800	-1.91801100
C	-2.81685700	-5.08236800	4.12098900	C	7.88725600	-3.17195300	0.19298400
C	-2.76225000	-3.92239100	3.31078900	C	6.45840400	-4.00885100	1.94235100
H	-3.83594700	-6.90927500	4.55710800	H	4.35440700	-3.99162100	1.58081000
H	-2.05744700	-5.21863500	4.89079200	H	5.91475800	-1.74776400	-3.71370800
C	-1.71766700	-2.98032500	3.42941700	H	7.90497300	-2.15494600	-2.28639000
H	-0.92575000	-3.19965200	4.14748200	C	7.74615800	-3.71191800	1.44597800
C	-3.18953800	-3.67370600	-1.06395700	H	8.87522100	-2.94639800	-0.20850200
H	-2.47411400	-3.80248100	-0.24995700	H	6.35070500	-4.45042800	2.93144100
C	-4.74203100	-4.72270400	2.11829800	H	8.62283000	-3.92040400	2.05609900
H	-5.49651000	-4.58687900	1.34481800	C	0.92613700	-1.84680100	2.63205000
H	-2.01627500	-4.80394000	-2.44551200	H	0.91224600	-2.59157400	3.44023800
H	-5.54445000	-6.58854200	2.77491000	H	1.76347900	-1.18682300	2.89414000
C	-2.71654200	-1.56778600	1.74922500	P	3.40590100	-0.68710900	0.80045400
C	-5.89742000	-1.70536400	0.61544300	P	-3.26438300	0.13349100	1.25414000
P	-1.93676700	1.05820100	0.00272700	C	-0.37301300	-1.02108100	2.69013200
C	-1.62997000	-1.85632900	2.63963300	H	-0.35000300	-0.42847000	3.61967300
H	-7.75335400	-1.04189800	-0.28106300	H	-0.37127900	-0.29878600	1.86135700
H	-6.14348800	-1.30138100	1.59752100	Pd	-0.05541600	-0.01583100	-1.02448200
C	1.26507100	-2.57777800	1.34918700	C	-1.39456600	-1.10305900	-2.42957900
C	0.54299400	-3.68782000	0.96579700	C	0.99275400	-1.24883300	-2.54462600
C	2.43807900	-2.25049800	0.59474900	C	-0.22919200	-1.86155400	-2.25282700
C	0.93768300	-4.50825900	-0.11533500	H	1.04925100	-0.48067000	-3.31928500
H	-0.34653100	-3.98008700	1.52639900	H	1.92122400	-1.73669700	-2.26687700
C	2.94431800	-3.12284700	-0.36639600	H	-0.25559500	-2.78248400	-1.66431100
C	2.18466700	-4.26142100	-0.76411700	H	-2.34396200	-1.48261500	-2.05723000
C	0.13830100	-5.59876600	-0.54109200	H	-1.44344800	-0.35510500	-3.22238200
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C	3.52412100	2.72389500	1.37969100	H	1.78770900	0.67031500	2.82652300
C	3.48476900	2.82800800	-1.08715900	H	1.26754200	1.90055900	3.96143800
C	4.62233200	3.59682600	1.34065800	C	4.03145900	1.76249000	3.67129000
C	4.53255300	3.73801200	-1.01635500	H	3.65005200	1.63824400	4.69485900
C	5.16339100	4.10138100	0.17370600	H	4.23586600	0.76228700	3.26247800
H	5.05925500	3.90121000	2.28639500	H	4.98425600	2.30271700	3.73528600
H	4.90587400	4.17528800	-1.93643500	C	2.72253900	3.88610000	3.44682700
C	-2.89823700	2.64894500	-0.23793600	H	3.61457400	4.51819400	3.51512600
C	-3.89523600	2.74613000	-1.24973200	H	1.96628400	4.44077600	2.87247600
C	-2.84343500	3.64827800	0.77723400	H	2.33707300	3.75519700	4.46720700
C	-4.94979200	3.64041300	-1.04797800	C	-0.34644700	3.81294200	0.78367300
C	-3.94311800	4.49220700	0.91746500	H	-0.14654800	2.78389600	0.45739600
C	-5.04196700	4.46868400	0.06386000	H	-0.43502000	4.43359400	-0.11997600
H	-5.73475200	3.68569300	-1.79508200	H	0.54065700	4.15107300	1.33602800
H	-3.93626700	5.21827400	1.72539500	C	-1.55051100	3.07336300	2.90880000
C	2.98984400	2.50044400	2.81886700	H	-1.36384900	2.01437000	2.69917400
C	2.93797600	2.50754100	-2.49563100	H	-0.75301000	3.42789400	3.57778600
C	6.35556600	5.05156800	0.14517000	H	-2.50253100	3.14381100	3.45435800
C	-1.60594600	3.94547400	1.64835200	C	-1.61156900	5.40389800	2.13721400
C	-6.23070000	5.38737700	0.32382700	H	-1.75408300	6.11528800	1.31246800
C	-3.84214200	2.00108100	-2.59725200	H	-2.37847500	5.59427400	2.89860000
C	1.41302600	2.67013600	-2.54765300	H	-0.64229000	5.62041800	2.60669200
H	1.02299700	2.32042100	-3.51575000	C	-2.42437000	2.12393200	-3.17506400
H	0.87732700	2.12167000	-1.76311100	H	-1.64073700	1.73577600	-2.51345100
H	1.13996800	3.72937500	-2.43591700	H	-2.35402600	1.58919900	-4.13399100
C	3.40164300	1.11184600	-2.93550900	H	-2.18792400	3.18132200	-3.36349400
H	4.49946700	1.05381100	-2.90863600	C	-4.31555800	0.55071300	-2.45961100
H	3.02257600	0.30570700	-2.30041600	H	-3.75363700	-0.02493800	-1.71901700
H	3.07597400	0.91110900	-3.96722800	H	-5.36821400	0.52974800	-2.14225600
C	3.46590900	3.46972900	-3.57053600	H	-4.24463900	0.02716600	-3.42570400
H	3.26229300	4.52047400	-3.32458500	C	-4.75703900	2.64191100	-3.65085900
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C	7.46429400	4.45327000	-0.72935700	H	-4.57305600	2.15136500	-4.61628300
H	7.13893000	4.29861400	-1.76631300	C	-7.35110400	5.19084600	-0.69510000
H	8.33032100	5.12977300	-0.75082500	H	-7.03448300	5.45698300	-1.71306900
H	7.79964400	3.48536700	-0.33148200	H	-7.71565600	4.15417000	-0.70586800
C	5.91317200	6.39914200	-0.43803000	H	-8.19872200	5.83926900	-0.43563600
H	6.76305500	7.09592600	-0.45981200	C	-5.77073500	6.84891100	0.25515200
H	5.53483700	6.30347700	-1.46423300	H	-4.99748000	7.07471200	1.00136000
H	5.11969800	6.84940400	0.17457100	H	-5.36199000	7.08440200	-0.73743100
C	6.93382800	5.30107300	1.53670200	H	-6.62089300	7.52046900	0.44134200
H	6.20371400	5.77467300	2.20801200	C	-6.79847400	5.09351900	1.71774500
H	7.28359400	4.37125600	2.00680400	H	-7.65529300	5.75122900	1.92117200
H	7.79535600	5.97747500	1.45835400	H	-7.14444400	4.05288200	1.78864500
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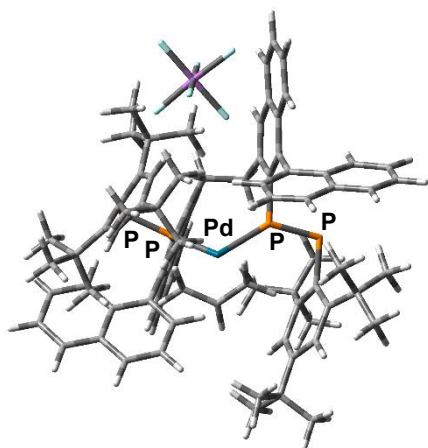
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F	4.35473300	-4.90182900	1.98730100	H	-0.92266800	-3.27831900	-3.70369200
F	4.70722400	-2.80733100	3.62050900	C	-0.92181200	-0.85808800	-4.68591200
F	4.03064000	-1.16289800	1.65117200	C	4.02312000	-1.17570500	-3.01775300
F	5.98160000	-2.90420400	1.25644300	C	-0.61728800	3.83390600	-2.01741400
F	3.66607000	-3.24873600	0.01690000	H	3.70233900	1.28256200	2.38377100
C	2.38461400	7.34962000	0.05812000	C	0.86305900	-5.08357800	-2.61731000
C	5.29939500	3.64764000	-3.01442700	H	1.70594200	2.41652800	1.41137000
C	1.49349800	5.24159300	-0.75143300	C	-3.90887600	1.97427800	-1.77360500
C	3.97870100	3.12521400	-1.04402300	C	-4.79495000	1.97104400	-2.82331900
C	2.73940800	3.10274600	-0.33516300	C	-3.78667700	0.79787200	-0.96877100
C	1.55635600	3.82110100	-0.88305200	C	-5.55508300	0.82856100	-3.15821500
C	3.79273700	1.82256800	1.44336000	H	-4.90297700	2.86882300	-3.43634000
C	5.00412600	1.87994500	0.80455700	C	-4.52021700	-0.34339500	-1.26091100
C	5.12716700	2.52290100	-0.44941700	C	-5.40912900	-0.35490100	-2.37859500
C	6.35391200	2.52682500	-1.15732700	C	-6.43583900	0.82507900	-4.26717400
C	6.43989100	3.06948700	-2.41522600	C	-4.41074100	-1.57298100	-0.42617500
H	7.38451800	3.05314900	-2.95579100	P	-3.70957800	1.47831700	2.00387000
H	7.22420100	2.06593700	-0.68921500	C	-6.14705100	-1.50768200	-2.75172200
H	5.88096400	1.39686100	1.23615200	C	-7.13805300	-0.30559300	-4.60112800
C	1.28329100	8.03841700	-0.49638000	H	-6.53816500	1.73819700	-4.85352600
C	0.30312000	7.34612400	-1.16176500	C	-5.41645000	-1.86245600	0.54691800
C	0.37756800	5.93834900	-1.29826000	C	-3.37675600	-2.46487800	-0.62306400
H	1.21345100	9.11940000	-0.39014100	C	-2.39362600	1.43579600	3.31569900
H	-0.55554700	7.86567700	-1.58699400	C	-6.98823300	-1.48352300	-3.83679100
C	-0.65077100	5.20452400	-1.92913800	H	-6.03616700	-2.42111600	-2.16965400
H	-1.50738800	5.74828600	-2.33418500	H	-7.80951900	-0.29949100	-5.45773600
C	4.10180000	3.68478800	-2.34163600	C	-5.33349000	-3.07846200	1.28801100
H	3.22831900	4.13824100	-2.80943600	C	-6.49597600	-0.98085600	0.80856400
C	2.48987300	5.98668700	-0.06957100	C	-3.29183800	-3.66233600	0.12298300
H	3.34039200	5.46319700	0.36398400	H	-2.61285500	-2.24148500	-1.37127900
H	5.37208500	4.07035400	-4.01492400	C	-2.23967200	0.27024100	4.11518300
H	3.15427700	7.90477800	0.59105500	C	-1.39511800	2.44273100	3.35226100
C	0.51926800	3.13756700	-1.49990600	H	-7.54350200	-2.37834700	-4.11167300
C	2.66007100	2.44626700	0.87783900	C	-4.25300000	-3.96478200	1.05345900
P	1.56529100	0.98371700	-3.38089400	C	-6.32844000	-3.36804300	2.25338500
C	1.45755500	-0.86581000	-3.50872800	C	-7.44627300	-1.29069500	1.75156700
C	2.56654900	-1.68024900	-3.12034900	H	-6.56675700	-0.04807600	0.24996300
C	0.22580200	-1.47730700	-3.85369000	H	-2.46133800	-4.34710100	-0.04947900
C	2.31631500	-3.02304900	-2.84661100	C	-0.97657200	0.01609800	4.65233200
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C	-1.56589100	3.91833100	2.92921400	C	-1.19678300	-1.79942700	-5.87657700
H	-4.19804000	-4.88721100	1.63197200	H	-2.00647100	-1.38348800	-6.49191300
C	-7.36464100	-2.49638900	2.48085600	H	-1.50436400	-2.80606300	-5.57322100
H	-6.25147600	-4.29968800	2.81471300	H	-0.30403500	-1.89526500	-6.51029300
H	-8.26799000	-0.60189800	1.93910900	C	2.44986100	1.67798700	5.06079400
C	0.10147700	0.89071200	4.52487300	H	2.09874600	2.47111700	5.73642700
H	-0.82597500	-0.91617800	5.19444900	H	2.59966600	2.12196700	4.06677300
H	0.61864500	2.87827100	3.92428900	H	3.43258800	1.34185100	5.41848300
H	-8.12373500	-2.73044600	3.22493600	C	1.40721800	-0.07608100	6.45171700
C	1.48543100	0.49339800	5.03109200	H	0.80665800	-0.99292200	6.50631500
C	-3.00748400	3.15993600	-1.57863700	H	0.97560700	0.65630400	7.14830000
H	-3.56165100	4.09724500	-1.72921900	H	2.41646900	-0.32842800	6.80585700
H	-2.62093800	3.19699100	-0.55027300	C	2.04129100	-0.57435100	4.08215100
P	-2.60119200	0.76743100	0.44094200	H	2.09000000	-0.19480600	3.04988300
P	0.58726500	1.30289700	-1.61202700	H	1.42114800	-1.48142300	4.07350000
C	-1.81413300	3.10330500	-2.55769000	H	3.05974400	-0.87817200	4.36544900
H	-1.56909700	2.04890700	-2.74843500	C	-3.32436400	-0.83492700	6.06622500
H	-2.12299400	3.51774500	-3.52914800	H	-3.46596800	0.14552700	6.54202200
C	4.27858800	-0.40073100	-1.72209700	H	-2.38777500	-1.26091300	6.44368800
H	4.14319400	-1.03994300	-0.83966900	H	-4.13861600	-1.49411700	6.39720300
H	3.63200800	0.47944300	-1.61314200	C	-4.77912000	-0.24835200	4.19428000
H	5.31701200	-0.03683400	-1.71572500	H	-5.49696300	-0.89943500	4.71311700
C	4.38065300	-0.30058800	-4.22708100	H	-5.02245200	-0.32995100	3.12556400
H	5.44991700	-0.04828600	-4.19366400	H	-4.96946000	0.78238800	4.52686400
H	3.84043300	0.65617200	-4.24936200	C	-3.14744100	-2.09058000	3.91037400
H	4.18173200	-0.82681500	-5.17129100	H	-2.15104000	-2.49757000	4.13227900
C	5.02191400	-2.34180400	-3.02298900	H	-3.27420400	-2.05256000	2.81930400
H	4.88135400	-3.00565600	-3.88764200	H	-3.89592400	-2.79842800	4.29723400
H	4.96294800	-2.93578900	-2.10225600	C	-2.96913100	4.32574000	2.47663000
H	6.03946600	-1.93223400	-3.07691300	H	-3.01066500	5.42168400	2.40422200
C	1.73257000	-5.92025900	-3.56613900	H	-3.74296700	4.02011800	3.19538400
H	1.58706100	-6.99152800	-3.36633500	H	-3.23803100	3.94519100	1.48288400
H	2.80110400	-5.69922300	-3.44432400	C	-0.57869100	4.29259200	1.82097700
H	1.46371000	-5.72841300	-4.61446000	H	-0.72658100	3.67070300	0.92433700
C	1.28985200	-5.36073000	-1.17053400	H	0.46686200	4.17759000	2.14005100
H	0.59440200	-4.89770900	-0.45468000	H	-0.71487700	5.34492500	1.52758300
H	2.29486000	-4.98560800	-0.94364400	C	-1.27788100	4.78294700	4.17225900
H	1.27760600	-6.44365600	-0.98105900	H	-1.39140800	5.84558100	3.91615900
C	-0.58634300	-5.53692800	-2.77894800	H	-0.26335500	4.64611000	4.56348100
H	-0.92750400	-5.47107400	-3.82169000	H	-1.98604900	4.55031400	4.97989700
H	-1.27320500	-4.94343200	-2.15646300	Pd	-0.42193400	-0.08358200	0.02489800
H	-0.67928300	-6.58612900	-2.46741900	C	1.37092800	-1.36397800	0.15149700
C	-2.19648800	-0.73698700	-3.84625400	C	-0.60509800	-1.72916500	1.49402500
H	-2.02639500	-0.14070800	-2.93643500	C	0.24029900	-2.13504400	0.45298100
H	-2.57531400	-1.72111200	-3.53478800	H	-0.20652600	-1.20274500	2.36671000
H	-2.99494000	-0.24844500	-4.42590000	H	-1.57722700	-2.20383400	1.61625300
C	-0.62884400	0.49958900	-5.33129200	H	-0.12043900	-2.85264500	-0.28941000
H	-1.41668200	0.71472400	-6.06695300	H	1.93117200	-1.57319800	-0.75580700
H	0.32768600	0.50100600	-5.87346400	H	1.90508300	-0.82045500	0.93424700

