Electronic Supplementary Information (ESI)

Electrophilic Fluorination of Cationic Pt-aryl Complexes

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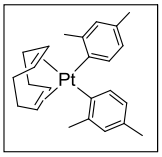
S1. General consideration

All air and moisture sensitive reactions were performed under an inert atmosphere of dry N_2 with standard Schlenk techniques or in a glove box unless otherwise noted. All commercially available reagents (Aldrich and Strem) were used as received without further purification. The deuterated solvents methylene chloride-d_2 and acetonitrile-d_3 were dried over CaH_2; chloroform-d_1 was used as received. NMR spectra were recorded on a Bruker 400, 500 or 600 MHz Avance spectrometer. NMR chemical shifts (δ) were referenced to the residual solvent peaks (^{1}H, ^{13}C) or to an external standard (85% H_3PO_4 for ^{31}P, CF_3Ph for ^{19}F NMR). All chemical shifts are reported in parts per million (ppm). GC-MS data was obtained on an Agilent G2570A GC/MSD system containing a 6850 GC with an HP-5MS column (length 30 m; I. D. 0.250 mm) connected to an Agilent 5983N MSD. HRMS was performed by the Mass Spectrometry Laboratories of University of Illinois and Department of Chemistry, University of North Carolina at Chapel Hill. (COD)$PtCl_2$, (COD)PtI_2, (COD)$PtPh_2$ and (COD)Pt(Ph)(Cl) (COD = cycloocta-1,5-diene),[1] chloro(2-phenylpyridine)[2-(2-pyridyl)phenyl-C,N]platinum,[2] and [(triphos)Pt-(NCC_6F_5)]$(BF_4)_2$[3] were prepared using literature procedures.

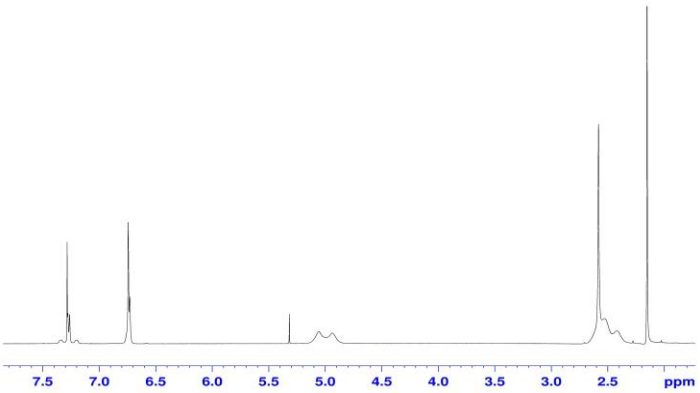
S2. Synthesis and characterization data of Pt^{II} precursors and complexes 1-6.

(COD)Pt(2,4-Me_2Ph)$_2$



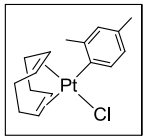
This complex was prepared similarly to that reported for (COD)$PtPh_2$.[1] To a suspension of (COD)$PtCl_2$ (0.30 g, 0.81 mmol) in dry Et_2O (10 mL) was slowly added 2,4-dimethylphenylmagnesium bromide (Aldrich Grignard reagent; 0.5 M in THF) (6.4 mL, 3.2 mmol) under N_2 at room temperature. After stirring for 20 hours, the mixture was cooled down to – 20 °C and then poured slowly into an ice-cold saturated NH_4Cl solution (10 mL) to quench the excess amount of the Grignard reagent. After separation of organic layer and extraction of the aqueous with CH_2Cl_2 (10 mL x 2), the organic layer was dried with $MgSO_4$. After removal of the solvent, the residue was recrystallized with a mixed CH_2Cl_2/hexanes solvent to afford (COD)Pt(2,4-Me_2Ph)$_2$ as a white solid (0.28 g, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26 (d, with Pt satellites, 2H, J_{Pt-H} = 70 Hz, $^3J_{H-H}$ = 7.5 Hz), 6.73 (m, 4H), 5.09 (br, 2H), 4.92 (br, 2H), 2.61-2.36 (br, 14H), 2.19 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.3, 141.1, 134.8, 131.4, 130.2 (J_{Pt-H} = 32 Hz), 125.6 (J_{Pt-H} = 75 Hz), 105.7, 101.7, 30.4, 29.7, 24.8, 20.3 ppm. HRMS (EI) for $C_{24}H_{30}Pt$ ($[M]^+$/z) calc. 513.1995, found 513.2001.

^{1}H NMR spectrum of (COD)Pt(2,4-Me_2Ph)$_2$:



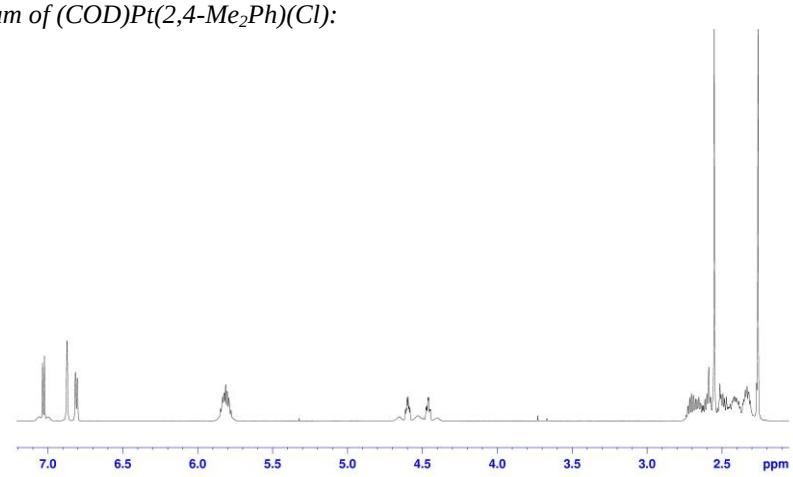
[1] (a) H. C. Clark and L. E. Manzer, *J. Organomet. Chem.*, 1973, **59**, 411; (b) M. Hackett and G. M. Whitesides, *J. Am. Chem. Soc.*, 1988, **110**, 1449.
[2] N. Godbert, T. Pugliese, I. Aiello, A. Bellusci, A. Crispini and M. Ghedini, *Eur. J. Inorg. Chem.*, 2007, 5105.
[3] J. H. Koh and M. R. Gagné, *Angew. Chem. Int. Ed.*, 2004, **43**, 3459.

(COD)Pt(2,4-Me_2Ph)(Cl)

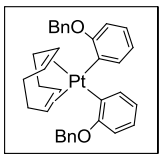


This complex was synthesized using a modified method as reported for (COD)PtPh(Cl).[1] A freshly prepared dry MeOH (3 mL) solution of phenylacetyl chloride (81 mg, 0.52 mmol) was added slowly to a stirred solution of (COD)Pt(2,4-Me_2Ph)$_2$ (0.25 g, 0.50 mmol) in mixed CH_2Cl_2 (5 mL)/MeOH (2 mL) at room temperature. The mixture was stirred for 2 hours. After removal of the solvent, the residuals were recrystallized with a mixed Et_2O/hexanes solvent to afford (COD)Pt(2,4-Me_2Ph)(Cl) as a pale yellow solid (0.20 g, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.03 (d, 1H, with satellites, J_{Pt-H} = 40 Hz, J = 7.6 Hz), 6.87 (s, 1H), 6.80 (d, 1H, J = 7.6 Hz), 5.82 (m, 2H), 4.60 (m, with satellites, J_{Pt-H} = 74 Hz), 4.47 (m, with satellites, J_{Pt-H} = 78 Hz), 2.75-2.62 (m, 2H), 2.55 (s, 3H), 2.50 (m, 2H), 2.43 (m, 2H), 2.34 (m, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.4, 134.0, 133.5, 133.2, 131.3, 126.7, 115.8, 88.0, 83.9, 32.8, 32.7, 28.2, 27.8, 24.8, 20.7 ppm. HRMS (EI) for $C_{16}H_{21}ClPt$ ($[M]^+$/z) calc. 443.0980, found 443.0981.

^{1}H NMR spectrum of (COD)Pt(2,4-Me_2Ph)(Cl):

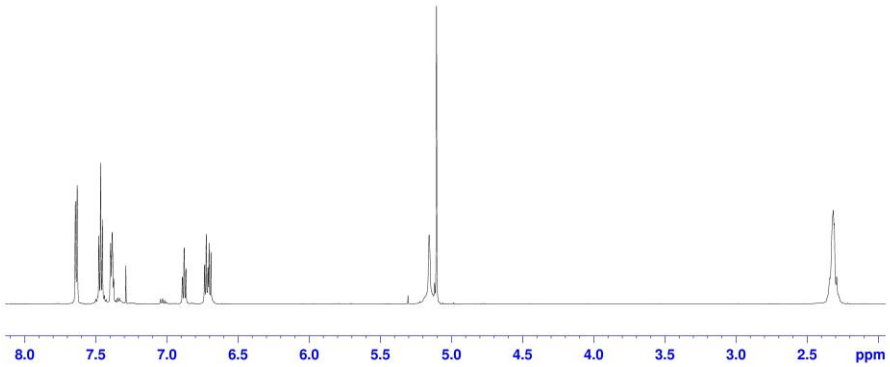


(COD)Pt(2-*BnO*Ph)$_2$

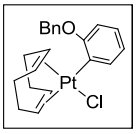


This compound was synthesized similarly as described above for (COD)Pt(2,4-Me_2Ph)$_2$ using (COD)$PtCl_2$ and 2-benzyloxyphenylmagnesium bromide solution (Aldrich Grignard reagent; 1.0 M in THF) (white solid, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, 4H, J = 7.2 Hz), 7.46 (m, 4H), 7.36 (m, 4H), 6.85 (t, 2H, J = 7.0 Hz), 7.69 (m, 4H), 5.19 (s, 4H), 5.09 (s, 4H), 2.30 (m, br, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 142.1, 138.9, 135.9, 128.3, 127.4, 127.3, 123.6, 121.4, 111.2, 102.3, 69.8, 29.9 ppm. HRMS (EI) for $C_{34}H_{34}O_2Pt$ ($[M]^+$/z) calc. 669.2207, found 669.2220.

^{1}H NMR spectrum of (COD)Pt(2-BnOPh)$_2$:

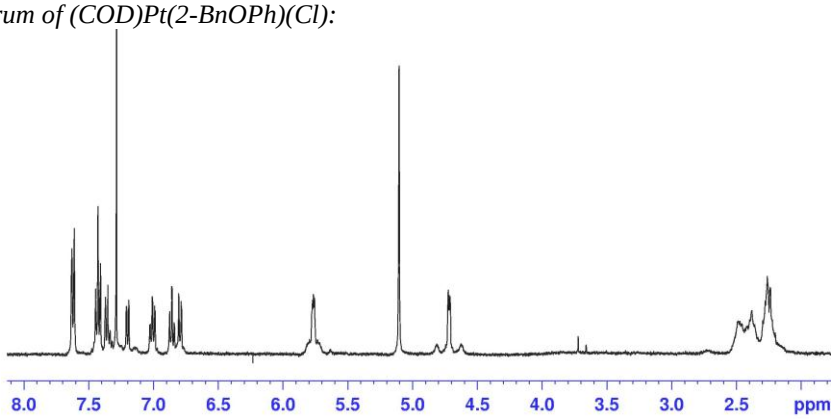


(COD)Pt(2-*BnO*Ph)(Cl)

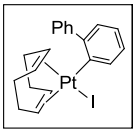


This compound was synthesized similarly as described above for (COD)Pt(2,4-Me_2Ph)(Cl) (pale yellow solid, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (d, 2H, J = 7.2 Hz), 7.42 (t, 2H, J = 7.2 Hz), 7.35 (d, 1H, J = 7.2 Hz), 7.20 (dd, with satellites, 1H, J_{Pt-H} = 56 Hz, $^4J_{H-H}$ = 1.6, $^4J_{H-H}$ = 7.6 Hz), 7.00 (m, 1H), 6.85 (m, 1H), 6.79 (m, 1H), 5.76 (m, with satellites, 2H, J_{Pt-H} = 32 Hz), 5.14 (s, 2H), 4.72 (m, with satellites, J_{Pt-H} = 75 Hz), 2.58-2.49 (m, 4H), 2.47-2.19 (m, 4H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4, 138.3, 135.0, 133.0, 128.3, 127.6, 127.5, 125.2, 121.9, 114.6, 112.8, 86.8, 70.5, 32.1, 27.9 ppm. HRMS (EI) for $C_{21}H_{23}ClOPt$ ([M]$^+$/z) calc. 521.1085, found 521.1077.

^{1}H NMR spectrum of (COD)Pt(2-BnOPh)(Cl):

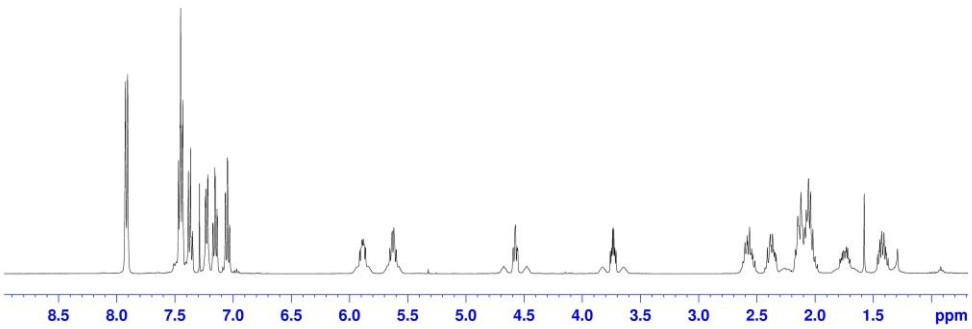


(C**OD)Pt(2-*Ph*Ph)(I)**

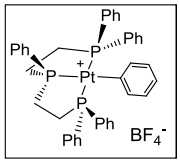


To a suspension of (COD)PtI_2 (0.90 g, 1.6 mmol) in dry Et_2O (60 mL) was slowly added the Grignard reagent 2-biphenylmagnesium bromide (0.5 M in Et_2O, 9.7 mL, 4.8 mmol) under N_2 at room temperature. After stirring for 20 hours, the mixture was cooled down to – 20 °C and then poured slowly into a saturated NH_4Cl solution (20 mL) to quench the excess amount of Grignard reagent. After separation of the organic layer and extraction of the aqueous with CH_2Cl_2 (10 mL x 2), the organic layer was dried with $MgSO_4$ and concentrated. The residue was purified by flash chromatography on silica gel using CH_2Cl_2/EtOAc (5 : 1) as the eluent to afford (COD)Pt(2-*Ph*Ph)(I) as a pale yellow solid (0.54 g, 57% yield). (Even with 3 equiv. of 2-biphenylmagnesium bromide reagent, the above reaction gave mainly the mono-substitution product.) ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, 2H, J = 7.6 Hz), 7.46 (d, 1H, J = 7.6 Hz), 7.42 (t, 2H, J = 8.4 Hz), 7.33 (t, 1H, J = 8.4 Hz), 7.21 (d, 1H, J = 7.6 Hz), 7.10 (t, 1H, J = 7.6 Hz), 6.99 (t, 1H, J = 7.6 Hz), 5.89 (m, br, 1H), 5.61 (m, br, 1H), 4.72 (br, with Pt satellites, 1H, J_{Pt-H} = 84 Hz), 3.84 (br, with Pt satellites, 1H, J_{Pt-H} = 76 Hz), 2.50 (m, 1H), 2.31 (m, 1H), 1.70-2.20 (m, 4H), 1.67 (m, 1H), 1.35 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.0, 145.0, 142.8, 135.4, 129.9, 129.8, 127.9, 127.2, 126.4, 124.4, 114.3, 113.9, 89.7, 86.4, 33.1, 29.9, 28.8, 26.9 ppm. HRMS (ESI) for $C_{20}H_{21}IPtCs$ ([M+Cs]$^+$/z) calc. 715.9390, found 715.9363.

^{1}H NMR spectrum of (COD)Pt(2-PhPh)(I):

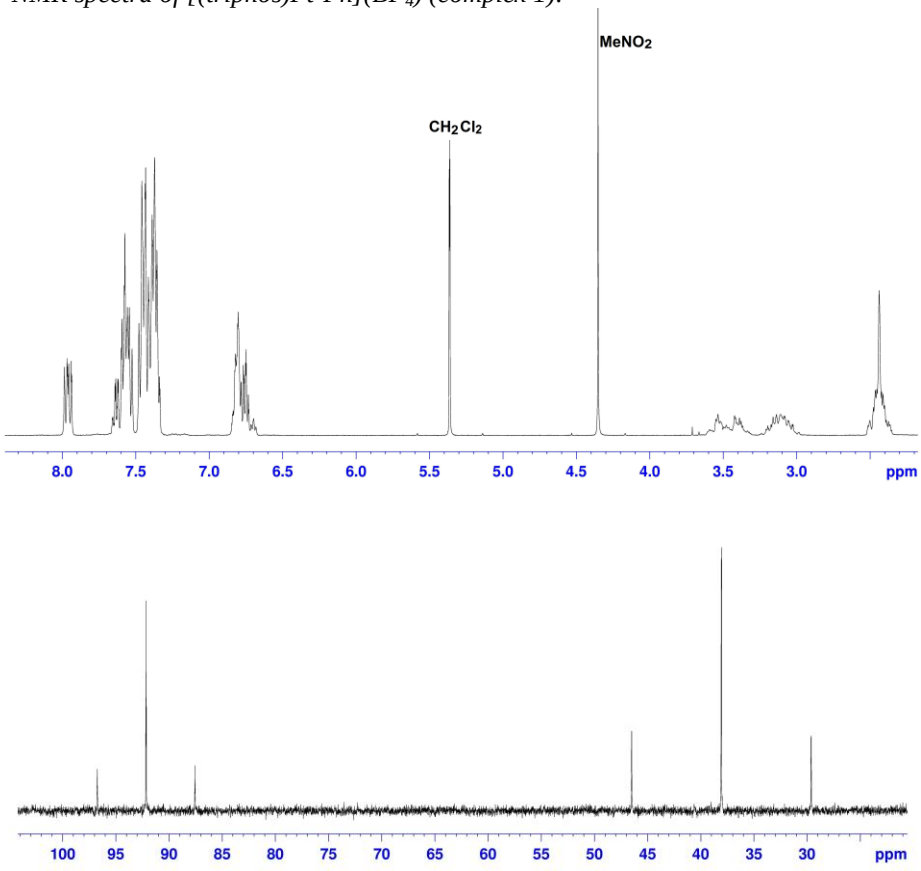


[(triphos)Pt-Ph](BF$_4$) (complex **1**)

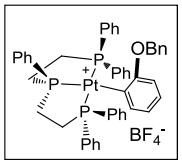


A mixture of triphos (0.15 g, 0.28 mmol) and (COD)Pt(Ph)(Cl) complex (0.11 g, 0.27 mmol) in 5 mL dry CH_2Cl_2 was stirred under N_2 for 30 min at room temperature. An aqueous solution of $NaBF_4$ (0.25 g, 2.3 mmol, in 5 mL H_2O) was added, and the resulting mixture was stirred for 15 min. After separation of the organic layer, extraction with CH_2Cl_2 (5 mL x 2) and removal of the solvent, the residue was purified by flash chromatography on silica gel using CH_2Cl_2/$MeNO_2$ (1 : 1) as the eluent to afford the [(triphos)Pt-Ph]BF_4 as a white solid, which was then recrystallized using a CH_2Cl_2/ hexanes mixed solvent (0.21 g, 86% yield). ^{1}H NMR: (400 MHz, CD_3CN) δ 7.99 (m, 2H), 7.62-46 (m, 19H), 7.30 (m, 4H), 6.75 (m, 5H), 3.59 (dd, 3H), 2.91 (m, 2H), 2.66 (m, 2H), 2.45 (m, 2H) ppm. ^{31}P NMR: (161.9 MHz, CD_3CN) δ 93.9 (s, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1504 Hz), 39.7 (s, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 2722 Hz). HRMS (ESI) for $C_{40}H_{38}P_3Pt$ ([M-BF_4]$^+$/z) calc. 806.1834, found 806.1833. Elemental Anal. Calcd for $C_{40}H_{38}BF_4P_3Pt$: C 53.77%, H 4.29%. Found: C 53.02%, H 4.25%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-Ph](BF$_4$) (complex 1):

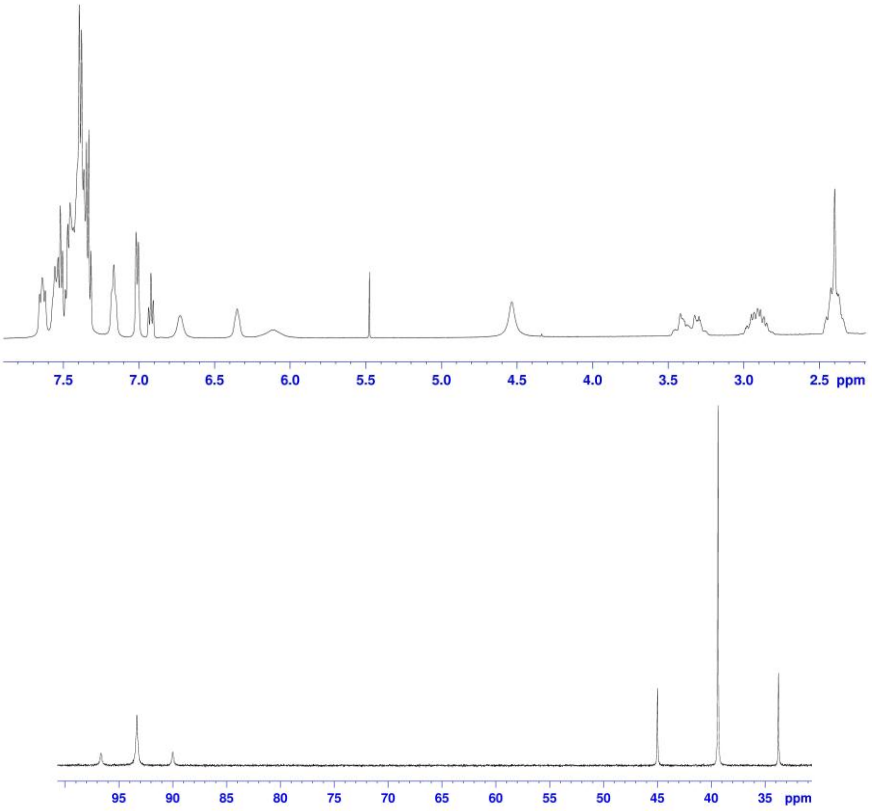


[(triphos)Pt-(2-*BnO*)Ph](BF$_4$) (complex **2**)

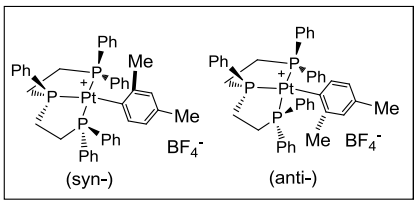


This complex was synthesized similarly as descried above for complex **1** using triphos and (COD)Pt(2-*BnO*Ph)(Cl) (obtained as a white powder, 81% yield). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.68 (m, 2H), 7.67-7.26 (m, 24H), 2.19 (br, 2H), 7.02 (d, 2H, J = 8.0 Hz), 6.92 (t, 1H, J = 8.0 Hz), 6.72 (br, 1H), 6.36 (br, 1H), 6.13 (br, 1H), 4.55 (br, 2H), 3.41-3.28 (m, 2H), 2.98-2.79 (m, 2H), 2.40 (m, 4H) ppm. ^{31}P NMR: (202.4 MHz, CD_2Cl_2): δ 91.9 (s, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1627 Hz), 37.9 (s, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 2730 Hz) ppm. HRMS (ESI) for $C_{47}H_{44}OP_3Pt$ ([M-BF_4]$^+$/z) calc. 912.2253, found 912.2247. Elemental Anal. Calcd for $C_{47}H_{44}BF_4OP_3Pt$: C 56.47%, H 4.44%. Found: C 56.21%, H 4.12%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-(2-BnO)Ph](BF$_4$) (complex 2):



[(triphos)Pt-(2,4-*Me*$_2$)Ph](BF$_4$) (complex **3**)



This complex was synthesized as descried for complex **1** (obtained as a white powder, 65% yield). This complex exists as a mixture of its *syn*- and *anti*- rotamers with a ratio of ~2.7 : 1.

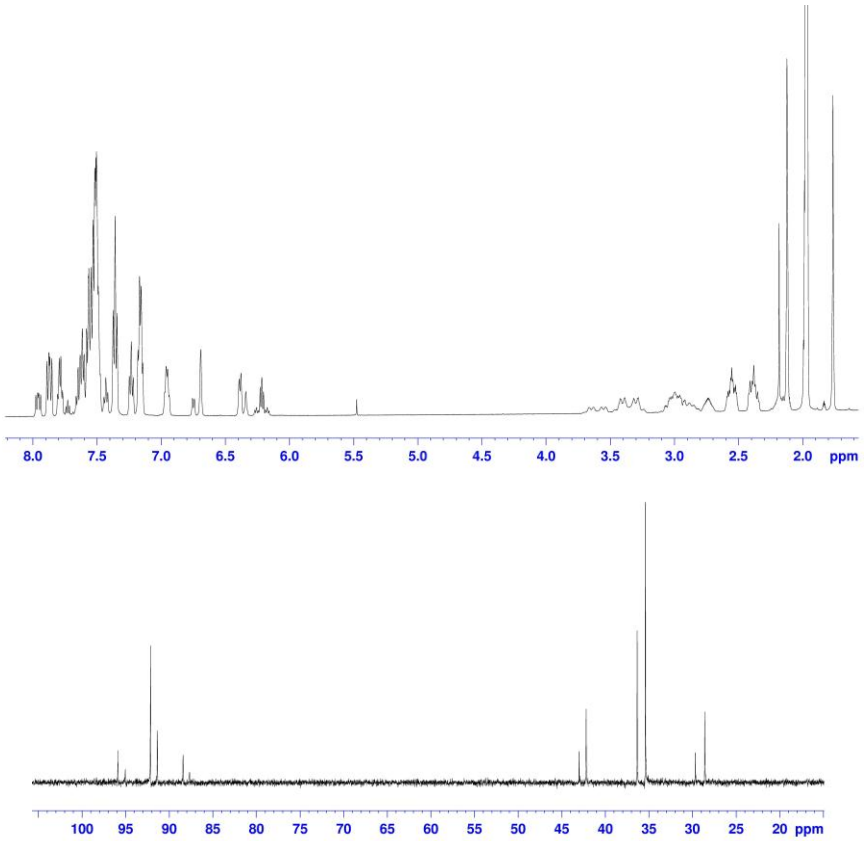
Note: By analogy to **4**, the major species is assigned as the *syn*- rotamer.

For the *syn*- rotamer, ^{1}H NMR (400 MHz, CD_3CN): δ 7.87 (m, 2H), 7.76 (m, 2H), 7.69-7.48 (m, 13H), 7.38 (m, 4H), 7.23 (m, 4H), 6.70 (s, 1H), 6.41 (d, J = 4.0, 1H), 6.21 (m, with satellites, 1H), 3.47-3.28 (m, 2H), 3.00 (m, 2H), 2.59 (m, 2H), 2.39 (m, 2H), 2.18 (2, 3H), 1.73 (s, 3H) ppm; ^{31}P NMR: (161.9 MHz, CD_3CN): δ 92.2 (s, with Pt satellites, 1P, J_{Pt-P} = 1508 Hz), 35.40 (s, with Pt satellites, 2P, J_{Pt-P} = 2747 Hz) ppm.

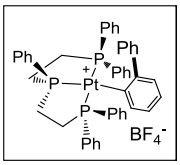
For the *anti*-rotamer, ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.98 (m, 2H), 7.69 (m, with satellite, 1H), 7.69-7.48 (m, 13H), 7.48 (m, 1H), 7.32 (m, 4H), 6.96 (m, 4H), 6.76 (d, J = 3.6 Hz), 6.37 (s, 1H), 3.69-3.50 (m, 2H), 2.98-2.80 (m, 2H), 2.77-2.70 (m, 2H), 2.30 (m, 5H), 0.43 (s, 3H) ppm; 91.4 (s, with Pt satellites, 1P, J_{Pt-P} = 1491 Hz), 35.40 (s, with Pt satellites, 2P, J_{Pt-P} = 2700 Hz) ppm.

HRMS (ESI) for $C_{42}H_{42}P_3Pt$ ($[M-BF_4]^+/z$) calc. 834.2147, found 834.2144. Elemental Anal. Calcd for $C_{42}H_{42}BF_4P_3Pt$: C 54.74%, H 4.59%. Found: C 54.29%, H 4.28%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-(2,4-Me_2)Ph](BF_4) (complex 3):

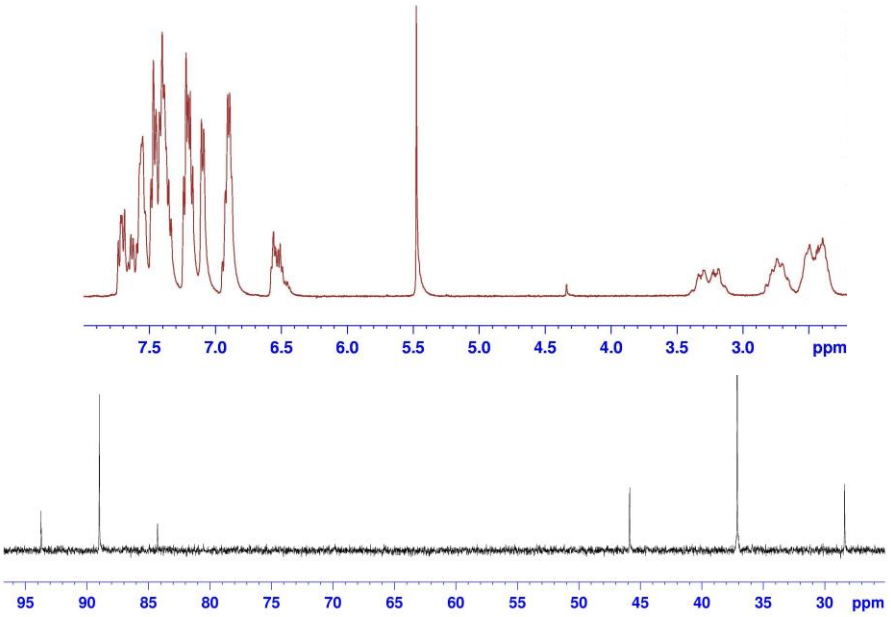


[(triphos)Pt-(2-*Ph*)Ph](BF_4) (complex **4**)

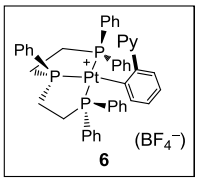


This complex was synthesized similarly as descried for complex **1** using triphos and (COD)Pt(2-*Ph*Ph)(I) (white powder, 75% yield). ^{1}H NMR: (400 MHz, CD_2Cl_2) δ 7.79 (m, 2H), 7.58 (m, 6H), 7.28-7.48 (m, 10H), 7.17 (m, 6H), 7.09 (d, 3H, *J* = 7.6 Hz), 6.90 (m, 5H), 6.50-6.60 (m, 2H), 3.15-3.24 (m, 2H), 2.76 (m, 2H), 2.26-2.40 (m, 4H) ppm. ^{31}P NMR: (161.9 MHz, CD_2Cl_2) δ 89.0 (s, with Pt satellites, 1P, J_{Pt-P} = 1534 Hz), 36.3 (s, with Pt satellites, 2P, J_{Pt-P} = 2815 Hz). HRMS (ESI) for $C_{46}H_{42}P_3Pt$ ($[M-BF_4]^+/z$) calc. 882.2147, found 882.2104. Elemental Anal. Calcd for $C_{46}H_{42}BF_4P_3Pt$: C 56.98%, H 4.37%. Found: C 57.04%, H 3.97%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-(2-Ph)Ph](BF_4) (complex 4):



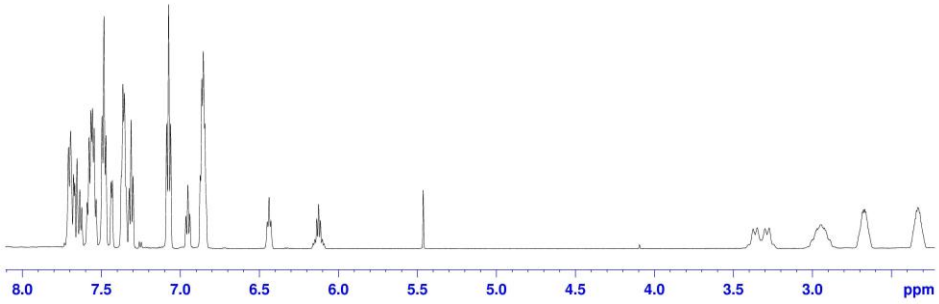
[(triphos)Pt-(2-*Py*)Ph](BF$_4$) (complex **5**)

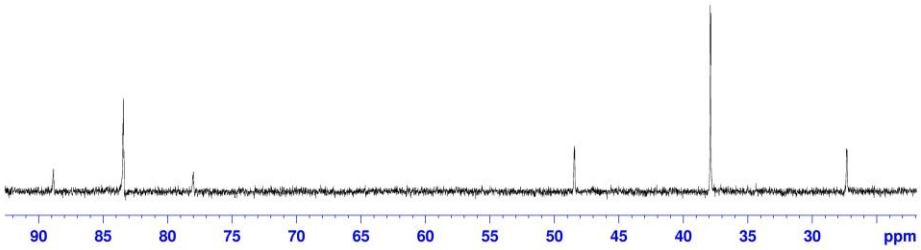


6

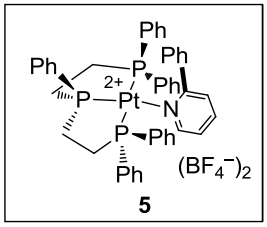
A $MeNO_2/H_2O$ (5 : 1) (6 mL) solution of chloro(2-phenylpyridine)[2-(2-pyridyl)phenyl-C,N]platinum[2] (0.25 g, 0.47 mmol), triphos (0.27 g, 0.50 mmol) and $NaBF_4$ (0.30 g, 2.7 mmol) was heated at 70 °C for 3 h under N_2. After removal of the solvent, the residual was purified by flash chromatography on silica gel using $CH_2Cl_2/MeNO_2$ (1 : 1) as the eluent to afford complex **5** as pale yellow solid (0.35 g, 78% yield). ^{1}H NMR (600 MHz, CD_3CN): δ 7.70-7.60 (m, 5H), 7.57 (m, 5), 7.53 (m, 4H), 7.46 (d, 1H), 7.38 (m, 4H), 7.32 (t, 2H), 7.12 (t, 4H), 6.93 (t, 1H), 6.85 (m, 5H), 6.43 (t, 1H), 6.12 (m, 1H), 3.31 (dd, 2H), 2.98 (m, 2H), 2.68 (m, 2H), 2.34 (m, 2H) ppm. ^{31}P NMR: (161.9 MHz, CD_3CN): δ 83.4 (t, with Pt satellites, 1P, J_{Pt-P} = 1755 Hz, J_{P-P} = 8 Hz), 37.9 (d, with Pt satellites, 2P, J_{Pt-P} = 4322 Hz, J_{P-P} = 8 Hz) ppm. HRMS (ESI) for $C_{45}H_{41}NP_3Pt$ ($[M-BF_4]^+/z$) calc. 883.2100, found 883.2102. Elemental Anal. Calcd for $C_{45}H_{41}BF_4NP_3Pt$: C 55.68%, H 4.26%, N 1.44%. Found: C 55.35%, H 3.94%, N 1.41%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-(2-Py)Ph](BF$_4$) (complex 7):





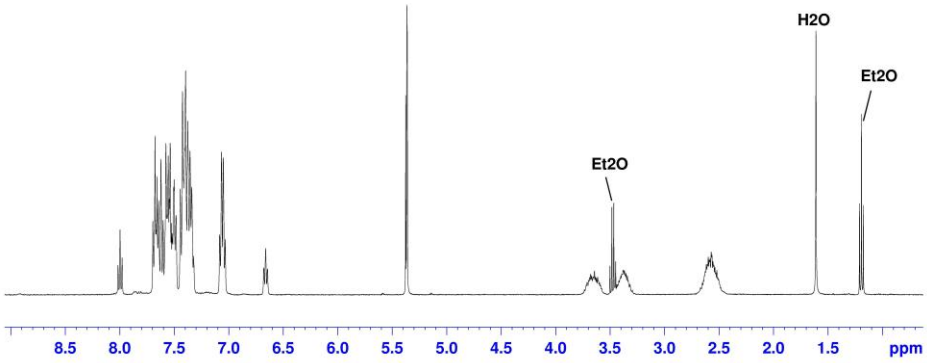
[(triphos)Pt-(2-*Ph*)Py](BF$_4$)$_2$ (complex **6**)

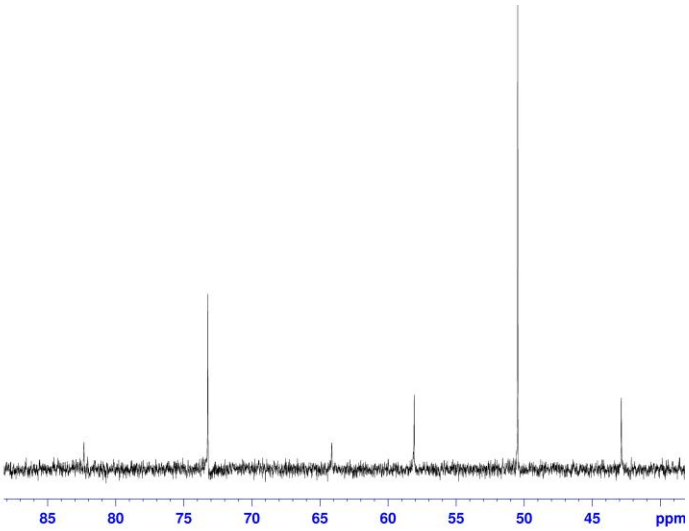


5

[(triphos)Pt-(NCC$_6$F$_5$)](BF$_4$)$_2$ (0.21 g, 0.19 mmol) and 2-phenylpyridine (0.062 g, 0.40 mmol) were dissolved in dry CH_2Cl_2 (5 mL) and stirred at room temperature for 1 h. After removal of the solvent, the residue was washed with Et_2O (3 mL x 3). Recrystallization from CH_2Cl_2 and hexanes led to complex **6** as white solid (0.18 g, ~93% yield). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.98 (m, 2H), 7.73 (m, 2H), 7.67-7.30 (m, 25H), 7.05 (m, 4H), 6.72 (t, J = 7.0 Hz, 1H), 3.71 (m, 2H), 3.43 (m, 2H), 2.70 (m, 4H) ppm. ^{31}P NMR: (161.9 MHz, CD_2Cl_2): δ 73.2 (s, with Pt satellites, 1P, J_{Pt-P} = 2950 Hz), 50.5 (s, with Pt satellites, 2P, J_{Pt-P} = 2465 Hz) ppm. HRMS (ESI) for $C_{45}H_{42}BF_4NP_3Pt$ ([M-BF$_4$]$^+$/z) calc. 971.2202, found 971.1828. Elemental Anal. Calcd for $C_{45}H_{42}B_2F_8NP_3Pt$: C 51.06%, H 4.00%, N 1.32%. Found: C 50.90%, H 3.73%, N 1.28%.

^{1}H and ^{31}P NMR spectra of [(triphos)Pt-(2-Ph)Py](BF$_4$)$_2$ (complex 6):





S3. Fluorination of complexes 1-6 by XeF_2 and Selectfluor® and supporting spectra.

General procedure:

For reactions with **XeF_2**:

In a typical experiment, solid XeF_2 (3.3 mg, 0.02 mmol) was added to a solution of the corresponding [(triphos)Pt^+-Ar](BF_4) complex (~10 mg, 0.01 mmol, in 0.5 mL CD_3CN) in an NMR tube. The reaction was then monitored by NMR spectroscopy at room temperature until its completion. The organometallic Pt(IV) products were characterized in situ, NMR yields of these complexes were calculated using ^{31}P NMR determined ratios of all the metal products.

For reactions with **Selectfluor®**:

In a typical experiment, Selectfluor® (5.3 mg, 0.015 mmol), the corresponding (triphos)Pt-aryl$^+$ complex (~10 mg, 0.01 mmol) and CF_3Ph (2 uL, internal ^{19}F NMR standard) were dissolved with CD_3CN (0.5 mL) in an NMR tube. The sample was inserted into an NMR spectrometer and monitored by NMR spectroscopy at the designated temperature until complete consumption of the Pt-aryl$^+$ complex.

(S3.1) For [(triphos)Pt-Ph](BF_4) (complex 1):

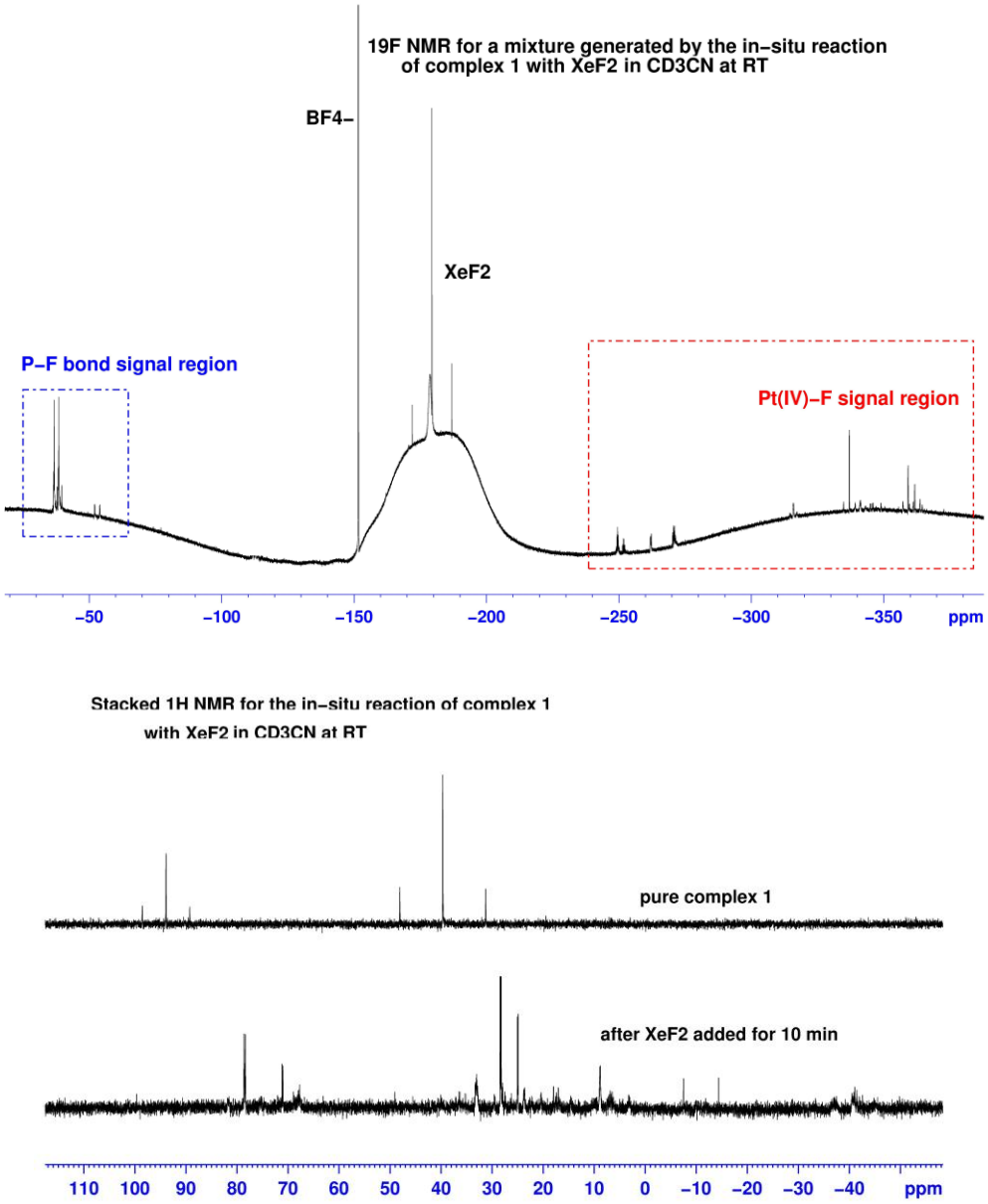
***XeF_2*:**

When reacting with XeF_2, complex **1** exhibited similar reaction pattern as previously demonstrated for its methyl derivative ([(triphos)Pt-Me](BF_4)).[4] According to ^{31}P and ^{19}F NMR monitoring, the reaction quickly produces a mixture of Pt(IV)-F species (RT, <20 min), comparable to the mixture of Pt(IV)-F complexes generated by reactions of [(triphos)Pt-Me](BF_4) with XeF_2.[4]

No C-F coupling product (Ph-F) was observed even with prolonged heating of the product mixture at 80 ^oC (> 30h).

Supporting ^{31}P and ^{19}F NMR spectra:

[4] S.-B. Zhao, J. J. Becker and M. R. Gagné, *Organometallics*, 2011, **30**, 3926.



Selectfluor®:

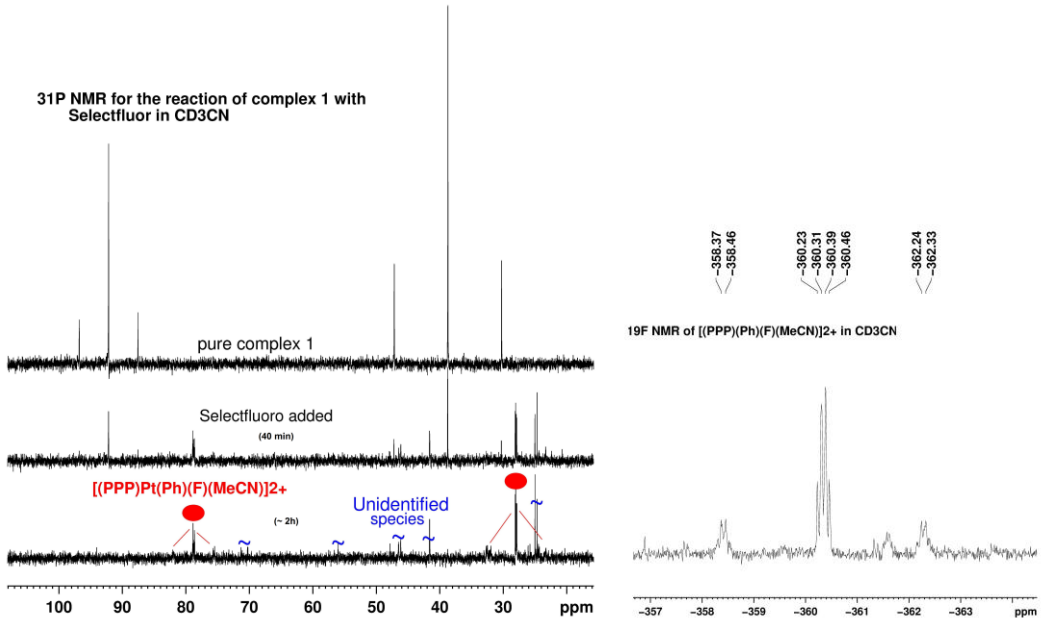
Reactions of **1** with Selectfluor® proceeded to completion within 2 h at RT, producing one Pt(IV) fluoro complex (60~70% NMR yield). The ^{31}P and ^{19}F NMR data of this complex match very well with one of the products generated by reactions of **1** with XeF_2; other Pt species were also noticed.

Again, no C-F coupling product Ph-F was generated even after prolonged heating of the reaction mixture at 80 ^{o}C (> 30h).

Diagnostic NMR data of this Pt^{IV}-F complex:

^{1}H NMR signals (400 MHz, CD_3CN): δ 6.95 (br, 2H), 6.80 (m, 2H) ppm; ^{31}P NMR (202 MHz, CD_3CN): δ 78.7 (doublet of triplet, with Pt satellites, 1P, J_{Pt-P} = 1033 Hz, J_{P-F} = 35 Hz, J_{P-P} = 10 Hz), 27.8 (doublet of doublet, with Pt satellites, 2P, J_{Pt-P} = 1497 Hz, J_{P-F} = 27 Hz, J_{P-P} = 10 Hz) ppm; ^{19}F NMR (376 MHz, CD_3CN): δ -360.3 (m, with Pt satellites, J_{Pt-F} = 1453 Hz, J_{P-F} = 30 Hz, J_{P-F} = 27 Hz) ppm.

Supporting NMR spectra:



(3.2) For [(triphos)Pt-(2-*BnO*)Ph](BF$_4$) (complex 2):

***XeF$_2$*:**

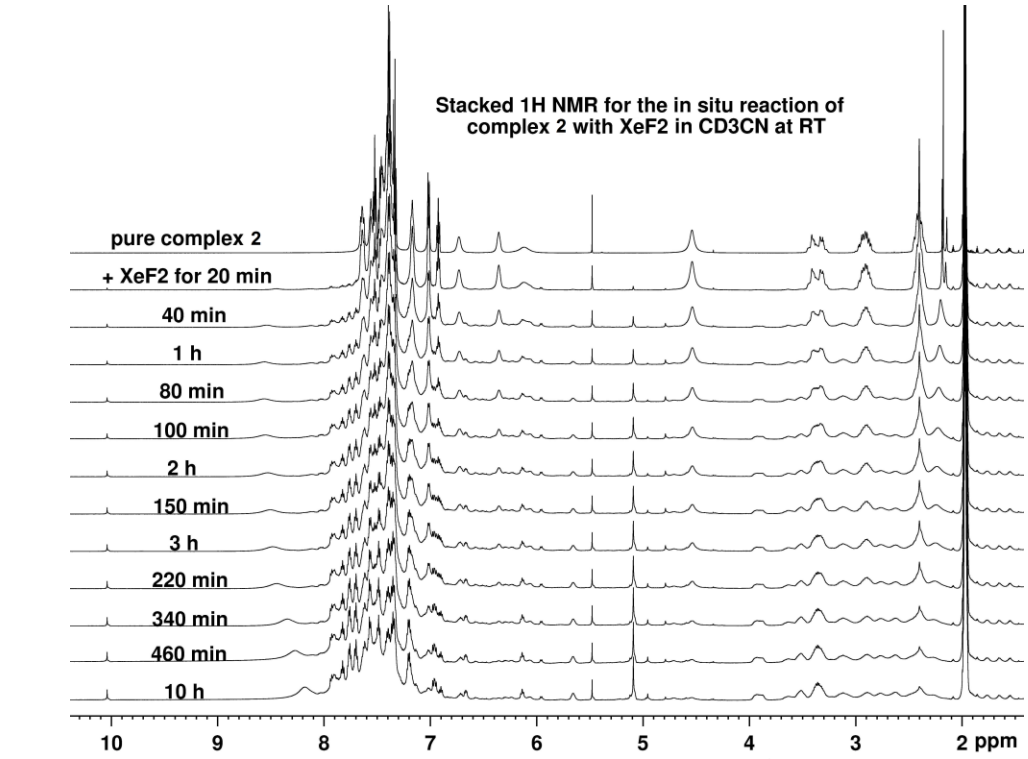
Reactions of **2** with XeF_2 proceeded to completion after 12 h at RT, leading to the formation of one major Pt complex (~75% NMR yield), which was identified by ^{31}P and ^{19}F NMR to be a Pt(IV)-F species. However, efforts to crystallize this product were unsuccessful; its structure remains unclear.

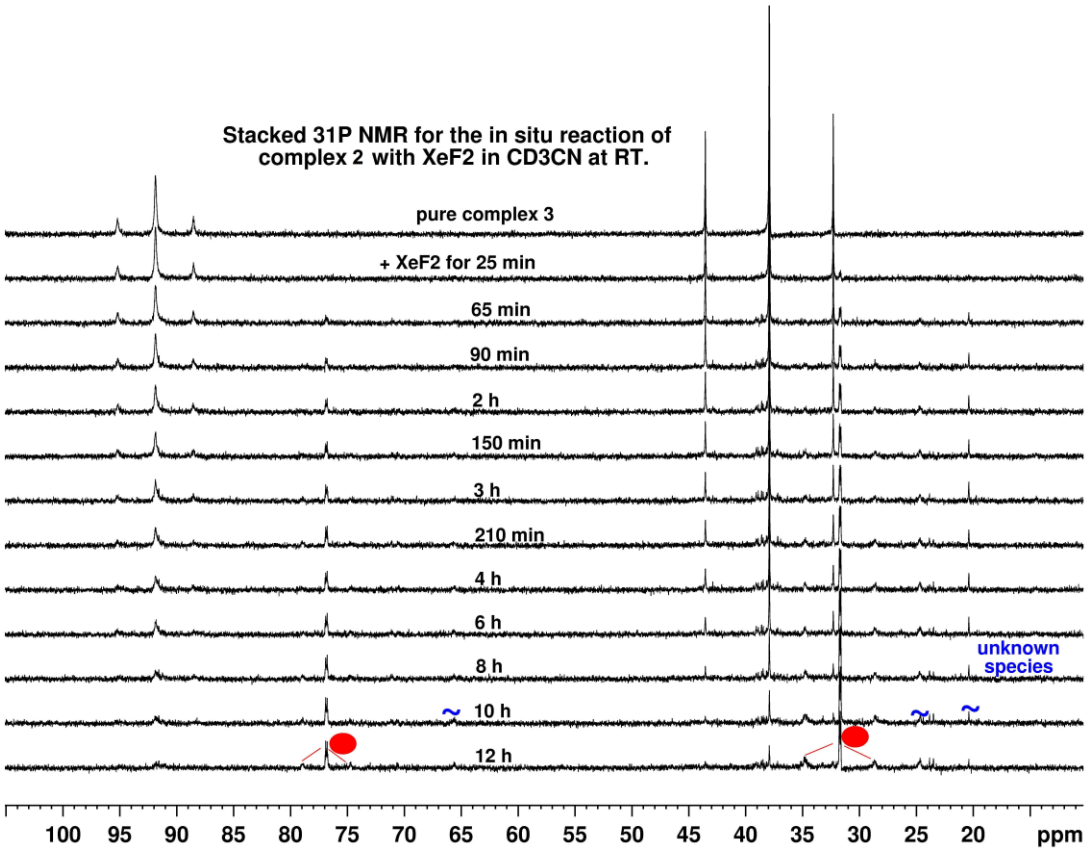
Only trace amount of the C-F coupling product (2-fluorophenyl)benzyl ether (< 5% GC-MS yield) was obtained after heating a freshly prepared reaction mixture containing this Pt(IV)–F complex.