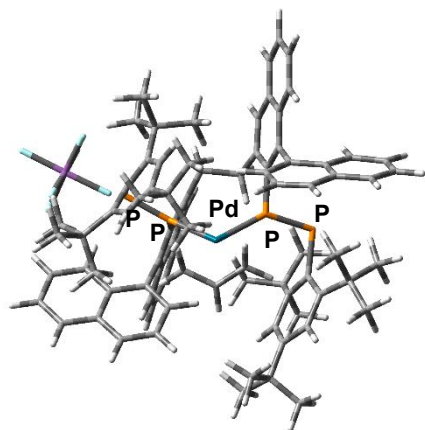
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C	-3.83461900	5.60310000	1.46275200	H	2.02334100	3.68159800	3.67943500
C	0.94448300	7.04734100	-1.30533000	C	6.62269700	-0.77217000	-2.22279300
C	-2.32102600	4.05947700	0.36115500	H	0.17418000	2.60789100	2.39800300
C	0.72213300	5.31676100	0.38327000	C	-1.69855600	-1.95038600	-1.60231500
C	0.13756800	4.10666700	0.86758800	C	-2.13594400	-2.58310000	-2.74050300
C	-1.02283500	3.50181800	0.15613100	C	-0.57275400	-2.48881500	-0.90785300
C	1.66285000	4.14724400	2.76235700	C	-1.46528000	-3.70964300	-3.26782200
C	2.20398500	5.33440700	2.33916400	H	-3.01570600	-2.19387000	-3.25938800
C	1.75376900	5.94350900	1.14342800	C	0.12029600	-3.58632600	-1.39287500
C	2.33815800	7.13980700	0.66152300	C	-0.30707500	-4.21101500	-2.60271000
C	1.94877000	7.67903900	-0.53976000	C	-1.89793300	-4.33177300	-4.46430300
H	2.41361500	8.59215800	-0.90695000	C	1.31359100	-4.10783600	-0.66914400
H	3.11996700	7.61271600	1.25649600	P	-1.23062200	-2.67663900	2.03296000
H	2.99689500	5.81961800	2.90842400	C	0.38449900	-5.30868500	-3.17600000
C	-4.93333900	5.02169500	0.79083000	C	-1.20993100	-5.39572100	-4.99150200
C	-4.73482500	3.98604900	-0.08740700	H	-2.78580600	-3.94083400	-4.96095400
C	-3.43041000	3.48741000	-0.32499800	C	1.21329400	-5.27957000	0.14133800
H	-5.93847100	5.39507000	0.97888900	C	2.52981700	-3.46344700	-0.78519900
H	-5.56906300	3.50419100	-0.59838100	C	-0.80142500	-1.71707100	3.56142900
C	-3.22610100	2.38799000	-1.18466100	C	-0.05514300	-5.88535200	-4.34208600
H	-4.08823200	1.94273000	-1.67560000	H	1.27658000	-5.69027700	-2.68146800
C	0.33814800	5.90072400	-0.85023100	H	-1.54961600	-5.86320800	-5.91387900
H	-0.44255800	5.42375600	-1.44212100	C	2.38596600	-5.78555600	0.77726800
C	-2.56021200	5.13566500	1.25426000	C	-0.02125600	-5.93801100	0.37082000
H	-1.72254700	5.58180000	1.78842000	C	3.68173600	-3.95414100	-0.13118600
H	0.64510300	7.47596600	-2.26004000	H	2.60351400	-2.56124600	-1.39692500
H	-4.00243300	6.42341700	2.15848800	C	0.23030600	-2.17680200	4.43093700
C	-0.87075000	2.39963600	-0.67224000	C	-1.36006400	-0.42951500	3.75553500
C	0.61894100	3.53731300	2.03047400	H	0.48885900	-6.72509300	-4.77054400
P	1.51091800	2.63748800	-2.53244400	C	3.61484000	-5.09924600	0.62111300
C	3.12364100	1.75255200	-2.77651700	C	2.28752000	-6.94295000	1.58743200
C	4.33331100	2.30965000	-2.25885600	C	-0.08839000	-7.04486100	1.18268200
C	3.13607000	0.45652700	-3.34694900	H	-0.92445100	-5.54998400	-0.09941500
C	5.41475900	1.44933300	-2.08528400	H	4.62894100	-3.42506800	-0.23895500
C	4.25467500	-0.35475700	-3.10225900	C	0.86663800	-1.22961700	5.23064200
C	5.38592000	0.09610800	-2.43857000	C	0.65591600	-3.65396700	4.57966400
H	6.33669800	1.84557600	-1.66799800	C	-0.66237500	0.46490500	4.57877100
H	4.24161800	-1.37245000	-3.48450800	C	-2.73737600	0.06611300	3.25986500
C	2.10848600	-0.12844400	-4.34432300	H	4.50152300	-5.49211200	1.11879500
C	4.53873800	3.81353600	-1.96259300	C	1.07755300	-7.55889800	1.79110000
C	-1.98940900	1.81340700	-1.34222700	H	3.19254000	-7.32397200	2.06141900

H	-1.04610400	-7.53244600	1.35548900	H	-0.32127300	2.45303500	6.64057900
C	0.48971200	0.11528200	5.26970100	H	0.49140800	2.93028100	5.13351400
H	1.70041300	-1.54772200	5.85199100	H	1.29292500	3.18729200	6.69211700
H	-1.05690400	1.47229500	4.68735000	C	1.52050700	0.63454700	7.50553000
H	1.01191000	-8.44161100	2.42446500	H	2.06327400	-0.31789200	7.55404400
C	1.31439200	1.12043400	6.06658300	H	0.55666300	0.50251100	8.01617500
C	-2.33456400	-0.66023500	-1.18109100	H	2.10521700	1.37459900	8.06991600
H	-3.42578700	-0.72707100	-1.21232600	C	2.67819700	1.26604900	5.37866200
H	-2.07753100	-0.41991800	-0.13970600	H	2.55328000	1.58271900	4.33041800
P	-0.05613200	-1.70717400	0.66945200	H	3.23792100	0.32023500	5.37814100
P	0.79459200	1.65952800	-0.88678200	H	3.29198400	2.02127300	5.89088700
C	-1.87698300	0.50933700	-2.07946700	C	1.17534500	-3.92578800	6.00062300
H	-0.84158100	0.32580400	-2.40220400	H	0.44947500	-3.61501500	6.76452100
H	-2.49444900	0.52015600	-2.98760600	H	2.13133200	-3.43085600	6.21077500
C	3.98474600	4.22727600	-0.59642600	H	1.34903800	-5.00377000	6.11635600
H	4.52198800	3.72400300	0.22126000	C	-0.52048800	-4.61757400	4.37938200
H	2.91339200	4.01722600	-0.48154900	H	-0.21281500	-5.63337600	4.66401400
H	4.11640500	5.31051800	-0.45804200	H	-0.85526700	-4.68785100	3.33615200
C	3.90156500	4.67807100	-3.05980100	H	-1.38231300	-4.33393800	4.99925700
H	4.17612200	5.73046200	-2.90299800	C	1.77781000	-4.01166600	3.60380400
H	2.80419500	4.64572500	-3.06046500	H	2.67743900	-3.41123200	3.80552100
H	4.25288200	4.37596600	-4.05607000	H	1.47949200	-3.85389200	2.55793000
C	6.03017200	4.17941900	-1.96190900	H	2.04958900	-5.07242100	3.71083400
H	6.52937700	3.87226900	-2.89133500	C	-3.60186100	-0.96098500	2.52529600
H	6.57400000	3.74331400	-1.11413800	H	-4.61504700	-0.55132000	2.41518100
H	6.12681700	5.26932400	-1.87159900	H	-3.68861900	-1.90426200	3.08393600
C	7.78952000	-0.18129100	-3.02650800	H	-3.26720400	-1.17419100	1.50255100
H	8.68034400	-0.81641400	-2.91947200	C	-2.59044200	1.30019300	2.36580800
H	8.05714500	0.82799600	-2.68722100	H	-1.95860000	1.09002100	1.48955700
H	7.53783400	-0.12393400	-4.09460800	H	-2.14636900	2.15195500	2.90119500
C	6.99951600	-0.80273800	-0.73783300	H	-3.57513300	1.62072900	1.99319900
H	6.24611200	-1.34769200	-0.15027700	C	-3.55193900	0.44908900	4.51184200
H	7.10067500	0.20333400	-0.30917800	H	-4.54203300	0.81425100	4.20600800
H	7.95786400	-1.32360500	-0.60204700	H	-3.07935900	1.23869800	5.10719000
C	6.41139300	-2.21094200	-2.68922200	H	-3.69819600	-0.42430900	5.16294600
H	6.24309900	-2.27143600	-3.77352200	Pd	1.59869400	-0.01938200	0.58446900
H	5.55629700	-2.68561900	-2.18520000	C	3.45988000	1.09721200	1.06065000
H	7.30507300	-2.80692000	-2.46027700	C	2.85898000	-1.02633600	2.08285600
C	1.42194200	-1.36832500	-3.76681600	C	3.68686900	-0.27471500	1.23223600
H	0.88554700	-1.13752700	-2.83368100	H	2.42003000	-0.58753400	2.98500500
H	2.13853700	-2.17428000	-3.55308000	H	2.91790700	-2.11325000	2.05596200
H	0.68897500	-1.76603500	-4.48495800	H	4.29830500	-0.79364500	0.48961400
C	1.02899300	0.83625600	-4.84158800	H	3.97577400	1.62290700	0.25898300
H	0.51001600	0.37164800	-5.69168100	H	3.05031200	1.71205300	1.86731900
H	1.45454000	1.78330500	-5.20337800	Sb	-6.31227000	-0.08765900	-1.54914900
H	0.25227100	1.05637800	-4.09932200	F	-6.70348100	1.74449200	-1.78918200
C	2.88434700	-0.53374500	-5.61477700	F	-5.17362100	0.38513000	-0.11717100
H	2.18357000	-0.94111000	-6.35635400	F	-5.79367300	-1.88244300	-1.32378500
H	3.64577100	-1.30004700	-5.43184800	F	-7.72551300	-0.28028400	-0.33040000
H	3.38207000	0.33836400	-6.06141200	F	-7.45772300	-0.54765500	-2.96306800
C	0.65122300	2.49505500	6.13028100	F	-4.89769100	0.10669300	-2.79838300

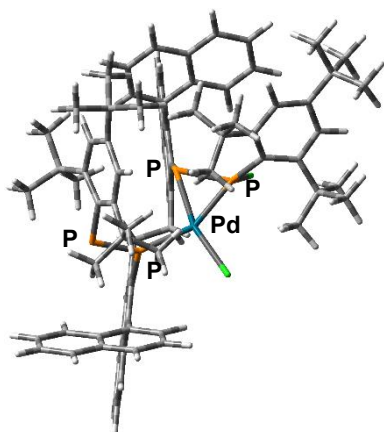
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Sb	6.09901400	-1.13876600	-1.41321100	C	-3.32053700	4.63343300	1.01681000
F	5.09697000	-2.73308200	-1.47909700	H	-5.17858800	4.00486100	1.86396700
F	4.50354600	-0.15891000	-1.68072700	H	-1.67382700	5.20443700	-0.21922100
F	6.34256500	-1.17700800	-3.27756000	C	-1.99832100	3.92360300	-2.46755800
F	7.69094500	-2.11348900	-1.19868800	C	-6.17859400	2.22379600	0.11967000
F	7.03704100	0.49556300	-1.29578800	C	-1.42449200	-1.46978800	-3.18125100
F	5.90448800	-1.09744400	0.45923300	H	-4.16584700	-2.90587500	2.75610500
C	-3.64025700	-6.02466800	-2.99458100	C	-3.04567400	5.63458500	2.13563500
C	-7.35343300	-1.83951400	-2.34518700	H	-2.56662800	-2.77970400	0.84850500
C	-3.04126500	-3.71462100	-2.55066000	C	1.71183900	0.53542300	-2.53906600
C	-5.48968600	-2.33067800	-0.86901100	C	2.23275700	1.33746700	-3.52351000
C	-4.09036800	-2.48873500	-0.62896700	C	1.79051500	0.97053000	-1.17948500
C	-3.13949800	-2.51953200	-1.77489100	C	2.81047100	2.59351100	-3.23600100
C	-4.54478200	-2.75222300	1.74606200	H	2.18726000	1.00911000	-4.56447700
C	-5.89570300	-2.66369700	1.52777600	C	2.34459100	2.19900600	-0.85538800
C	-6.39970300	-2.44303000	0.22340400	C	2.85485600	3.04483000	-1.88583800
C	-7.78661900	-2.28214600	-0.01309800	C	3.30372200	3.43299900	-4.26483800
C	-8.25554600	-1.97942400	-1.26749900	C	2.40926900	2.67125900	0.55567000
H	-9.32225900	-1.84285000	-1.43529000	P	2.70457400	-1.34861100	0.60677000
H	-8.47272900	-2.38053700	0.82842600	C	3.38377600	4.33416900	-1.61891300
H	-6.60033800	-2.74268500	2.35560400	C	3.80874500	4.67552800	-3.97467400
C	-2.76322100	-6.04814700	-4.10172200	H	3.26446600	3.07355100	-5.29315100
C	-2.03593400	-4.93126900	-4.42785200	C	3.63429300	2.57570000	1.28599200
C	-2.14874200	-3.74514000	-3.66180900	C	1.30394100	3.24852000	1.14765900
H	-2.66449100	-6.95706000	-4.69221200	C	1.85812300	-2.38118000	1.90185800
H	-1.35066500	-4.93999000	-5.27528800	C	3.84482800	5.13053900	-2.63802400
C	-1.36499400	-2.60602900	-3.95018200	H	3.41392300	4.69320900	-0.59123900
H	-0.67319000	-2.64735800	-4.79449600	H	4.17993500	5.31566000	-4.77299300
C	-6.00509600	-2.02399200	-2.15383400	C	3.69347400	3.10912500	2.60933800
H	-5.31473600	-1.92481800	-2.99111000	C	4.78723300	1.94397600	0.75466800
C	-3.77920800	-4.88606300	-2.24051500	C	1.36056500	3.74571700	2.46980100
H	-4.45202800	-4.87767300	-1.38431800	H	0.36949900	3.32346500	0.58540700
H	-7.73140600	-1.59061400	-3.33510300	C	1.94444700	-2.01906200	3.27533400
H	-4.20799200	-6.91704100	-2.73776600	C	0.96968600	-3.41441500	1.51026600
C	-2.34637700	-1.42694600	-2.08888100	H	4.24201300	6.11949000	-2.41651200
C	-3.63950900	-2.67619300	0.66292400	C	2.53296200	3.68881700	3.17975200
P	-3.89809000	1.17437400	-2.01124300	C	4.90575600	3.01870900	3.33597000
C	-3.85957700	2.73085600	-1.00104800	C	5.94445800	1.86264800	1.49073600
C	-4.80308100	2.92622100	0.05447700	H	4.75377300	1.49010600	-0.23430700
C	-2.80219500	3.65649400	-1.17361300	H	0.46996900	4.18850000	2.91803700
C	-4.48592500	3.85914900	1.03918900	C	0.93012200	-2.46239300	4.12504600
C	-2.52881500	4.54019700	-0.11822600	C	3.09779700	-1.22669800	3.92999500

C	-0.01271700	-3.81673900	2.42362500	H	-2.13378500	2.08447200	-3.69438700
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H	2.58963600	4.08111700	4.19555600	H	-1.68064400	5.64076900	-3.76089800
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H	4.93907600	3.43347100	4.34408200	H	-3.29464800	5.59936000	-3.01690300
H	6.80093000	1.35122300	1.05669100	C	-2.15177900	-4.74743400	4.11307900
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H	-0.72863100	-4.56844000	2.10125600	H	-2.96164100	-4.94620700	4.82799900
H	6.93485500	2.34431900	3.35982600	C	-0.68453100	-4.15383000	6.01020500
C	-1.23703400	-3.65726500	4.66927900	H	-0.08187800	-3.39422100	6.52393900
C	0.96769500	-0.70941700	-2.93036200	H	-0.05845300	-5.04557200	5.86902200
H	1.50895900	-1.25855600	-3.71405300	H	-1.51327500	-4.42336700	6.68000200
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P	-2.44975700	0.08928000	-1.05933100	H	-1.48095100	-1.59524200	5.37968800
C	-0.45081300	-0.35425100	-3.43085400	H	-2.93299800	-2.60699800	5.54989900
H	-0.77329100	0.56185700	-2.91605300	C	3.48740800	-1.91583000	5.25104800
H	-0.41031600	-0.09994800	-4.50021800	H	3.74039800	-2.97228000	5.08584400
C	-6.08251100	0.80656200	0.69084300	H	2.70126400	-1.86941200	6.01378600
H	-5.76393000	0.82127600	1.74378300	H	4.37057300	-1.41746400	5.67315800
H	-5.38616500	0.16754100	0.13186400	C	4.37405300	-1.18726100	3.09134100
H	-7.06994100	0.32369100	0.64947400	H	5.19570400	-0.78113900	3.69925000
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H	-6.33375100	1.48179900	-1.96223100	C	2.67854300	0.21234700	4.23450100
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C	-1.73703300	6.39377400	1.92551600	H	0.29977700	-6.08000500	1.18946700
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C	-0.50263400	3.69086500	-2.24704000	C	-0.53991800	0.59891000	2.97812700
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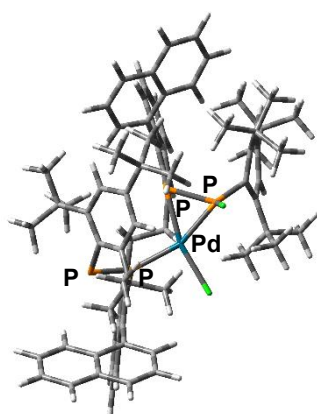
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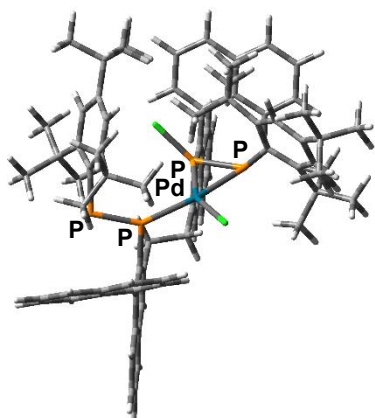
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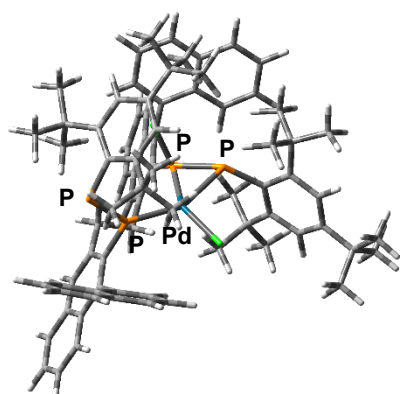
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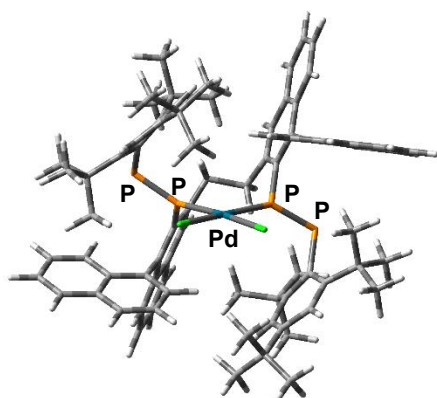
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8D