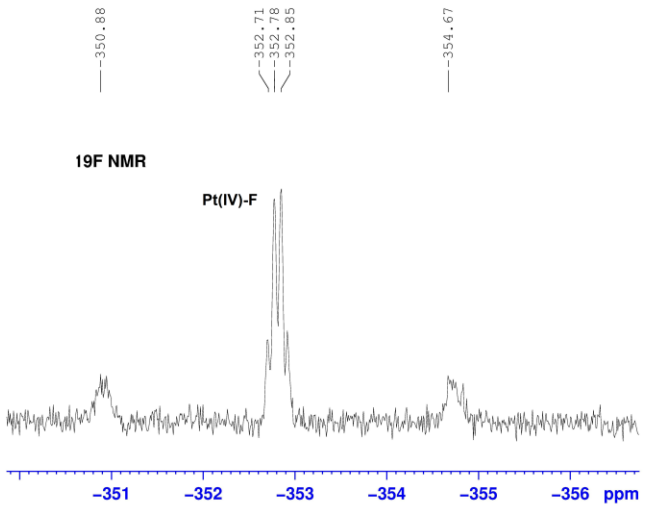
NMR data of this Pt(IV)-F complex:

Diagnostic ^1H NMR signals (400 MHz, CD_3CN): δ 6.90 (dd, J = 8.0 Hz, 1H), 6.67 (dd, J = 8.0 Hz, 1H), 6.14 (t, J = 8.0 Hz, 1H), 5.66 (br, 1H), 5.09 (br, 2H) ppm. ^{31}P NMR (202 MHz, CD_3CN): δ 76.8 (doublet of triplet, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1026 Hz, $J_{P\text{-}F}$ = 30 Hz, $J_{P\text{-}P}$ = 11 Hz), 31.7 (doublet of doublet, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 1495 Hz, $J_{P\text{-}F}$ = 23 Hz, $J_{P\text{-}P}$ = 11 Hz) ppm. ^{19}F NMR (376 MHz, CD_3CN): δ -352.8 (doublet of triplet, with Pt satellites, $J_{Pt\text{-}F}$ = 1442 Hz, $J_{P\text{-}F}$ = 29 Hz, $J_{P\text{-}F}$ = 27 Hz).

Supporting ^1H, ^{31}P and ^{19}F NMR spectra:





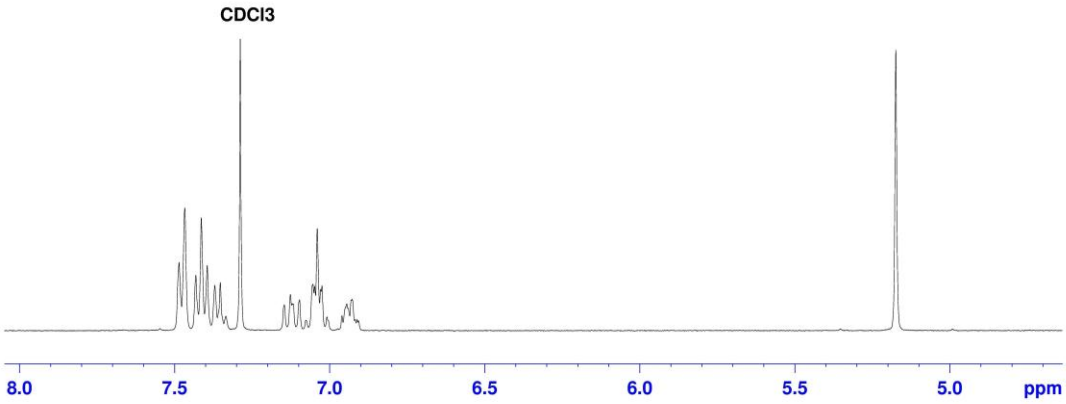


Selectfluor®:

Reactions of **2** with Selectfluor® at 80 °C in CD_3CN proceeded to completion within 1 h. According to ^{1}H, ^{31}P, ^{19}F NMR and GC-MS analysis, these reactions led directly to the C-F coupling product (2-fluorophenyl)benzyl ether, along with the corresponding generation of $[(triphos)Pt\text{-}MeCN]^{2+}$ (this is a known complex, *see:* Reference 4, i.e., S.-B. Zhao, *et al. Organometallics*, 2011, **30**, 3926) as the by-product for the metal complex. (2-fluorophenyl)benzyl ether was produced in ~91% yield based on ^{19}F NMR (δ_F ~ -135.3 ppm) and GC-MS (m/z = 202) analyses using CF_3Ph as internal standard.

(2-fluorophenyl)benzyl ether is a known compound.[5] We were also able to isolate the fluorination product (2-fluorophenyl)benzyl ether by preparative TLC. NMR data of this product: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, 2H, J = 7.6 Hz), 7.37 (dd, 2H, J_1 = 7.6 Hz, J_2 = 7.2 Hz), 7.35 (t, 1H, J = 7.2 Hz), 7.11 (m, 1H), 7.04 (m, 2H), 6.91 (m, 1H), 5.17 (s, 2H) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ -135.3 ppm. These data match the literature reported values.[5]

^{1}H NMR spectrum of (2-fluorophenyl)benzyl ether:



[5] A. Kim, J. D. Powers and J. F. Toczko, *J. Org. Chem.*, 2006, **71**, 2170.

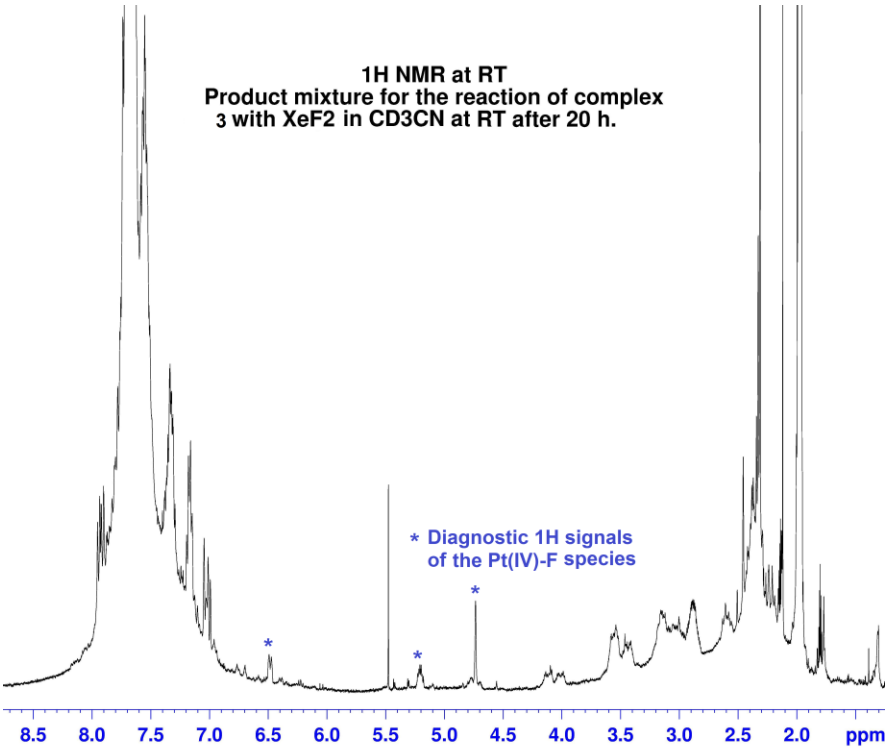
(3.3) For [(triphos)Pt-(2,4-*Me*$_2$)Ph](BF$_4$) (complex 3):

***XeF$_2$*:**

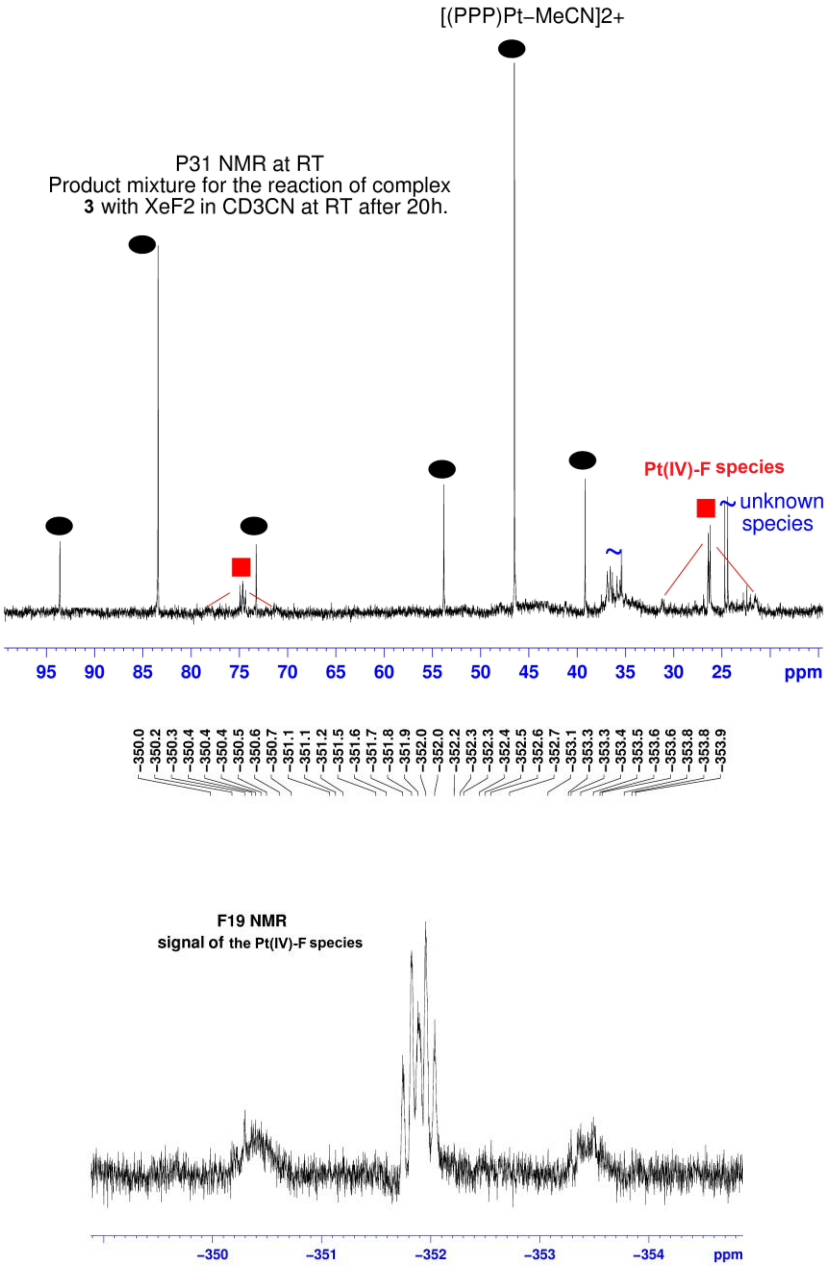
Reactions of **3** with XeF_2 proceeded to completion after 15 h at RT. According to ^{31}P and ^{19}F NMR analysis, these reactions directly yielded the C-F coupling product 1-fluoro-2,4-dimethylbenzene (~55% NMR yield), along with the corresponding $[(triphos)Pt\text{-}MeCN]^{2+}$ by-product. 1-fluoro-2,4-dimethylbenzene is a known compound.[6] Its formation was confirmed by ^{19}F NMR (δ_F ~ -123.6 ppm) and GC-MS (m/z = 124).

The formation of other Pt species was also noticed, including one identified to be a Pt(IV)-F complex. NMR data of this complex: Diagnostic ^1H NMR signals (400 MHz, CD_3CN): δ 6.48 (d, J = 8.0 Hz, 1H), 5.21 (br, 1H), 4.73 (s, with Pt satellites, $^2J_{Pt\text{-}H}$= 32.0 Hz, 2H) ppm. ^{31}P NMR (202 MHz, CD_3CN): δ 74.7 (doublet of triplet, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1134 Hz, $J_{P\text{-}F}$ = 10 Hz, $J_{P\text{-}P}$ = 6 Hz), 26.3 (doublet of doublet, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 1556 Hz, $J_{P\text{-}F}$ = 30 Hz, $J_{P\text{-}P}$ = 6 Hz) ppm. ^{19}F NMR (376 MHz, CD_3CN): δ -351.9 (doublet of triplet, with Pt satellites, $J_{Pt\text{-}F}$ = 1146 Hz, $J_{P\text{-}F}$ = 50 Hz, $J_{P\text{-}F}$ = 29 Hz) ppm.

Supporting ^1H, ^{31}P and ^{19}F NMR spectra for these reactions:



[6] S. Singh, D. D. DesMarteau, S. S. Zuberi, M. Witz and H.-N. Huang, *J. Am. Chem. Soc*., 1987, **109**, 7194.

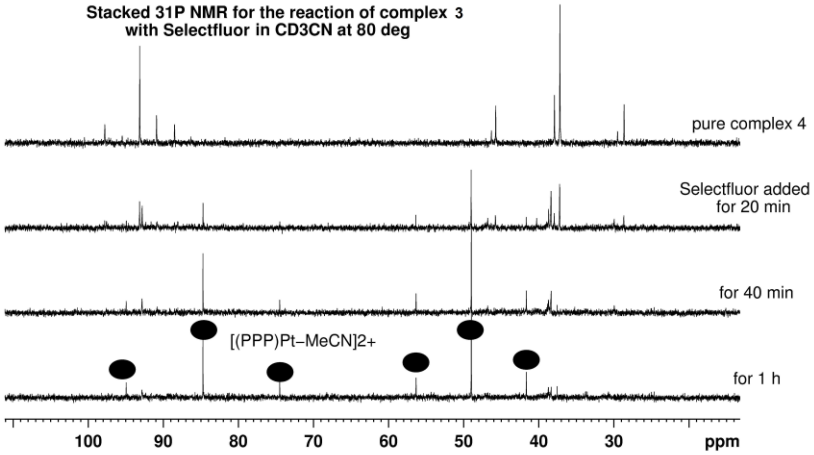


Selectfluor®:

Reactions of **3** with Selectfluor® at 80 °C in CD_3CN proceeded to completion within 2 h, which directly produced the C-F coupling product 1-fluoro-2,4-dimethylbenzene, along with the formation of corresponding $[(triphos)Pt\text{-}MeCN]^{2+}$ by-product.

1-fluoro-2,4-dimethylbenzene was confirmed by ^{19}F NMR and GC-MS analyses. Its yield was estimated based on based on ^{19}F NMR and GC-MS analyses using CF_3Ph as internal standard. As mentioned above, *the occurrence of C-F coupling and the formation of* $[(triphos)Pt\text{-}MeCN]^{2+}$ *corresponds with each other very well for these reactions.* Analyses of the composition of Pt species after these reactions were also carried out to further verify the yields for these reactions. According to these analyses, these fluorination reactions occurred typically in >95% yield.

Representative ^{31}P spectra for these reactions:



(3.4) For [(triphos)Pt-(2-*Ph*)Ph](BF$_4$) (complex 4):

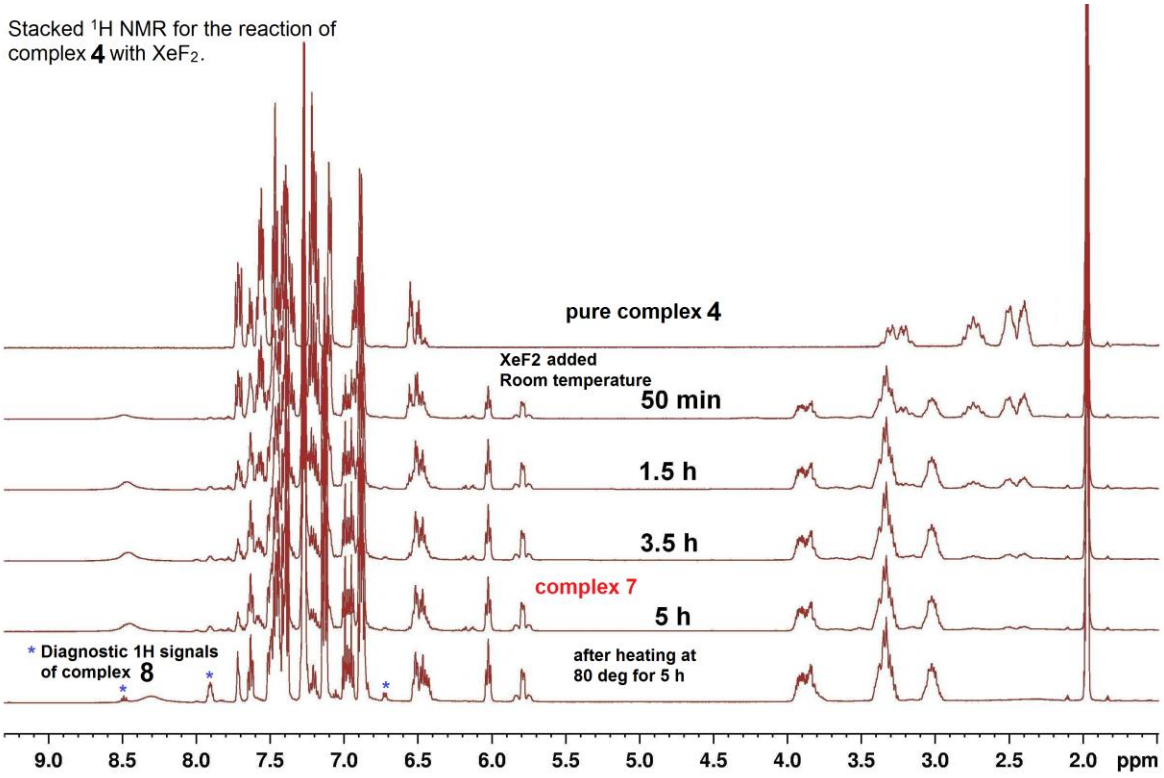
***XeF$_2$*:**

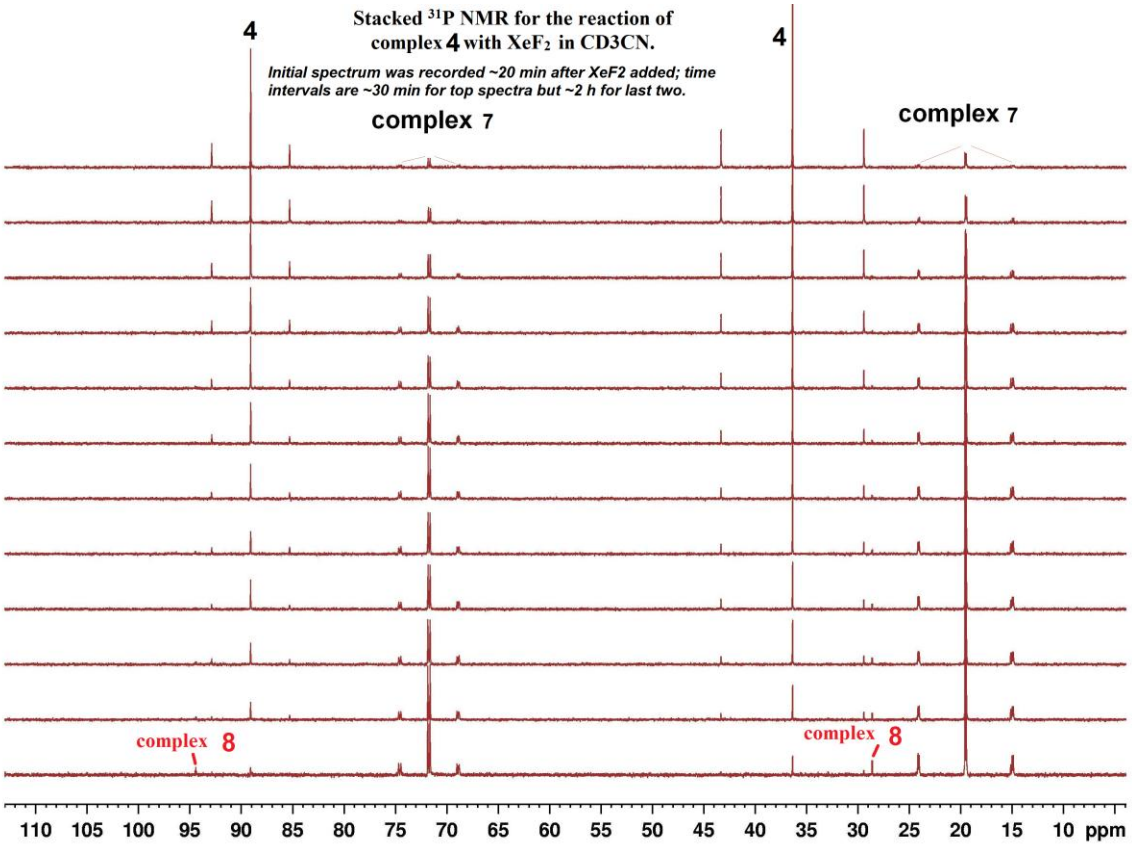
Reactions of **4** with XeF_2 proceeded to completion within ~ 5 h at room temperature, leading to two Pt(IV) complexes, identified to be **7** (>95% yield) and **8** (<5% yield), respectively. Complexes **7** and **8** were fully characterized by ^1H, ^{31}P, and ^{19}F NMR as well as HRMS; both their structures were verified by X-ray diffraction analysis.

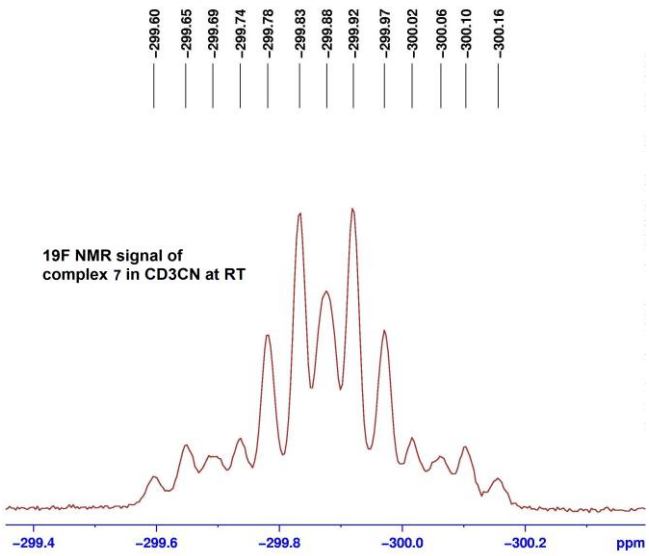
Note: Heating a solution of complex **7** in CD_3CN at 80 ^oC led to its slow conversion into complex **8** (~40% conv., 18 h).

*Characterization data of **7**:* ^1H NMR (500 MHz, CD_3CN): δ 7.90 (br, 1H) 7.70 (br, 1H),7.63 (t, 1H), 7.57-7.31 (m, 10H), 7.12 (m, 8H), 7.04 (t, 4H), 6.95 (m, 2H), 6.92 (m, 4H), 6.44 (m, 2H), 6.0 (t, 1H), 5.87 (d, with satellites, 1H), 3.95-3.70 (m, 2H), 3.40-3.20 (m, 4H), 3.02 (m, 2H) ppm. ^{31}P NMR (202 MHz, CD_3CN): δ 71.7 (d, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1151 Hz, $J_{P\text{-}F}$ = 41 Hz, $J_{P\text{-}P}$ = 5 Hz), 19.5 (d, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 1822 Hz, $J_{P\text{-}F}$ = 25 Hz, $J_{P\text{-}P}$ = 5 Hz) ppm. ^{19}F NMR (470 MHz, CD_3CN): δ -299.9 (doublet of triplet, with Pt satellites, $J_{Pt\text{-}F}$ = 173 Hz, $J_{P\text{-}F}$ = 52 Hz, $J_{P\text{-}F}$ = 24 Hz). HRMS (ESI) for $[C_{46}H_{41}FP_3Pt]^+$: calc. 900.2047, found 900.2030.

Supporting ^1H, ^{31}P and ^{19}F NMR spectra:


Stacked ^{1}H NMR for the reaction of complex 4 with XeF_2.
pure complex 4
XeF2 added
Room temperature
50 min
1.5 h
3.5 h
complex 7
5 h
after heating at
80 deg for 5 h
* Diagnostic 1H signals of complex 8
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm


Stacked ^{31}P NMR for the reaction of complex 4 with XeF_2 in CD3CN.
Initial spectrum was recorded ~20 min after XeF2 added; time intervals are ~30 min for top spectra but ~2 h for last two.
4
4
complex 7
complex 7
complex 8
complex 8
110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 ppm



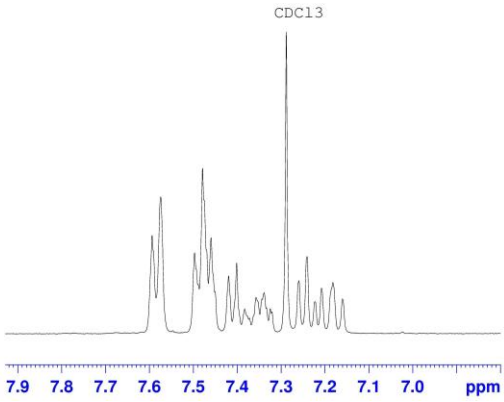
Selectfluor®:

Reactions of complex **4** with Selectfluor® proceeded to completion within 5 h at 80 °C, leading mainly to the Pt(IV) product complex **8** (~85% NMR yield). According to ^{31}P, ^{19}F NMR and GC-MS analysis, these reactions also produced the C-F coupling product 2-fluorobiphenyl (15% NMR yield), along with the corresponding by-product $[(triphos)Pt\text{-}MeCN]^{2+}$. 2-fluorobiphenyl was confirmed by GC-MS (m/z = 172) and NMR analyses.

*Characterization data of complex **8***: Diagnostic ^{1}H NMR signals (400 MHz, CD_3CN): δ 8.47 (t, J = 7.0 Hz, 1H), 7.05 (m, 1H), 6.72 (d, J = 7.8 Hz) ppm. ^{31}P NMR (202 MHz, CD_3CN): δ 94.4 (t, with Pt satellites, 1P, $J_{Pt\text{-}P}$ = 1172 Hz, $J_{P\text{-}P}$ = 16 Hz), 28.6 (d, with Pt satellites, 2P, $J_{Pt\text{-}P}$ = 1734 Hz, $J_{P\text{-}P}$ = 16 Hz) ppm. HRMS (ESI) for $C_{46}H_{41}FP_3Pt$ ($[M\text{-}MeCN\text{-}2(BF_4)]^{2+}/2$): calc. 440.6029, found 440.5959.