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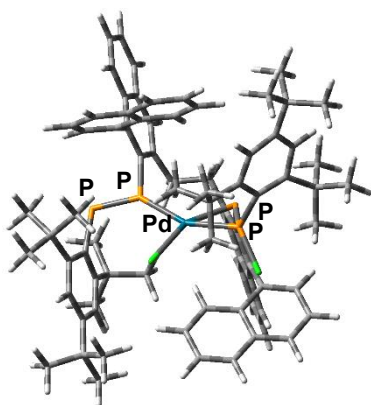
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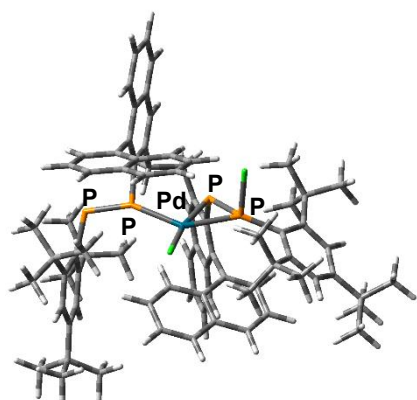
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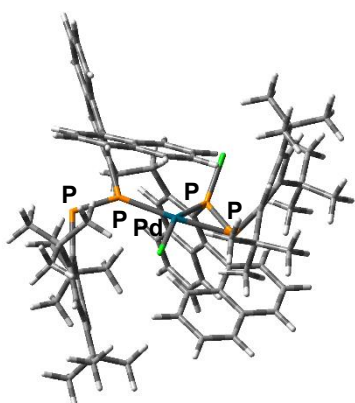
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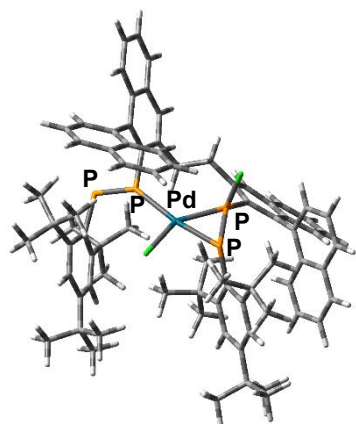
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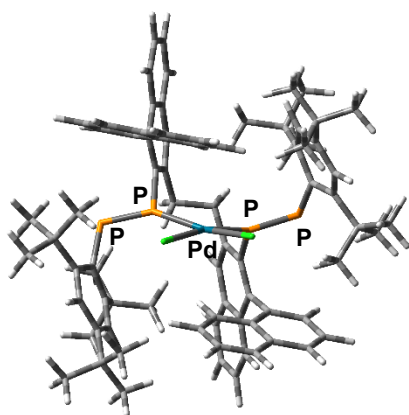
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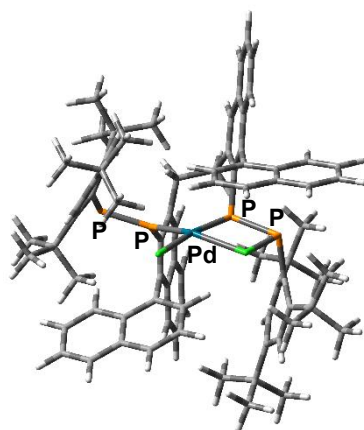
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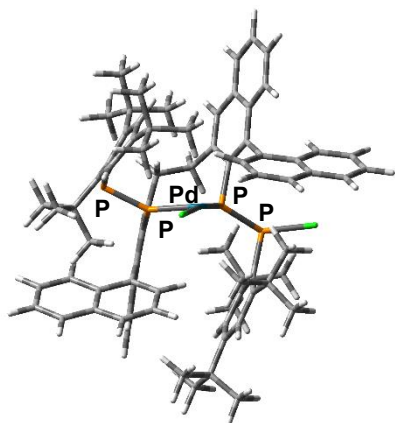
Int-1



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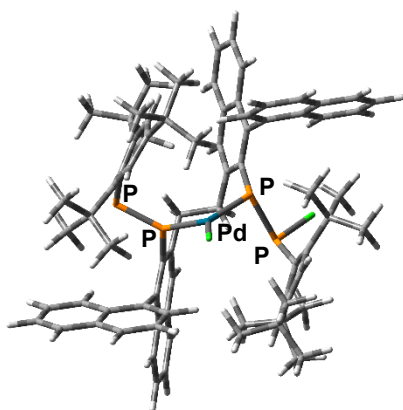
Int-2



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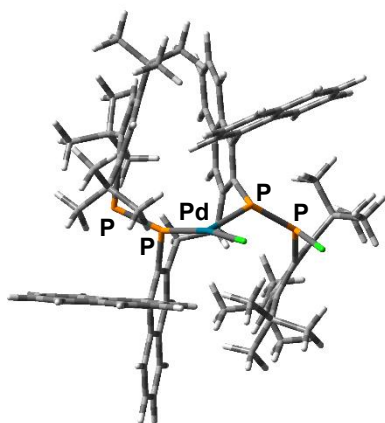
Int-3A



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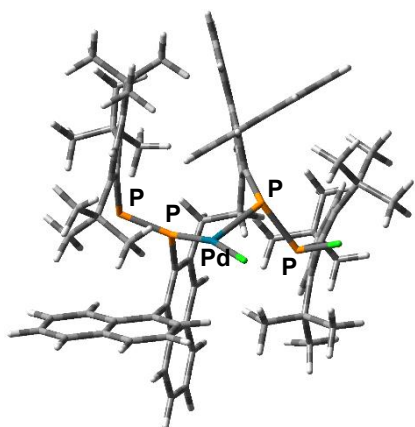
Int-3B



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C	3.813879609321	-1.943875160593	-0.928678660926	C	-0.309316968570	5.746570136208	1.053185213564
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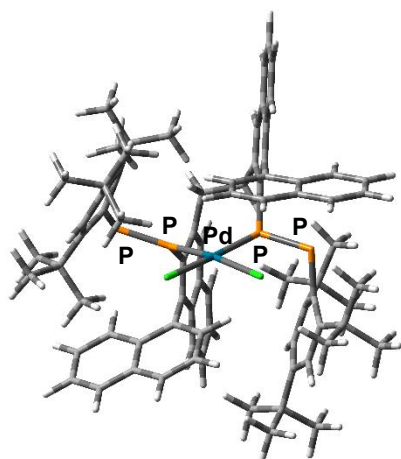
Int-4_B



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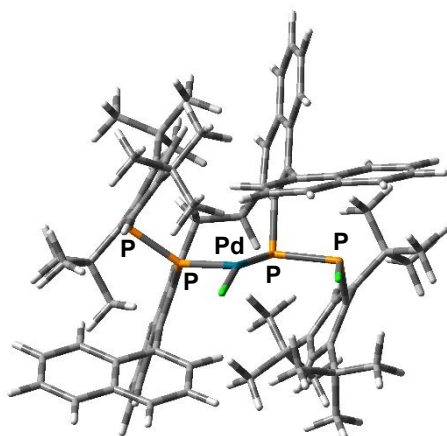
TS-1



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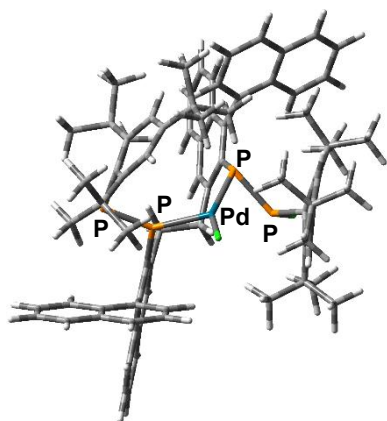
TS-2



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C	4.208587521483	-2.102631633726	-1.513848649423	C	-0.575059148409	-2.784630953381	3.746451024994
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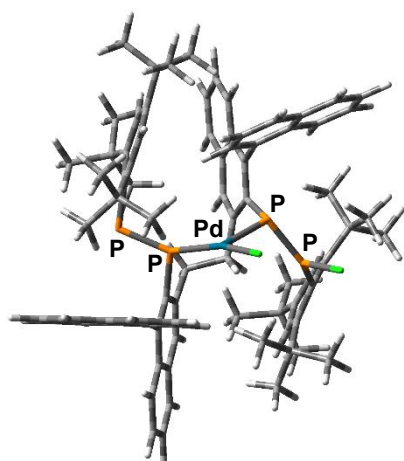
TS-3A



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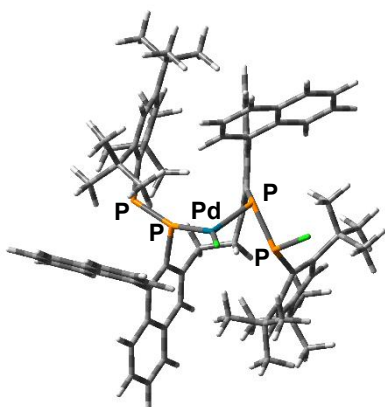
TS-3B



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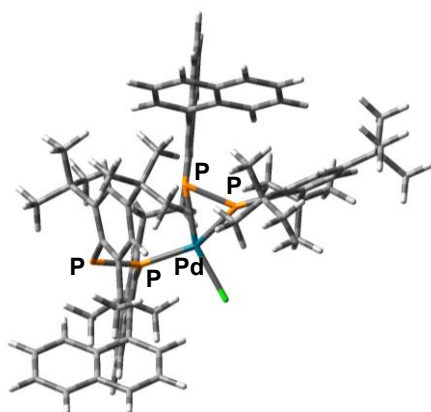
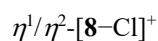
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H	6.622817244860	-2.755683132290	4.299558725718	H	-7.670110323657	-2.679371424346	-1.049717034943
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TS-4B



C	-2.603393021393	2.500987576686	1.119710457687	H	1.449243046173	-6.620409862260	-2.735660332810
C	-3.331724412527	1.698591090293	2.060699685591	C	1.484179969836	-6.451835345538	-0.066798275978
C	-3.278541524799	3.046891635051	-0.006988021898	H	0.807718437321	-7.211853196224	-0.478516982229
C	-4.608877599505	1.280158190061	1.696608775538	H	2.462370037499	-6.931004667615	0.068109942488
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C	-2.733478811752	4.173711605599	-0.916025794876	H	3.431142809183	-1.286159935527	-3.782350818337
C	-6.658973385675	1.180174871896	0.226926305337	C	6.239734816063	-1.268484376459	-1.806381713084
C	-2.880229244009	1.391786223015	3.511056427987	H	6.693096192440	-0.639795208909	-2.583339512719
C	2.824176915680	-2.977687990926	-1.292183986243	H	6.578189278604	-0.863320529392	-0.844318195202
C	2.511779428806	-4.167033665947	-0.563996331351	H	6.639694590714	-2.285663578883	-1.917736917153
C	4.051103073105	-2.284250616340	-1.042020967162	C	4.265853519142	0.194988068106	-1.618116400574
C	3.278145607631	-4.431361107605	0.571694968971	H	4.835904804160	0.924298174590	-2.214531992753
C	4.745434841417	-2.615468665575	0.122069193237	H	3.197852974702	0.361820034262	-1.816738531022
C	4.337987467828	-3.626049857531	0.985932326481	H	4.450621671668	0.406898353152	-0.554827049532
H	3.029899272304	-5.294711493978	1.176619860969	C	-3.878499739764	4.922866097930	-1.619079370670
H	5.641454724523	-2.053987406527	0.372007047104	H	-4.374750921630	4.316731512161	-2.387940678333
C	4.708570900973	-1.229388870837	-1.971529151234	H	-4.638419014315	5.278109468999	-0.909611774192
C	5.089060977256	-3.867573581223	2.290580665342	H	-3.461207833628	5.798570544159	-2.132755230633
C	1.534970951221	-5.266144647596	-1.039056065976	C	-1.990144075542	5.242662791447	-0.106478029711
C	4.379177046609	-4.879363324286	3.188631606775	H	-1.034711880587	4.900821896202	0.315189317972
H	4.347429072391	-5.882237945691	2.741713275913	H	-1.736101050126	6.089202171600	-0.759894891300
H	4.918650246778	-4.964835711050	4.141384632959	H	-2.612919380725	5.620436038622	0.717210784085
H	3.348149178463	-4.567352118845	3.412899107374	C	-1.830070439993	3.621589982388	-2.023550398082
C	5.204113676074	-2.551972926822	3.069847234865	H	-0.896694735820	3.199411035221	-1.635730401168
H	5.749240442924	-1.779527695687	2.510800124392	H	-2.344795485891	2.832942831489	-2.594709635423
H	4.207135753150	-2.155571103780	3.318246751850	H	-1.556390059874	4.426264021347	-2.723098755274
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C	6.492337489227	-4.396266406615	1.969896856845	H	-8.147995362891	1.167584040668	-1.334463189189
H	7.049437574282	-4.579162182360	2.899818309791	H	-7.197327012604	2.658231580012	-1.300755201050
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H	7.069202604807	-3.683417832885	1.365654981341	C	-7.608146305462	1.816941600712	1.251680044021
C	0.078148178113	-4.831431965276	-1.217464446820	H	-7.575851903967	2.913608116440	1.184824260885
H	-0.326841917181	-4.425885505723	-0.279123486520	H	-8.642150332012	1.493599886701	1.063402763559
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H	-0.525459897578	-5.709968945100	-1.485926754837	C	-6.739609551875	-0.346845177927	0.348250977852
C	2.092154860636	-5.809039135777	-2.365042672210	H	-6.079634979669	-0.837853350644	-0.381767439491
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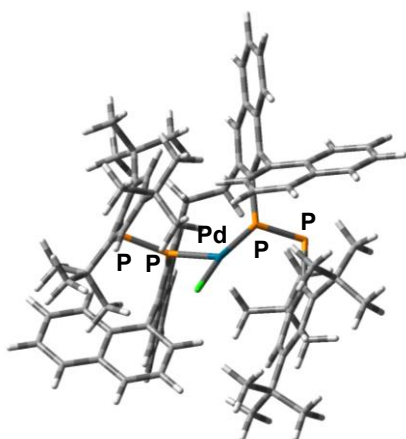
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H	-3.541723818158	0.383084555310	5.292647686640	H	4.277635718958	0.228690585308	2.824365917183
H	-4.889068017148	1.010539753860	4.339015598694	C	2.833232819673	2.904741890763	0.385623536652
C	-2.778368696984	2.722004993775	4.272208525836	C	4.210487790766	2.966923723611	0.761053289990
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C	-1.553710248983	0.630934484402	3.607699646806	H	6.500205051443	1.219970278947	2.629038420299
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H	-1.495674826941	-0.160425411959	2.849135186922	H	4.691691455269	4.744170068632	-0.383721518720
H	-0.684306352240	1.288826999964	3.492892765369	H	7.990290490258	2.988403297811	1.738716761363
C	-4.399789910154	-3.232552403276	3.234676109794	H	7.072340642839	4.752557132301	0.239801700066
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C	-2.589737861388	-2.575071869333	1.759703274591	C	1.810546491083	5.188752795776	0.019502583705
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C	-4.348060640685	-2.595761002682	-2.566913984946	C	0.848646680199	7.413199606334	-0.348251907738
C	-4.881357890219	-3.648381259790	-3.350313817221	C	1.307161428454	5.928969322271	-2.269005714564
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H	-3.817815195435	-3.884638941016	5.219086030864	H	0.482670631878	8.594330280632	1.397084368899
H	-1.398805613020	-3.539004733003	4.828053444534	C	2.551950688017	0.893726717603	1.763134337480
C	-0.283425972262	-2.554821458906	2.584193969809	C	1.685933950331	-0.204169721008	2.310653345607
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C	-3.380252931617	-4.275978783184	-1.078517573897	H	2.078988039616	-0.526930745573	3.285570064031
H	-2.793997212888	-4.530491016933	-0.196054988157	C	1.565098566216	-1.431245355548	1.374459340884
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H	-4.689879572372	-2.550016686883	1.225262284460	H	1.829971050621	-1.129069402638	0.355349747825
H	-3.731719229010	-6.316541840229	-1.598538266343	P	0.316088863049	1.672131978044	0.198016999116
H	-5.462850516499	-3.376335546595	3.418677326610	P	-0.809253630413	2.803551581062	1.491372058296
C	-0.741785679109	-1.853284481217	0.325749794560	P	-0.379452773373	-1.444476685863	-1.425730102574
C	-3.286506008412	-0.535663141323	-0.995203415107	Pd	0.544328642131	0.624304081020	-1.843259657303
C	0.177095239459	-2.005434469140	1.411328332893	Cl	0.855359481554	1.307840212207	-4.202779053532
H	-4.152204586349	0.813074273810	-2.445773638816	P	1.636395764043	-1.917488648393	-2.204702489810
H	-2.860069793665	0.275465767088	-0.401561345750	Cl	1.052948937752	-2.816431493347	-4.032361246125
C	3.874594082021	0.963340104359	2.124084464486				