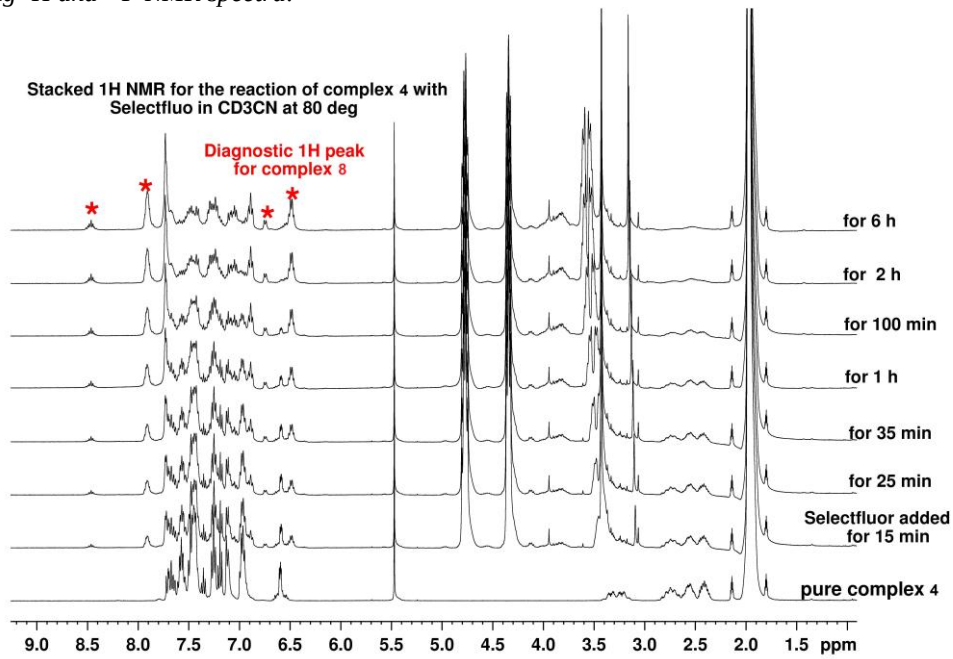
Characterization data of 2-fluoro-biphenyl: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, J = 8.0 Hz, 2H), 7.48 (m, 3H), 7.42-7.31 (m, 2H), 7.25 (d, J = 7.6 Hz, 1H), 7.22-7.15 (m, 1H) ppm. ^{19}F NMR (376 MHz, CD_3CN): δ -119.5 ppm.

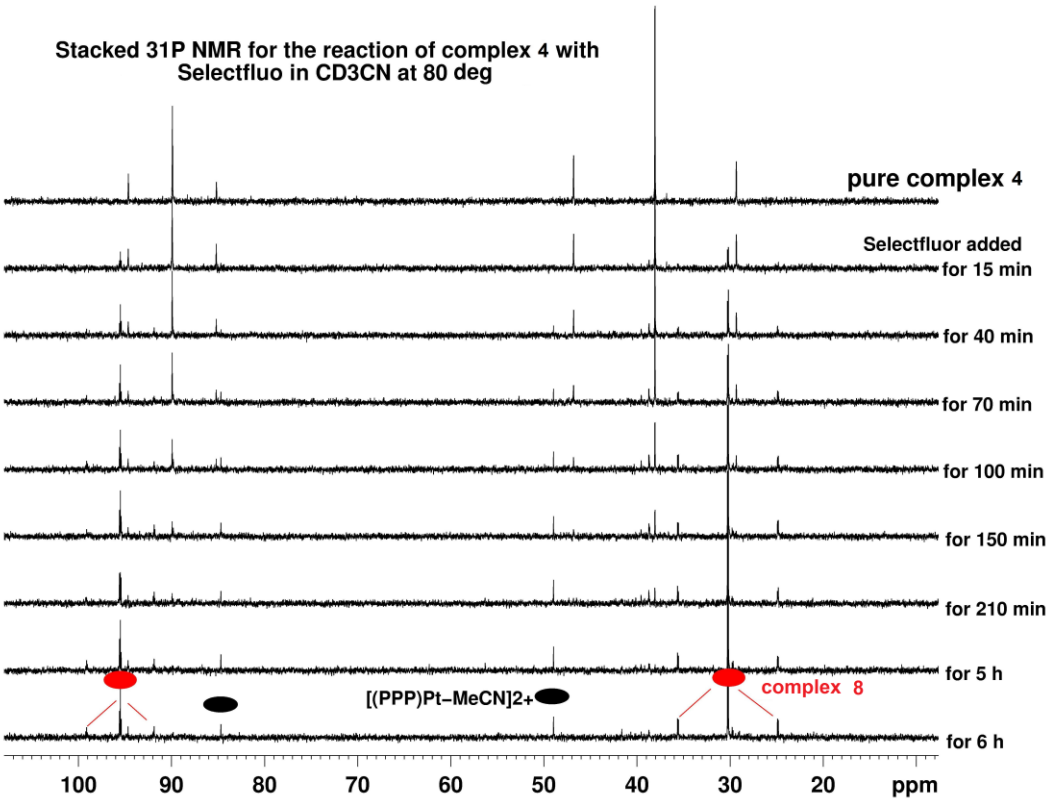
^{1}H NMR of 2-fluoro-biphenyl:



Note: Different from above reactions of **4** with XeF_2, no signs for the formation of the Pt(IV)-F complex **7** were observed for reactions of **4** with Selectfluor®.

Supporting ^{1}H and ^{31}P NMR spectra:

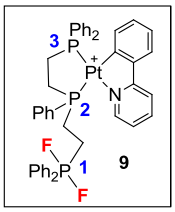




(3.5) For [(triphos)Pt-(2-*Py*)Ph](BF$_4$) (complex 5) and [(triphos)Pt-(2-*Ph*)Py](BF$_4$)$_2$ (complex 6):

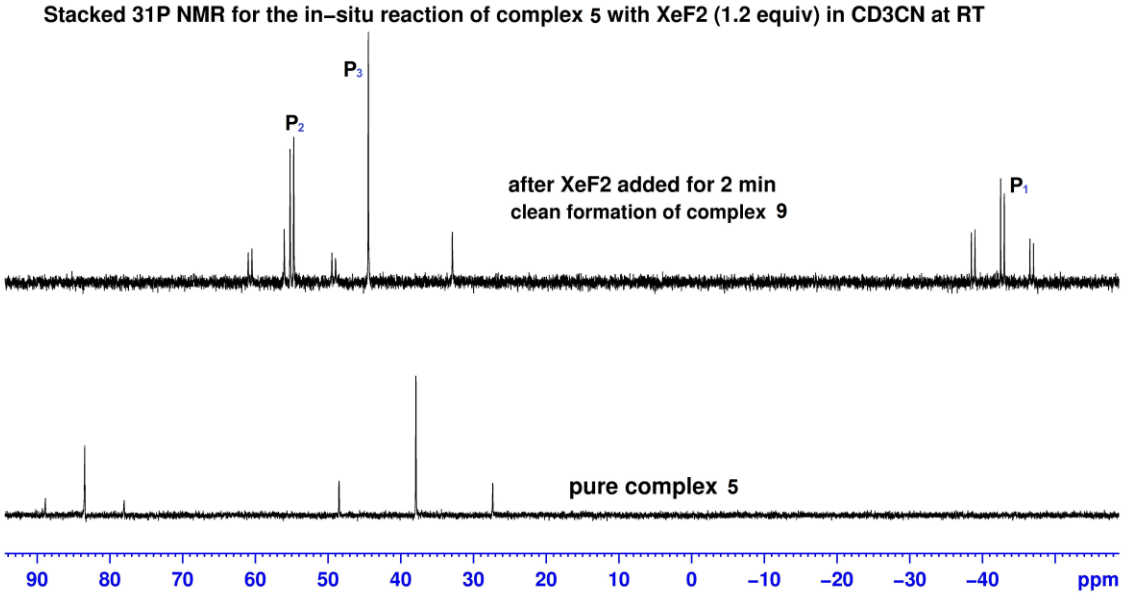
***XeF$_2$*:**

Reactions of complex **5** with XeF_2 (~1.2 equiv.) proceeded to completion within 3 min, generating complex **9** cleanly. No reaction between complex **6** and XeF_2 was observed under the reaction conditions.



Characterization data of complex **9**: ^{1}H NMR (400 MHz, CD_3CN): δ 8.06 (br, 6H), 7.95-7.70 (m, 10H), 7.52-7.30 (m, 18H), 7.20-7.09 (m, 2H), 7.02 (m, 1H), 6.62 (br, 1H), 3.33 (m, 1H), 2.80 (m, 2H), 2.70-1.98 (br, m, 5H) ppm. ^{31}P NMR (202 MHz, CD_3CN): δ 54.0 (d, with Pt satellites, for P_2, J_{Pt-P} = 1863 Hz, J_{P-P} = 16 Hz), 43.5 (doublet, with Pt satellites, for P_3, J_{Pt-P} = 3745 Hz, J_{P-P} = 80 Hz), -43.7 (triplet of doublet, for P_1, J_{P-F} = 652 Hz, J_{P-P} = 80 Hz) ppm. ^{19}F NMR (376 MHz, CD_3CN): δ -37.9 (d, J_{P-F} = 652 Hz) ppm.

Note: ^{31}P NMR data of this complex support the *trans*-configuration of the pyridyl moiety to the P_3 atom (J_{Pt-P3} = 3745 Hz), not the P_2 atom (J_{Pt-P2} = 1863 Hz, J_{P2-P1} = 80 Hz).



***Selectfluor*®**:

Reactions of complexes **5** and **6** with Selectfluor® were not examined after the observations of their above reaction modes with XeF_2.

S4. X-ray structure determinations and data tables for complexes 4, 7 and 8.

X-ray quality crystals of **4** were grown by slow evaporation of a CH_2Cl_2 solution of **4** at room temperature; those of **7** were obtained by slow diffusion of Et_2O into its MeCN solution at room temperature; crystals of complex **8** were obtained by slow evaporation of its MeCN solution at room temperature. Single crystals of these complexes were mounted in inert oil on the end of a fiber and transferred to the cold gas stream of the diffractometer. Intensity data for complex **4** were collected on a Siemens SMART diffractometer with CCD detection using Cu Kα radiation of wavelength 1.54178 Å (to scan mode). Intensity data for complexes **7** and **8** was performed on a Bruker SMART APEX II X-ray diffractometer with graphite-monochromated Mo K_α radiation of wavelength λ = 0.71073 Å.

Data were processed on a PC using the Bruker AXS Crystal Structure Analysis Package:[1] Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT (Bruker, 2005); structure solution: XPREP (Bruker, 2005) and SHELXTL (Bruker, 2000); structure refinement: SHELXTL; molecular graphics: SHELXTL; publication materials: SHELXTL. Neutral atom scattering factors were taken from Cromer and Waber.[2] The structure was solved by direct methods and refined by least-squares techniques on F^2. All non-hydrogen atoms were refined anisotropically. Full-matrix least-square refinements minimizing the function $\sum w (F_o^2 - F_c^2)^2$ were applied to the compound. All non-hydrogen atoms were refined anisotropically. All H atoms were placed in geometrically calculated positions, with C-H = 0.95 (aromatic), 0.99(CH_2), and 0.98(CH_3) Å, and refined as riding atoms, with Uiso(H) = 1.5UeqC(CH_3) or 1.2 UeqC(other C).

Special refinement details for the structure of complex **8**: The crystal used was non-merohedrally twinned *via* a 3.5 ° rotation about the real axis (0,1,0). This was determined with the program *CELL_NOW* (Bruker, 2008/2). Integration of the raw intensity data for the two twin components was accomplished with *SAINT* (Bruker, 2005) as controlled by the two-component orientation matrix generated by *CELL_NOW* and the data were further corrected for absorption and decay effects with *TWINABS* (Bruker, 2008/4). Solution and refinement of the structure was accomplished with the HKL4 format reflections, which included contributions of the single reflections from both twin components. Difference electron density maps revealed the presence of disordered BF_4^-, PF_6^-, F^- and lattice water molecules, which were ultimately modeled through the use of the SQUEEZE subroutine of the PLATON software suite. PLATON (Reference: P. v. d. Sluis & A.L. Spek. Acta Cryst. (1990), A46, 194.). One accessible void per lattice was found, comprising a total volume of 1249 $Å^3$ and contributing a total of 423 electrons. The void was assigned to four BF_4^-, two PF_6^-, ten F^- and 5.5 water molecules, which contribute 4 x 41 + 2 x 52 + 10 x 10 + 5.5 x 10 = 423 electrons, and occupy about 1000 $Å^3$ in space. The larger volume of the void may be a result of the disorder. The contributions have been included in all derived crystal quantities. Note: The PF_6^- anion and water molecules were accidentally introduced to the complex when we were trying different conditions in order to crystallize **8**. Also, one of the phenyl rings is disordered, which was refined into two orientations with the occupancies refined to 0.63 and 0.37. SHELX restraints: "SADI P3 C29a P3 C29b" and "EADP C29a > C34b" were applied to refined the disorder.

Crystallographic data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters, and torsion angles of these complexes are given in the following tables. The crystal structures of complexes **4**, **7** and **8** have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers **CCDC 838071 – 838073**, respectively.

S6.1 Labeling diagram and data tables for complex 4 (CCDC 838071).

ORTEP drawing of compound **4** with thermal ellipsoids drawn at 30% probability level. (all H atoms, the BF_4^- anion and solvent molecules are omitted for clarity)

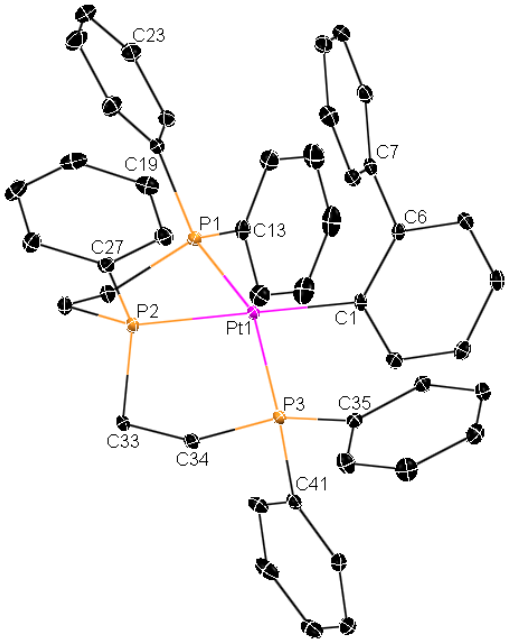


Table 1. Crystal data and structure refinement for complex **4**

Identification code	x1103019
Empirical formula	$C_{47}H_{44}BCl_2F_4P_3Pt$
Formula weight	1054.53
Temperature / K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a / Å, b / Å, c / Å	11.1844(10), 15.4199(2), 24.7809(3)
α/°, β/°, γ/°	90.00, 91.93(1), 90.00
Volume / $Å^3$	4271.35(8)
Z	4
ρ_{calc} / mg mm^{-3}	1.640
μ / mm^{-1}	8.785
F(000)	2096
Crystal size / mm^3	0.36 ×0.16 ×0.11
2θ range for data collection	3.56 to 144.32 °
Index ranges	$-13 \le h \le 12$, $-18 \le k \le 17$, $-29 \le l \le 30$
Reflections collected	36354
Independent reflections	8252[R(int) = 0.0182]
Data/restraints/parameters	8252/0/524
Goodness-of-fit on F^2	1.080
Final R indexes [I>2σ (I)]	R_1 = 0.0241, wR_2 = 0.0604
Final R indexes [all data]	R_1 = 0.0245, wR_2 = 0.0607
Largest diff. peak/hole / e $Å^{-3}$	1.665/-1.347

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for complex 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt1	6541.83(8)	2240.95(6)	1045.62(4)	10.31(4)
P1	5764.9(5)	3592.1(4)	847.5(2)	12.21(12)
P2	4576.2(5)	1848.5(4)	967.2(2)	12.88(12)
P3	6937.2(5)	793.2(4)	943.9(2)	11.37(12)
C1	8318(2)	2659.7(16)	1068.2(10)	12.5(5)
C2	9093(2)	2491.0(18)	648.7(11)	16.2(5)
C3	10237(2)	2856.1(18)	633.6(11)	17.7(5)
C4	10623(2)	3424.5(18)	1034.2(11)	18.1(5)
C5	9888(2)	3591.6(18)	1460.5(11)	17.5(5)
C6	8753(2)	3209.6(17)	1485.3(10)	13.5(5)
C7	8037(2)	3386.6(18)	1970.3(10)	14.9(5)
C8	7889(2)	4236.0(18)	2160.1(11)	17.8(5)
C9	7262(2)	4392.0(19)	2624.4(11)	20.4(5)
C10	6771(2)	3711(2)	2906.0(11)	20.9(6)
C11	6911(3)	2864.9(19)	2723.4(11)	20.5(6)
C12	7541(2)	2705.1(17)	2259.8(11)	16.9(5)
C13	6767(2)	4354.3(18)	546.2(11)	16.9(5)
C14	7299(3)	4126(2)	63.5(12)	23.9(6)
C15	8170(3)	4656(2)	-146.4(13)	29.7(7)
C16	8516(3)	5404(2)	124.7(14)	30.7(7)
C17	7985(3)	5640(2)	596.5(14)	29.2(7)
C18	7106(2)	5113.9(19)	809.8(12)	21.4(6)
C19	4910(2)	4170.7(17)	1343(1)	14.9(5)
C20	4289(3)	4927.0(19)	1200.8(11)	22.5(6)
C21	3531(3)	5308(2)	1563.3(13)	28.1(6)
C22	3386(3)	4936(2)	2069.9(12)	26.3(6)
C23	4013(3)	4197(2)	2215.6(11)	22.8(6)
C24	4778(2)	3811.0(18)	1852.6(10)	17.0(5)
C25	4609(2)	3324.5(18)	326.4(10)	16.5(5)
C26	3738(2)	2654.5(17)	555.3(11)	16.8(5)
C27	3802(2)	1720.8(17)	1598(1)	15.8(5)
C28	2567(2)	1843.3(18)	1627.6(12)	20.8(6)
C29	2037(3)	1829.4(19)	2126.3(13)	25.4(6)
C30	2722(3)	1680.3(19)	2595.5(12)	26.1(6)
C31	3940(3)	1533.7(19)	2567.9(12)	24.0(6)
C32	4480(2)	1560.5(18)	2071.7(11)	19.7(5)
C33	4538(2)	793.0(17)	632.2(11)	16.2(5)
C34	5482(2)	218.7(17)	922.5(10)	15.2(5)
C35	7888(2)	179.3(17)	1411.1(10)	14.1(5)
C36	7644(3)	-688.2(19)	1515.8(11)	21.6(6)
C37	8427(3)	-1168(2)	1846.0(12)	24.7(6)
C38	9449(2)	-785(2)	2070.8(11)	21.0(6)
C39	9690(2)	80.6(19)	1972.7(11)	19.8(5)
C40	8909(2)	570.7(18)	1644.4(10)	16.6(5)
C41	7532(2)	562.3(18)	280.6(10)	15.1(5)
C42	8263(2)	-152(2)	193.4(11)	20.8(6)
C43	8682(2)	-317(2)	-322.7(12)	26.8(7)
C44	8366(3)	230(2)	-747.8(12)	28.2(7)
C45	7624(3)	937(2)	-662.8(11)	26.0(6)
C46	7208(2)	1105.9(18)	-152.7(11)	19.2(5)
Cl1	10059.9(12)	2550.8(9)	4200.4(4)	65.5(4)

Cl2	9544.4(8)	1450.4(7)	3259.8(4)	49.9(2)
C51	9068(3)	2342(2)	3651.5(16)	37.7(8)
F1	5968(2)	2343.8(14)	4046.2(9)	42.6(5)
F2	4056(2)	1862.8(14)	3967.9(9)	47.6(6)
F3	4612.0(16)	3049.7(13)	3502.7(7)	30.4(4)
F4	4460.3(18)	3127.3(12)	4410.8(7)	32.0(4)
B1	4759(3)	2590(2)	3978.0(13)	22.5(6)

Table 3. Bond lengths for complex 4.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Pt1	P1	2.3040(6)	C19	C20	1.397(4)
Pt1	P2	2.2822(6)	C19	C24	1.392(4)
Pt1	P3	2.2913(6)	C20	C21	1.386(4)
Pt1	C1	2.088(2)	C21	C22	1.395(4)
P1	C13	1.803(3)	C22	C23	1.381(4)
P1	C19	1.816(3)	C23	C24	1.396(4)
P1	C25	1.843(3)	C25	C26	1.541(4)
P2	C26	1.844(3)	C27	C28	1.399(4)
P2	C27	1.823(3)	C27	C32	1.398(4)
P2	C33	1.827(3)	C28	C29	1.389(4)
P3	C34	1.852(2)	C29	C30	1.390(5)
P3	C35	1.813(3)	C30	C31	1.385(4)
P3	C41	1.829(3)	C31	C32	1.388(4)
C1	C2	1.400(4)	C33	C34	1.538(4)
C1	C6	1.411(4)	C35	C36	1.391(4)
C2	C3	1.400(4)	C35	C40	1.399(4)
C3	C4	1.383(4)	C36	C37	1.391(4)
C4	C5	1.385(4)	C37	C38	1.387(4)
C5	C6	1.402(4)	C38	C39	1.384(4)
C6	C7	1.492(3)	C39	C40	1.396(4)
C7	C8	1.403(4)	C41	C42	1.393(4)
C7	C12	1.398(4)	C41	C46	1.400(4)
C8	C9	1.388(4)	C42	C43	1.400(4)
C9	C10	1.384(4)	C43	C44	1.386(5)
C10	C11	1.392(4)	C44	C45	1.390(5)
C11	C12	1.390(4)	C45	C46	1.386(4)
C13	C14	1.399(4)	Cl1	C51	1.756(4)
C13	C18	1.388(4)	Cl2	C51	1.775(4)
C14	C15	1.386(4)	F1	B1	1.409(4)
C15	C16	1.384(5)	F2	B1	1.368(4)
C16	C17	1.378(5)	F3	B1	1.380(4)
C17	C18	1.392(4)	F4	B1	1.405(4)

Table 4. Bond Angles for complex 4.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
P2	Pt1	P1	82.32(2)	C17	C16	C15	120.7(3)
P2	Pt1	P3	85.48(2)	C16	C17	C18	119.9(3)
P3	Pt1	P1	158.49(2)	C13	C18	C17	119.9(3)
C1	Pt1	P1	94.45(7)	C20	C19	P1	120.6(2)

C1	Pt1	P2	175.76(7)	C24	C19	P1	119.5(2)
C1	Pt1	P3	96.74(7)	C24	C19	C20	119.7(2)
C13	P1	Pt1	116.25(9)	C21	C20	C19	120.0(3)
C13	P1	C19	107.98(12)	C20	C21	C22	120.1(3)
C13	P1	C25	106.68(12)	C23	C22	C21	120.1(3)
C19	P1	Pt1	120.24(9)	C22	C23	C24	120.0(3)
C19	P1	C25	102.17(12)	C19	C24	C23	120.1(3)
C25	P1	Pt1	101.39(9)	C26	C25	P1	109.22(18)
C26	P2	Pt1	109.79(9)	C25	C26	P2	109.88(18)
C27	P2	Pt1	116.07(9)	C28	C27	P2	121.9(2)
C27	P2	C26	107.48(12)	C32	C27	P2	118.68(19)
C27	P2	C33	106.80(12)	C32	C27	C28	119.2(2)
C33	P2	Pt1	106.40(8)	C29	C28	C27	119.8(3)
C33	P2	C26	110.21(12)	C28	C29	C30	120.5(3)
C34	P3	Pt1	107.25(9)	C31	C30	C29	120.1(3)
C35	P3	Pt1	123.36(9)	C30	C31	C32	119.8(3)
C35	P3	C34	105.34(12)	C31	C32	C27	120.7(3)
C35	P3	C41	104.43(12)	C34	C33	P2	107.18(17)
C41	P3	Pt1	111.47(9)	C33	C34	P3	109.05(17)
C41	P3	C34	103.12(11)	C36	C35	P3	120.4(2)
C2	C1	Pt1	122.34(19)	C36	C35	C40	120.0(2)
C2	C1	C6	116.6(2)	C40	C35	P3	119.5(2)
C6	C1	Pt1	120.68(18)	C37	C36	C35	119.8(3)
C3	C2	C1	122.3(2)	C38	C37	C36	120.2(3)
C4	C3	C2	120.0(2)	C39	C38	C37	120.2(3)
C3	C4	C5	119.1(2)	C38	C39	C40	120.2(3)
C4	C5	C6	121.1(2)	C39	C40	C35	119.5(3)
C1	C6	C7	121.2(2)	C42	C41	P3	121.8(2)
C5	C6	C1	120.7(2)	C42	C41	C46	119.5(2)
C5	C6	C7	118.0(2)	C46	C41	P3	118.7(2)
C8	C7	C6	120.9(2)	C41	C42	C43	120.1(3)
C12	C7	C6	120.6(2)	C44	C43	C42	119.9(3)
C12	C7	C8	118.5(2)	C43	C44	C45	120.0(3)
C9	C8	C7	120.5(3)	C46	C45	C44	120.4(3)
C10	C9	C8	120.4(3)	C45	C46	C41	120.1(3)
C9	C10	C11	119.8(3)	Cl1	C51	Cl2	111.8(2)
C12	C11	C10	120.0(3)	F2	B1	F1	109.3(3)
C11	C12	C7	120.8(3)	F2	B1	F3	110.7(3)
C14	C13	P1	118.5(2)	F2	B1	F4	110.3(3)
C18	C13	P1	121.3(2)	F3	B1	F1	109.1(3)
C18	C13	C14	119.9(3)	F3	B1	F4	108.9(3)
C15	C14	C13	119.8(3)	F4	B1	F1	108.6(3)
C16	C15	C14	119.9(3)				

Table 5. Torsion angles for complex 4.