C	-4.38918200	-3.03474700	5.35048500	H	-2.90320700	3.09108500	4.53099100
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H	-4.96386500	3.53799300	3.22616200	C	7.39858200	-4.66047400	-0.79810800
C	-3.73465000	-4.28604900	5.33598600	H	7.11134900	-2.74704700	-1.70592700
C	-2.66206200	-4.49414000	4.50544600	H	7.44955600	-6.54969600	0.26530200
C	-2.20173000	-3.46175500	3.65452900	H	8.31162600	-4.86519400	-1.35378800
H	-4.08348700	-5.08413000	5.98835300	C	5.31165100	-0.97256200	-1.44490300
H	-2.14638100	-5.45387200	4.48884800	C	6.38117800	-0.08323600	-1.12283500
C	-1.09159200	-3.64756800	2.80285800	C	4.74722900	-0.93727300	-2.70175700
H	-0.57924700	-4.61152500	2.82718800	C	6.85096900	0.81776400	-2.12514100
C	-4.81570000	-0.59390100	1.19734800	C	6.97665000	-0.03906800	0.16294400
H	-4.31676800	-1.55810100	1.09760300	C	5.20603100	-0.03415600	-3.68467700
C	-3.96374300	-2.01496200	4.53561600	H	3.92494000	-1.61256900	-2.93670400
H	-4.47332200	-1.05338100	4.55577200	C	7.89603400	1.71836000	-1.80669300
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H	-5.23699900	-2.87883400	6.01450900	C	7.97960900	0.85752500	0.44486400
C	-1.31034700	-1.40910300	1.94193000	H	6.62481600	-0.72394000	0.93437700
C	-2.61810700	1.11532000	3.69479800	H	4.72758600	-0.02400300	-4.66286500
C	-3.24133800	-0.63161800	-1.98671500	C	8.44650600	1.74433400	-0.54894000
C	-3.92161500	0.53658600	-2.40346000	H	8.24589900	2.40215400	-2.58064400
C	-3.79085400	-1.92963000	-2.23925900	H	6.60936300	1.51764600	-4.15677500
C	-5.21118600	0.38722400	-2.91617300	H	8.42044300	0.88237200	1.43978500
C	-5.07005100	-1.98167400	-2.77032500	H	9.24349800	2.44748000	-0.31431900
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H	0.89935000	4.72531100	-1.15368900	H	0.71944100	0.50333800	3.36971800
H	-0.16220500	3.89237200	2.86349300	H	2.47798600	0.24771100	3.24972300
C	3.22474300	3.48585300	-1.32057900	H	1.74069900	0.54860400	4.82327800
C	-1.02148000	5.27341100	0.74302600	C	0.95068700	2.97780600	4.65365400
C	1.88018500	2.34159900	3.61143600	H	1.25509300	2.63668700	5.65137600
C	3.15257500	-2.72433400	1.18699300	H	1.00534400	4.07451900	4.64821500
C	1.87702900	-2.51273600	1.95272700	H	-0.09857400	2.68026100	4.51498300
H	1.75532200	-1.45502300	2.22883000	C	-1.85431700	1.95187700	-2.15187200
H	1.91920000	-3.06814500	2.90111400	H	-1.43142500	2.96880500	-2.14941200
C	0.63017500	-2.97585300	1.18406800	H	-1.58053200	1.61233800	-1.12936400
H	0.69996500	-4.06197700	1.02527300	H	-1.31196000	1.39095100	-2.92663400
H	0.62121300	-2.52607800	0.17786400	C	-4.03338900	2.71875200	-1.20795100
P	-0.90337800	0.05197300	0.87287800	H	-3.65708200	3.75052900	-1.16149400
Pd	0.58001300	-0.39487600	-1.01507300	H	-5.12123400	2.76118000	-1.34771500
Cl	1.27897700	-0.76298000	-3.28753300	H	-3.84620700	2.23666100	-0.23601400
P	-1.66310500	-0.51526100	-1.08758800	C	-3.60806900	2.68819900	-3.67914700
C	4.67994700	3.25000100	-0.90110300	H	-4.67182200	2.86934100	-3.86876800
H	4.92241800	2.19899000	-0.69735600	H	-3.11671900	3.67028600	-3.64785600
H	5.34636400	3.54074700	-1.72540300	H	-3.19617200	2.12631800	-4.52773900
H	4.95143000	3.85087700	-0.02095000	C	-7.89498600	0.34593500	-3.92730600
C	2.84665200	2.52280700	-2.45034700	H	-7.96400900	0.98100800	-3.03272200
H	2.94468300	1.47069000	-2.15434600	H	-7.35365000	0.89979000	-4.70676300
H	1.80665600	2.68232300	-2.77451200	H	-8.91679300	0.17820300	-4.29197300
H	3.50402400	2.68267200	-3.31852600	C	-7.20262800	-1.82147500	-4.91653600
C	3.20443100	4.91318200	-1.90200500	H	-6.57893700	-1.33028200	-5.67586600
H	3.35490400	5.67207600	-1.12187900	H	-6.81024000	-2.83402300	-4.75720500
H	4.01850000	5.01125000	-2.63173600	H	-8.21878100	-1.92033900	-5.32245400
H	2.27795100	5.14901800	-2.43880200	C	-8.09996300	-1.72319700	-2.57828600
C	-2.24735700	4.58666800	1.35245200	H	-9.11292000	-1.87961600	-2.97414500
H	-2.15202900	4.46155600	2.43832400	H	-7.69131300	-2.70599900	-2.30884300
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H	-2.40452200	3.58582100	0.92211800	C	-3.85130700	-4.48164200	-2.25800700
C	-1.35147100	5.70230200	-0.68541500	H	-3.23803200	-5.36588500	-2.04266500
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H	-2.25266900	6.33039900	-0.68205300	C	-1.83462800	-3.26704900	-3.01984500
C	-0.70168700	6.53905700	1.55059000	H	-1.27331800	-4.20343100	-2.89638900
H	-1.56039400	7.22586100	1.53555600	H	-2.20705100	-3.22339700	-4.05177100
H	-0.47507700	6.30409300	2.59932300	H	-1.12068800	-2.43982700	-2.89002700
H	0.16437500	7.06570500	1.12586500	C	-2.49350400	-3.31271800	-0.60021700
C	3.30413300	2.74532100	4.02173200	H	-1.87881600	-2.42983100	-0.31311200
H	4.08329700	2.28977200	3.39691900	H	-3.30364100	-3.36978000	0.14104900
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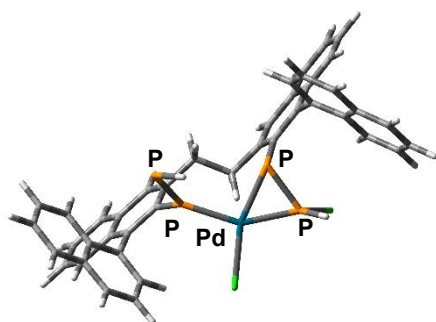
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C	4.38236500	-0.93494700	2.48357200	C	-2.74267600	4.83883000	-2.87937800
C	4.92142200	1.45900200	0.30854000	H	3.43193000	-1.39363200	-0.86206300
C	4.14310200	0.25961500	0.29722100	C	-1.98999000	-0.98776300	3.46062500
C	3.54946600	-0.22068700	1.57341100	C	-2.90370500	-0.59117600	4.40258400
C	4.67974200	-0.06189900	-2.04845900	C	-2.37333000	-0.96771400	2.08209900
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C	5.58283800	1.86231300	-0.88818600	H	-2.62633800	-0.60134200	5.45811900
C	6.34265000	3.05695000	-0.89053200	C	-3.62072100	-0.50426400	1.68238800
C	6.44092500	3.83114400	0.23911700	C	-4.55416900	-0.05963800	2.66892800
H	7.02313400	4.75052500	0.22444600	C	-5.10565100	0.32285500	5.02661800
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C	5.95067600	-2.39668000	4.30389300	C	-5.81962500	0.48252600	2.32699900
C	4.66975500	-2.04609500	4.64988700	C	-6.32698800	0.83391600	4.66420200
C	3.85545600	-1.31660400	3.75117200	H	-4.81514000	0.26385800	6.07518900
H	6.56751500	-2.96442900	4.99771400	C	-4.93696900	-1.30721700	-0.33079400
H	4.25542700	-2.33041100	5.61669100	C	-3.43737200	0.59245400	-0.53618100
C	2.52603700	-0.97168200	4.07852300	C	-0.19721200	-3.91419400	-0.71831500
H	2.14463600	-1.24667000	5.06406000	C	-6.68315800	0.91921800	3.30098900
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H	7.49162500	-2.30771000	2.78173200	H	-2.72183000	1.28993900	-0.09729000
C	2.23333700	0.05986300	1.92177200	C	-0.58061600	-3.73397300	-2.07822200
C	4.02393600	-0.47285800	-0.86564200	C	1.15834900	-4.17935700	-0.39451100
P	1.41549300	2.93694300	1.17152200	H	-7.64820300	1.33676300	3.02114000
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C	0.64131100	4.35836800	-1.14756500	C	-6.26533600	-2.00889000	-2.26836400
C	-1.13763900	3.91558500	0.50861300	C	-6.41186700	-3.23086600	-0.19302700
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H	-0.07038700	5.01573200	-3.04952300	C	-2.00962600	-3.76886800	-2.65818700
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C	-1.67834100	3.92088600	1.95774900	C	1.71505900	-4.70076500	0.94633200
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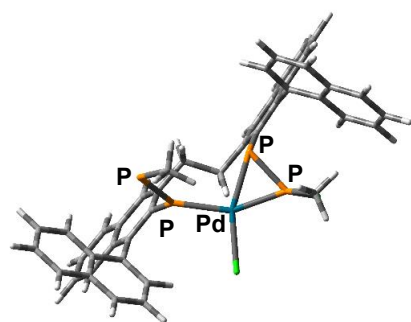
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C	2.82479800	-3.47161400	-3.81037600	H	-3.24139200	5.41394000	1.48852200
C	-0.57094600	-1.27545400	3.85025500	H	-1.68694800	6.10855600	1.99139600
H	-0.51594900	-1.56757400	4.90671800	C	4.25589500	-3.57328200	-3.28606800
H	-0.16220500	-2.11956600	3.27589200	H	4.47949000	-4.57964400	-2.90558000
P	-1.20165900	-1.54291400	0.80499700	H	4.46065500	-2.85507100	-2.47945900
P	1.19341100	0.95512800	0.71506700	H	4.96198200	-3.36672400	-4.10175200
Pd	-0.15265500	-0.18123200	-0.72654600	C	2.63968100	-4.55519400	-4.88079200
Cl	0.49686300	0.92779800	-2.67537100	H	1.64042300	-4.52088000	-5.33498100
C	0.28752100	-0.01464900	3.59899200	H	2.78318000	-5.55705200	-4.45272500
H	-0.20172800	0.59449100	2.82508800	H	3.37722500	-4.41933200	-5.68457600
H	0.27250500	0.61038300	4.50451800	C	2.61976100	-2.09086000	-4.44623400
C	2.83473400	3.46558800	-2.08222300	H	2.64483100	-1.29345200	-3.68925600
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H	3.10766500	4.50221400	0.44468000	H	-3.05283500	-4.84031500	-4.22834800
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H	1.78981200	5.42607600	-3.57850900	H	-2.83117400	-5.19489800	-1.20593600
H	3.19543900	6.08417700	-2.74928700	C	-2.39164800	-2.38381500	-3.18707600
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H	-2.80230200	6.95929500	-2.36583200	C	0.67819500	-5.05335400	2.01205900
C	-2.46832800	3.99117300	-4.12751300	H	1.18311500	-5.57091100	2.83976700
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H	-1.46774000	4.17215000	-4.54077800	H	0.19853600	-4.17353300	2.46288100
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8A-H



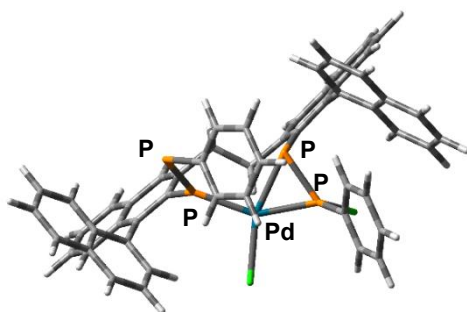
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C	4.40245000	-0.34535900	1.40817900	H	-6.64412100	5.25252400	-1.33678600
C	3.76484800	0.89289300	0.87317000	H	-7.83490400	3.06675600	-1.37522400
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H	6.98415100	-4.10576900	0.69896700	H	-3.83600300	-1.08842600	-2.05610000
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C	5.81369700	4.59586000	1.07813500	C	-5.68293200	-3.17321700	-0.12336900
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C	5.63732000	-0.74911800	-0.71927600	H	-6.60558200	0.04931500	3.99970500
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H	7.42515200	3.48188100	2.00705100	C	-0.52123800	2.21008700	0.56836700
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H	4.39902400	-2.24676100	4.23460100	H	0.28911300	2.96549100	-1.28270500
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C	-6.11124500	1.93939200	-0.81094500				

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C	5.88120500	-2.06757200	1.20838700	C	-5.00653200	-2.47692500	-1.53060600
C	6.70439200	-2.90884500	0.41971100	H	-3.77759400	-0.81823900	-2.18183500
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H	7.11437900	-3.81003700	0.87603100	C	-6.71796800	-0.62514700	2.85086000
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C	4.46488300	4.73597900	0.14661400	C	-7.27556400	-1.91493400	2.71744800
C	3.79261900	3.49153900	0.21041900	H	-7.41317800	-3.67393300	1.49833000
H	6.25984600	5.82123000	0.55859600	H	-6.26276300	-3.96415700	-0.63215000
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C	2.46538400	3.34070900	-0.24501500	H	-7.92360000	-2.30721100	3.49912600
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C	5.65287700	-0.58581600	-0.72388400	P	-2.29350800	-1.19201800	2.38396000
H	5.25286800	0.32378100	-1.17052300	C	-2.02637000	2.22724900	0.27393500
C	5.78787200	2.52566500	1.23938300	C	-0.56771600	2.29114800	0.62887800
H	6.30564300	1.66911200	1.66830300	H	-0.31178600	1.52680000	1.37949300
H	6.68878600	-1.17192600	-2.49740400	H	-0.34424600	3.26138600	1.09676700
H	7.43433100	3.85284600	1.53262800	C	0.34621300	2.13417500	-0.59836000
C	2.47588100	0.99563500	0.32364900	H	0.15096100	2.97149400	-1.28405600
C	4.24118700	-0.38345900	2.72977800	H	0.08481600	1.21619500	-1.15023000
C	1.79277000	2.14140500	-0.19494600	P	1.80225200	-0.73927300	0.46768400
H	4.60110900	-1.76488500	4.35717500	Pd	-0.09502400	-1.23067000	-0.96768400
H	3.58687200	0.25678300	3.32213400	Cl	-1.32576500	-2.23049900	-2.80725700
C	-2.71086100	3.38530800	-0.00425900	P	2.10876100	-1.47258400	-1.52949700
C	-2.72498200	0.98364400	0.18177800	Cl	2.97124100	-0.20501100	-2.90371100
C	-4.07118600	3.38081800	-0.38897100	C	2.99875500	-3.04916000	-1.71079500
H	-2.19448100	4.34453700	0.07424400	H	4.07845300	-2.89054500	-1.59730700
C	-4.05935400	0.93352300	-0.19702200	H	2.63189700	-3.71452500	-0.91965700
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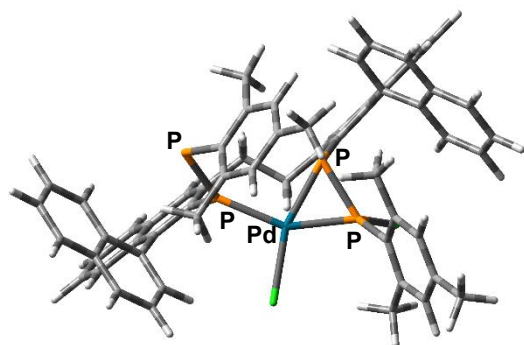


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C	-6.67754500	-1.57928100	-0.60658600	C	5.73405600	-0.97821200	-0.64931100
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H	-7.16922100	-2.43403800	-1.07218100	C	6.21452600	-0.20179700	-1.73482100
H	-5.86642800	-2.12164500	-3.11257000	C	4.75619600	-2.62653600	1.42020200
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H	-3.00238300	6.52751700	0.14752800	H	5.97995900	0.86150000	-1.77064900
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C	-5.40541400	0.61906100	0.56043100	H	7.02719600	-4.00055200	-1.63888300
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C	-5.08465500	3.64353200	-1.42282200	H	7.32689300	-0.16216200	-3.55732300
H	-5.66737500	2.83923400	-1.86907200	H	7.86742800	-2.59315900	-3.49477200
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C	4.79242300	3.39701300	0.59304400	H	0.35956700	1.80163800	1.21622500
H	3.07097000	4.61707700	0.12339800	P	-1.47597600	0.01248300	-0.47172000
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P	-1.98705900	-0.68785300	1.49578600
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H	-4.57122200	-4.45878000	-0.33847500

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8A-Mes

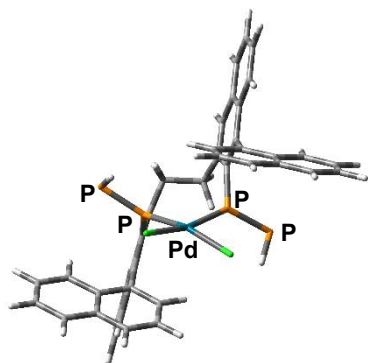


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C	-2.08368100	-1.48641000	4.46172700
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C	7.21944800	-2.16975200	-2.72265000
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H	1.48677500	4.04282600	-0.65572900	H	0.91375200	0.46867400	-4.37592900
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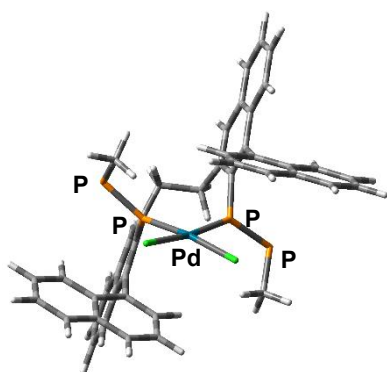
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H	-4.45500600	4.30552300	0.69619900	H	-2.48667000	0.79382800	2.21406700
C	-5.99620700	-3.70579600	2.22385600	C	1.84863400	-2.82937200	0.15771300
C	-4.84034000	-4.15734900	1.63780000	C	2.73029800	-3.69386800	-0.44329200
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H	-6.68462700	-4.41050000	2.68643200	C	3.93847400	-3.25167600	-1.02944400
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C	4.84087200	-4.15727300	-1.63748100	H	4.45426000	4.30571300	-0.69664700
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P	1.54216700	-0.44600500	3.10985800	H	5.76974000	4.17734300	1.35823600
C	5.44447000	-1.42318500	-1.64865500	H	6.18886500	0.42634700	3.42173900
C	5.99673900	-3.70566700	-2.22349100	H	6.68027700	2.86162200	3.24760600
H	4.59673200	-5.21931500	-1.63174300	C	0.50138300	-3.32183000	0.59492400
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H	6.68524100	-4.41035000	-2.68597800	Pd	0.00005600	1.36954700	-0.00005400
C	4.74471700	2.50220600	0.45804600	Cl	-0.79651200	3.02518500	-1.53311400
C	4.99985000	0.37818800	1.64786100	Cl	0.79616300	3.02507700	1.53334800
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H	2.48656900	0.79351500	-2.21418300	H	-0.10486800	-2.69927000	-1.40889100
H	7.21981200	-1.97862700	-2.69597400	H	-0.57949400	-4.33721400	-1.00465100
C	4.21708700	3.24423700	-0.62702400	H	0.66501500	0.63148900	3.42896100
C	5.55637000	3.11208100	1.44617500	H	-0.66505300	0.63128300	-3.42923800
C	5.78006200	1.00068300	2.59250400				

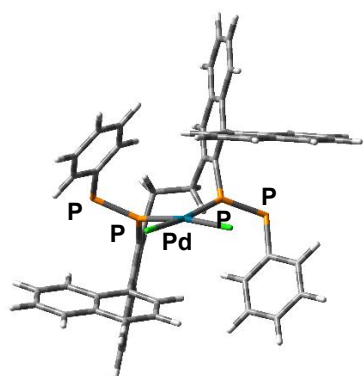
8E-Me



C	-6.38758200	-2.36424500	2.14302100	H	-2.56512000	-4.81865100	0.45879500
C	-5.44715700	1.25755800	-2.66499800	C	-4.81242900	0.53080100	-1.68746400
C	-4.29643000	-1.90852500	1.00232100	H	-4.68199400	-0.54557500	-1.80335000
C	-4.31879700	1.16450700	-0.51965300	C	-5.50467300	-1.46478200	1.59829100
C	-3.61178600	0.45674500	0.49459300	H	-5.72806000	-0.39930000	1.61427500
C	-3.36581900	-1.00840300	0.40543700	H	-5.81488600	0.75866100	-3.55989800
C	-3.39209700	2.50673800	1.78441300	H	-7.31377000	-2.01076200	2.59191600
C	-4.05089700	3.21304100	0.80888900	C	-2.22139400	-1.49911100	-0.20947200
C	-4.52431500	2.56773800	-0.35839200	C	-3.17076900	1.12419700	1.62088600
C	-5.18937100	3.28613500	-1.38244300	P	-1.40412000	-0.72513200	-3.09803400
C	-5.63356000	2.65035200	-2.51448500	C	-1.89645700	-2.89436700	-0.16516700
H	-6.13709600	3.21386400	-3.29778000	H	-3.02823500	3.00629400	2.68071800
H	-5.33536600	4.35870500	-1.25369500	H	-2.64344800	0.56351300	2.39485300
H	-4.22034200	4.28436000	0.91748600	C	1.79808400	-2.84018900	0.18913100
C	-6.10328000	-3.74762200	2.12269100	C	2.68156700	-3.72249800	-0.38485800
C	-4.94101900	-4.20650400	1.55465400	C	2.15413700	-1.45402400	0.22215400
C	-4.01355900	-3.30463900	0.98047000	C	3.90319900	-3.30457000	-0.95933100
H	-6.81166000	-4.44971800	2.55850900	H	2.42820500	-4.78435700	-0.41503100
H	-4.71201600	-5.27182800	1.53678900	C	3.31919100	-0.99477300	-0.37658900
C	-2.79874100	-3.75303300	0.41352500	C	4.22411600	-1.91636300	-0.97815600