A	B	C	D	Angle/°
Pt1	P1	C13	C14	57.3(2)
Pt1	P1	C13	C18	-116.2(2)
Pt1	P1	C19	C20	-170.48(19)
Pt1	P1	C19	C24	3.2(2)
Pt1	P1	C25	C26	56.47(18)
Pt1	P2	C26	C25	5.8(2)
Pt1	P2	C27	C28	152.7(2)
Pt1	P2	C27	C32	-22.4(2)
Pt1	P2	C33	C34	47.88(18)
Pt1	P3	C34	C33	35.12(18)
Pt1	P3	C35	C36	146.11(19)
Pt1	P3	C35	C40	-37.3(2)
Pt1	P3	C41	C42	153.98(19)
Pt1	P3	C41	C46	-28.0(2)
Pt1	C1	C2	C3	172.3(2)
Pt1	C1	C6	C5	-170.75(19)
Pt1	C1	C6	C7	10.6(3)
P1	Pt1	P2	C26	22.23(10)
P1	Pt1	P2	C27	-99.87(10)
P1	Pt1	P2	C33	141.48(9)
P1	Pt1	P3	C34	-60.18(11)
P1	Pt1	P3	C35	177.41(10)
P1	Pt1	P3	C41	52.00(11)
P1	Pt1	C1	C2	-104.2(2)
P1	Pt1	C1	C6	68.9(2)
P1	C13	C14	C15	-173.1(2)
P1	C13	C18	C17	172.6(2)
P1	C19	C20	C21	172.6(2)
P1	C19	C24	C23	-172.6(2)
P1	C25	C26	P2	-40.0(2)
P2	Pt1	P1	C13	-155.26(10)
P2	Pt1	P1	C19	71.44(10)
P2	Pt1	P1	C25	-40.05(9)
P2	Pt1	P3	C34	-4.67(9)
P2	Pt1	P3	C35	-127.09(10)
P2	Pt1	P3	C41	107.50(9)
P2	Pt1	C1	C2	-64.0(11)
P2	Pt1	C1	C6	109.1(10)
P2	C27	C28	C29	-173.2(2)
P2	C27	C32	C31	174.4(2)
P2	C33	C34	P3	-53.1(2)
P3	Pt1	P1	C13	-99.26(11)
P3	Pt1	P1	C19	127.44(10)
P3	Pt1	P1	C25	15.95(11)
P3	Pt1	P2	C26	-140.02(10)
P3	Pt1	P2	C27	97.88(10)
P3	Pt1	P2	C33	-20.77(9)
P3	Pt1	C1	C2	57.4(2)
P3	Pt1	C1	C6	-129.48(19)
P3	C35	C36	C37	175.5(2)
P3	C35	C40	C39	-175.3(2)

P3	C41	C42	C43	178.8(2)
P3	C41	C46	C45	-178.7(2)
C1	Pt1	P1	C13	21.99(12)
C1	Pt1	P1	C19	-111.31(12)
C1	Pt1	P1	C25	137.19(11)
C1	Pt1	P2	C26	-18.3(10)
C1	Pt1	P2	C27	-140.3(10)
C1	Pt1	P2	C33	101.0(10)
C1	Pt1	P3	C34	178.95(11)
C1	Pt1	P3	C35	56.54(12)
C1	Pt1	P3	C41	-68.87(11)
C1	C2	C3	C4	-1.9(4)
C1	C6	C7	C8	-132.8(3)
C1	C6	C7	C12	50.0(3)
C2	C1	C6	C5	2.8(4)
C2	C1	C6	C7	-175.9(2)
C2	C3	C4	C5	3.1(4)
C3	C4	C5	C6	-1.4(4)
C4	C5	C6	C1	-1.6(4)
C4	C5	C6	C7	177.1(2)
C5	C6	C7	C8	48.5(3)
C5	C6	C7	C12	-128.6(3)
C6	C1	C2	C3	-1.0(4)
C6	C7	C8	C9	-177.4(2)
C6	C7	C12	C11	177.6(2)
C7	C8	C9	C10	-0.1(4)
C8	C7	C12	C11	0.4(4)
C8	C9	C10	C11	0.2(4)
C9	C10	C11	C12	0.0(4)
C10	C11	C12	C7	-0.3(4)
C12	C7	C8	C9	-0.2(4)
C13	P1	C19	C20	52.8(2)
C13	P1	C19	C24	-133.5(2)
C13	P1	C25	C26	178.57(18)
C13	C14	C15	C16	0.6(5)
C14	C13	C18	C17	-0.8(4)
C14	C15	C16	C17	-1.5(5)
C15	C16	C17	C18	1.2(5)
C16	C17	C18	C13	-0.1(4)
C18	C13	C14	C15	0.5(4)
C19	P1	C13	C14	-164.1(2)
C19	P1	C13	C18	22.4(3)
C19	P1	C25	C26	-68.2(2)
C19	C20	C21	C22	-0.1(5)
C20	C19	C24	C23	1.1(4)
C20	C21	C22	C23	1.1(5)
C21	C22	C23	C24	-1.0(5)
C22	C23	C24	C19	-0.1(4)
C24	C19	C20	C21	-1.0(4)
C25	P1	C13	C14	-54.9(2)
C25	P1	C13	C18	131.6(2)
C25	P1	C19	C20	-59.4(2)
C25	P1	C19	C24	114.3(2)
C26	P2	C27	C28	29.4(3)
C26	P2	C27	C32	-145.7(2)
C26	P2	C33	C34	166.86(17)

C27	P2	C26	C25	132.86(19)
C27	P2	C33	C34	-76.69(19)
C27	C28	C29	C30	-1.1(4)
C28	C27	C32	C31	-0.8(4)
C28	C29	C30	C31	-0.8(5)
C29	C30	C31	C32	1.8(5)
C30	C31	C32	C27	-1.0(4)
C32	C27	C28	C29	1.9(4)
C33	P2	C26	C25	-111.11(19)
C33	P2	C27	C28	-88.8(2)
C33	P2	C27	C32	96.1(2)
C34	P3	C35	C36	22.8(2)
C34	P3	C35	C40	-160.6(2)
C34	P3	C41	C42	-91.3(2)
C34	P3	C41	C46	86.7(2)
C35	P3	C34	C33	168.14(17)
C35	P3	C41	C42	18.6(2)
C35	P3	C41	C46	-163.4(2)
C35	C36	C37	C38	0.0(4)
C36	C35	C40	C39	1.3(4)
C36	C37	C38	C39	0.7(4)
C37	C38	C39	C40	-0.4(4)
C38	C39	C40	C35	-0.6(4)
C40	C35	C36	C37	-1.0(4)
C41	P3	C34	C33	-82.64(19)
C41	P3	C35	C36	-85.4(2)
C41	P3	C35	C40	91.1(2)
C41	C42	C43	C44	-0.2(4)
C42	C41	C46	C45	-0.7(4)
C42	C43	C44	C45	-0.6(4)
C43	C44	C45	C46	0.7(4)
C44	C45	C46	C41	-0.1(4)
C46	C41	C42	C43	0.8(4)

Table 6. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for complex 4.

Atom	***x***	***y***	***z***	**U(eq)**
H2	8833	2115	364	19
H3	10748	2713	348	21
H4	11383	3697	1017	22
H5	10156	3972	1741	21
H8	8221	4708	1970	21
H9	7169	4970	2749	24
H10	6341	3822	3223	25
H11	6575	2396	2916	25
H12	7636	2126	2138	20
H14	7065	3608	-120	29
H15	8528	4506	-476	36
H16	9126	5759	-16	37
H17	8218	6160	776	35
H18	6739	5275	1135	26
H20	4385	5180	856	27
H21	3109	5823	1466	34

H22	2855	5193	2315	32
H23	3923	3950	2563	27
H24	5210	3302	1954	20
H25A	4167	3856	217	20
H25B	4989	3084	4	20
H26A	3297	2359	255	20
H26B	3149	2952	780	20
H28	2092	1936	1308	25
H29	1200	1923	2147	31
H30	2354	1679	2936	31
H31	4405	1415	2887	29
H32	5317	1469	2054	24
H33A	3735	529	655	19
H33B	4724	858	246	19
H34A	5558	-338	728	18
H34B	5235	92	1294	18
H36	6945	-952	1362	26
H37	8261	-1760	1918	30
H38	9985	-1117	2293	25
H39	10388	342	2129	24
H40	9070	1166	1580	20
H42	8478	-527	485	25
H43	9183	-803	-381	32
H44	8656	122	-1097	34
H45	7401	1307	-956	31
H46	6702	1591	-97	23
H51A	9006	2865	3420	45
H51B	8263	2218	3787	45

Table 7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for complex 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt1	8.91(6)	9.83(6)	12.18(6)	-0.71(3)	0.07(4)	-1.36(3)
P1	11.9(3)	10.6(3)	14.0(3)	0.1(2)	0.5(2)	-0.5(2)
P2	9.4(3)	12.8(3)	16.4(3)	-1.0(2)	-0.1(2)	-1.7(2)
P3	10.7(3)	10.9(3)	12.5(3)	-0.6(2)	0.2(2)	-1.2(2)
C1	8.9(11)	11.1(12)	17.4(12)	3.8(9)	-1.0(9)	-2.9(9)
C2	15.9(12)	14.7(13)	18.0(12)	-1.2(10)	-0.2(10)	-1.6(10)
C3	14.7(12)	19.7(14)	18.9(13)	2.9(10)	4.3(10)	0.4(10)
C4	11.9(11)	19.8(14)	22.6(13)	3.2(11)	-0.2(10)	-4(1)
C5	16.0(12)	19.2(13)	17.2(12)	-1.9(10)	-2.8(10)	-3(1)
C6	11.7(11)	13.3(12)	15.3(11)	2.3(9)	-1.2(9)	0.2(9)
C7	11.4(11)	19.0(13)	14.3(11)	-0.2(10)	-3.4(9)	-1.9(10)
C8	15.6(12)	17.6(13)	20.1(13)	-1.1(10)	-2(1)	-3.1(10)
C9	18.5(12)	20.1(14)	22.4(13)	-6.4(11)	-3.1(10)	0.4(11)
C10	18.1(12)	29.8(16)	14.7(12)	-4.0(11)	0.6(10)	-0.3(11)
C11	22.3(14)	23.7(15)	15.4(13)	4(1)	-0.5(11)	-3.9(11)
C12	16.9(13)	16.4(14)	17.3(13)	-0.1(9)	-2.7(10)	-0.8(10)
C13	13.5(11)	15.6(13)	21.5(13)	4.5(10)	-1.1(10)	-1(1)
C14	24.3(14)	24.7(15)	22.8(14)	1.4(11)	2.9(11)	-3.3(12)
C15	24.2(14)	38.4(19)	26.8(15)	10.5(13)	7.0(12)	-2.3(13)
C16	19.8(13)	29.0(17)	43.1(18)	18.3(14)	1.6(12)	-6.1(12)
C17	26.1(15)	19.3(15)	42.0(18)	4.4(13)	-2.2(13)	-8.3(12)
C18	20.4(13)	17.2(14)	26.5(14)	1.3(11)	1.2(11)	-2.6(11)

C19	12.3(11)	15.0(13)	17.4(12)	-3.2(10)	-0.1(9)	-0.8(9)
C20	23.7(14)	21.8(15)	22.2(13)	2.5(11)	1.2(11)	4.8(11)
C21	28.5(15)	22.4(15)	33.5(16)	-0.8(12)	1.6(12)	11.2(12)
C22	22.6(14)	29.2(17)	27.4(15)	-7.8(12)	5.5(11)	5.5(12)
C23	22.0(13)	28.6(16)	18.1(13)	-3.0(11)	3.7(10)	-0.6(12)
C24	17.1(12)	14.8(13)	18.9(12)	-0.8(10)	-1.5(10)	0.1(10)
C25	14.3(11)	19.2(13)	16.1(12)	0.7(10)	-1.9(9)	-0.7(10)
C26	13.2(12)	16.1(13)	20.9(13)	1(1)	-2(1)	-0.1(10)
C27	15.6(12)	12.3(12)	19.6(12)	-1.3(10)	2.9(10)	-2.1(10)
C28	16.8(13)	16.1(14)	29.7(14)	2.1(11)	3.3(11)	-1.5(10)
C29	21.1(13)	17.9(14)	38.2(16)	0.9(12)	12.8(12)	1.2(11)
C30	36.3(16)	16.0(14)	27.1(15)	-2.2(11)	15.9(12)	-1.4(12)
C31	30.4(15)	21.6(15)	20.1(13)	-1.7(11)	2.1(11)	-3.3(12)
C32	18.8(13)	18.1(14)	22.3(13)	-1.2(11)	1.3(10)	-3.5(10)
C33	11.3(11)	16.8(13)	20.5(12)	-4.1(10)	-1.6(9)	-2.5(10)
C34	13.2(11)	14.3(12)	18.2(12)	-2.4(10)	0.8(9)	-4(1)
C35	14.7(11)	14.8(13)	12.7(11)	0.9(9)	1.4(9)	1.3(10)
C36	21.7(13)	18.1(14)	24.6(14)	3.7(11)	-2.7(11)	-5.0(11)
C37	28.8(15)	18.9(14)	26.4(14)	8.3(11)	0.4(12)	-1.3(12)
C38	21.4(13)	25.2(15)	16.3(12)	5.4(11)	-0.2(10)	6.1(11)
C39	16.3(12)	24.1(15)	18.6(12)	-2.1(11)	-3.7(10)	2.4(11)
C40	16.7(12)	14.9(13)	18.2(12)	-0.6(10)	-0.3(10)	1.4(10)
C41	12.6(11)	18.4(13)	14.2(12)	-3(1)	0.3(9)	-4.6(10)
C42	14.3(12)	26.1(15)	22.1(13)	-5.8(11)	0.4(10)	-1.2(11)
C43	14.6(12)	36.2(18)	29.9(15)	-15.6(13)	4.5(11)	-1.4(12)
C44	23.4(14)	41.5(19)	20.1(13)	-12.9(13)	9.2(11)	-15.1(13)
C45	33.4(16)	28.5(16)	16.3(13)	0.6(11)	1.5(11)	-17.7(13)
C46	22.8(13)	16.9(13)	17.9(13)	-2.5(10)	-0.6(10)	-6.2(10)
Cl1	83.3(8)	72.8(7)	38.9(5)	-13.3(5)	-20.3(5)	51.3(7)
Cl2	38.2(4)	53.0(6)	58.4(6)	-17.4(5)	3.0(4)	7.3(4)
C51	36.3(19)	34(2)	42(2)	1.9(15)	4.0(15)	6.6(15)
F1	42.8(12)	40.2(12)	43.8(12)	-5.2(9)	-12.1(9)	19.8(9)
F2	67.9(15)	29.8(11)	46.0(12)	-9.0(9)	13.2(10)	-22.8(11)
F3	32.6(9)	35.7(11)	23.5(8)	10.3(8)	8.4(7)	11.2(8)
F4	55.7(12)	19.5(9)	21.0(8)	-1.2(7)	4.2(8)	4.4(8)
B1	32.8(17)	15.6(15)	18.8(15)	1.2(12)	-1.1(13)	0.5(13)

S6.2 Labeling diagram and data tables for complex 7 (CCDC 838072).

ORTEP drawing of compound **7** with thermal ellipsoids drawn at 30% probability level. (all H atoms, the BF_4^- anion and solvent moleclues are omitted for clarity)

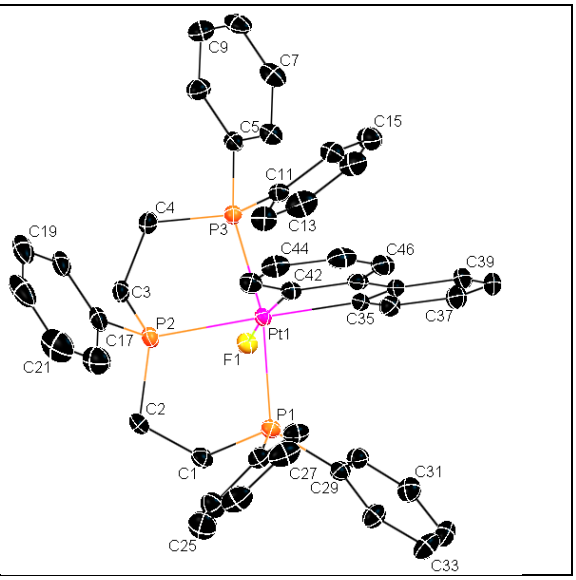


Table 1. Crystal data and structure refinement for complex **7.**

Identification code	zsnew01a	
Empirical formula	C49 H48 B F5 N O2 P3 Pt	
Formula weight	1076.69	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 31.7695(19) Å	α= 90 °.
	b = 10.0332(6) Å	β= 116.680(1) °.
	c = 33.988(3) Å	γ = 90 °.
Volume	9680.2(12) $Å^3$	
Z	8	
Density (calculated)	1.478 Mg/m^3	
Absorption coefficient	3.056 mm^{-1}	
F(000)	4304	
Crystal size	0.25 x 0.10 x 0.08 mm^3	
Theta range for data collection	3.57 to 26.00 °.	
Index ranges	-35<=h<=39, -12<=k<=12, -41<=l<=41	
Reflections collected	18908	
Independent reflections	9401 [R(int) = 0.0255]	
Completeness to theta = 26.00 °	98.7 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7921 and 0.5155	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9401 / 46 / 514	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0302, wR2 = 0.0685	
R indices (all data)	R1 = 0.0374, wR2 = 0.0707	
Largest diff. peak and hole	0.915 and -0.641 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for complex 7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	1658(1)	8472(1)	977(1)	24(1)
P(1)	1804(1)	9874(1)	496(1)	28(1)
P(2)	860(1)	9058(1)	520(1)	30(1)
P(3)	1373(1)	7552(1)	1447(1)	26(1)
F(1)	1632(1)	10253(2)	1289(1)	32(1)
C(1)	1366(1)	11182(4)	397(1)	34(1)
C(2)	869(1)	10632(4)	248(1)	38(1)
C(3)	653(1)	9412(4)	931(1)	33(1)
C(4)	785(1)	8306(4)	1275(1)	37(1)
C(5)	1278(1)	5782(4)	1490(1)	29(1)
C(6)	1502(1)	4800(4)	1371(1)	35(1)
C(7)	1441(2)	3462(4)	1446(1)	43(1)
C(8)	1158(2)	3123(4)	1642(1)	46(1)
C(9)	934(2)	4099(5)	1761(2)	50(1)
C(10)	992(2)	5425(4)	1685(1)	42(1)
C(11)	1735(1)	8054(4)	2012(1)	29(1)
C(12)	1686(2)	9317(4)	2152(1)	42(1)
C(13)	1980(2)	9708(5)	2580(2)	54(1)
C(14)	2316(2)	8853(5)	2865(1)	51(1)
C(15)	2369(2)	7604(5)	2727(1)	47(1)
C(16)	2076(1)	7202(4)	2299(1)	38(1)
C(17)	422(1)	8010(4)	100(1)	38(1)
C(18)	106(1)	7280(4)	183(2)	43(1)
C(19)	-222(2)	6448(4)	-138(2)	56(1)
C(20)	-226(2)	6346(5)	-543(2)	67(2)
C(21)	84(2)	7070(6)	-633(2)	77(2)
C(22)	414(2)	7910(5)	-311(1)	59(1)
C(23)	1692(1)	9212(4)	-40(1)	35(1)
C(24)	1393(2)	9901(5)	-422(1)	47(1)
C(25)	1294(2)	9380(6)	-829(2)	61(1)
C(26)	1488(2)	8178(5)	-861(2)	57(1)
C(27)	1793(2)	7522(5)	-488(2)	53(1)
C(28)	1899(2)	8034(4)	-74(1)	40(1)
C(29)	2364(1)	10743(4)	714(1)	32(1)
C(30)	2523(1)	11370(4)	1120(1)	36(1)
C(31)	2943(2)	12054(4)	1295(1)	43(1)
C(32)	3212(2)	12116(5)	1067(2)	49(1)
C(33)	3052(2)	11498(5)	665(2)	50(1)
C(34)	2627(1)	10820(4)	482(1)	40(1)
C(35)	2357(1)	8160(4)	1417(1)	28(1)
C(36)	2614(1)	8955(4)	1782(1)	37(1)
C(37)	3090(2)	8677(5)	2045(1)	47(1)
C(38)	3299(1)	7615(5)	1946(1)	49(1)
C(39)	3042(1)	6799(4)	1591(1)	42(1)
C(40)	2566(1)	7082(4)	1321(1)	30(1)
C(41)	2243(1)	6287(4)	940(1)	31(1)
C(42)	1772(1)	6744(3)	729(1)	28(1)
C(43)	1441(1)	6031(4)	381(1)	35(1)
C(44)	1564(2)	4871(4)	233(1)	43(1)
C(45)	2029(2)	4434(4)	439(2)	45(1)
C(46)	2366(2)	5132(4)	787(1)	40(1)

B(1)	4508(2)	12429(7)	979(2)	65(2)
F(2)	4655(1)	13625(4)	879(1)	82(1)
F(3A)	4853(2)	11483(7)	1099(3)	77(1)
F(4A)	4093(2)	12084(7)	612(2)	77(1)
F(5A)	4368(3)	12708(6)	1314(2)	77(1)
F(3B)	4903(5)	11850(20)	1306(6)	77(1)
F(4B)	4283(7)	12040(20)	531(4)	77(1)
F(5B)	4155(6)	12400(20)	1093(8)	77(1)
F(3C)	4761(7)	11348(18)	930(7)	77(1)
F(4C)	4063(5)	11960(20)	800(8)	77(1)
F(5C)	4651(7)	12592(19)	1429(4)	77(1)

Table 3. Bond lengths [Å] and angles [°] for complex 7.

Pt(1)-C(42)	2.031(3)	C(12)-H(12)	0.9500
Pt(1)-C(35)	2.070(3)	C(13)-C(14)	1.373(7)
Pt(1)-F(1)	2.097(2)	C(13)-H(13)	0.9500
Pt(1)-P(3)	2.3492(9)	C(14)-C(15)	1.374(7)
Pt(1)-P(1)	2.3569(10)	C(14)-H(14)	0.9500
Pt(1)-P(2)	2.3775(9)	C(15)-C(16)	1.389(5)
P(1)-C(29)	1.814(4)	C(15)-H(15)	0.9500
P(1)-C(23)	1.817(4)	C(16)-H(16)	0.9500
P(1)-C(1)	1.831(4)	C(17)-C(18)	1.372(6)
P(2)-C(17)	1.816(4)	C(17)-C(22)	1.390(6)
P(2)-C(3)	1.824(4)	C(18)-C(19)	1.398(6)
P(2)-C(2)	1.836(4)	C(18)-H(18)	0.9500
P(3)-C(11)	1.813(4)	C(19)-C(20)	1.375(8)
P(3)-C(5)	1.819(4)	C(19)-H(19)	0.9500
P(3)-C(4)	1.850(4)	C(20)-C(21)	1.363(8)
C(1)-C(2)	1.527(5)	C(20)-H(20)	0.9500
C(1)-H(1A)	0.9900	C(21)-C(22)	1.405(7)
C(1)-H(1B)	0.9900	C(21)-H(21)	0.9500
C(2)-H(2A)	0.9900	C(22)-H(22)	0.9500
C(2)-H(2B)	0.9900	C(23)-C(28)	1.383(6)
C(3)-C(4)	1.528(5)	C(23)-C(24)	1.399(6)
C(3)-H(3A)	0.9900	C(24)-C(25)	1.376(6)
C(3)-H(3B)	0.9900	C(24)-H(24)	0.9500
C(4)-H(4A)	0.9900	C(25)-C(26)	1.380(7)
C(4)-H(4B)	0.9900	C(25)-H(25)	0.9500
C(5)-C(6)	1.380(5)	C(26)-C(27)	1.369(7)
C(5)-C(10)	1.389(5)	C(26)-H(26)	0.9500
C(6)-C(7)	1.397(6)	C(27)-C(28)	1.390(6)
C(6)-H(6)	0.9500	C(27)-H(27)	0.9500
C(7)-C(8)	1.382(6)	C(28)-H(28)	0.9500
C(7)-H(7)	0.9500	C(29)-C(34)	1.388(5)
C(8)-C(9)	1.374(7)	C(29)-C(30)	1.388(5)
C(8)-H(8)	0.9500	C(30)-C(31)	1.374(6)
C(9)-C(10)	1.383(6)	C(30)-H(30)	0.9500
C(9)-H(9)	0.9500	C(31)-C(32)	1.392(6)
C(10)-H(10)	0.9500	C(31)-H(31)	0.9500
C(11)-C(16)	1.382(5)	C(32)-C(33)	1.373(6)
C(11)-C(12)	1.385(5)	C(32)-H(32)	0.9500
C(12)-C(13)	1.386(6)	C(33)-C(34)	1.384(6)

C(33)-H(33)	0.9500	C(17)-P(2)-C(2)	106.35(19)
C(34)-H(34)	0.9500	C(3)-P(2)-C(2)	108.07(19)
C(35)-C(40)	1.383(5)	C(17)-P(2)-Pt(1)	125.87(13)
C(35)-C(36)	1.390(5)	C(3)-P(2)-Pt(1)	101.14(12)
C(36)-C(37)	1.394(6)	C(2)-P(2)-Pt(1)	106.76(13)
C(36)-H(36)	0.9500	C(11)-P(3)-C(5)	103.57(17)
C(37)-C(38)	1.375(7)	C(11)-P(3)-C(4)	106.98(19)
C(37)-H(37)	0.9500	C(5)-P(3)-C(4)	104.15(18)
C(38)-C(39)	1.383(6)	C(11)-P(3)-Pt(1)	110.87(12)
C(38)-H(38)	0.9500	C(5)-P(3)-Pt(1)	124.55(12)
C(39)-C(40)	1.400(5)	C(4)-P(3)-Pt(1)	105.52(13)
C(39)-H(39)	0.9500	C(2)-C(1)-P(1)	112.9(3)
C(40)-C(41)	1.475(5)	C(2)-C(1)-H(1A)	109.0
C(41)-C(46)	1.396(5)	P(1)-C(1)-H(1A)	109.0
C(41)-C(42)	1.414(5)	C(2)-C(1)-H(1B)	109.0
C(42)-C(43)	1.377(5)	P(1)-C(1)-H(1B)	109.0
C(43)-C(44)	1.391(6)	H(1A)-C(1)-H(1B)	107.8
C(43)-H(43)	0.9500	C(1)-C(2)-P(2)	113.1(3)
C(44)-C(45)	1.393(6)	C(1)-C(2)-H(2A)	109.0
C(44)-H(44)	0.9500	P(2)-C(2)-H(2A)	109.0
C(45)-C(46)	1.378(6)	C(1)-C(2)-H(2B)	109.0
C(45)-H(45)	0.9500	P(2)-C(2)-H(2B)	109.0
C(46)-H(46)	0.9500	H(2A)-C(2)-H(2B)	107.8
B(1)-F(5B)	1.343(12)	C(4)-C(3)-P(2)	112.0(3)
B(1)-F(4C)	1.349(12)	C(4)-C(3)-H(3A)	109.2
B(1)-F(3A)	1.367(8)	P(2)-C(3)-H(3A)	109.2
B(1)-F(3B)	1.377(13)	C(4)-C(3)-H(3B)	109.2
B(1)-F(2)	1.383(6)	P(2)-C(3)-H(3B)	109.2
B(1)-F(4A)	1.392(7)	H(3A)-C(3)-H(3B)	107.9
B(1)-F(5C)	1.397(12)	C(3)-C(4)-P(3)	115.4(3)
B(1)-F(3C)	1.402(13)	C(3)-C(4)-H(4A)	108.4
B(1)-F(4B)	1.416(13)	P(3)-C(4)-H(4A)	108.4
B(1)-F(5A)	1.426(7)	C(3)-C(4)-H(4B)	108.4
		P(3)-C(4)-H(4B)	108.4
C(42)-Pt(1)-C(35)	80.66(15)	H(4A)-C(4)-H(4B)	107.5
C(42)-Pt(1)-F(1)	172.72(12)	C(6)-C(5)-C(10)	119.4(4)
C(35)-Pt(1)-F(1)	92.10(12)	C(6)-C(5)-P(3)	123.1(3)
C(42)-Pt(1)-P(3)	98.22(10)	C(10)-C(5)-P(3)	117.2(3)
C(35)-Pt(1)-P(3)	93.80(10)	C(5)-C(6)-C(7)	120.0(4)
F(1)-Pt(1)-P(3)	82.94(6)	C(5)-C(6)-H(6)	120.0
C(42)-Pt(1)-P(1)	95.35(10)	C(7)-C(6)-H(6)	120.0
C(35)-Pt(1)-P(1)	96.34(10)	C(8)-C(7)-C(6)	119.9(4)
F(1)-Pt(1)-P(1)	84.62(6)	C(8)-C(7)-H(7)	120.1
P(3)-Pt(1)-P(1)	164.21(3)	C(6)-C(7)-H(7)	120.1
C(42)-Pt(1)-P(2)	106.06(11)	C(9)-C(8)-C(7)	120.2(4)
C(35)-Pt(1)-P(2)	173.28(11)	C(9)-C(8)-H(8)	119.9
F(1)-Pt(1)-P(2)	81.18(6)	C(7)-C(8)-H(8)	119.9
P(3)-Pt(1)-P(2)	85.25(3)	C(8)-C(9)-C(10)	120.1(4)
P(1)-Pt(1)-P(2)	83.27(3)	C(8)-C(9)-H(9)	120.0
C(29)-P(1)-C(23)	107.51(18)	C(10)-C(9)-H(9)	120.0
C(29)-P(1)-C(1)	104.82(18)	C(9)-C(10)-C(5)	120.4(4)
C(23)-P(1)-C(1)	106.75(18)	C(9)-C(10)-H(10)	119.8
C(29)-P(1)-Pt(1)	117.71(12)	C(5)-C(10)-H(10)	119.8
C(23)-P(1)-Pt(1)	117.81(13)	C(16)-C(11)-C(12)	119.8(3)
C(1)-P(1)-Pt(1)	100.63(13)	C(16)-C(11)-P(3)	120.0(3)
C(17)-P(2)-C(3)	107.67(19)	C(12)-C(11)-P(3)	120.2(3)