C	4.80674000	-4.22973800	-1.53584000	H	5.73599600	4.14796900	1.37534400
C	3.61784600	0.46222500	-0.41157000	H	6.19126700	0.39665300	3.43105000
P	1.42325600	-0.51850900	3.08866800	H	6.67080000	2.83407700	3.25378200
C	5.43989100	-1.50279100	-1.58058400	C	0.45109600	-3.33662400	0.62908200
C	5.97812200	-3.80017900	-2.10725200	H	0.54818800	-4.33295500	1.08022400
H	4.55118200	-5.28900700	-1.51719300	H	0.03529200	-2.69190300	1.41328500
C	4.44727200	1.06998600	0.57619300	P	1.14960500	-0.20348500	1.10252400
C	3.10318000	1.22313700	-1.44235400	P	-1.19774800	-0.29075300	-1.12535000
C	6.29647400	-2.42385700	-2.13029800	Pd	-0.04365400	1.37615600	-0.05850300
H	5.68828000	-0.44277300	-1.59901200	Cl	-1.06410800	2.99617300	-1.50513400
H	6.66766900	-4.51950900	-2.54515000	Cl	0.93034100	3.12043500	1.26003600
C	4.72014700	2.46692900	0.47542400	C	-0.54488300	-3.41135600	-0.56482800
C	4.99684000	0.34225800	1.66058000	H	-0.14188400	-2.84641500	-1.41382300
C	3.37407600	2.60313700	-1.53652200	H	-0.62724000	-4.45184700	-0.90475100
H	2.47866800	0.73895200	-2.19493000	C	0.27506800	0.71913800	3.84950900
H	7.22786100	-2.09381800	-2.58622700	H	-0.17543000	1.40298100	3.12143100
C	4.16820900	3.20958500	-0.59680500	H	-0.51003100	0.16937500	4.38407400
C	5.53278700	3.08036800	1.46051700	H	0.83896000	1.30433900	4.58560000
C	5.77740200	0.96834300	2.60239600	C	-0.22885200	0.46169200	-3.89677100
H	4.79055500	-0.72521300	1.74182500	H	0.02790100	1.31478100	-3.25699200
H	2.94368900	3.17907700	-2.35420600	H	0.68010600	-0.08691600	-4.17558700
H	4.38343300	4.27645900	-0.65658100	H	-0.69510000	0.83157500	-4.81729700
C	6.05023500	2.35051800	2.50169800				

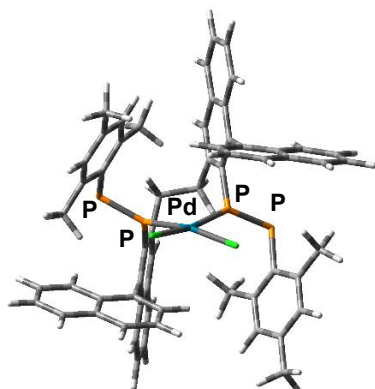
8E-Ph



C	-6.29473800	2.42593100	2.70076900	C	-3.89633000	1.21124300	3.50882800
C	-6.10283100	-2.53749100	-0.44454300	H	-6.52157300	2.97559400	4.78590900
C	-4.29847200	1.16874800	2.14164000	H	-4.40586200	1.90232900	5.49183400
C	-4.72945000	-0.55812200	-0.73877500	C	-2.68087000	0.59983800	3.89294800
C	-3.85080000	0.44668400	-0.23647200	H	-2.37985500	0.65139100	4.94148400
C	-3.46615800	0.49561000	1.20161600	C	-5.28224500	-1.57006700	0.08499800
C	-3.67367100	1.41150200	-2.46446200	H	-5.04866400	-1.57644900	1.14985600
C	-4.50887000	0.44950100	-2.97118600	C	-5.51623800	1.79101600	1.76562100
C	-5.05166700	-0.55312700	-2.12969400	H	-5.82521500	1.76053300	0.72192400
C	-5.90398600	-1.56182300	-2.64185900	H	-6.51698400	-3.30895600	0.20210900
C	-6.41703700	-2.53537400	-1.82078900	H	-7.22663700	2.90036600	2.39946800
H	-7.06916800	-3.30639700	-2.22677900	C	-2.28858500	-0.10396300	1.62584300
H	-6.14204300	-1.54972400	-3.70551800	C	-3.35034400	1.40507200	-1.09361000
H	-4.76452300	0.43516500	-4.03064100	P	-1.91506900	-2.98635600	0.68254400
C	-5.89435000	2.46848400	4.05517100	C	-0.82146100	-3.88245300	-0.46815700
C	-4.72205100	1.87404300	4.44931000	C	-1.41326900	-4.70344500	-1.43580800

C	0.57450500	-3.81659900	-0.37861100	H	7.24599000	-2.88828600	2.37661000
C	-0.62030000	-5.40679700	-2.33454700	C	4.43885600	-0.47604700	-2.98792100
C	1.36410100	-4.53208100	-1.27345500	C	5.85269200	1.52603100	-2.68264400
C	0.76804000	-5.31542000	-2.25907500	C	6.09088800	2.50374100	-0.48993500
H	-1.08614400	-6.02825800	-3.09676000	H	5.05701000	1.54955600	1.12208200
H	2.45014200	-4.48293600	-1.19950700	H	3.15932100	-2.19350300	-3.10604200
C	-1.86957000	-0.04708800	2.99214800	C	0.69225200	5.50304800	-2.23481300
H	-3.24437100	2.17536200	-3.11178700	C	-1.31009200	4.50018000	-1.33152400
H	-2.68165700	2.16607500	-0.69494900	H	4.67638600	-0.46325000	-4.05162400
C	1.87496100	0.02772200	3.00119600	C	6.38341300	2.49810800	-1.87103900
C	2.69621400	-0.61220000	3.89778000	H	6.07339800	1.51202300	-3.75003400
C	2.28538800	0.08525700	1.63246300	H	6.51828500	3.27466500	0.14865300
C	3.91338200	-1.21659200	3.50651000	C	-0.69361300	5.35890500	-2.23913400
H	2.40283700	-0.66300500	4.94848000	H	-2.39591600	4.40879800	-1.32007500
C	3.46052200	-0.51309200	1.20020400	H	7.03262600	3.26547200	-2.28847300
C	4.30333200	-1.17905400	2.13569400	C	0.53835600	0.54610300	3.44765000
C	4.75279300	-1.86735200	4.44313100	H	0.61283200	0.96765200	4.45915700
C	3.82805800	-0.46891300	-0.24240600	H	0.20495300	1.37143000	2.80363200
P	1.92651300	2.97182300	0.70866800	P	1.35358200	1.04322600	0.38298000
C	5.52129000	-1.79586300	1.75164600	P	-1.35284900	-1.05220400	0.37104500
C	5.92622200	-2.45493600	4.04175400	Pd	-0.00669000	0.01371300	-1.16639100
H	4.44680900	-1.89156200	5.48881000	Cl	-1.10668600	-1.24395400	-2.87283900
C	4.70484800	0.52974900	-0.75961000	Cl	1.08680000	1.31641000	-2.84232800
C	3.30598500	-1.42395200	-1.09060600	C	-0.53438000	-0.57317600	3.43464900
C	0.85384600	3.88499300	-0.44486500	H	-0.19905600	-1.38752100	2.77779800
C	6.31345100	-2.41867100	2.68343300	H	-0.61312900	-1.01322400	4.43797100
H	5.81981100	-1.76922000	0.70473700	H	-1.29750600	5.93068800	-2.94106800
H	6.56445100	-2.95174800	4.77003300	H	1.17243600	6.18238900	-2.93633300
C	5.00363200	0.52232700	-2.15578500	H	2.54856200	4.89112900	-1.33374400
C	5.27477900	1.54037000	0.05386000	H	-1.01989000	3.09810300	0.28441200
C	3.60528500	-1.43200500	-2.46702900	H	1.03971700	-3.21167100	0.40268000
H	2.63683400	-2.17936300	-0.68167700	H	1.38855900	-5.87095300	-2.95956800
C	1.46377000	4.77994100	-1.33292900	H	-2.49962800	-4.77244500	-1.49996900
C	-0.54114700	3.76486400	-0.43588700				

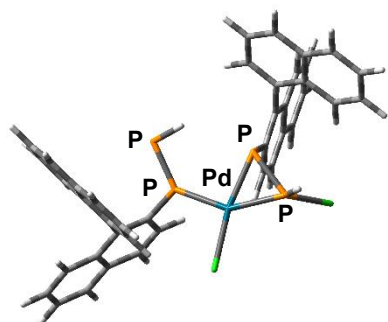
8E-Mes



C	-6.38206700	1.95073900	2.32914500	C	-3.37247400	0.04840600	1.19292800
C	-5.30218600	-3.55367900	-0.20306000	C	-3.69932900	0.63845800	-2.53314100
C	-4.29825100	0.75181700	2.01427700	C	-4.30871300	-0.51312400	-2.96308900
C	-4.34955000	-1.36924100	-0.66223300	C	-4.64536100	-1.54041100	-2.04773400
C	-3.69445600	-0.17328000	-0.24278800	C	-5.26414200	-2.74138600	-2.47520300

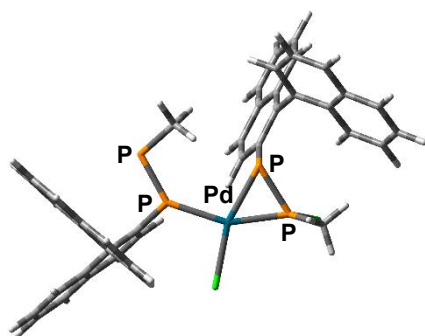
C	-5.58128200	-3.72990000	-1.57653200	C	4.70754900	2.39213100	0.24786600
H	-6.05207600	-4.64980600	-1.91843300	C	3.69639100	-0.64696500	-2.52588200
H	-5.48056200	-2.86488300	-3.53651100	H	2.90932600	-1.73503100	-0.82702500
H	-4.53989400	-0.65901200	-4.01838200	C	0.50990000	4.70078100	-1.27457900
C	-6.04502600	2.19200400	3.68004600	C	-1.38307100	3.99251300	0.10745700
C	-4.86525900	1.71536500	4.19445600	H	7.31455300	-2.33629600	1.94553500
C	-3.96569800	0.98541000	3.37989600	C	4.30890200	0.50259100	-2.95690400
H	-6.72682700	2.75756900	4.31240600	C	5.26894300	2.72944400	-2.47116200
H	-4.59876500	1.89478800	5.23585800	C	5.30753900	3.54456000	-0.19998300
C	-2.73882800	0.49763100	3.88297700	H	4.49850000	2.26147100	1.30991400
H	-2.49599500	0.68524900	4.93123400	H	3.43056900	-1.43406000	-3.23027600
C	-4.70542600	-2.39915600	0.24372700	C	-0.39011400	5.30672200	-2.15061000
H	-4.49749200	-2.26673300	1.30576800	C	1.97729800	4.74743200	-1.57618000
C	-5.53153800	1.24480600	1.51552000	C	-2.24172200	4.60138900	-0.80503200
H	-5.79490100	1.06039700	0.47539100	C	-1.95497900	3.34595100	1.33532400
H	-5.56555500	-4.33713900	0.50545500	H	4.54164900	0.64642900	-4.01213600
H	-7.32345500	2.32765800	1.93396000	C	5.58785400	3.71833600	-1.57351900
C	-2.17634300	-0.41464600	1.72779800	H	5.48640400	2.85111200	-3.53246700
C	-3.39590700	0.80828200	-1.16746300	H	5.57243900	4.32828200	0.50767300
P	-1.19592300	-3.26560600	1.00904600	C	-1.76607100	5.25493300	-1.94409400
C	0.00110100	-4.01656500	-0.15412400	H	-0.00140300	5.82552500	-3.02892600
C	-0.50059700	-4.69582600	-1.28078200	H	-3.31719300	4.57706300	-0.61413900
C	1.38641000	-3.98813500	0.10913500	H	6.06113100	4.63664900	-1.91627200
C	0.40277500	-5.29744000	-2.15558800	C	-2.71793500	5.91493400	-2.89466900
C	2.24929800	-4.59202000	-0.80350900	C	0.50796700	0.58478200	3.69234600
C	1.77897700	-5.23677800	-1.94912600	H	0.66233000	0.92508300	4.72457900
H	0.01724300	-5.82089200	-3.03261400	H	0.08573500	1.44391700	3.15646200
H	3.32348000	-4.57142500	-0.60567300	P	1.05648300	1.28170700	0.56719600
C	1.95339300	-3.35137700	1.34446000	P	-1.05920100	-1.28325000	0.56474300
C	-1.96770400	-4.74995200	-1.58272900	Pd	-0.00043500	0.00019200	-1.03365600
C	-1.84088200	-0.18990900	3.10001200	Cl	-0.67646500	-1.53720800	-2.73245900
H	-3.43455900	1.42428600	-3.23920200	Cl	0.67880200	1.53990500	-2.72911400
C	2.73451600	-5.84847900	-2.92777400	C	-0.51663700	-0.58692400	3.69118700
H	-2.91690900	1.73171300	-0.83518200	H	-0.09315500	-1.44589800	3.15601200
C	1.83322500	0.18756100	3.10363300	H	-0.67300000	-0.92744800	4.72304800
C	2.72948600	-0.50053100	3.88803200	H	-3.03620600	3.52337000	1.40635300
C	2.17101400	0.41206400	1.73195600	H	-1.49188100	3.72986900	2.25688900
C	3.95673200	-0.98927900	3.38682900	H	-1.80373500	2.25634500	1.33837200
H	2.48479100	-0.68821100	4.93584200	H	2.19404600	5.48303300	-2.35998200
C	3.36771800	-0.05167800	1.19899400	H	2.58117600	5.01069300	-0.69521200
C	4.29166700	-0.75585000	2.02176200	H	2.33279100	3.76710900	-1.92957800
C	4.85395800	-1.72079200	4.20256100	H	-2.22504700	6.18194000	-3.83668000
C	3.69140000	0.16830900	-0.23660200	H	-3.13221800	6.83751500	-2.46442300
P	1.19655200	3.26358100	1.01236100	H	-3.56921100	5.26190600	-3.12636900
C	5.52499000	-1.25049000	1.52475600	H	1.80564800	-2.26134700	1.35326400
C	6.03371400	-2.19919900	3.68977400	H	1.48428100	-3.73944300	2.26119500
H	4.58556400	-1.90016500	5.24348100	H	3.03376900	-3.53216600	1.41996400
C	4.34980900	1.36198700	-0.65706000	H	3.59182100	-6.30898800	-2.42094700
C	3.39114100	-0.81357000	-1.16025800	H	3.13710700	-5.08780900	-3.61167600
C	0.00377900	4.02080500	-0.15086900	H	2.24585200	-6.61345500	-3.54278100
C	6.37317700	-1.95802200	2.33945600	H	-2.57119800	-5.01553100	-0.70217200
H	5.79020100	-1.06625400	0.48506800	H	-2.32738700	-3.77134500	-1.93664900
H	6.71361700	-2.76614900	4.32293900	H	-2.18051000	-5.48658900	-2.36665100
C	4.64704200	1.53045500	-2.04262600				

10A-H



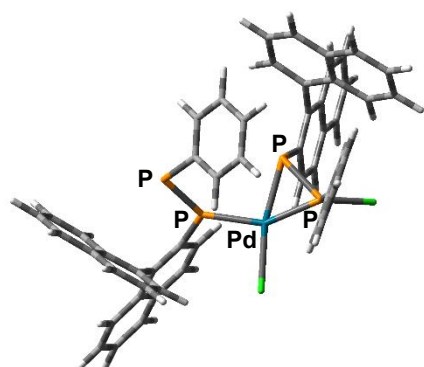
C	5.70098600	2.43219500	3.50859900	C	-6.55710900	0.95215200	0.15846700
C	6.48753800	-1.18696600	-1.56929400	C	-7.36883700	3.19241800	0.56799600
C	4.10915600	1.59133700	1.88143400	H	-5.88892200	4.71060200	0.89318400
C	5.03996400	-1.39091600	0.36885200	C	-7.60608000	1.82713700	0.29656900
C	4.07517500	-0.85754600	1.27514900	H	-6.74517500	-0.09892100	-0.05516200
C	3.55485200	0.52706200	1.10764100	H	-8.20923000	3.87557500	0.67497700
C	4.01980800	-2.97539500	2.46514800	H	-8.62821300	1.46758100	0.19410900
C	4.92854400	-3.51741100	1.59131400	C	-4.29321400	-0.92062900	-0.18542900
C	5.45800400	-2.74625800	0.52788000	C	-4.67197400	-1.87371500	0.80590700
C	6.39295400	-3.28937800	-0.38787700	C	-4.03378800	-1.33653200	-1.47636600
C	6.89294500	-2.53212000	-1.41745500	C	-4.79437300	-3.24518700	0.42956100
H	7.60667500	-2.96248700	-2.11753100	C	-4.89179600	-1.52015700	2.16120800
H	6.70502300	-4.32580500	-0.25828100	C	-4.14990400	-2.69578300	-1.84099700
H	5.25876800	-4.55035900	1.70113400	H	-3.72558700	-0.60010900	-2.22101000
C	5.15941500	3.72981500	3.38072000	C	-5.16719700	-4.19858300	1.40813800
C	4.11815600	3.95953700	2.51621500	C	-4.52774400	-3.62791000	-0.90936200
C	3.57295200	2.90570600	1.74469300	C	-5.24383700	-2.47068000	3.08911100
H	5.57360400	4.54765100	3.96733400	H	-4.77397700	-0.47984300	2.46378500
H	3.69518000	4.95796200	2.40541200	H	-3.94224200	-2.99307600	-2.86715200
C	2.50890400	3.12643100	0.83636500	C	-5.39158900	-3.82219800	2.70922500
H	2.09956800	4.13199000	0.74005500	H	-5.26447200	-5.24152900	1.10628900
C	5.58909400	-0.62892400	-0.69335900	H	-4.62393700	-4.67947600	-1.17985900
H	5.29259500	0.41387800	-0.80528700	H	-5.40981200	-2.18125400	4.12518200
C	5.18833100	1.38801400	2.77861000	H	-5.67556600	-4.56441900	3.45289400
H	5.60927800	0.38909600	2.88097300	P	-1.38689200	-0.07780400	0.07474500
H	6.89300300	-0.58787000	-2.38298100	P	-1.13944500	-1.10383500	1.81440600
H	6.53067800	2.26016300	4.19160800	P	1.88076000	-0.66859700	-0.72214400
C	2.52740100	0.78432800	0.20969800	Pd	-0.07828800	0.16955700	-1.81840100
C	3.59349000	-1.64033200	2.30320500	Cl	-1.76772300	1.03813700	-3.32231200
H	3.61777700	-3.57178900	3.28173100	P	2.04730500	0.00031100	-2.77530700
H	2.85940200	-1.21853500	2.99096700	Cl	3.43788800	1.45222300	-3.21942300
C	-3.64719400	3.25333800	0.65783100	C	-2.58845600	2.39709900	0.51610500
C	-2.82311400	1.01790100	0.28219000	H	-1.56477200	2.76646500	0.58903600
C	-4.97959000	2.78126000	0.55346300	C	2.00222300	2.10015200	0.08602000
H	-3.47952400	4.31281600	0.84994000	H	1.18256000	2.29143700	-0.60822000
C	-4.10611900	0.51557900	0.15244600	H	0.03146900	-1.75981300	1.32083200
C	-5.21800800	1.39939300	0.28967700	H	2.49772100	-1.06703000	-3.57290700
C	-6.08319700	3.65746900	0.69059600				