C(11)-C(12)-C(13)	119.5(4)	C(29)-C(30)-H(30)	119.7
C(11)-C(12)-H(12)	120.2	C(30)-C(31)-C(32)	120.0(4)
C(13)-C(12)-H(12)	120.2	C(30)-C(31)-H(31)	120.0
C(14)-C(13)-C(12)	120.5(4)	C(32)-C(31)-H(31)	120.0
C(14)-C(13)-H(13)	119.8	C(33)-C(32)-C(31)	119.2(4)
C(12)-C(13)-H(13)	119.8	C(33)-C(32)-H(32)	120.4
C(13)-C(14)-C(15)	120.4(4)	C(31)-C(32)-H(32)	120.4
C(13)-C(14)-H(14)	119.8	C(32)-C(33)-C(34)	121.4(4)
C(15)-C(14)-H(14)	119.8	C(32)-C(33)-H(33)	119.3
C(14)-C(15)-C(16)	119.6(4)	C(34)-C(33)-H(33)	119.3
C(14)-C(15)-H(15)	120.2	C(33)-C(34)-C(29)	119.1(4)
C(16)-C(15)-H(15)	120.2	C(33)-C(34)-H(34)	120.4
C(11)-C(16)-C(15)	120.2(4)	C(29)-C(34)-H(34)	120.4
C(11)-C(16)-H(16)	119.9	C(40)-C(35)-C(36)	120.5(3)
C(15)-C(16)-H(16)	119.9	C(40)-C(35)-Pt(1)	114.9(3)
C(18)-C(17)-C(22)	119.0(4)	C(36)-C(35)-Pt(1)	124.6(3)
C(18)-C(17)-P(2)	121.3(3)	C(35)-C(36)-C(37)	119.3(4)
C(22)-C(17)-P(2)	119.7(4)	C(35)-C(36)-H(36)	120.3
C(17)-C(18)-C(19)	121.0(5)	C(37)-C(36)-H(36)	120.3
C(17)-C(18)-H(18)	119.5	C(38)-C(37)-C(36)	120.2(4)
C(19)-C(18)-H(18)	119.5	C(38)-C(37)-H(37)	119.9
C(20)-C(19)-C(18)	119.7(5)	C(36)-C(37)-H(37)	119.9
C(20)-C(19)-H(19)	120.2	C(37)-C(38)-C(39)	120.7(4)
C(18)-C(19)-H(19)	120.2	C(37)-C(38)-H(38)	119.7
C(21)-C(20)-C(19)	120.0(5)	C(39)-C(38)-H(38)	119.7
C(21)-C(20)-H(20)	120.0	C(38)-C(39)-C(40)	119.5(4)
C(19)-C(20)-H(20)	120.0	C(38)-C(39)-H(39)	120.2
C(20)-C(21)-C(22)	120.6(5)	C(40)-C(39)-H(39)	120.2
C(20)-C(21)-H(21)	119.7	C(35)-C(40)-C(39)	119.7(4)
C(22)-C(21)-H(21)	119.7	C(35)-C(40)-C(41)	114.4(3)
C(17)-C(22)-C(21)	119.7(5)	C(39)-C(40)-C(41)	125.9(4)
C(17)-C(22)-H(22)	120.1	C(46)-C(41)-C(42)	119.4(4)
C(21)-C(22)-H(22)	120.1	C(46)-C(41)-C(40)	125.1(4)
C(28)-C(23)-C(24)	119.6(4)	C(42)-C(41)-C(40)	115.5(3)
C(28)-C(23)-P(1)	120.7(3)	C(43)-C(42)-C(41)	119.6(3)
C(24)-C(23)-P(1)	119.8(3)	C(43)-C(42)-Pt(1)	126.1(3)
C(25)-C(24)-C(23)	120.1(5)	C(41)-C(42)-Pt(1)	114.3(3)
C(25)-C(24)-H(24)	120.0	C(42)-C(43)-C(44)	120.9(4)
C(23)-C(24)-H(24)	120.0	C(42)-C(43)-H(43)	119.5
C(24)-C(25)-C(26)	120.0(5)	C(44)-C(43)-H(43)	119.5
C(24)-C(25)-H(25)	120.0	C(43)-C(44)-C(45)	119.3(4)
C(26)-C(25)-H(25)	120.0	C(43)-C(44)-H(44)	120.4
C(27)-C(26)-C(25)	120.2(4)	C(45)-C(44)-H(44)	120.4
C(27)-C(26)-H(26)	119.9	C(46)-C(45)-C(44)	120.8(4)
C(25)-C(26)-H(26)	119.9	C(46)-C(45)-H(45)	119.6
C(26)-C(27)-C(28)	120.6(5)	C(44)-C(45)-H(45)	119.6
C(26)-C(27)-H(27)	119.7	C(45)-C(46)-C(41)	120.1(4)
C(28)-C(27)-H(27)	119.7	C(45)-C(46)-H(46)	119.9
C(23)-C(28)-C(27)	119.5(4)	C(41)-C(46)-H(46)	119.9
C(23)-C(28)-H(28)	120.3	F(5B)-B(1)-F(4C)	43.9(11)
C(27)-C(28)-H(28)	120.3	F(5B)-B(1)-F(3A)	124.1(10)
C(34)-C(29)-C(30)	119.7(4)	F(4C)-B(1)-F(3A)	115.5(11)
C(34)-C(29)-P(1)	121.7(3)	F(5B)-B(1)-F(3B)	109.4(12)
C(30)-C(29)-P(1)	118.6(3)	F(4C)-B(1)-F(3B)	127.3(14)
C(31)-C(30)-C(29)	120.5(4)	F(3A)-B(1)-F(3B)	31.7(9)
C(31)-C(30)-H(30)	119.7	F(5B)-B(1)-F(2)	120.5(11)

F(4C)-B(1)-F(2)	126.4(10)	F(4A)-B(1)-F(3C)	93.7(9)
F(3A)-B(1)-F(2)	111.2(5)	F(5C)-B(1)-F(3C)	107.4(12)
F(3B)-B(1)-F(2)	106.2(10)	F(5B)-B(1)-F(4B)	102.8(13)
F(5B)-B(1)-F(4A)	71.0(11)	F(4C)-B(1)-F(4B)	59.9(12)
F(4C)-B(1)-F(4A)	29.4(9)	F(3A)-B(1)-F(4B)	94.6(10)
F(3A)-B(1)-F(4A)	113.9(6)	F(3B)-B(1)-F(4B)	126.3(13)
F(3B)-B(1)-F(4A)	140.6(12)	F(2)-B(1)-F(4B)	92.1(9)
F(2)-B(1)-F(4A)	106.6(5)	F(4A)-B(1)-F(4B)	31.9(7)
F(5B)-B(1)-F(5C)	65.6(12)	F(5C)-B(1)-F(4B)	165.8(12)
F(4C)-B(1)-F(5C)	107.0(12)	F(3C)-B(1)-F(4B)	72.5(12)
F(3A)-B(1)-F(5C)	86.2(9)	F(5B)-B(1)-F(5A)	34.0(10)
F(3B)-B(1)-F(5C)	55.5(12)	F(4C)-B(1)-F(5A)	77.7(10)
F(2)-B(1)-F(5C)	100.9(9)	F(3A)-B(1)-F(5A)	113.3(5)
F(4A)-B(1)-F(5C)	136.0(9)	F(3B)-B(1)-F(5A)	86.2(10)
F(5B)-B(1)-F(3C)	127.8(14)	F(2)-B(1)-F(5A)	106.6(5)
F(4C)-B(1)-F(3C)	102.5(13)	F(4A)-B(1)-F(5A)	104.7(5)
F(3A)-B(1)-F(3C)	22.1(8)	F(5C)-B(1)-F(5A)	33.3(7)
F(3B)-B(1)-F(3C)	53.7(12)	F(3C)-B(1)-F(5A)	130.3(10)
F(2)-B(1)-F(3C)	111.6(10)	F(4B)-B(1)-F(5A)	136.6(9)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for complex 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	23(1)	20(1)	26(1)	-1(1)	9(1)	2(1)
P(1)	31(1)	23(1)	30(1)	0(1)	14(1)	1(1)
P(2)	24(1)	27(1)	34(1)	2(1)	8(1)	5(1)
P(3)	25(1)	23(1)	29(1)	-1(1)	11(1)	0(1)
F(1)	35(1)	24(1)	36(1)	-5(1)	15(1)	2(1)
C(1)	37(2)	26(2)	38(2)	4(2)	16(2)	8(2)
C(2)	35(2)	31(2)	43(2)	10(2)	14(2)	9(2)
C(3)	25(2)	29(2)	43(2)	1(2)	13(2)	5(2)
C(4)	29(2)	37(2)	45(2)	5(2)	18(2)	4(2)
C(5)	30(2)	22(2)	29(2)	-2(2)	7(2)	-3(2)
C(6)	42(2)	30(2)	30(2)	-2(2)	13(2)	3(2)
C(7)	55(3)	27(2)	36(2)	-3(2)	11(2)	4(2)
C(8)	57(3)	25(2)	41(2)	4(2)	9(2)	-9(2)
C(9)	50(3)	46(3)	56(3)	7(2)	25(2)	-9(2)
C(10)	45(2)	35(2)	50(2)	3(2)	25(2)	-2(2)
C(11)	32(2)	28(2)	28(2)	-3(2)	13(2)	-5(2)
C(12)	52(3)	34(2)	40(2)	-10(2)	22(2)	-1(2)
C(13)	76(3)	46(3)	51(3)	-21(2)	38(3)	-15(3)
C(14)	59(3)	57(3)	31(2)	-11(2)	15(2)	-22(2)
C(15)	47(3)	51(3)	35(2)	3(2)	9(2)	-9(2)
C(16)	45(2)	29(2)	33(2)	-3(2)	13(2)	-4(2)
C(17)	27(2)	34(2)	36(2)	1(2)	0(2)	5(2)
C(18)	29(2)	28(2)	57(3)	2(2)	6(2)	7(2)
C(19)	37(2)	29(2)	75(3)	3(2)	2(2)	5(2)
C(20)	58(3)	37(3)	58(3)	-3(2)	-17(3)	0(2)
C(21)	84(4)	77(4)	40(3)	-10(3)	3(3)	-7(4)

C(22)	57(3)	62(3)	40(2)	-2(2)	7(2)	-11(3)
C(23)	37(2)	36(2)	33(2)	-3(2)	17(2)	-4(2)
C(24)	50(3)	52(3)	38(2)	4(2)	18(2)	7(2)
C(25)	64(3)	81(4)	37(2)	3(3)	21(2)	0(3)
C(26)	72(3)	68(4)	41(2)	-16(2)	34(3)	-21(3)
C(27)	75(3)	43(3)	59(3)	-12(2)	47(3)	-8(2)
C(28)	53(3)	33(2)	43(2)	-2(2)	31(2)	-1(2)
C(29)	34(2)	24(2)	38(2)	2(2)	18(2)	3(2)
C(30)	38(2)	32(2)	39(2)	2(2)	20(2)	-2(2)
C(31)	41(2)	38(2)	46(2)	-8(2)	17(2)	-6(2)
C(32)	36(2)	47(3)	65(3)	-7(2)	25(2)	-9(2)
C(33)	48(3)	51(3)	64(3)	-12(2)	38(2)	-11(2)
C(34)	40(2)	41(3)	46(2)	-8(2)	25(2)	-4(2)
C(35)	25(2)	29(2)	27(2)	5(2)	9(2)	-2(2)
C(36)	36(2)	37(2)	36(2)	2(2)	14(2)	-4(2)
C(37)	31(2)	60(3)	35(2)	6(2)	3(2)	-9(2)
C(38)	23(2)	66(3)	49(2)	21(2)	9(2)	3(2)
C(39)	32(2)	48(3)	50(2)	20(2)	22(2)	13(2)
C(40)	26(2)	31(2)	34(2)	10(2)	15(2)	3(2)
C(41)	38(2)	24(2)	38(2)	8(2)	25(2)	7(2)
C(42)	35(2)	21(2)	33(2)	-1(2)	19(2)	3(2)
C(43)	41(2)	28(2)	36(2)	-2(2)	18(2)	1(2)
C(44)	63(3)	30(2)	46(2)	-7(2)	32(2)	-7(2)
C(45)	71(3)	23(2)	61(3)	-1(2)	47(3)	4(2)
C(46)	46(2)	30(2)	55(2)	9(2)	33(2)	12(2)
B(1)	37(3)	91(5)	67(4)	13(4)	24(3)	5(3)
F(2)	52(2)	93(3)	105(3)	26(2)	40(2)	-3(2)
F(3A)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(4A)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(5A)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(3B)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(4B)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(5B)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(3C)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(4C)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)
F(5C)	47(2)	98(2)	82(3)	9(2)	25(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex 7.

	x	y	z	U(eq)
H(1A)	1457	11700	672	41
H(1B)	1364	11797	169	41
H(2A)	721	10488	-74	45
H(2B)	678	11301	311	45
H(3A)	792	10263	1080	40
H(3B)	306	9519	782	40
H(4A)	545	7592	1155	44
H(4B)	770	8671	1539	44
H(6)	1698	5035	1237	42
H(7)	1594	2785	1362	52
H(8)	1119	2213	1695	55

H(9)	739	3862	1895	60
H(10)	836	6096	1767	50
H(12)	1454	9910	1956	50
H(13)	1949	10574	2677	65
H(14)	2513	9126	3158	61
H(15)	2605	7018	2924	57
H(16)	2111	6338	2203	45
H(18)	110	7341	464	52
H(19)	-441	5955	-77	67
H(20)	-445	5771	-761	81
H(21)	77	7005	-914	92
H(22)	630	8408	-375	70
H(24)	1260	10728	-401	57
H(25)	1091	9848	-1089	73
H(26)	1409	7805	-1142	68
H(27)	1932	6709	-513	63
H(28)	2113	7579	184	47
H(30)	2341	11327	1278	43
H(31)	3049	12485	1573	51
H(32)	3504	12579	1188	58
H(33)	3236	11538	509	60
H(34)	2518	10412	201	48
H(36)	2468	9680	1852	44
H(37)	3269	9224	2292	56
H(38)	3624	7440	2124	59
H(39)	3187	6052	1530	50
H(43)	1124	6336	241	41
H(44)	1332	4382	-5	52
H(45)	2115	3646	337	54
H(46)	2683	4827	923	48

Table 6. Torsion angles [º] for complex 7.

C(42)-Pt(1)-P(1)-C(29)	-103.92(18)
C(35)-Pt(1)-P(1)-C(29)	-22.75(17)
F(1)-Pt(1)-P(1)-C(29)	68.77(15)
P(3)-Pt(1)-P(1)-C(29)	106.88(18)
P(2)-Pt(1)-P(1)-C(29)	150.49(14)
C(42)-Pt(1)-P(1)-C(23)	27.48(18)
C(35)-Pt(1)-P(1)-C(23)	108.64(18)
F(1)-Pt(1)-P(1)-C(23)	-159.83(16)
P(3)-Pt(1)-P(1)-C(23)	-121.73(18)
P(2)-Pt(1)-P(1)-C(23)	-78.11(15)
C(42)-Pt(1)-P(1)-C(1)	142.97(17)
C(35)-Pt(1)-P(1)-C(1)	-135.86(17)
F(1)-Pt(1)-P(1)-C(1)	-44.33(14)
P(3)-Pt(1)-P(1)-C(1)	-6.23(19)
P(2)-Pt(1)-P(1)-C(1)	37.38(13)
C(42)-Pt(1)-P(2)-C(17)	9.8(2)
C(35)-Pt(1)-P(2)-C(17)	-169.5(9)
F(1)-Pt(1)-P(2)-C(17)	-170.95(19)
P(3)-Pt(1)-P(2)-C(17)	-87.38(18)
P(1)-Pt(1)-P(2)-C(17)	103.48(18)

C(42)-Pt(1)-P(2)-C(3)	131.43(17)
C(35)-Pt(1)-P(2)-C(3)	-47.9(9)
F(1)-Pt(1)-P(2)-C(3)	-49.34(14)
P(3)-Pt(1)-P(2)-C(3)	34.23(13)
P(1)-Pt(1)-P(2)-C(3)	-134.92(14)
C(42)-Pt(1)-P(2)-C(2)	-115.65(18)
C(35)-Pt(1)-P(2)-C(2)	65.0(9)
F(1)-Pt(1)-P(2)-C(2)	63.57(16)
P(3)-Pt(1)-P(2)-C(2)	147.14(15)
P(1)-Pt(1)-P(2)-C(2)	-22.00(15)
C(42)-Pt(1)-P(3)-C(11)	121.32(17)
C(35)-Pt(1)-P(3)-C(11)	40.22(17)
F(1)-Pt(1)-P(3)-C(11)	-51.44(15)
P(1)-Pt(1)-P(3)-C(11)	-89.69(18)
P(2)-Pt(1)-P(3)-C(11)	-133.11(14)
C(42)-Pt(1)-P(3)-C(5)	-3.25(18)
C(35)-Pt(1)-P(3)-C(5)	-84.35(17)
F(1)-Pt(1)-P(3)-C(5)	-176.00(15)
P(1)-Pt(1)-P(3)-C(5)	145.74(17)
P(2)-Pt(1)-P(3)-C(5)	102.32(14)
C(42)-Pt(1)-P(3)-C(4)	-123.20(18)
C(35)-Pt(1)-P(3)-C(4)	155.69(18)
F(1)-Pt(1)-P(3)-C(4)	64.04(15)
P(1)-Pt(1)-P(3)-C(4)	25.8(2)
P(2)-Pt(1)-P(3)-C(4)	-17.63(14)
C(29)-P(1)-C(1)-C(2)	-174.9(3)
C(23)-P(1)-C(1)-C(2)	71.2(3)
Pt(1)-P(1)-C(1)-C(2)	-52.3(3)
P(1)-C(1)-C(2)-P(2)	36.9(4)
C(17)-P(2)-C(2)-C(1)	-139.5(3)
C(3)-P(2)-C(2)-C(1)	105.1(3)
Pt(1)-P(2)-C(2)-C(1)	-3.0(3)
C(17)-P(2)-C(3)-C(4)	84.6(3)
C(2)-P(2)-C(3)-C(4)	-160.9(3)
Pt(1)-P(2)-C(3)-C(4)	-49.0(3)
P(2)-C(3)-C(4)-P(3)	38.2(4)
C(11)-P(3)-C(4)-C(3)	110.9(3)
C(5)-P(3)-C(4)-C(3)	-139.8(3)
Pt(1)-P(3)-C(4)-C(3)	-7.2(3)
C(11)-P(3)-C(5)-C(6)	-105.4(3)
C(4)-P(3)-C(5)-C(6)	142.8(3)
Pt(1)-P(3)-C(5)-C(6)	22.2(4)
C(11)-P(3)-C(5)-C(10)	69.5(3)
C(4)-P(3)-C(5)-C(10)	-42.2(3)
Pt(1)-P(3)-C(5)-C(10)	-162.8(2)
C(10)-C(5)-C(6)-C(7)	0.0(5)
P(3)-C(5)-C(6)-C(7)	174.9(3)
C(5)-C(6)-C(7)-C(8)	-0.4(6)
C(6)-C(7)-C(8)-C(9)	0.5(6)
C(7)-C(8)-C(9)-C(10)	-0.2(7)
C(8)-C(9)-C(10)-C(5)	-0.2(7)
C(6)-C(5)-C(10)-C(9)	0.3(6)
P(3)-C(5)-C(10)-C(9)	-174.9(3)
C(5)-P(3)-C(11)-C(16)	37.0(4)
C(4)-P(3)-C(11)-C(16)	146.6(3)
Pt(1)-P(3)-C(11)-C(16)	-98.8(3)

C(5)-P(3)-C(11)-C(12)	-146.3(3)
C(4)-P(3)-C(11)-C(12)	-36.7(4)
Pt(1)-P(3)-C(11)-C(12)	77.9(3)
C(16)-C(11)-C(12)-C(13)	-0.4(6)
P(3)-C(11)-C(12)-C(13)	-177.1(3)
C(11)-C(12)-C(13)-C(14)	-0.2(7)
C(12)-C(13)-C(14)-C(15)	0.8(7)
C(13)-C(14)-C(15)-C(16)	-0.8(7)
C(12)-C(11)-C(16)-C(15)	0.4(6)
P(3)-C(11)-C(16)-C(15)	177.1(3)
C(14)-C(15)-C(16)-C(11)	0.2(6)
C(3)-P(2)-C(17)-C(18)	-20.9(4)
C(2)-P(2)-C(17)-C(18)	-136.6(3)
Pt(1)-P(2)-C(17)-C(18)	97.8(3)
C(3)-P(2)-C(17)-C(22)	160.9(4)
C(2)-P(2)-C(17)-C(22)	45.3(4)
Pt(1)-P(2)-C(17)-C(22)	-80.4(4)
C(22)-C(17)-C(18)-C(19)	-0.1(6)
P(2)-C(17)-C(18)-C(19)	-178.3(3)
C(17)-C(18)-C(19)-C(20)	0.7(6)
C(18)-C(19)-C(20)-C(21)	-1.0(7)
C(19)-C(20)-C(21)-C(22)	0.9(9)
C(18)-C(17)-C(22)-C(21)	0.0(7)
P(2)-C(17)-C(22)-C(21)	178.2(4)
C(20)-C(21)-C(22)-C(17)	-0.4(9)
C(29)-P(1)-C(23)-C(28)	81.3(4)
C(1)-P(1)-C(23)-C(28)	-166.7(3)
Pt(1)-P(1)-C(23)-C(28)	-54.6(4)
C(29)-P(1)-C(23)-C(24)	-98.6(4)
C(1)-P(1)-C(23)-C(24)	13.4(4)
Pt(1)-P(1)-C(23)-C(24)	125.5(3)
C(28)-C(23)-C(24)-C(25)	2.5(7)
P(1)-C(23)-C(24)-C(25)	-177.6(4)
C(23)-C(24)-C(25)-C(26)	0.0(8)
C(24)-C(25)-C(26)-C(27)	-2.3(8)
C(25)-C(26)-C(27)-C(28)	2.0(7)
C(24)-C(23)-C(28)-C(27)	-2.7(6)
P(1)-C(23)-C(28)-C(27)	177.4(3)
C(26)-C(27)-C(28)-C(23)	0.5(7)
C(23)-P(1)-C(29)-C(34)	0.0(4)
C(1)-P(1)-C(29)-C(34)	-113.3(4)
Pt(1)-P(1)-C(29)-C(34)	135.9(3)
C(23)-P(1)-C(29)-C(30)	178.5(3)
C(1)-P(1)-C(29)-C(30)	65.1(3)
Pt(1)-P(1)-C(29)-C(30)	-45.6(3)
C(34)-C(29)-C(30)-C(31)	-0.7(6)
P(1)-C(29)-C(30)-C(31)	-179.2(3)
C(29)-C(30)-C(31)-C(32)	-0.4(7)
C(30)-C(31)-C(32)-C(33)	0.6(7)
C(31)-C(32)-C(33)-C(34)	0.1(8)
C(32)-C(33)-C(34)-C(29)	-1.2(7)
C(30)-C(29)-C(34)-C(33)	1.4(6)
P(1)-C(29)-C(34)-C(33)	179.9(3)
C(42)-Pt(1)-C(35)-C(40)	4.9(3)
F(1)-Pt(1)-C(35)-C(40)	-174.3(3)
P(3)-Pt(1)-C(35)-C(40)	102.6(3)

P(1)-Pt(1)-C(35)-C(40)	-89.5(3)
P(2)-Pt(1)-C(35)-C(40)	-175.8(7)
C(42)-Pt(1)-C(35)-C(36)	-176.0(3)
F(1)-Pt(1)-C(35)-C(36)	4.8(3)
P(3)-Pt(1)-C(35)-C(36)	-78.3(3)
P(1)-Pt(1)-C(35)-C(36)	89.6(3)
P(2)-Pt(1)-C(35)-C(36)	3.3(11)
C(40)-C(35)-C(36)-C(37)	1.8(6)
Pt(1)-C(35)-C(36)-C(37)	-177.3(3)
C(35)-C(36)-C(37)-C(38)	-1.0(6)
C(36)-C(37)-C(38)-C(39)	-0.8(7)
C(37)-C(38)-C(39)-C(40)	1.8(6)
C(36)-C(35)-C(40)-C(39)	-0.8(6)
Pt(1)-C(35)-C(40)-C(39)	178.3(3)
C(36)-C(35)-C(40)-C(41)	176.7(3)
Pt(1)-C(35)-C(40)-C(41)	-4.2(4)
C(38)-C(39)-C(40)-C(35)	-1.0(6)
C(38)-C(39)-C(40)-C(41)	-178.2(4)
C(35)-C(40)-C(41)-C(46)	-177.9(4)
C(39)-C(40)-C(41)-C(46)	-0.6(6)
C(35)-C(40)-C(41)-C(42)	0.2(5)
C(39)-C(40)-C(41)-C(42)	177.6(4)
C(46)-C(41)-C(42)-C(43)	1.1(5)
C(40)-C(41)-C(42)-C(43)	-177.1(3)
C(46)-C(41)-C(42)-Pt(1)	-177.9(3)
C(40)-C(41)-C(42)-Pt(1)	3.9(4)
C(35)-Pt(1)-C(42)-C(43)	176.4(3)
F(1)-Pt(1)-C(42)-C(43)	-177(6)
P(3)-Pt(1)-C(42)-C(43)	83.9(3)
P(1)-Pt(1)-C(42)-C(43)	-88.0(3)
P(2)-Pt(1)-C(42)-C(43)	-3.5(3)
C(35)-Pt(1)-C(42)-C(41)	-4.7(3)
F(1)-Pt(1)-C(42)-C(41)	1.5(11)
P(3)-Pt(1)-C(42)-C(41)	-97.2(3)
P(1)-Pt(1)-C(42)-C(41)	90.9(3)
P(2)-Pt(1)-C(42)-C(41)	175.4(2)
C(41)-C(42)-C(43)-C(44)	-0.3(6)
Pt(1)-C(42)-C(43)-C(44)	178.6(3)
C(42)-C(43)-C(44)-C(45)	-0.5(6)
C(43)-C(44)-C(45)-C(46)	0.5(6)
C(44)-C(45)-C(46)-C(41)	0.4(6)
C(42)-C(41)-C(46)-C(45)	-1.1(6)
C(40)-C(41)-C(46)-C(45)	176.9(4)

Symmetry transformations used to generate equivalent atoms.