10A-Me



C	5.89372300	3.46662100	2.63701200	C	-7.80894400	1.60215000	-0.95007500
C	6.27654900	-1.07072700	-1.82221500	H	-6.92097100	-0.25323700	-0.36250500
C	4.21622000	2.12682000	1.50435600	H	-8.44330600	3.58843000	-1.54558300
C	5.27719500	-1.00595400	0.39026600	H	-8.81772000	1.19409300	-0.97359900
C	4.44658200	-0.38729600	1.37335100	C	-4.47838400	-0.95181000	0.09331900
C	3.71125200	0.86834600	1.05932100	C	-4.92108000	-1.39238900	1.37547500
C	4.89828500	-2.21943500	2.90424100	C	-4.15712300	-1.87825600	-0.87819800
C	5.66605200	-2.85278600	1.96002300	C	-5.02940100	-2.79399000	1.62170800
C	5.87361900	-2.26827200	0.68654700	C	-5.23142800	-0.49224700	2.42596200
C	6.65676200	-2.90915900	-0.30583700	C	-4.26559000	-3.26392500	-0.62936100
C	6.84822100	-2.33130700	-1.53614800	H	-3.80033300	-1.52501000	-1.84723300
H	7.44685500	-2.83684300	-2.29153300	C	-5.46194900	-3.23836500	2.89486800
H	7.10330900	-3.87558900	-0.07129200	C	-4.69566100	-3.71107400	0.59368400
H	6.13009000	-3.81559900	2.17441300	C	-5.64173200	-0.95543700	3.65324200
C	5.16043700	4.64007800	2.35455700	H	-5.14017400	0.57918200	2.24889000
C	3.98228800	4.56365000	1.65461400	H	-4.00892700	-3.97066400	-1.41627000
C	3.48514600	3.31570900	1.20824300	C	-5.76374100	-2.34183800	3.88999000
H	5.53525200	5.60458600	2.69208700	H	-5.54579600	-4.31126200	3.06936100
H	3.41096900	5.46302900	1.42487700	H	-4.78547600	-4.77826000	0.79741800
C	2.28317100	3.22208100	0.46604300	H	-5.87532800	-0.24970700	4.44836000
H	1.73342800	4.13525900	0.23789000	H	-6.09450100	-2.69679500	4.86439200
C	5.51575900	-0.42266400	-0.87967200	P	-1.60055400	0.03920300	0.28343700
H	5.08650800	0.55448200	-1.10137400	P	-1.53927500	0.23378200	2.31094000
C	5.43410000	2.24061300	2.22297600	P	1.94113800	-0.86220000	-0.16689800
H	6.00396500	1.33955100	2.44376200	Pd	-0.08239900	-0.51898400	-1.43551300
H	6.44132500	-0.60865500	-2.79488600	Cl	-1.65554400	-0.36822800	-3.28073100
H	6.83099800	3.53652000	3.18598200	P	2.02848400	-0.79426200	-2.31092200
C	2.53251800	0.81578600	0.32471600	Cl	3.01447400	0.76714800	-3.22096900
C	4.28438100	-0.98447800	2.60554500	C	-2.84019100	2.41488200	-0.53058000
H	4.74711700	-2.67069700	3.88299200	H	-1.83081900	2.82743700	-0.51431300
H	3.65395400	-0.49884900	3.35125600	C	1.82050700	2.00880500	0.03150200
C	-3.90271100	3.20361500	-0.88133400	H	0.90048900	1.94884000	-0.55062600
C	-3.04718700	1.05609800	-0.17908300	C	0.00544700	-0.70331700	2.74523900
C	-5.21786300	2.67697500	-0.90316800	H	0.26170300	-1.48277200	2.01824600
H	-3.75164500	4.25050500	-1.14399700	H	0.84211900	0.00560400	2.82075500
C	-4.31143900	0.49519500	-0.21016800	H	-0.13358700	-1.16690600	3.72834700
C	-5.43045000	1.30581300	-0.56883700	C	2.74502700	-2.28652200	-3.06907000
C	-6.32776600	3.48235400	-1.25466400	H	2.28531400	-3.14967700	-2.57248900
C	-6.75245100	0.79430700	-0.60821300	H	2.50941800	-2.31245100	-4.13770600
C	-7.59671100	2.95998700	-1.27542900	H	3.83042800	-2.30041000	-2.91223200
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10A-Ph

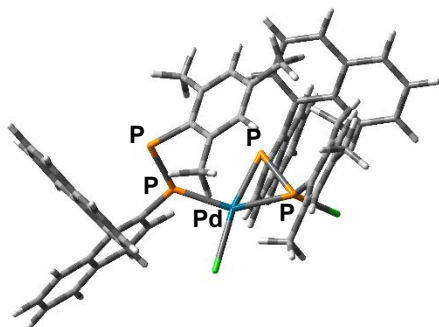


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C	4.90808400	0.13365000	1.12884100	C	-6.90591200	1.40914500	-0.73440600
C	3.93066500	1.00961900	1.69156400	C	-7.51802600	3.66563500	-1.34918000
C	3.29986000	2.07023000	0.85679700	H	-5.93695500	5.11363000	-1.39992000
C	4.01318200	-0.24396100	3.77104900	C	-7.86427900	2.31770800	-1.10908800
C	4.90279400	-1.13710000	3.22871700	H	-7.17639600	0.37010400	-0.55350700
C	5.37094700	-0.97348000	1.90175200	H	-8.28720600	4.37576500	-1.64678400
C	6.30351100	-1.87264200	1.32627900	H	-8.89843500	1.99847300	-1.22341800
C	6.78219100	-1.67488200	0.05442300	C	-4.86885400	-0.55746900	0.02428800
H	7.50137800	-2.37084300	-0.37384400	C	-5.39091700	-0.99090400	1.27783800
H	6.64225700	-2.72090400	1.92149400	C	-4.59055300	-1.47872600	-0.96302600
H	5.26843300	-1.98234200	3.81236000	C	-5.57930200	-2.38815900	1.49830100
C	4.63623600	6.09136000	1.02444400	C	-5.67994500	-0.09060300	2.33531400
C	3.58807900	5.75272500	0.20516400	C	-4.79568300	-2.85891100	-0.74603500
C	3.13001300	4.41541900	0.13055700	H	-4.16671600	-1.13622500	-1.90917200
H	4.98189200	7.12229500	1.07215300	C	-6.05108600	-2.82880400	2.75941900
H	3.09193000	6.50754500	-0.40484300	C	-5.27087300	-3.30383600	0.46144700
C	2.05896300	4.04444900	-0.71901200	C	-6.13275800	-0.54942800	3.54765500
H	1.57742200	4.81383000	-1.32265200	H	-5.52763900	0.97674800	2.17666800
C	5.43082800	0.31827500	-0.17617600	H	-4.56487500	-3.56568500	-1.54104400
H	5.10413400	1.17798100	-0.76068500	C	-6.32090300	-1.93302000	3.76358400
C	4.84946600	3.79714700	1.75820800	H	-6.19008200	-3.89860100	2.91697900
H	5.34461300	3.03666200	2.36020400	H	-5.42049200	-4.36819500	0.64391100
H	6.73964600	-0.40244600	-1.70292100	H	-6.34597000	0.15547900	4.34920800
H	6.11043800	5.37782400	2.44465200	H	-6.67907000	-2.28545900	4.72920100
C	2.25467200	1.73838800	0.00246300	P	-1.82437900	0.20136000	0.25447000
C	3.51827800	0.82473500	2.99397600	P	-2.05145500	-0.76316000	2.04451900
C	2.42708800	-2.34080300	-2.14929600	C	-0.57932200	-1.84554500	1.91874000
C	3.57569400	-2.81848500	-1.50788500	C	-0.34738300	-2.70183100	0.83069100
C	1.56780400	-3.21720100	-2.81998100	C	0.34563100	-1.81748100	2.97165600
C	3.86233200	-4.17668900	-1.54141600	C	0.81343000	-3.46810200	0.77496200
C	1.86275100	-4.57744900	-2.84561400	C	1.50707200	-2.57819800	2.90681700
C	3.00553100	-5.05382300	-2.20732700	C	1.75373400	-3.38716100	1.79935200
H	4.75244100	-4.55268400	-1.03961700	H	0.99017500	-4.11966500	-0.08093400
H	1.19753700	-5.26575300	-3.36261000	H	2.23164800	-2.52828300	3.71722900
H	3.66376400	-0.36804700	4.79479200	P	1.71678100	-0.02613300	0.04114900
H	2.77652400	1.50387700	3.41564000	Pd	-0.22403900	-0.12934000	-1.41099900
C	-3.85242300	3.56880800	-0.70452400	Cl	-1.79510700	-0.44406300	-3.24355600
C	-3.22403700	1.31434300	-0.07826800	P	1.95118400	-0.60380700	-2.02414500
C	-5.20426200	3.16396000	-0.82809300	Cl	3.28056100	0.46847200	-3.20056900
H	-3.59451300	4.60855600	-0.90434700	C	-2.88507400	2.66782500	-0.35227700

H	-1.84438600	2.98491100	-0.27547100
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H	0.80475200	2.47323800	-1.44148900
H	2.67523000	-3.96575900	1.73922700
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H	0.16974500	-1.17113900	3.83262800
H	0.66823100	-2.83473200	-3.30327300
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10_A-Mes



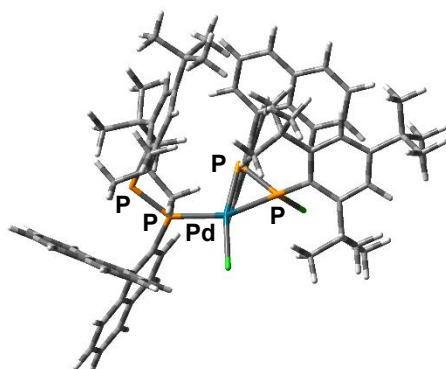
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C	3.82352900	1.63775500	1.46648500
C	2.97681200	2.51267800	0.60942700
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C	5.40980100	0.00591700	3.12480000
C	5.89667900	0.36759600	1.84434200
C	7.16075200	-0.07597000	1.38146300
C	7.61611300	0.27284600	0.13465700
H	8.58752700	-0.07616000	-0.21094500
H	7.76409800	-0.70359800	2.03784100
H	6.03092300	-0.62461900	3.76124300
C	3.78191700	6.67789700	0.39222800
C	2.75788100	6.13971900	-0.34603400
C	2.47557300	4.75365000	-0.28942100
H	3.99234200	7.74453700	0.34112000
H	2.14358800	6.76941800	-0.98967500
C	1.42612600	4.18124900	-1.04773000
H	0.82903400	4.82587000	-1.69291100
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C	4.31481400	4.50048000	1.29950900
H	4.92226500	3.86728400	1.94432500
H	7.18989100	1.35573400	-1.69562800
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C	1.93008200	1.98480700	-0.13608500
C	3.39462300	1.27027700	2.72452100
C	2.32229500	-2.34879300	-1.86994100
C	3.39597800	-2.79702100	-1.06834500
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C	1.88625200	-4.61412200	-2.57058500
C	2.91844500	-5.08725000	-1.75931700
H	4.50610600	-4.51558700	-0.43103300

H	1.31324800	-5.32336800	-3.17054500
H	3.81952300	0.17909300	4.54641900
H	2.42364500	1.62011000	3.07956500
C	-3.98336600	3.68614600	-0.72360600
C	-3.40832800	1.41655500	-0.09403800
C	-5.34031600	3.30840700	-0.86864400
H	-3.70134500	4.72073100	-0.91763400
C	-4.72658200	1.00365000	-0.23423700
C	-5.71804300	1.95371200	-0.62707900
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C	-7.63482100	3.85990000	-1.42319900
H	-6.02229700	5.27365100	-1.44852500
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C	-5.10228000	-0.41923400	-0.01822600
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H	-4.44091100	-1.00004100	-1.96237000
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Pd	-0.38028900	-0.03140800	-1.35529000
Cl	-1.99964000	-0.18482100	-3.17857100
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C	-1.44633000	-3.21767500	0.08542500
H	-2.48332900	-3.23068300	0.45173500
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H	0.03425000	0.78276900	3.28526300
C	2.92740600	-3.96684400	2.41887300
H	2.94105600	-4.47816600	3.39139700
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H	5.14393100	-2.40612300	0.10611700
C	0.50837300	-2.82659800	-3.61625500
H	-0.39103200	-2.45493000	-3.10681100
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H	0.20899000	-3.66483500	-4.25569900
C	3.22320300	-6.55136700	-1.69390600
H	2.32432800	-7.13204700	-1.44908100
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10A-Mes*



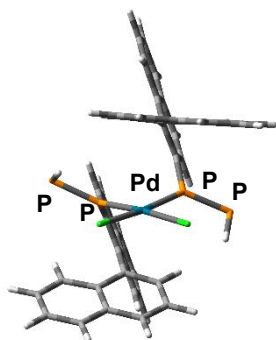
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C	-4.80815800	2.21272600	1.79461200
C	-6.05838300	1.92670600	1.19116700
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C	-0.86337700	-0.93279900	5.20134600
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H	-0.10015100	-1.95225100	6.94462700
C	-0.02885900	-1.61381300	4.28264500
H	0.66739300	-2.36494300	4.65771700
C	-4.47151600	-0.19378200	2.08474400
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H	-3.35003300	1.42792200	5.28535100
H	-6.01561200	-1.46839500	1.34395900
H	-3.23098400	0.90327200	7.68388400
C	-0.99753500	-0.36345200	2.43843700
C	-2.32892500	2.72997800	2.98229300
C	-3.23828000	-1.66674400	-1.48626500
C	-3.86342900	-0.47452300	-1.94354200
C	-3.91889000	-2.91319300	-1.64140300
C	-5.24369400	-0.51350200	-2.15453200
C	-5.29589000	-2.85852700	-1.84255900
C	-6.00153600	-1.67197300	-2.02973700
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C	-3.14304400	0.82341200	-2.35193600	C	2.16950700	0.73596000	-3.26718300
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P	2.59247000	-0.33505500	0.11217000	H	-1.52410500	-0.20749500	-3.40015600
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H	4.45171800	1.82784800	-2.06148400	H	-7.79564000	-3.31577500	-0.75643400

H	-7.99981500	-1.68237600	-0.08954800	C	-1.75488200	-4.34934000	-1.81037200
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10E-H

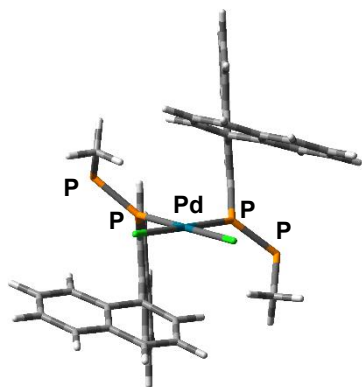


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H	-4.92469000	-4.20627700	0.41556300	C	3.76958300	-0.97007100	-0.37202300
H	-4.09316500	-3.62465900	-1.79185500	C	2.93454100	-0.42524500	1.84380600
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C	-1.61370000	1.37988000	0.84063000	H	4.09465100	-3.62395800	1.79145200
C	-2.93508700	-0.42519600	-1.84400500	C	4.97095900	-2.86206100	-2.08696100
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P	0.77973000	-0.10801800	-1.44462700
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H	-0.31110500	2.69813500	1.98122900
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10E-Me



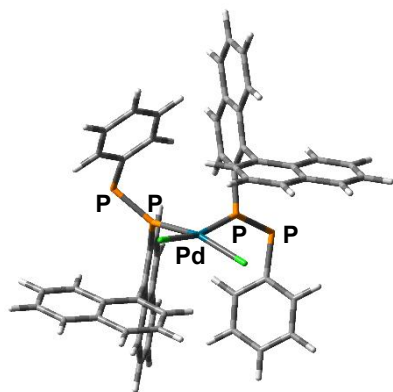
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H	5.26680800	5.50250200	2.26731400
H	3.31481100	5.80629800	0.77468800
C	1.92595100	3.85875200	-0.43657900
H	1.57350300	4.86688200	-0.65461300
C	4.32215100	-0.42526600	-1.76856500
H	4.10749300	0.61412900	-2.01580700
C	4.62833500	2.23720800	1.58086600
H	5.00592400	1.24000800	1.79828700
H	5.21210700	-0.83416200	-3.66489300
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C	1.74721700	1.45980800	-0.68235300
C	3.03488500	-0.65421500	1.73916000
P	0.72555500	0.36986200	-3.37665200
H	3.17080100	-2.36631400	3.05808900
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C	-4.93688900	-3.07832300	1.13560200
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H	-5.73216500	-3.20886200	3.11520600
P	-0.85796200	0.03845500	1.37689900
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C	-1.30106500	2.77374800	0.98938400
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10E-Ph

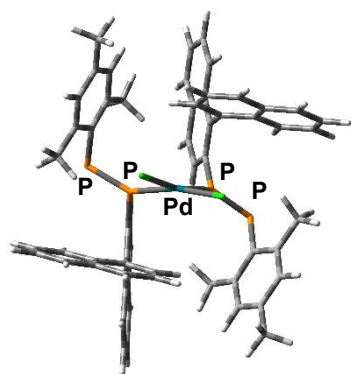


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C	4.31658400	1.60230200	-0.94154700
C	3.66654500	0.38242700	-0.58228400
C	3.43843400	0.05477000	0.85071200
C	3.55666300	-0.25351800	-2.92522500
C	4.18069900	0.90968700	-3.29495600
C	4.56786000	1.86407300	-2.32212900
C	5.20895900	3.07314300	-2.68818200
C	5.59220600	3.98456200	-1.73608700
H	6.08402000	4.90990100	-2.03023300
H	5.39296700	3.26368300	-3.74567900
H	4.38532500	1.12280200	-4.34426700
C	6.29233600	-2.22199800	3.00628800
C	5.14447200	-1.80221800	3.63007900
C	4.18761800	-1.02296800	2.93637400
H	7.02073300	-2.82117600	3.54899600
H	4.95016200	-2.05948500	4.67096800
C	3.00470400	-0.57061700	3.57036500
H	2.84188100	-0.81687000	4.61914500
C	4.73492600	2.55792000	0.01891000
H	4.56212400	2.36007200	1.07690500
C	5.62826500	-1.12200900	0.95764100
H	5.81876500	-0.85869900	-0.08160300
H	5.66821200	4.44447500	0.38120600
H	7.45702900	-2.20140600	1.17789900
C	2.29009700	0.47021900	1.50827400
C	3.30107500	-0.51655000	-1.56359600
P	0.83089700	3.18593300	1.36622200
C	-0.68452100	3.81405500	0.56615400
C	-0.59419900	4.98509000	-0.19782400
C	-1.93621600	3.22213300	0.77877200
C	-1.73622000	5.53319100	-0.77035700

C	-3.07839600	3.78822300	0.22126100
C	-2.97789000	4.93653000	-0.56049400
H	-1.65895800	6.43342200	-1.37678400
H	-4.05037800	3.32502900	0.39793500
H	3.24702400	-0.97870600	-3.67568100
H	2.81004000	-1.44914000	-1.27957600
C	-3.00421800	0.57074400	3.57073300
C	-2.28989700	-0.47021200	1.50860300
C	-4.18718500	1.02312400	2.93685900
H	-2.84126200	0.81702300	4.61948700
C	-3.43828100	-0.05472600	0.85115300
C	-4.42230100	0.68793000	1.56888000
C	-5.14393100	1.80243500	3.63064600
C	-3.66659100	-0.38244900	-0.58179800
P	-0.83069300	-3.18598400	1.36646800
C	-5.62805500	1.12214900	0.95828700
C	-6.29185300	2.22223100	3.00697200
H	-4.94949300	2.05973200	4.67150400
C	-4.31680200	-1.60227900	-0.94089800
C	-3.30116000	0.51643400	-1.56321000
C	0.68470300	-3.81401600	0.56627600
C	-6.53823100	1.87265200	1.66058000
H	-5.81867700	0.85881100	-0.08092800
H	-7.02016500	2.82145200	3.54974600
C	-4.56831200	-1.86409200	-2.32143000
C	-4.73508100	-2.55781400	0.01966800
C	-3.55697800	0.25335900	-2.92478800
H	-2.80997600	1.44898000	-1.27930500
C	0.59438200	-4.98500600	-0.19776800
C	1.93638700	-3.22207300	0.77889600
H	-7.45675800	2.20161600	1.17872100
C	-4.18120200	-0.90979400	-3.29436500
C	-5.20961100	-3.07310300	-2.68732700
C	-5.35421100	-3.72127600	-0.36840500

H	-4.56207200	-2.35994400	1.07762400	Pd	-0.00010200	-0.00008300	-1.02921500
H	-3.24739400	0.97848200	-3.67533000	Cl	0.43563100	1.68528200	-2.67368400
C	1.73639600	-5.53303900	-0.77037700	Cl	-0.43600800	-1.68573300	-2.67338400
C	3.07856200	-3.78809900	0.22130200	C	2.07985100	0.16727800	2.88080400
H	-4.38601700	-1.12293800	-4.34363300	H	1.17490900	0.51579700	3.37722800
C	-5.59281900	-3.98443000	-1.73512700	C	-2.07947900	-0.16722300	2.88109700
H	-5.39380300	-3.26367300	-3.74478600	H	-1.17450200	-0.51577500	3.37743600
H	-5.66852300	-4.44424700	0.38219500	H	-3.87233200	5.37463900	-0.99916000
C	2.97805800	-4.93635900	-0.56052000	H	-2.01922400	2.32451300	1.39358500
H	1.65913600	-6.43323000	-1.37686500	H	0.37425400	5.46050300	-0.35382100
H	4.05053800	-3.32488600	0.39795800	H	3.87249600	-5.37441900	-0.99924200
H	-6.08480100	-4.90972000	-2.02914900	H	-0.37406800	-5.46042100	-0.35377800
P	-0.98143700	-1.31853100	0.57466100	H	2.01939500	-2.32447500	1.39374200
P	0.98148700	1.31844600	0.57443700				

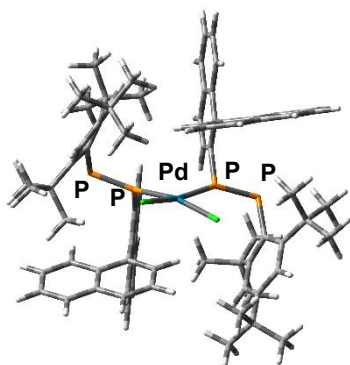
10E-Mes



C	-6.39994700	0.21774200	2.67517900	H	-7.41993300	0.39878700	2.34177600
C	-3.94314000	-4.68581600	-0.53381100	C	-1.81658300	-1.08444900	1.74218600
C	-4.11743000	-0.44989300	2.19198100	C	-3.48105600	0.12973400	-0.97291600
C	-3.70827600	-2.27740800	-0.72691400	P	0.02494700	-3.43923700	1.15178500
C	-3.42475400	-0.99318100	-0.17110900	C	1.42562000	-3.83617300	0.04468300
C	-3.10069600	-0.84539400	1.27324100	C	1.18329400	-4.59232400	-1.11991100
C	-3.80901700	0.03599700	-2.34099800	C	2.73649100	-3.48717600	0.41837200
C	-4.07261900	-1.18907200	-2.90080100	C	2.26431600	-4.92260200	-1.93221600
C	-4.01997000	-2.36850800	-2.11804500	C	3.78589300	-3.83371800	-0.43381000
C	-4.26823500	-3.64320500	-2.68539500	C	3.56858600	-4.53541700	-1.61814200
C	-4.22408800	-4.77855800	-1.91544800	H	2.08335100	-5.49833200	-2.84231500
H	-4.41180900	-5.75229400	-2.36419700	H	4.80408800	-3.54981100	-0.15889700
H	-4.49592800	-3.70162600	-3.74981300	C	3.02775400	-2.77560600	1.70738300
H	-4.32091200	-1.27555900	-3.95861400	C	-0.20149000	-5.02509800	-1.49672400
C	-6.05997600	0.42790000	4.03005000	H	-3.83693700	0.94181300	-2.94571800
C	-4.78093000	0.18606200	4.46558600	C	4.70469900	-4.88925200	-2.52893100
C	-3.78327900	-0.26284900	3.56739600	H	-3.27178700	1.10957800	-0.53990200
H	-6.81792500	0.77682600	4.72872200	C	2.46060500	0.52044200	4.00338500
H	-4.51142100	0.33572300	5.51083400	C	1.81658500	1.08451200	1.74221100
C	-2.46059800	-0.52033700	4.00335400	C	3.78327500	0.26290200	3.56742200
H	-2.21898400	-0.38729000	5.05760400	H	2.21899800	0.38742100	5.05763900
C	-3.69627100	-3.46555000	0.04666400	C	3.10069300	0.84543000	1.27326500
H	-3.49081200	-3.40135000	1.11515000	C	4.11742100	0.44990700	2.19200100
C	-5.45371500	-0.21287400	1.77828800	C	4.78091200	-0.18604800	4.46560900
H	-5.72034900	-0.37073300	0.73466900	C	3.42475000	0.99320100	-0.17108700
H	-3.92546600	-5.58854800	0.07450300	P	-0.02503000	3.43920900	1.15175500

C	5.45368100	0.21278600	1.77829100	H	-4.80417900	3.55006200	-0.15884000
C	6.05993600	-0.42797400	4.03005900	H	4.41183500	5.75233200	-2.36413100
H	4.51140700	-0.33567300	5.51086300	C	-4.70474600	4.88938200	-2.52894000
C	3.70827600	2.27743400	-0.72687900	P	0.51154700	1.56411500	0.56839400
C	3.48106200	-0.12970300	-0.97290300	P	-0.51150700	-1.56410900	0.56842700
C	-1.42567700	3.83614400	0.04463100	Pd	0.00004100	-0.00001900	-1.05169200
C	6.39989800	-0.21787300	2.67517700	Cl	-0.07454600	-1.68602300	-2.73729900
H	5.72030900	0.37059700	0.73466300	Cl	0.07466100	1.68583200	-2.73746000
H	6.81787400	-0.77693100	4.72872700	C	-1.50014800	-0.93512400	3.11938000
C	4.02000000	2.36854500	-2.11800200	H	-0.48485200	-1.13574200	3.46217800
C	3.69625600	3.46557000	0.04670400	C	1.50015400	0.93522300	3.11940900
C	3.80906800	-0.03595800	-2.34097500	H	0.48486100	1.13585100	3.46220700
H	3.27177400	-1.10954800	-0.53990500	H	0.82347100	4.15652800	-1.75984300
C	-1.18332500	4.59221600	-1.12001400	H	0.70769400	5.55095600	-0.67346900
C	-2.73656900	3.48727600	0.41836800	H	0.18240900	5.69836300	-2.36173700
H	7.41986600	-0.39900000	2.34176200	H	-4.57061300	4.43999000	-3.52229900
C	4.07267700	1.18911300	-2.90076500	H	-4.77183500	5.97516900	-2.67969500
C	4.26827200	3.64324400	-2.68534300	H	-5.66521900	4.54289300	-2.13014200
C	3.94313800	4.68583900	-0.53375900	H	-4.10511700	2.60589500	1.83208700
H	3.49077900	3.40136900	1.11518700	H	-2.67936900	3.35392200	2.57619700
H	3.83701200	-0.94177900	-2.94568900	H	-2.53244800	1.79549000	1.76233600
C	-2.26434000	4.92252500	-1.93231300	H	4.10501600	-2.60572400	1.83207400
C	0.20147700	5.02489400	-1.49686900	H	2.67919200	-3.35361200	2.57619000
C	-3.78596800	3.83386700	-0.43379700	H	2.53239300	-1.79525700	1.76217200
C	-3.02785700	2.77581000	1.70743000	H	4.77169200	-5.97501400	-2.67989800
H	4.32100300	1.27560900	-3.95857000	H	4.57064700	-4.43965200	-3.52220700
C	4.22410800	4.77859300	-1.91539100	H	5.66518800	-4.54292300	-2.13003300
H	4.49598300	3.70166900	-3.74975700	H	-0.82351000	-4.15677400	-1.75979000
H	3.92545800	5.58856600	0.07456300	H	-0.70770500	-5.55108900	-0.67327700
C	-3.56863600	4.53547600	-1.61817500	H	-0.18239900	-5.69864800	-2.36152800
H	-2.08335300	5.49818100	-2.84245500				

10_E-Mes*

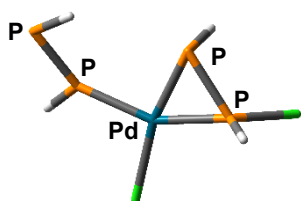


C	-6.25850900	0.66618400	-3.39637100	C	-4.90756600	4.00432100	2.02165800
C	-4.55259600	4.99009500	-0.15118100	C	-5.00269500	5.08748900	1.18344000
C	-3.96442000	1.02904900	-2.69032200	H	-5.41874800	6.02562100	1.54634400
C	-3.93801200	2.66821800	0.20900300	H	-5.24246700	4.07181000	3.05693000
C	-3.42159800	1.41953600	-0.25331300	H	-4.58248200	1.75569900	3.46087000
C	-2.99263500	1.26480200	-1.67104600	C	-5.83162000	0.50506800	-4.73299900
C	-3.74768800	0.46949400	1.96213100	C	-4.49977700	0.60856200	-5.04725000
C	-4.25609600	1.65571800	2.42570800	C	-3.53697300	0.87126100	-4.04293600
C	-4.37112500	2.77544600	1.56522700	H	-6.56323800	0.29999000	-5.51221700

H	-4.15914800	0.48759100	-6.07545900	C	-3.56932800	-3.69134700	0.68439800
C	-2.15986500	0.96963700	-4.35386300	C	-3.19180100	-3.57414100	-1.79430300
H	-1.84409100	0.85759300	-5.39101300	H	4.58245300	-1.75547400	3.46091800
C	-4.03443500	3.80966500	-0.62724400	C	5.00271600	-5.08733800	1.18360200
H	-3.69189800	3.74139600	-1.65977600	H	5.24243300	-4.07160500	3.05706900
C	-5.34925300	0.92436400	-2.40094900	H	4.62019500	-5.85579800	-0.80755500
H	-5.68452300	1.03934600	-1.37120500	C	-3.28234000	-4.10614900	1.97852900
H	-4.62011100	5.85589200	-0.80772800	H	-1.87127100	-5.19035200	3.15938100
H	-7.31663000	0.58332800	-3.15550400	H	-4.55932700	-3.30010100	0.46408100
C	-1.65391400	1.35683700	-2.01914000	H	5.41878100	-6.02545100	1.54653800
C	-3.34039000	0.34994500	0.61649800	C	-4.27394200	-3.97710000	3.12970400
P	-0.06725900	3.69807500	-1.13192500	P	0.37882100	-1.70862400	-0.75376500
C	1.32659300	4.18713100	-0.03457900	P	-0.37881800	1.70855800	-0.75376200
C	1.06260300	4.81753000	1.21603600	Pd	0.00002000	-0.00003500	0.79119500
C	2.64532700	3.78754100	-0.36371400	Cl	0.12432200	1.66101800	2.48886300
C	2.05770400	4.74709100	2.18473800	Cl	-0.12420200	-1.66109400	2.48887400
C	3.56934600	3.69136400	0.68436600	C	-1.39542300	4.72884800	1.91197100
C	3.28236100	4.10613900	1.97850600	H	-1.14687400	4.11222700	2.78556500
H	1.87127300	5.19028300	3.15938800	H	-1.69940600	4.04816300	1.10550800
H	4.55935300	3.30014700	0.46403400	H	-2.26737700	5.35272000	2.15758900
C	3.19179300	3.57416100	-1.79433300	C	-0.60711600	6.49749800	0.32037100
C	-0.21737400	5.62408900	1.52091900	H	-1.45185100	7.14520300	0.59427600
H	-3.64822800	-0.38997200	2.62506800	H	-0.93755700	5.91657000	-0.55186400
C	4.27397300	3.97708800	3.12967300	H	0.22876300	7.13747800	0.00485400
H	-2.95579700	-0.60776000	0.26157800	C	0.00847300	6.59487800	2.68830200
C	2.15988500	-0.96972600	-4.35386100	H	0.88094800	7.24239000	2.52367600
C	1.65391900	-1.35688900	-2.01913600	H	0.13539600	6.07675500	3.64759200
C	3.53698500	-0.87128500	-4.04291700	H	-0.87502900	7.23886000	2.78993600
H	1.84412100	-0.85771900	-5.39101800	C	4.70495100	5.37610500	3.58758300
C	2.99263000	-1.26478100	-1.67102400	H	5.42575000	5.29796100	4.41417400
C	3.96442000	-1.02902000	-2.69029400	H	3.85456700	5.97395600	3.94108000
C	4.49979300	-0.60857700	-5.04722500	H	5.18660600	5.92484800	2.76611400
C	3.42158400	-1.41945500	-0.25328100	C	3.60617500	3.24329500	4.29870400
P	0.06726400	-3.69814200	-1.13192500	H	3.29578900	2.23035000	4.00411300
C	5.34924600	-0.92428300	-2.40090600	H	2.71391300	3.76856000	4.66349700
C	5.83162800	-0.50502900	-4.73296100	H	4.30911800	3.15306100	5.13905200
H	4.15917200	-0.48764600	-6.07544200	C	5.52777700	3.19981700	2.73300900
C	3.93800400	-2.66811600	0.20908200	H	6.10451200	3.71860300	1.95457900
C	3.34037600	-0.34983000	0.61648800	H	5.28785800	2.19092500	2.36601800
C	-1.32659600	-4.18717700	-0.03458000	H	6.18265200	3.08887900	3.60778200
C	6.25850700	-0.66609800	-3.39632300	C	3.44279700	2.09638400	-2.08760900
H	5.68450800	-1.03923000	-1.37115500	H	2.51005500	1.51219400	-2.05707500
H	6.56324900	-0.29994600	-5.51217400	H	4.14476900	1.65638900	-1.36530800
C	4.37110100	-2.77529600	1.56531400	H	3.88120300	1.97465300	-3.09021100
C	4.03446500	-3.80958200	-0.62713300	C	2.30856300	4.15473500	-2.90352000
C	3.74768000	-0.46932200	1.96212400	H	2.87848900	4.16907900	-3.84279500
H	2.95577800	0.60786100	0.26153300	H	2.00117900	5.18786400	-2.68616800
C	-1.06261300	-4.81760200	1.21602300	H	1.41011300	3.55861400	-3.10823600
C	-2.64532100	-3.78753800	-0.36369300	C	4.53028600	4.32867400	-1.91608100
H	7.31662300	-0.58320300	-3.15544500	H	4.89864900	4.24876500	-2.94783900
C	4.25607100	-1.65553300	2.42575000	H	5.31466900	3.92665600	-1.26527500
C	4.90754900	-4.00415000	2.02178900	H	4.40523200	5.39472200	-1.68103500
C	4.55264500	-4.98998700	-0.15103100	C	-5.52771800	-3.19976500	2.73307600
H	3.69194900	-3.74134600	-1.65967300	H	-6.10448300	-3.71850600	1.95463800
H	3.64824100	0.39018000	2.62502000	H	-5.28776500	-2.19087400	2.36611000
C	-2.05769900	-4.74713900	2.18473900	H	-6.18258000	-3.08882600	3.60785900
C	0.21733700	-5.62421500	1.52087700	C	-4.70497700	-5.37611800	3.58755600

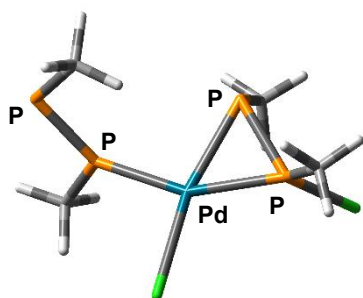
H	-3.85461500	-5.97401900	3.94102400	C	-2.30858000	-4.15466200	-2.90351500
H	-5.18665800	-5.92480700	2.76606600	H	-2.87852200	-4.16899900	-3.84278100
H	-5.42577000	-5.29798000	4.41415400	H	-2.00116900	-5.18778400	-2.68619500
C	-3.60611100	-3.24338500	4.29876600	H	-1.41015400	-3.55851700	-3.10823100
H	-3.29566600	-2.23044700	4.00421200	C	-3.44285100	-2.09637300	-2.08755100
H	-2.71388200	-3.76871400	4.66354500	H	-2.51012500	-1.51216100	-2.05702700
H	-4.30905300	-3.15314400	5.13911200	H	-4.14481800	-1.65640500	-1.36523300
C	-0.00854700	-6.59504300	2.68822200	H	-3.88127600	-1.97464000	-3.09014400
H	-0.88104800	-7.24251900	2.52356400	C	-4.53026100	-4.32869500	-1.91604100
H	-0.13545500	-6.07695300	3.64753300	H	-4.89865900	-4.24877200	-2.94778600
H	0.87493400	-7.23906200	2.78983700	H	-5.31463200	-3.92673300	-1.26519900
C	0.60705800	-6.49758900	0.32029400	H	-4.40515500	-5.39473600	-1.68103100
H	1.45170100	-7.14540400	0.59420400	C	-1.23942100	1.21421200	-3.36983000
H	0.93761400	-5.91664000	-0.55187900	H	-0.18080500	1.29902400	-3.61823900
H	-0.22886700	-7.13745700	0.00468400	C	1.23943800	-1.21431800	-3.36983500
C	1.39541200	-4.72902200	1.91196700	H	0.18082700	-1.29917600	-3.61825500
H	1.14688400	-4.11244000	2.78559400				
H	1.69940400	-4.04830200	1.10553400				
H	2.26735300	-5.35292900	2.15755000				

11A-H



P	2.33215100	0.15264300	-0.38387500	Cl	-3.62346700	-0.44991000	-0.69829800
P	3.75311200	-1.26322800	-0.09626700	H	2.80217600	-2.19960300	0.40639200
P	-0.50911600	-1.96677000	0.27486200	H	-2.63354300	-0.55216300	1.82700800
Pd	0.07414000	0.37326700	0.09663600	H	-0.85924900	-2.12850800	-1.09904900
Cl	0.14140600	2.78115000	0.10202900	H	3.06682200	1.24993700	-0.88975700
P	-2.01558800	-0.46738000	0.56839600				