S6.2 Labeling diagram and data tables for complex 8 (CCDC 838073).

ORTEP drawing of compound **8** with
thermal ellipsoids drawn at 50% probability level.
(all H atoms, the anions and solvent moleclues are omitted for clarity)

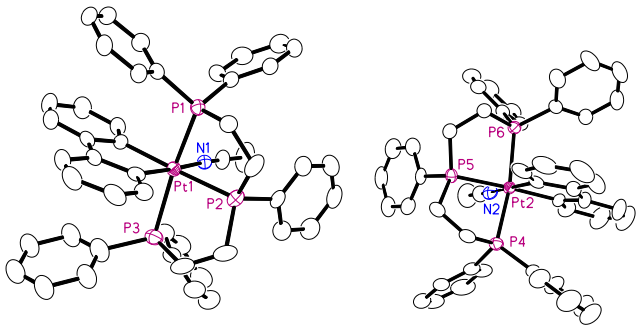


Table 1. Crystal data and structure refinement for complex **8**.

Identification code	zsnew02c	
Empirical formula	C48 H46.75 B F9.50 N O1.38 P3.50 Pt	
Formula weight	1154.41	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.666(1) Å	α= 95.002(1) °.
	b = 17.484(2) Å	β= 113.180(1) °.
	c = 22.340(2) Å	γ = 96.172(1) °.
Volume	4829.3(8) $Å^3$	
Z	4	
Density (calculated)	1.588 Mg/m^3	
Absorption coefficient	3.096 mm^{-1}	
F(000)	2295	
Crystal size	0.25 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.00 to 26.00 °.	
Index ranges	-16<=h<=15, -21<=k<=21, 0<=l<=27	
Reflections collected	18829	
Independent reflections	18829 [R(int) = 0.0454]	
Completeness to theta = 26.00 °	99.2 %	
Absorption correction	Twinabs	
Max. and min. transmission	0.7471 and 0.5116	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18829 / 14 / 905	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0841	
R indices (all data)	R1 = 0.0483, wR2 = 0.0876	
Largest diff. peak and hole	1.756 and -1.170 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for complex 8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	5761(1)	10070(1)	7648(1)	23(1)
Pt(2)	8861(1)	5119(1)	2347(1)	24(1)
P(1)	4027(1)	9354(1)	7232(1)	26(1)
P(2)	5205(1)	10443(1)	6584(1)	30(1)
P(3)	7188(1)	11098(1)	7934(1)	32(1)
P(4)	9623(1)	6436(1)	2535(1)	28(1)
P(5)	9018(1)	5392(1)	3449(1)	26(1)
P(6)	7715(1)	3999(1)	2313(1)	26(1)
N(1)	6500(3)	9217(2)	7339(2)	26(1)
N(2)	10291(3)	4638(2)	2727(2)	31(1)
C(1)	3965(4)	8383(3)	6835(2)	34(1)
C(2)	3213(4)	8109(3)	6202(2)	40(1)
C(3)	3235(5)	7378(3)	5897(2)	52(2)
C(4)	3991(5)	6937(3)	6227(3)	52(1)
C(5)	4725(4)	7202(3)	6857(3)	47(1)
C(6)	4713(4)	7920(3)	7168(2)	37(1)
C(7)	3430(3)	9259(2)	7823(2)	29(1)
C(8)	3599(4)	8641(3)	8184(2)	36(1)
C(9)	3194(4)	8588(3)	8659(2)	44(1)
C(10)	2623(4)	9128(3)	8778(2)	40(1)
C(11)	2455(4)	9747(3)	8432(2)	37(1)
C(12)	2861(3)	9816(3)	7955(2)	32(1)
C(13)	3197(3)	9910(2)	6622(2)	30(1)
C(14)	3726(4)	10318(3)	6214(2)	42(1)
C(15)	5577(4)	9861(3)	6012(2)	31(1)
C(16)	4908(4)	9189(3)	5642(2)	43(1)
C(17)	5241(4)	8707(3)	5256(2)	52(1)
C(18)	6200(4)	8896(3)	5216(2)	44(1)
C(19)	6862(4)	9568(3)	5582(2)	48(1)
C(20)	6561(4)	10045(3)	5977(2)	43(1)
C(21)	5852(4)	11443(3)	6662(2)	42(1)
C(22)	6565(4)	11770(2)	7333(2)	42(1)
C(23)	8313(3)	10808(3)	7792(2)	32(1)
C(24)	8722(4)	11196(3)	7400(2)	42(1)
C(25)	9534(4)	10933(3)	7260(3)	50(1)
C(26)	9965(4)	10293(3)	7512(3)	53(1)
C(27)	9568(4)	9909(3)	7908(3)	49(1)
C(28)	8749(4)	10160(3)	8045(2)	43(1)
C(29A)	7658(2)	11659(2)	8743(1)	58(1)
C(30A)	7472(2)	12419(2)	8790(2)	58(1)
C(31A)	7821(3)	12862(2)	9399(2)	58(1)
C(32A)	8356(3)	12545(3)	9963(2)	58(1)
C(33A)	8542(3)	11785(3)	9916(2)	58(1)
C(34A)	8193(2)	11343(2)	9306(2)	58(1)
C(29B)	7755(2)	11601(2)	8785(1)	58(1)
C(30B)	7470(2)	12299(1)	8980(1)	58(1)
C(31B)	7901(3)	12615(2)	9648(2)	58(1)
C(32B)	8619(3)	12233(3)	10121(2)	58(1)
C(33B)	8904(3)	11535(3)	9927(2)	58(1)
C(34B)	8473(2)	11219(2)	9259(2)	58(1)

C(35)	5143(2)	10857(2)	8049(1)	27(1)
C(36)	4581(2)	11460(2)	7790(2)	34(1)
C(37)	4207(4)	11963(3)	8094(2)	40(1)
C(38)	4385(4)	11895(3)	8744(2)	44(1)
C(39)	4925(4)	11326(3)	9050(2)	38(1)
C(40)	5288(3)	10801(2)	8716(2)	30(1)
C(41)	5858(3)	10163(3)	8993(2)	31(1)
C(42)	6053(4)	9958(3)	9614(2)	40(1)
C(43)	6572(4)	9338(3)	9816(2)	49(1)
C(44)	6911(4)	8916(3)	9405(2)	47(1)
C(45)	6732(4)	9110(2)	8782(2)	35(1)
C(46)	6197(3)	9727(2)	8579(2)	26(1)
C(47)	6866(4)	8775(3)	7129(2)	34(1)
C(48)	7334(5)	8224(3)	6854(3)	66(2)
C(49)	6558(4)	3605(2)	1555(2)	32(1)
C(50)	6683(4)	3427(3)	972(2)	37(1)
C(51)	5817(5)	3095(3)	406(2)	50(1)
C(52)	4805(5)	2935(3)	404(3)	62(2)
C(53)	4653(4)	3105(4)	972(3)	64(2)
C(54)	5545(4)	3439(3)	1557(2)	50(1)
C(55)	8435(3)	3184(2)	2564(2)	30(1)
C(56)	9024(4)	2934(3)	2218(2)	36(1)
C(57)	9554(4)	2304(3)	2381(2)	44(1)
C(58)	9506(4)	1924(3)	2882(3)	51(1)
C(59)	8923(4)	2166(3)	3229(3)	48(1)
C(60)	8370(4)	2794(2)	3067(2)	36(1)
C(61)	7121(3)	4281(2)	2889(2)	30(1)
C(95)	11041(4)	4356(3)	2935(2)	38(1)
C(62)	7837(3)	4857(2)	3508(2)	31(1)
C(63)	10188(4)	5088(2)	4065(2)	30(1)
C(64)	10123(4)	4363(3)	4273(2)	42(1)
C(65)	11040(5)	4111(3)	4698(2)	53(1)
C(66)	12016(4)	4564(3)	4919(2)	48(1)
C(67)	12105(4)	5281(3)	4724(2)	51(1)
C(68)	11185(4)	5540(3)	4298(2)	40(1)
C(69)	9134(4)	6452(2)	3651(2)	32(1)
C(70)	9051(3)	6881(2)	3064(2)	31(1)
C(71)	11076(4)	6622(3)	2987(2)	35(1)
C(72)	11533(4)	7169(3)	3545(2)	42(1)
C(73)	12640(4)	7274(3)	3920(3)	56(2)
C(74)	13273(4)	6842(4)	3741(3)	61(2)
C(75)	12836(5)	6311(3)	3171(3)	63(2)
C(76)	11742(4)	6189(3)	2801(3)	47(1)
C(77)	9298(4)	6941(2)	1820(2)	34(1)
C(78)	8591(4)	7463(3)	1697(3)	55(1)
C(79)	8380(5)	7843(4)	1150(3)	77(2)
C(80)	8866(6)	7695(4)	732(3)	81(2)
C(81)	9569(6)	7166(4)	842(3)	77(2)
C(82)	9807(5)	6798(3)	1404(3)	55(1)
C(83)	8765(4)	4923(2)	1393(2)	37(1)
C(84)	9523(5)	4613(3)	1217(3)	52(1)
C(85)	9403(7)	4531(4)	559(3)	84(2)
C(86)	8520(8)	4760(5)	90(4)	101(3)
C(87)	7755(6)	5069(4)	257(3)	79(2)
C(88)	7879(5)	5147(3)	917(2)	50(1)
C(89)	7118(4)	5438(3)	1153(2)	45(1)

C(90)	6127(5)	5641(3)	769(3)	67(2)
C(91)	5469(5)	5899(3)	1051(3)	75(2)
C(92)	5781(4)	5973(3)	1721(3)	59(2)
C(93)	6766(4)	5782(2)	2124(3)	43(1)
C(94)	7431(3)	5504(2)	1846(2)	31(1)
C(96)	11997(5)	4002(4)	3206(3)	67(2)

Table 3. Bond lengths [Å] and angles [º] for complex 8.

Pt(1)-C(35)	2.009(3)	C(7)-C(8)	1.389(6)
Pt(1)-C(46)	2.087(4)	C(8)-C(9)	1.381(6)
Pt(1)-N(1)	2.101(4)	C(8)-H(8A)	0.9500
Pt(1)-P(1)	2.3383(11)	C(9)-C(10)	1.361(7)
Pt(1)-P(3)	2.3473(11)	C(9)-H(9A)	0.9500
Pt(1)-P(2)	2.3695(11)	C(10)-C(11)	1.373(6)
Pt(2)-C(94)	2.053(4)	C(10)-H(10A)	0.9500
Pt(2)-C(83)	2.078(4)	C(11)-C(12)	1.390(6)
Pt(2)-N(2)	2.102(4)	C(11)-H(11A)	0.9500
Pt(2)-P(6)	2.3491(11)	C(12)-H(12A)	0.9500
Pt(2)-P(4)	2.3514(11)	C(13)-C(14)	1.543(6)
Pt(2)-P(5)	2.3861(11)	C(13)-H(13A)	0.9900
P(1)-C(7)	1.816(4)	C(13)-H(13B)	0.9900
P(1)-C(1)	1.822(4)	C(14)-H(14A)	0.9900
P(1)-C(13)	1.828(4)	C(14)-H(14B)	0.9900
P(2)-C(15)	1.823(5)	C(15)-C(16)	1.380(6)
P(2)-C(21)	1.833(4)	C(15)-C(20)	1.382(6)
P(2)-C(14)	1.836(5)	C(16)-C(17)	1.387(7)
P(3)-C(23)	1.801(5)	C(16)-H(16A)	0.9500
P(3)-C(29A)	1.811(2)	C(17)-C(18)	1.357(7)
P(3)-C(29B)	1.842(2)	C(17)-H(17A)	0.9500
P(3)-C(22)	1.871(4)	C(18)-C(19)	1.375(7)
P(4)-C(77)	1.816(4)	C(18)-H(18A)	0.9500
P(4)-C(71)	1.816(5)	C(19)-C(20)	1.369(6)
P(4)-C(70)	1.820(4)	C(19)-H(19A)	0.9500
P(5)-C(63)	1.820(4)	C(20)-H(20A)	0.9500
P(5)-C(62)	1.833(4)	C(21)-C(22)	1.450(6)
P(5)-C(69)	1.844(4)	C(21)-H(21A)	0.9900
P(6)-C(49)	1.814(4)	C(21)-H(21B)	0.9900
P(6)-C(55)	1.822(4)	C(22)-H(22A)	0.9900
P(6)-C(61)	1.832(4)	C(22)-H(22B)	0.9900
N(1)-C(47)	1.129(5)	C(23)-C(24)	1.394(6)
N(2)-C(95)	1.133(6)	C(23)-C(28)	1.397(6)
C(1)-C(2)	1.386(6)	C(24)-C(25)	1.378(7)
C(1)-C(6)	1.391(6)	C(24)-H(24A)	0.9500
C(2)-C(3)	1.403(7)	C(25)-C(26)	1.381(7)
C(2)-H(2A)	0.9500	C(25)-H(25A)	0.9500
C(3)-C(4)	1.369(8)	C(26)-C(27)	1.390(7)
C(3)-H(3A)	0.9500	C(26)-H(26A)	0.9500
C(4)-C(5)	1.370(7)	C(27)-C(28)	1.376(7)
C(4)-H(4A)	0.9500	C(27)-H(27A)	0.9500
C(5)-C(6)	1.386(6)	C(28)-H(28A)	0.9500
C(5)-H(5A)	0.9500	C(29A)-C(30A)	1.3813(11)
C(6)-H(6A)	0.9500	C(29A)-C(34A)	1.3814(11)
C(7)-C(12)	1.389(6)	C(30A)-C(31A)	1.3814(11)

C(30A)-H(30A)	0.9500	C(55)-C(56)	1.393(6)
C(31A)-C(32A)	1.3814(11)	C(56)-C(57)	1.381(6)
C(31A)-H(31A)	0.9500	C(56)-H(56A)	0.9500
C(32A)-C(33A)	1.3814(12)	C(57)-C(58)	1.369(7)
C(32A)-H(32A)	0.9500	C(57)-H(57A)	0.9500
C(33A)-C(34A)	1.3814(11)	C(58)-C(59)	1.384(7)
C(33A)-H(33A)	0.9500	C(58)-H(58A)	0.9500
C(34A)-H(34A)	0.9500	C(59)-C(60)	1.392(6)
C(29B)-C(30B)	1.4045(12)	C(59)-H(59A)	0.9500
C(29B)-C(34B)	1.4046(12)	C(60)-H(60A)	0.9500
C(30B)-C(31B)	1.4045(12)	C(61)-C(62)	1.537(5)
C(30B)-H(30B)	0.9500	C(61)-H(61A)	0.9900
C(31B)-C(32B)	1.4044(12)	C(61)-H(61B)	0.9900
C(31B)-H(31B)	0.9500	C(95)-C(96)	1.440(7)
C(32B)-C(33B)	1.4047(12)	C(62)-H(62A)	0.9900
C(32B)-H(32B)	0.9500	C(62)-H(62B)	0.9900
C(33B)-C(34B)	1.4045(12)	C(63)-C(68)	1.374(6)
C(33B)-H(33B)	0.9500	C(63)-C(64)	1.394(6)
C(34B)-H(34B)	0.9500	C(64)-C(65)	1.385(7)
C(35)-C(36)	1.4027(11)	C(64)-H(64A)	0.9500
C(35)-C(40)	1.439(5)	C(65)-C(66)	1.356(7)
C(36)-C(37)	1.328(5)	C(65)-H(65A)	0.9500
C(36)-H(36A)	0.9500	C(66)-C(67)	1.372(7)
C(37)-C(38)	1.391(6)	C(66)-H(66A)	0.9500
C(37)-H(37A)	0.9500	C(67)-C(68)	1.395(6)
C(38)-C(39)	1.372(7)	C(67)-H(67A)	0.9500
C(38)-H(38A)	0.9500	C(68)-H(68A)	0.9500
C(39)-C(40)	1.385(6)	C(69)-C(70)	1.540(6)
C(39)-H(39A)	0.9500	C(69)-H(69A)	0.9900
C(40)-C(41)	1.469(6)	C(69)-H(69B)	0.9900
C(41)-C(42)	1.393(6)	C(70)-H(70A)	0.9900
C(41)-C(46)	1.394(6)	C(70)-H(70B)	0.9900
C(42)-C(43)	1.372(7)	C(71)-C(72)	1.383(6)
C(42)-H(42A)	0.9500	C(71)-C(76)	1.401(7)
C(43)-C(44)	1.376(7)	C(72)-C(73)	1.392(7)
C(43)-H(43A)	0.9500	C(72)-H(72A)	0.9500
C(44)-C(45)	1.393(6)	C(73)-C(74)	1.355(8)
C(44)-H(44A)	0.9500	C(73)-H(73A)	0.9500
C(45)-C(46)	1.377(6)	C(74)-C(75)	1.385(8)
C(45)-H(45A)	0.9500	C(74)-H(74A)	0.9500
C(47)-C(48)	1.433(6)	C(75)-C(76)	1.375(7)
C(48)-H(48A)	0.9800	C(75)-H(75A)	0.9500
C(48)-H(48B)	0.9800	C(76)-H(76A)	0.9500
C(48)-H(48C)	0.9800	C(77)-C(78)	1.366(7)
C(49)-C(54)	1.385(6)	C(77)-C(82)	1.385(7)
C(49)-C(50)	1.392(6)	C(78)-C(79)	1.387(7)
C(50)-C(51)	1.372(6)	C(78)-H(78A)	0.9500
C(50)-H(50A)	0.9500	C(79)-C(80)	1.363(9)
C(51)-C(52)	1.380(7)	C(79)-H(79A)	0.9500
C(51)-H(51A)	0.9500	C(80)-C(81)	1.371(9)
C(52)-C(53)	1.379(8)	C(80)-H(80A)	0.9500
C(52)-H(52A)	0.9500	C(81)-C(82)	1.399(7)
C(53)-C(54)	1.412(7)	C(81)-H(81A)	0.9500
C(53)-H(53A)	0.9500	C(82)-H(82A)	0.9500
C(54)-H(54A)	0.9500	C(83)-C(88)	1.383(7)
C(55)-C(60)	1.391(6)	C(83)-C(84)	1.389(7)

C(84)-C(85)	1.405(7)	C(7)-P(1)-Pt(1)	115.44(13)
C(84)-H(84A)	0.9500	C(1)-P(1)-Pt(1)	112.27(16)
C(85)-C(86)	1.377(11)	C(13)-P(1)-Pt(1)	104.61(14)
C(85)-H(85A)	0.9500	C(15)-P(2)-C(21)	106.2(2)
C(86)-C(87)	1.384(10)	C(15)-P(2)-C(14)	105.8(2)
C(86)-H(86A)	0.9500	C(21)-P(2)-C(14)	113.8(2)
C(87)-C(88)	1.410(7)	C(15)-P(2)-Pt(1)	114.97(14)
C(87)-H(87A)	0.9500	C(21)-P(2)-Pt(1)	108.31(16)
C(88)-C(89)	1.454(8)	C(14)-P(2)-Pt(1)	107.94(14)
C(89)-C(90)	1.392(7)	C(23)-P(3)-C(29A)	110.04(17)
C(89)-C(94)	1.424(6)	C(23)-P(3)-C(29B)	105.86(17)
C(90)-C(91)	1.376(9)	C(29A)-P(3)-C(29B)	5.5
C(90)-H(90A)	0.9500	C(23)-P(3)-C(22)	108.0(2)
C(91)-C(92)	1.375(9)	C(29A)-P(3)-C(22)	106.06(16)
C(91)-H(91A)	0.9500	C(29B)-P(3)-C(22)	111.17(16)
C(92)-C(93)	1.388(6)	C(23)-P(3)-Pt(1)	112.67(15)
C(92)-H(92A)	0.9500	C(29A)-P(3)-Pt(1)	117.36(9)
C(93)-C(94)	1.391(7)	C(29B)-P(3)-Pt(1)	117.13(9)
C(93)-H(93A)	0.9500	C(22)-P(3)-Pt(1)	101.83(14)
C(96)-H(96A)	0.9800	C(77)-P(4)-C(71)	107.4(2)
C(96)-H(96B)	0.9800	C(77)-P(4)-C(70)	107.7(2)
C(96)-H(96C)	0.9800	C(71)-P(4)-C(70)	106.9(2)
		C(77)-P(4)-Pt(2)	116.88(14)
C(35)-Pt(1)-C(46)	80.86(14)	C(71)-P(4)-Pt(2)	114.29(15)
C(35)-Pt(1)-N(1)	173.42(12)	C(70)-P(4)-Pt(2)	102.95(14)
C(46)-Pt(1)-N(1)	92.71(14)	C(63)-P(5)-C(62)	106.1(2)
C(35)-Pt(1)-P(1)	84.93(8)	C(63)-P(5)-C(69)	107.1(2)
C(46)-Pt(1)-P(1)	93.91(11)	C(62)-P(5)-C(69)	112.6(2)
N(1)-Pt(1)-P(1)	96.99(9)	C(63)-P(5)-Pt(2)	114.50(14)
C(35)-Pt(1)-P(3)	82.91(8)	C(62)-P(5)-Pt(2)	108.48(13)
C(46)-Pt(1)-P(3)	97.22(11)	C(69)-P(5)-Pt(2)	108.10(14)
N(1)-Pt(1)-P(3)	96.59(9)	C(49)-P(6)-C(55)	105.21(19)
P(1)-Pt(1)-P(3)	161.99(4)	C(49)-P(6)-C(61)	104.0(2)
C(35)-Pt(1)-P(2)	98.52(9)	C(55)-P(6)-C(61)	110.0(2)
C(46)-Pt(1)-P(2)	178.08(12)	C(49)-P(6)-Pt(2)	119.81(14)
N(1)-Pt(1)-P(2)	87.95(9)	C(55)-P(6)-Pt(2)	112.48(14)
P(1)-Pt(1)-P(2)	84.23(4)	C(61)-P(6)-Pt(2)	104.91(14)
P(3)-Pt(1)-P(2)	84.49(4)	C(47)-N(1)-Pt(1)	174.9(3)
C(94)-Pt(2)-C(83)	79.97(19)	C(95)-N(2)-Pt(2)	177.5(4)
C(94)-Pt(2)-N(2)	171.61(15)	C(2)-C(1)-C(6)	119.5(4)
C(83)-Pt(2)-N(2)	92.10(17)	C(2)-C(1)-P(1)	121.3(4)
C(94)-Pt(2)-P(6)	82.95(11)	C(6)-C(1)-P(1)	119.2(3)
C(83)-Pt(2)-P(6)	98.56(12)	C(1)-C(2)-C(3)	119.6(5)
N(2)-Pt(2)-P(6)	95.65(10)	C(1)-C(2)-H(2A)	120.2
C(94)-Pt(2)-P(4)	84.82(11)	C(3)-C(2)-H(2A)	120.2
C(83)-Pt(2)-P(4)	94.86(12)	C(4)-C(3)-C(2)	120.2(5)
N(2)-Pt(2)-P(4)	98.67(10)	C(4)-C(3)-H(3A)	119.9
P(6)-Pt(2)-P(4)	159.96(4)	C(2)-C(3)-H(3A)	119.9
C(94)-Pt(2)-P(5)	100.37(13)	C(3)-C(4)-C(5)	120.3(5)
C(83)-Pt(2)-P(5)	177.76(12)	C(3)-C(4)-H(4A)	119.8
N(2)-Pt(2)-P(5)	87.66(9)	C(5)-C(4)-H(4A)	119.8
P(6)-Pt(2)-P(5)	83.68(4)	C(4)-C(5)-C(6)	120.5(5)
P(4)-Pt(2)-P(5)	82.97(4)	C(4)-C(5)-H(5A)	119.8
C(7)-P(1)-C(1)	108.10(19)	C(6)-C(5)-H(5A)	119.8
C(7)-P(1)-C(13)	106.58(19)	C(5)-C(6)-C(1)	119.9(4)
C(1)-P(1)-C(13)	109.5(2)	C(5)-C(6)-H(6A)	120.0

C(1)-C(6)-H(6A)	120.0	C(21)-C(22)-H(22A)	107.6
C(12)-C(7)-C(8)	118.7(4)	P(3)-C(22)-H(22A)	107.6
C(12)-C(7)-P(1)	121.7(3)	C(21)-C(22)-H(22B)	107.6
C(8)-C(7)-P(1)	119.4(3)	P(3)-C(22)-H(22B)	107.6
C(9)-C(8)-C(7)	119.8(4)	H(22A)-C(22)-H(22B)	107.0
C(9)-C(8)-H(8A)	120.1	C(24)-C(23)-C(28)	119.0(4)
C(7)-C(8)-H(8A)	120.1	C(24)-C(23)-P(3)	121.0(4)
C(10)-C(9)-C(8)	121.2(4)	C(28)-C(23)-P(3)	119.9(3)
C(10)-C(9)-H(9A)	119.4	C(25)-C(24)-C(23)	120.1(5)
C(8)-C(9)-H(9A)	119.4	C(25)-C(24)-H(24A)	119.9
C(9)-C(10)-C(11)	120.0(4)	C(23)-C(24)-H(24A)	119.9
C(9)-C(10)-H(10A)	120.0	C(24)-C(25)-C(26)	120.7(5)
C(11)-C(10)-H(10A)	120.0	C(24)-C(25)-H(25A)	119.6
C(10)-C(11)-C(12)	119.7(4)	C(26)-C(25)-H(25A)	119.6
C(10)-C(11)-H(11A)	120.1	C(25)-C(26)-C(27)	119.4(5)
C(12)-C(11)-H(11A)	120.1	C(25)-C(26)-H(26A)	120.3
C(7)-C(12)-C(11)	120.5(4)	C(27)-C(26)-H(26A)	120.3
C(7)-C(12)-H(12A)	119.7	C(28)-C(27)-C(26)	120.4(5)
C(11)-C(12)-H(12A)	119.7	C(28)-C(27)-H(27A)	119.8
C(14)-C(13)-P(1)	116.7(3)	C(26)-C(27)-H(27A)	119.8
C(14)-C(13)-H(13A)	108.1	C(27)-C(28)-C(23)	120.3(5)
P(1)-C(13)-H(13A)	108.1	C(27)-C(28)-H(28A)	119.8
C(14)-C(13)-H(13B)	108.1	C(23)-C(28)-H(28A)	119.8
P(1)-C(13)-H(13B)	108.1	C(30A)-C(29A)-C(34A)	120.0
H(13A)-C(13)-H(13B)	107.3	C(30A)-C(29A)-P(3)	118.67(16)
C(13)-C(14)-P(2)	114.0(3)	C(34A)-C(29A)-P(3)	121.33(16)
C(13)-C(14)-H(14A)	108.8	C(29A)-C(30A)-C(31A)	120.0
P(2)-C(14)-H(14A)	108.8	C(29A)-C(30A)-H(30A)	120.0
C(13)-C(14)-H(14B)	108.8	C(31A)-C(30A)-H(30A)	120.0
P(2)-C(14)-H(14B)	108.8	C(32A)-C(31A)-C(30A)	120.0
H(14A)-C(14)-H(14B)	107.7	C(32A)-C(31A)-H(31A)	120.0
C(16)-C(15)-C(20)	118.7(4)	C(30A)-C(31A)-H(31A)	120.0
C(16)-C(15)-P(2)	119.8(4)	C(31A)-C(32A)-C(33A)	120.0
C(20)-C(15)-P(2)	121.3(3)	C(31A)-C(32A)-H(32A)	120.0
C(15)-C(16)-C(17)	119.8(5)	C(33A)-C(32A)-H(32A)	120.0
C(15)-C(16)-H(16A)	120.1	C(32A)-C(33A)-C(34A)	120.0
C(17)-C(16)-H(16A)	120.1	C(32A)-C(33A)-H(33A)	120.0
C(18)-C(17)-C(16)	121.3(5)	C(34A)-C(33A)-H(33A)	120.0
C(18)-C(17)-H(17A)	119.4	C(33A)-C(34A)-C(29A)	120.0
C(16)-C(17)-H(17A)	119.4	C(33A)-C(34A)-H(34A)	120.0
C(17)-C(18)-C(19)	118.8(5)	C(29A)-C(34A)-H(34A)	120.0
C(17)-C(18)-H(18A)	120.6	C(30B)-C(29B)-C(34B)	120.0
C(19)-C(18)-H(18A)	120.6	C(30B)-C(29B)-P(3)	124.25(14)
C(20)-C(19)-C(18)	121.0(5)	C(34B)-C(29B)-P(3)	115.67(15)
C(20)-C(19)-H(19A)	119.5	C(29B)-C(30B)-C(31B)	120.0
C(18)-C(19)-H(19A)	119.5	C(29B)-C(30B)-H(30B)	120.0
C(19)-C(20)-C(15)	120.5(5)	C(31B)-C(30B)-H(30B)	120.0
C(19)-C(20)-H(20A)	119.8	C(32B)-C(31B)-C(30B)	120.0
C(15)-C(20)-H(20A)	119.8	C(32B)-C(31B)-H(31B)	120.0
C(22)-C(21)-P(2)	113.5(3)	C(30B)-C(31B)-H(31B)	120.0
C(22)-C(21)-H(21A)	108.9	C(31B)-C(32B)-C(33B)	120.0
P(2)-C(21)-H(21A)	108.9	C(31B)-C(32B)-H(32B)	120.0
C(22)-C(21)-H(21B)	108.9	C(33B)-C(32B)-H(32B)	120.0
P(2)-C(21)-H(21B)	108.9	C(34B)-C(33B)-C(32B)	120.0
H(21A)-C(21)-H(21B)	107.7	C(34B)-C(33B)-H(33B)	120.0
C(21)-C(22)-P(3)	118.9(3)	C(32B)-C(33B)-H(33B)	120.0

C(33B)-C(34B)-C(29B)	120.0	C(53)-C(52)-H(52A)	119.9
C(33B)-C(34B)-H(34B)	120.0	C(51)-C(52)-H(52A)	119.9
C(29B)-C(34B)-H(34B)	120.0	C(52)-C(53)-C(54)	119.3(5)
C(36)-C(35)-C(40)	113.2(3)	C(52)-C(53)-H(53A)	120.4
C(36)-C(35)-Pt(1)	131.22(16)	C(54)-C(53)-H(53A)	120.4
C(40)-C(35)-Pt(1)	115.6(2)	C(49)-C(54)-C(53)	120.3(5)
C(37)-C(36)-C(35)	127.3(3)	C(49)-C(54)-H(54A)	119.9
C(37)-C(36)-H(36A)	116.4	C(53)-C(54)-H(54A)	119.9
C(35)-C(36)-H(36A)	116.4	C(60)-C(55)-C(56)	120.2(4)
C(36)-C(37)-C(38)	117.4(4)	C(60)-C(55)-P(6)	121.7(3)
C(36)-C(37)-H(37A)	121.3	C(56)-C(55)-P(6)	118.1(3)
C(38)-C(37)-H(37A)	121.3	C(57)-C(56)-C(55)	119.8(4)
C(39)-C(38)-C(37)	120.6(4)	C(57)-C(56)-H(56A)	120.1
C(39)-C(38)-H(38A)	119.7	C(55)-C(56)-H(56A)	120.1
C(37)-C(38)-H(38A)	119.7	C(58)-C(57)-C(56)	120.4(5)
C(38)-C(39)-C(40)	120.6(4)	C(58)-C(57)-H(57A)	119.8
C(38)-C(39)-H(39A)	119.7	C(56)-C(57)-H(57A)	119.8
C(40)-C(39)-H(39A)	119.7	C(57)-C(58)-C(59)	120.3(5)
C(39)-C(40)-C(35)	120.8(4)	C(57)-C(58)-H(58A)	119.8
C(39)-C(40)-C(41)	125.1(4)	C(59)-C(58)-H(58A)	119.8
C(35)-C(40)-C(41)	114.1(3)	C(58)-C(59)-C(60)	120.3(5)
C(42)-C(41)-C(46)	118.9(4)	C(58)-C(59)-H(59A)	119.8
C(42)-C(41)-C(40)	125.6(4)	C(60)-C(59)-H(59A)	119.8
C(46)-C(41)-C(40)	115.5(4)	C(55)-C(60)-C(59)	119.0(5)
C(43)-C(42)-C(41)	120.6(4)	C(55)-C(60)-H(60A)	120.5
C(43)-C(42)-H(42A)	119.7	C(59)-C(60)-H(60A)	120.5
C(41)-C(42)-H(42A)	119.7	C(62)-C(61)-P(6)	117.4(3)
C(42)-C(43)-C(44)	120.0(4)	C(62)-C(61)-H(61A)	108.0
C(42)-C(43)-H(43A)	120.0	P(6)-C(61)-H(61A)	108.0
C(44)-C(43)-H(43A)	120.0	C(62)-C(61)-H(61B)	108.0
C(43)-C(44)-C(45)	120.7(5)	P(6)-C(61)-H(61B)	108.0
C(43)-C(44)-H(44A)	119.7	H(61A)-C(61)-H(61B)	107.2
C(45)-C(44)-H(44A)	119.7	N(2)-C(95)-C(96)	179.5(6)
C(46)-C(45)-C(44)	119.1(4)	C(61)-C(62)-P(5)	113.7(3)
C(46)-C(45)-H(45A)	120.5	C(61)-C(62)-H(62A)	108.8
C(44)-C(45)-H(45A)	120.5	P(5)-C(62)-H(62A)	108.8
C(45)-C(46)-C(41)	120.8(4)	C(61)-C(62)-H(62B)	108.8
C(45)-C(46)-Pt(1)	125.2(3)	P(5)-C(62)-H(62B)	108.8
C(41)-C(46)-Pt(1)	113.9(3)	H(62A)-C(62)-H(62B)	107.7
N(1)-C(47)-C(48)	179.0(5)	C(68)-C(63)-C(64)	117.8(4)
C(47)-C(48)-H(48A)	109.5	C(68)-C(63)-P(5)	120.8(3)
C(47)-C(48)-H(48B)	109.5	C(64)-C(63)-P(5)	121.1(3)
H(48A)-C(48)-H(48B)	109.5	C(65)-C(64)-C(63)	120.5(5)
C(47)-C(48)-H(48C)	109.5	C(65)-C(64)-H(64A)	119.7
H(48A)-C(48)-H(48C)	109.5	C(63)-C(64)-H(64A)	119.7
H(48B)-C(48)-H(48C)	109.5	C(66)-C(65)-C(64)	120.7(5)
C(54)-C(49)-C(50)	119.0(4)	C(66)-C(65)-H(65A)	119.6
C(54)-C(49)-P(6)	120.3(3)	C(64)-C(65)-H(65A)	119.6
C(50)-C(49)-P(6)	120.7(4)	C(65)-C(66)-C(67)	120.1(5)
C(51)-C(50)-C(49)	120.7(5)	C(65)-C(66)-H(66A)	120.0
C(51)-C(50)-H(50A)	119.6	C(67)-C(66)-H(66A)	120.0
C(49)-C(50)-H(50A)	119.6	C(66)-C(67)-C(68)	119.5(5)
C(50)-C(51)-C(52)	120.5(5)	C(66)-C(67)-H(67A)	120.2
C(50)-C(51)-H(51A)	119.7	C(68)-C(67)-H(67A)	120.2
C(52)-C(51)-H(51A)	119.7	C(63)-C(68)-C(67)	121.3(5)
C(53)-C(52)-C(51)	120.2(5)	C(63)-C(68)-H(68A)	119.3

C(67)-C(68)-H(68A)	119.3	C(77)-C(82)-C(81)	120.1(6)
C(70)-C(69)-P(5)	112.3(3)	C(77)-C(82)-H(82A)	120.0
C(70)-C(69)-H(69A)	109.1	C(81)-C(82)-H(82A)	120.0
P(5)-C(69)-H(69A)	109.1	C(88)-C(83)-C(84)	119.8(4)
C(70)-C(69)-H(69B)	109.1	C(88)-C(83)-Pt(2)	115.1(4)
P(5)-C(69)-H(69B)	109.1	C(84)-C(83)-Pt(2)	125.1(4)
H(69A)-C(69)-H(69B)	107.9	C(83)-C(84)-C(85)	120.6(6)
C(69)-C(70)-P(4)	114.1(3)	C(83)-C(84)-H(84A)	119.7
C(69)-C(70)-H(70A)	108.7	C(85)-C(84)-H(84A)	119.7
P(4)-C(70)-H(70A)	108.7	C(86)-C(85)-C(84)	119.2(7)
C(69)-C(70)-H(70B)	108.7	C(86)-C(85)-H(85A)	120.4
P(4)-C(70)-H(70B)	108.7	C(84)-C(85)-H(85A)	120.4
H(70A)-C(70)-H(70B)	107.6	C(85)-C(86)-C(87)	121.1(6)
C(72)-C(71)-C(76)	119.2(5)	C(85)-C(86)-H(86A)	119.5
C(72)-C(71)-P(4)	119.6(4)	C(87)-C(86)-H(86A)	119.5
C(76)-C(71)-P(4)	121.1(4)	C(86)-C(87)-C(88)	119.5(7)
C(71)-C(72)-C(73)	119.9(5)	C(86)-C(87)-H(87A)	120.2
C(71)-C(72)-H(72A)	120.1	C(88)-C(87)-H(87A)	120.2
C(73)-C(72)-H(72A)	120.1	C(83)-C(88)-C(87)	119.9(6)
C(74)-C(73)-C(72)	120.4(6)	C(83)-C(88)-C(89)	115.1(4)
C(74)-C(73)-H(73A)	119.8	C(87)-C(88)-C(89)	124.9(6)
C(72)-C(73)-H(73A)	119.8	C(90)-C(89)-C(94)	118.1(6)
C(73)-C(74)-C(75)	120.6(5)	C(90)-C(89)-C(88)	126.4(5)
C(73)-C(74)-H(74A)	119.7	C(94)-C(89)-C(88)	115.4(4)
C(75)-C(74)-H(74A)	119.7	C(91)-C(90)-C(89)	120.9(6)
C(76)-C(75)-C(74)	119.8(6)	C(91)-C(90)-H(90A)	119.5
C(76)-C(75)-H(75A)	120.1	C(89)-C(90)-H(90A)	119.5
C(74)-C(75)-H(75A)	120.1	C(92)-C(91)-C(90)	120.8(5)
C(75)-C(76)-C(71)	120.1(5)	C(92)-C(91)-H(91A)	119.6
C(75)-C(76)-H(76A)	119.9	C(90)-C(91)-H(91A)	119.6
C(71)-C(76)-H(76A)	119.9	C(91)-C(92)-C(93)	120.3(6)
C(78)-C(77)-C(82)	120.1(4)	C(91)-C(92)-H(92A)	119.9
C(78)-C(77)-P(4)	121.7(4)	C(93)-C(92)-H(92A)	119.9
C(82)-C(77)-P(4)	118.2(4)	C(92)-C(93)-C(94)	119.8(5)
C(77)-C(78)-C(79)	119.6(6)	C(92)-C(93)-H(93A)	120.1
C(77)-C(78)-H(78A)	120.2	C(94)-C(93)-H(93A)	120.1
C(79)-C(78)-H(78A)	120.2	C(93)-C(94)-C(89)	120.1(4)
C(80)-C(79)-C(78)	120.5(6)	C(93)-C(94)-Pt(2)	125.6(3)
C(80)-C(79)-H(79A)	119.7	C(89)-C(94)-Pt(2)	114.2(4)
C(78)-C(79)-H(79A)	119.7	C(95)-C(96)-H(96A)	109.5
C(79)-C(80)-C(81)	120.9(6)	C(95)-C(96)-H(96B)	109.5
C(79)-C(80)-H(80A)	119.6	H(96A)-C(96)-H(96B)	109.5
C(81)-C(80)-H(80A)	119.6	C(95)-C(96)-H(96C)	109.5
C(80)-C(81)-C(82)	118.8(6)	H(96A)-C(96)-H(96C)	109.5
C(80)-C(81)-H(81A)	120.6	H(96B)-C(96)-H(96C)	109.5
C(82)-C(81)-H(81A)	120.6		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex 8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	27(1)	20(1)	24(1)	2(1)	12(1)	4(1)
Pt(2)	30(1)	19(1)	23(1)	3(1)	12(1)	5(1)
P(1)	30(1)	25(1)	24(1)	2(1)	12(1)	4(1)
P(2)	34(1)	32(1)	31(1)	10(1)	18(1)	10(1)
P(3)	32(1)	26(1)	40(1)	-1(1)	20(1)	0(1)
P(4)	31(1)	23(1)	31(1)	4(1)	12(1)	3(1)
P(5)	29(1)	25(1)	23(1)	1(1)	10(1)	6(1)
P(6)	31(1)	21(1)	26(1)	2(1)	13(1)	3(1)
N(1)	32(2)	23(2)	24(2)	4(1)	11(2)	1(2)
N(2)	33(2)	32(2)	35(2)	3(2)	24(2)	6(2)
C(1)	45(3)	30(2)	31(2)	-1(2)	23(2)	-1(2)
C(2)	50(3)	39(3)	31(3)	-2(2)	22(2)	-7(2)
C(3)	70(4)	49(3)	33(3)	-10(2)	27(3)	-18(3)
C(4)	84(4)	30(3)	55(3)	-6(2)	46(3)	-1(3)
C(5)	57(3)	32(3)	61(3)	2(2)	35(3)	4(2)
C(6)	44(3)	29(2)	36(3)	-2(2)	19(2)	0(2)
C(7)	28(2)	32(2)	24(2)	-1(2)	9(2)	-2(2)
C(8)	48(3)	27(2)	37(3)	4(2)	20(2)	7(2)
C(9)	62(4)	37(3)	33(3)	7(2)	21(2)	-7(2)
C(10)	48(3)	46(3)	31(3)	-1(2)	25(2)	-5(2)
C(11)	39(3)	44(3)	30(2)	-4(2)	17(2)	4(2)
C(12)	34(3)	35(3)	29(2)	1(2)	15(2)	5(2)
C(13)	26(2)	34(2)	34(2)	2(2)	15(2)	4(2)
C(14)	34(3)	66(3)	34(3)	23(2)	17(2)	19(2)
C(15)	37(3)	37(3)	23(2)	14(2)	12(2)	10(2)
C(16)	43(3)	54(3)	35(3)	-2(2)	21(2)	0(2)
C(17)	53(3)	59(4)	37(3)	-7(2)	16(2)	-5(3)
C(18)	59(3)	52(3)	28(3)	11(2)	18(2)	24(3)
C(19)	46(3)	60(4)	48(3)	6(3)	28(2)	12(3)
C(20)	43(3)	48(3)	42(3)	0(2)	24(2)	5(2)
C(21)	48(2)	29(2)	63(2)	16(2)	36(2)	9(2)
C(22)	48(2)	29(2)	63(2)	16(2)	36(2)	9(2)
C(23)	26(2)	31(2)	39(3)	2(2)	16(2)	1(2)
C(24)	37(3)	38(3)	57(3)	8(2)	24(2)	6(2)
C(25)	42(3)	57(3)	61(3)	9(3)	33(3)	6(3)
C(26)	34(3)	56(4)	65(4)	-4(3)	22(3)	3(3)
C(27)	35(3)	42(3)	66(4)	8(3)	15(3)	11(2)
C(28)	41(3)	43(3)	44(3)	10(2)	14(2)	5(2)
C(29A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(30A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(31A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(32A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(33A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(34A)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(29B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(30B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(31B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(32B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(33B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)
C(34B)	70(2)	50(2)	51(2)	-14(1)	29(2)	1(2)

C(35)	26(2)	19(2)	39(3)	-4(2)	19(2)	1(2)
C(36)	29(2)	34(3)	35(3)	3(2)	12(2)	1(2)
C(37)	36(3)	26(2)	52(3)	-5(2)	13(2)	9(2)
C(38)	39(3)	41(3)	47(3)	-12(2)	17(2)	7(2)
C(39)	37(3)	45(3)	30(2)	-6(2)	13(2)	3(2)
C(40)	25(2)	31(2)	28(2)	-5(2)	10(2)	-3(2)
C(41)	26(2)	34(2)	27(2)	-6(2)	9(2)	-6(2)
C(42)	46(3)	43(3)	28(3)	-1(2)	15(2)	1(2)
C(43)	69(4)	50(3)	27(3)	8(2)	17(2)	5(3)
C(44)	59(3)	42(3)	33(3)	12(2)	8(2)	14(3)
C(45)	45(3)	30(2)	29(2)	1(2)	13(2)	6(2)
C(46)	30(2)	24(2)	22(2)	6(2)	9(2)	2(2)
C(47)	44(3)	34(3)	26(2)	6(2)	13(2)	15(2)
C(48)	95(5)	72(4)	50(3)	13(3)	38(3)	56(4)
C(49)	34(3)	26(2)	30(2)	4(2)	8(2)	1(2)
C(50)	44(3)	32(3)	32(3)	3(2)	13(2)	5(2)
C(51)	75(4)	37(3)	28(3)	-1(2)	12(3)	9(3)
C(52)	56(4)	64(4)	40(3)	-7(3)	0(3)	-5(3)
C(53)	38(3)	76(4)	57(4)	-16(3)	9(3)	-13(3)
C(54)	41(3)	61(4)	40(3)	-3(2)	13(2)	2(3)
C(55)	33(2)	23(2)	31(2)	2(2)	10(2)	2(2)
C(56)	37(3)	29(2)	43(3)	-2(2)	21(2)	2(2)
C(57)	42(3)	38(3)	50(3)	0(2)	18(2)	11(2)
C(58)	44(3)	35(3)	69(4)	9(3)	14(3)	16(2)
C(59)	45(3)	34(3)	57(3)	22(2)	10(3)	7(2)
C(60)	37(3)	27(2)	40(3)	6(2)	13(2)	3(2)
C(61)	31(2)	31(2)	32(2)	3(2)	16(2)	5(2)
C(95)	43(3)	36(3)	40(3)	0(2)	22(2)	10(2)
C(62)	33(2)	34(2)	30(2)	4(2)	15(2)	7(2)
C(63)	38(3)	33(2)	19(2)	2(2)	11(2)	13(2)
C(64)	45(3)	42(3)	36(3)	7(2)	9(2)	12(2)
C(65)	70(4)	44(3)	41(3)	14(2)	15(3)	24(3)
C(66)	51(3)	65(4)	26(3)	5(2)	7(2)	33(3)
C(67)	40(3)	71(4)	32(3)	8(3)	4(2)	14(3)
C(68)	37(3)	51(3)	33(3)	12(2)	13(2)	12(2)
C(69)	32(2)	25(2)	38(3)	-5(2)	14(2)	4(2)
C(70)	29(2)	19(2)	42(3)	0(2)	13(2)	3(2)
C(71)	35(3)	31(3)	43(3)	13(2)	18(2)	3(2)
C(72)	34(3)	43(3)	42(3)	12(2)	12(2)	-9(2)
C(73)	42(3)	65(4)	46(3)	23(3)	5(2)	-11(3)
C(74)	30(3)	62(4)	83(4)	37(3)	11(3)	-1(3)
C(75)	45(3)	55(4)	103(5)	34(4)	38(3)	17(3)
C(76)	42(3)	39(3)	69(4)	14(2)	31(3)	1(2)
C(77)	43(3)	23(2)	31(2)	7(2)	11(2)	-1(2)
C(78)	47(3)	56(4)	63(4)	28(3)	18(3)	17(3)
C(79)	63(4)	77(5)	88(5)	47(4)	18(4)	21(4)
C(80)	70(5)	95(5)	69(5)	57(4)	11(4)	8(4)
C(81)	105(6)	77(5)	56(4)	25(3)	38(4)	9(4)
C(82)	74(4)	48(3)	55(3)	26(3)	35(3)	16(3)
C(83)	59(3)	26(2)	24(2)	2(2)	19(2)	-6(2)
C(84)	77(4)	43(3)	49(3)	0(2)	43(3)	0(3)
C(85)	149(8)	71(5)	60(4)	0(3)	75(5)	10(5)
C(86)	180(10)	92(6)	51(5)	4(4)	72(6)	3(6)
C(87)	130(6)	58(4)	30(3)	13(3)	17(4)	-5(4)
C(88)	85(4)	29(3)	24(3)	1(2)	16(3)	-7(3)
C(89)	61(3)	25(2)	35(3)	9(2)	5(2)	-3(2)

C(90)	65(4)	39(3)	53(4)	16(3)	-20(3)	0(3)
C(91)	48(4)	42(3)	92(5)	19(3)	-20(3)	11(3)
C(92)	33(3)	36(3)	91(5)	18(3)	5(3)	8(2)
C(93)	34(3)	20(2)	59(3)	5(2)	3(2)	2(2)
C(94)	32(2)	13(2)	36(3)	5(2)	2(2)	-1(2)
C(96)	61(4)	77(4)	68(4)	10(3)	25(3)	43(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex 8.

	x	y	z	U(eq)
H(2A)	2686	8413	5974	47
H(3A)	2725	7188	5462	63
H(4A)	4007	6444	6017	63
H(5A)	5246	6892	7082	57
H(6A)	5213	8096	7609	44
H(8A)	3991	8257	8104	43
H(9A)	3317	8166	8907	53
H(10A)	2341	9076	9102	48
H(11A)	2063	10128	8518	45
H(12A)	2749	10246	7717	39
H(13A)	2543	9555	6314	36
H(13B)	2959	10311	6853	36
H(14A)	3498	10835	6158	50
H(14B)	3458	10010	5772	50
H(16A)	4222	9058	5651	52
H(17A)	4789	8235	5016	63
H(18A)	6410	8570	4939	53
H(19A)	7539	9703	5561	58
H(20A)	7031	10505	6228	51
H(21A)	6270	11453	6387	50
H(21B)	5287	11774	6490	50
H(22A)	6156	12083	7514	50
H(22B)	7157	12134	7315	50
H(24A)	8440	11642	7230	51
H(25A)	9800	11194	6986	59
H(26A)	10528	10117	7416	63
H(27A)	9864	9470	8085	59
H(28A)	8479	9892	8314	52
H(30A)	7104	12637	8402	69
H(31A)	7693	13384	9432	69
H(32A)	8596	12849	10382	69
H(33A)	8910	11568	10303	69
H(34A)	8321	10820	9274	69
H(30B)	6984	12557	8660	69
H(31B)	7708	13087	9779	69
H(32B)	8911	12447	10573	69
H(33B)	9390	11277	10247	69
H(34B)	8666	10747	9127	69
H(36A)	4453	11515	7347	40
H(37A)	3832	12354	7877	48

H(38A)	4130	12246	8977	52
H(39A)	5050	11292	9496	46
H(42A)	5824	10251	9900	48
H(43A)	6697	9200	10239	59
H(44A)	7272	8487	9547	57
H(45A)	6975	8821	8502	42
H(48A)	6761	7868	6493	98
H(48B)	7746	7927	7195	98
H(48C)	7815	8499	6686	98
H(50A)	7375	3536	967	44
H(51A)	5916	2974	13	60
H(52A)	4210	2707	9	74
H(53A)	3956	2999	971	76
H(54A)	5451	3550	1953	59
H(56A)	9061	3198	1872	43
H(57A)	9953	2132	2145	52
H(58A)	9875	1492	2992	61
H(59A)	8900	1904	3579	57
H(60A)	7954	2953	3297	43
H(61A)	6471	4511	2646	36
H(61B)	6879	3803	3032	36
H(62A)	8083	4568	3889	38
H(62B)	7399	5234	3592	38
H(64A)	9444	4038	4122	51
H(65A)	10984	3615	4835	63
H(66A)	12639	4386	5210	58
H(67A)	12788	5600	4877	61
H(68A)	11248	6039	4167	48
H(69A)	8556	6565	3792	39
H(69B)	9835	6649	4024	39
H(70A)	9424	7422	3233	37
H(70B)	8282	6903	2797	37
H(72A)	11093	7473	3673	50
H(73A)	12953	7651	4303	67
H(74A)	14023	6905	4010	74
H(75A)	13291	6031	3037	75
H(76A)	11438	5810	2419	57
H(78A)	8246	7565	1984	66
H(79A)	7893	8209	1065	92
H(80A)	8716	7961	361	97
H(81A)	9888	7052	543	92
H(82A)	10318	6449	1499	66
H(84A)	10129	4454	1544	63
H(85A)	9925	4322	440	101
H(86A)	8433	4704	-356	122
H(87A)	7152	5228	-71	94
H(90A)	5902	5602	306	80
H(91A)	4791	6028	780	89
H(92A)	5320	6155	1909	71
H(93A)	6985	5842	2587	52
H(96A)	12131	3736	2847	100
H(96B)	11897	3625	3485	100
H(96C)	12613	4404	3470	100