11A-Me

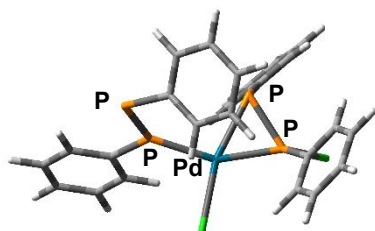


P	-2.22178400	0.17503500	0.44477300	C	-2.86475000	-1.97596600	-1.52844100
P	-3.74363500	-0.98990300	-0.22089200	H	-1.81092500	-1.69632300	-1.64972900
P	0.78370100	-1.79745300	0.21522200	H	-2.92931100	-3.04042200	-1.27289800
Pd	0.00591700	0.45631700	-0.16835300	H	-3.38433300	-1.82861900	-2.48282400
Cl	-0.21662400	2.83686400	-0.60441700	C	3.03546000	-0.68555200	-1.98841800
P	2.17702900	-0.29468400	-0.43061500	H	2.27746500	-1.06074800	-2.68701000
Cl	3.69832800	0.17410500	0.88454300	H	3.48461000	0.22444500	-2.39891400

H	3.80329700	-1.44899800	-1.82784300
C	1.04170600	-1.76381000	2.06368500
H	0.10812000	-2.10305400	2.52821200
H	1.84083600	-2.46630900	2.33006400
H	1.28628900	-0.77152300	2.45757000

C	-2.88846300	1.27489300	1.75341500
H	-3.96201200	1.12451500	1.91071600
H	-2.35033400	1.08427200	2.68944100
H	-2.69826500	2.31341400	1.45655400

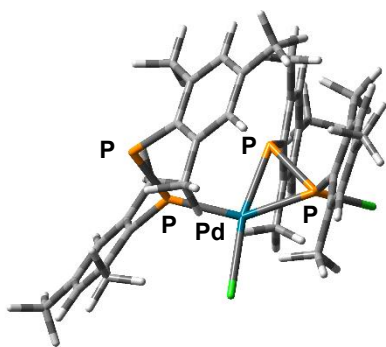
11A-Ph



C	0.90459200	4.77024000	2.26700800
C	1.22391800	3.43106800	2.07336800
C	-0.29614800	5.27774000	1.77613700
C	-1.17561200	4.44291500	1.09247800
H	-2.11534100	4.83614700	0.70830700
C	0.34902900	2.58638500	1.37835200
C	3.19887100	-0.12349000	-0.99091700
C	4.32790600	-0.03903600	-0.16843900
C	3.11120800	-1.09767800	-1.99127800
C	5.36867200	-0.94085100	-0.34689500
C	4.16212000	-1.99378100	-2.16358900
C	5.28370300	-1.91569100	-1.34137500
H	6.24711800	-0.88946700	0.29282700
H	4.10142300	-2.75610900	-2.93732700
C	-5.30690200	0.79422900	-1.43490200
C	-3.83107300	-0.67472800	-0.19644300
C	-6.40173800	0.04922500	-1.00878800
C	-4.94109800	-1.42165000	0.22574700
C	-6.21650400	-1.05799700	-0.17940800
P	-2.12677100	-1.02829800	0.28937300
P	-2.07409800	-2.61351900	1.58056100
C	-0.25670100	-2.74099300	1.76698800
C	0.63972100	-2.84478200	0.69216500
C	0.24367000	-2.77894600	3.07607200
C	2.00870100	-2.94047300	0.92851900
C	1.61219100	-2.86402400	3.30651500

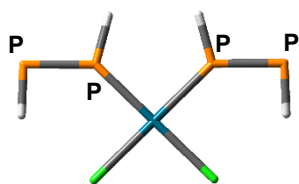
C	2.49696200	-2.93693100	2.23238000
H	2.69691700	-3.01362500	0.08627200
H	1.98892100	-2.87460300	4.32762100
P	0.86050100	0.82479500	1.20780800
Pd	-0.31545900	0.02005400	-0.75868300
Cl	-0.85039600	-0.73156800	-3.00742300
P	1.77958400	0.95626400	-0.73842000
Cl	2.34473600	2.84537800	-1.35015800
C	-4.02534600	0.43470500	-1.03226100
C	-0.85740800	3.10223200	0.89276300
H	-1.54740700	2.45510600	0.35034900
H	3.56849500	-3.00889600	2.41151500
H	0.26814300	-2.86260800	-0.33354400
H	-0.44385800	-2.72270900	3.92051500
H	2.21892700	-1.15562000	-2.61668800
H	6.10007300	-2.62284300	-1.47458900
H	4.38304100	0.72239500	0.60946900
H	2.16779000	3.03846600	2.45542700
H	1.59514300	5.41931500	2.80242300
H	-0.54695300	6.32592100	1.92821800
H	-3.16290300	1.00821400	-1.37574300
H	-5.44815600	1.65472300	-2.08546300
H	-7.40539200	0.32763200	-1.32420700
H	-7.07377800	-1.64261100	0.14844000
H	-4.80953000	-2.29082600	0.86942400

11A-Mes



C	-0.58165000	5.01024700	1.20738300	H	-0.72369100	0.78360500	3.31210200
C	0.06132900	3.77237000	1.18976400	C	4.60577600	-0.95291000	3.00412300
C	-1.54522600	5.35452500	0.26680000	H	4.87495100	-1.10168900	4.05892800
C	-1.86349000	4.41440100	-0.71039700	H	5.23788300	-1.61345000	2.39785200
H	-2.62588200	4.66391700	-1.45069100	H	4.86621300	0.08632200	2.75529800
C	-0.26405600	2.83003200	0.18156800	C	3.99780400	1.76950600	0.40200800
C	3.21347900	0.00368600	-1.28536000	H	3.48573300	2.56056300	-0.16106000
C	4.18078500	0.51110700	-0.39055900	H	3.40014900	1.56786100	1.30575100
C	3.46434900	-1.17413900	-2.02954400	H	4.96785100	2.16175500	0.72930800
C	5.35979700	-0.21037200	-0.21515200	C	2.52110900	-1.69616700	-3.07125200
C	4.64994300	-1.86400000	-1.79517900	H	1.60231000	-2.11231300	-2.63583900
C	5.59897800	-1.41120800	-0.87898300	H	2.19970400	-0.91014700	-3.76917200
H	6.11482500	0.17743800	0.47077900	H	3.00292800	-2.48608400	-3.65854200
H	4.84754100	-2.77761000	-2.35854400	C	6.83989700	-2.20312600	-0.61041000
C	-5.81841700	-0.41258700	0.32576700	H	6.61742900	-3.05362500	0.05036600
C	-3.62899200	-1.41593700	0.29998300	H	7.26162500	-2.61917500	-1.53380100
C	-6.37992900	-1.57209300	-0.20432500	H	7.60886900	-1.59654700	-0.11815500
H	-6.46299000	0.43982600	0.54753700	C	-3.31760500	-3.80510900	-0.52129000
C	-4.17124200	-2.60599300	-0.22877700	H	-2.92618600	-4.25706800	0.40137400
C	-5.54149000	-2.65602800	-0.47029200	H	-3.89391900	-4.57465300	-1.04779400
P	-1.83597600	-1.24928400	0.56354000	H	-2.45253200	-3.54161900	-1.14864000
P	-1.39398900	-2.12371500	2.34597300	C	-3.90316900	0.95786200	1.17618400
C	0.40999600	-1.75962800	2.43813900	H	-3.44231900	0.78146900	2.15905300
C	1.36429300	-2.51771000	1.73345600	H	-3.12866900	1.41672700	0.54229100
C	0.82288700	-0.72354300	3.30230300	H	-4.69607800	1.70266200	1.30997400
C	2.71947000	-2.22981700	1.91901900	C	-7.84835500	-1.66349700	-0.48786800
C	2.18341700	-0.47370400	3.45502000	H	-8.03562500	-1.83025200	-1.55728400
C	3.14880900	-1.22067900	2.77809200	H	-8.30610500	-2.50581000	0.04792800
H	3.46586800	-2.81922400	1.37990700	H	-8.37477300	-0.74840700	-0.19310600
H	2.50319900	0.32897100	4.12429300	C	-1.70495200	2.26050700	-1.89349500
P	0.62531400	1.21727600	0.39915300	H	-0.90214200	2.03454500	-2.60867700
Pd	-0.37183500	-0.41280200	-1.03525600	H	-2.08953900	1.29647600	-1.52368300
Cl	-1.11616900	-1.85235800	-2.87450000	H	-2.51631700	2.73309200	-2.45951200
P	1.59561500	0.78777200	-1.48332000	C	1.08888200	3.51505800	2.26047000
Cl	1.86909700	2.41389500	-2.76572600	H	0.87635400	2.60753300	2.84289300
C	-4.45181300	-0.30889900	0.58457900	H	2.09902200	3.39916800	1.84483000
C	-1.24933800	3.16400800	-0.78238200	H	1.12234700	4.35546000	2.96314000
C	0.97510400	-3.61397700	0.78372300	C	-2.21376700	6.69438000	0.29037200
H	0.18507600	-4.26044400	1.19230800	H	-3.28415300	6.61305300	0.06306600
H	0.58903200	-3.20496700	-0.16346500	H	-2.10468100	7.18145000	1.26664000
H	1.83850900	-4.24474800	0.53977900	H	-1.77772800	7.36609400	-0.46235500
C	-0.17123500	0.14246100	4.01924500	H	-0.32118800	5.72690600	1.98823200
H	-0.92632600	-0.44467600	4.56223000	H	-5.97036400	-3.57221400	-0.88143000
H	0.32572900	0.79772300	4.74490700				

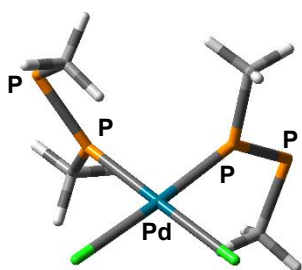
11E-H



P	-3.65884200	-1.28407800	-0.04687200
P	3.65874400	-1.28412400	0.04786000
P	1.64120800	-1.27518800	-0.03310400
P	-1.64126300	-1.27506500	0.03240900
Pd	0.00002200	0.32262900	-0.00013600
Cl	-1.69168300	1.96868800	0.07008300

Cl	1.69177100	1.96867600	-0.06996600
H	3.71402900	0.13885100	0.08752000
H	-3.71420100	0.13890400	-0.08629600
H	1.27392600	-2.63857600	-0.08079700
H	-1.27393400	-2.63846300	0.07943700

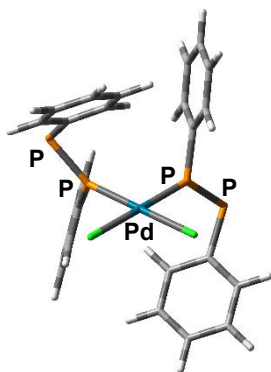
11E-Me



P	3.02690200	-1.70004300	0.24099000
P	-3.07448900	-1.64371700	-0.12303800
P	-1.45972500	-0.78484800	0.73511200
P	1.42209500	-0.89823100	-0.68892200
Pd	0.01346400	0.76465000	-0.03692200
Cl	1.63927800	2.34653500	-0.79286800
Cl	-1.55514200	2.42992900	0.66484900
C	-3.03507000	-0.82651700	-1.78975700
H	-3.99581800	-0.32049100	-1.94160500
H	-2.22600500	-0.09533300	-1.90937000
H	-2.93802600	-1.60308500	-2.55773400
C	3.04201400	-0.69238800	1.80104600

H	3.98711400	-0.13791500	1.84142300
H	2.20969100	0.01767000	1.88035900
H	3.01548000	-1.37843200	2.65583600
C	-1.19213600	-1.36441400	2.44367800
H	-1.97262300	-2.06899500	2.75008100
H	-0.20840800	-1.84614700	2.50674300
H	-1.19699300	-0.49282000	3.10943700
C	1.09938500	-1.69843300	-2.29733100
H	1.88639200	-2.42025500	-2.54085100
H	0.12996900	-2.21002200	-2.25475200
H	1.05267700	-0.92488500	-3.07277000

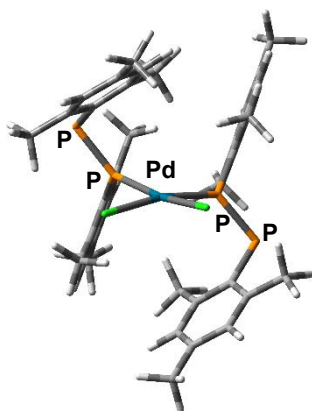
11E-Ph



C	-3.09204900	-3.36951500	1.38914200
C	-1.98229800	-2.90288700	0.69483700
C	-3.19424100	-3.15803300	2.76338000
C	-2.18239000	-2.49208200	3.45025900
H	-2.26627900	-2.32809400	4.52253200
C	-0.96022900	-2.23893100	1.38664200
P	2.15537900	-2.45655900	1.08447200
C	3.33890600	-1.54983700	0.02775800
C	4.13994700	-2.30067100	-0.84204400
C	3.46783900	-0.15596900	0.05658900
C	5.02545100	-1.65918700	-1.70126900
C	4.35886500	0.47931100	-0.80151800
C	5.13080600	-0.27014700	-1.68656100
H	5.63497900	-2.24667400	-2.38499900
H	4.45166900	1.56418000	-0.77465800
C	2.18246500	2.49077500	3.45092500
C	0.96022500	2.23847200	1.38725000
C	3.19429700	3.15699400	2.76427700
H	2.26638800	2.32634400	4.52312700
C	1.98227300	2.90270300	0.69567500
C	3.09205700	3.36902600	1.39012700
P	-2.15540300	2.45632000	1.08517000
C	-3.33893000	1.54991600	0.02816400
C	-4.13996700	2.30095000	-0.84146600
C	-3.46786900	0.15604000	0.05667600
C	-5.02548100	1.65966600	-1.70082800

C	-4.35891100	-0.47903600	-0.80157200
C	-5.13085600	0.27062700	-1.68643400
H	-5.63500800	2.24731400	-2.38442000
H	-4.45171900	-1.56391000	-0.77495100
P	-0.43423800	1.58781200	0.44147900
P	0.43419000	-1.58788500	0.44106600
Pd	0.00000900	0.00019900	-1.14927300
Cl	0.45856500	-1.66867400	-2.79342200
Cl	-0.45851200	1.66956700	-2.79291100
C	-1.06052200	-2.03252600	2.76780200
H	-0.26963000	-1.50580000	3.30132400
C	1.06056800	2.03150600	2.76831800
H	0.26968900	1.50457200	3.30165200
H	5.82547600	0.22878100	-2.35935300
H	2.87712300	0.43465600	0.75706200
H	4.05700500	-3.38735100	-0.86110400
H	-5.82554400	-0.22813300	-2.35933100
H	-4.05701000	3.38763200	-0.86028200
H	-2.87714500	-0.43476600	0.75699300
H	4.07070100	3.51172600	3.30280200
H	3.88295500	3.89360100	0.85736200
H	1.90622600	3.04787300	-0.38310000
H	-4.07061800	-3.51300200	3.30179300
H	-3.88294400	-3.89391600	0.85620300
H	-1.90627200	-3.04765100	-0.38399400

11E-Mes



C	-2.48377300	2.31725200	3.45068700
C	-1.62281200	1.32707200	2.98545700
C	-2.23326700	3.67088300	3.23167400
C	-1.08049400	4.02764300	2.53234500
H	-0.87748400	5.08423000	2.34783900
C	-0.46399800	1.71505400	2.27751200
P	2.40820000	0.49726300	2.55921100
C	3.33536200	-0.79617200	1.65078000
C	3.56912500	-2.02952800	2.28694900
C	3.84576100	-0.54546700	0.36016300
C	4.25293100	-3.02323300	1.58721500
C	4.51306800	-1.57331400	-0.30176100
C	4.71511300	-2.82280100	0.28849100

H	4.42501900	-3.98567600	2.07287400
H	4.90309800	-1.38785200	-1.30527100
C	3.71963000	0.79656100	-0.30166500
C	3.07692300	-2.30553100	3.67613800
C	5.45935600	-3.89821100	-0.44331200
C	1.03145000	4.08003600	-2.48102900
C	0.44194500	1.75706500	-2.25739800
C	2.19222900	3.74611100	-3.17810800
H	0.81451400	5.13170100	-2.28467400
C	1.60938300	1.39214200	-2.96386700
C	2.46073500	2.39832600	-3.41184600
P	-2.42057400	0.51452100	-2.55264700
C	-3.32819000	-0.80209500	-1.65776400

C	-3.55495900	-2.02814300	-2.31118900	H	5.17682700	-3.93065400	-1.50305600
C	-3.83477400	-0.57497400	-0.36179400	H	1.98268500	-2.41709000	3.68416900
C	-4.22467900	-3.03828600	-1.62234600	H	3.33274900	-1.49493100	4.37416800
C	-3.07326300	-2.27720100	-3.70910000	H	3.51104100	-3.23195200	4.06990800
C	-4.48838000	-1.61918200	0.28907700	C	1.94722800	-0.04150100	-3.24334800
C	-3.72432200	0.76030000	0.31638600	H	2.01283900	-0.63959300	-2.32136100
C	-4.67395300	-2.86418000	-0.31482800	H	1.18463100	-0.52440700	-3.87125600
H	-4.39612400	-3.99295000	-2.12341600	H	2.91041000	-0.12178000	-3.76097700
H	-4.88058000	-1.44962000	1.29440200	C	-1.09644800	3.57424200	-1.29410300
C	-5.34685100	-3.98006200	0.42500600	H	-1.29720200	2.99223400	-0.38351400
P	-0.61546600	0.42659200	-1.61686900	H	-0.99758200	4.62558600	-0.99772900
P	0.60737000	0.40618500	1.61569000	H	-1.99110400	3.49392200	-1.92660700
Pd	0.00327100	-1.11797200	-0.01305000	C	3.11578300	4.81092300	-3.68351400
Cl	0.18662400	-2.83196300	1.64767400	H	2.84070500	5.11303100	-4.70386700
Cl	-0.16846600	-2.80599800	-1.70145200	H	3.07493000	5.71030800	-3.05766300
C	-0.17693400	3.08049000	2.05471500	H	4.15389000	4.45958000	-3.71985300
C	0.13722300	3.11612500	-2.01933100	C	-1.94205700	-0.11404000	3.24758900
H	-1.97854900	-2.38324400	-3.72730000	H	-2.00526000	-0.70048800	2.31799800
H	-3.33837600	-1.45620000	-4.39127800	H	-1.17046100	-0.59610000	3.86511100
H	-3.50571400	-3.19911600	-4.11512100	H	-2.90150800	-0.21277800	3.76894900
H	-4.62295200	-4.53555000	1.03784600	C	1.04870300	3.56156600	1.33079900
H	-5.80926100	-4.69881900	-0.26208100	H	1.94704800	3.48019200	1.95795800
H	-6.12135700	-3.60379400	1.10472800	H	1.25076200	2.99545300	0.41045700
H	-4.34091900	0.78856700	1.22341600	H	0.93845400	4.61627400	1.05084200
H	-4.05362000	1.58040700	-0.33873200	C	-3.16659700	4.71845800	3.75490200
H	-2.69304200	0.99491700	0.61877400	H	-2.87728800	5.02623300	4.76961200
H	4.33933000	0.84471600	-1.20572300	H	-3.15429300	5.61835600	3.12848400
H	4.03583600	1.61218100	0.36540300	H	-4.19714800	4.34815200	3.81108700
H	2.68655000	1.02185000	-0.60469500	H	-3.38278800	2.02029800	3.99387100
H	6.54378600	-3.72261700	-0.40651300	H	3.36631600	2.11913700	-3.95356200
H	5.27187700	-4.88645500	-0.00741300				

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