Supporting Information for

Aerobic Oxidative Coupling of *o*-Xylene: Discovery of 2-Fluoropyridine as a Ligand to Support Selective Pd-Catalyzed C–H Functionalization

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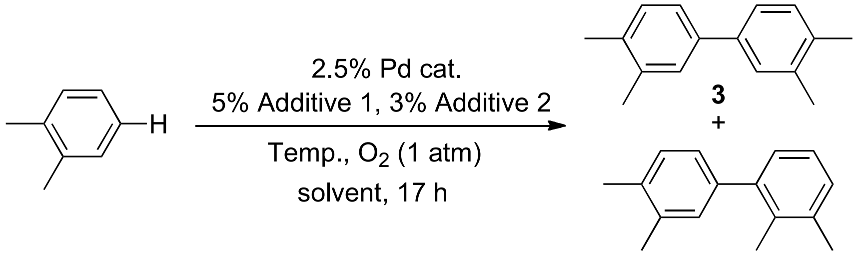
Table S1. Additional Reaction Optimization Data.



3

3'

Entry	Catalyst (2.5%)	Additive 1[a]	Additive 2	Solvent[b]	Temp °C	% yield (**3**+**3'**)[c]	% Regioselectivity(**3**)
1	$Pd(OAc)_2$	--	CF_3CO_2H	--	80	2.5	67
2	$Pd(TFA)_2$	--	--	--	80	2.8	68
3	$Pd(OAc)_2$	--	CF_3CO_2H	p.c.	80	11.1	67
4	$Pd(OAc)_2$	Py	CF_3CO_2H	p.c.	80	0.2	90
5	$Pd(OAc)_2$	2-OMe-py	CF_3CO_2H	p.c.	80	0.5	68
6	$Pd(OAc)_2$	2-OEt-py	CF_3CO_2H	p.c.	80	1.2	75
7	$Pd(OAc)_2$	2-OH-py	CF_3CO_2H	p.c.	80	1.8	70
8	$Pd(OAc)_2$	2-Me-py	CF_3CO_2H	p.c.	80	2.3	75
9	**$Pd(OAc)_2$**	**2-F-py**	CF_3CO_2H	**p.c.**	**80**	**27.4**	**88**
10	$Pd(OAc)_2$	2-Cl-py	CF_3CO_2H	p.c.	80	5.6	83
11	$Pd(OAc)_2$	2-CF_3-py	CF_3CO_2H	p.c.	80	10.2	65
12	$Pd(OAc)_2$	3-F-py	CF_3CO_2H	p.c.	80	3.2	90
13	$Pd(OAc)_2$	4-F-py	CF_3CO_2H	p.c.	80	7.7	86
14	$Pd(OAc)_2$	2,3,5-trifluoro-py	CF_3CO_2H	p.c.	80	16.3	68
15	$Pd(OAc)_2$	2,4,6-trifluoro-py	CF_3CO_2H	p.c.	80	21.9	58
16	$Pd(OAc)_2$	2-F,4-CF_3-py	CF_3CO_2H	p.c.	80	16.6	77
17	$Pd(OAc)_2$	2-F,6-CO_2Me-py	CF_3CO_2H	p.c.	80	19.2	71
18	$Pd(OAc)_2$	2,6-Di-^{t}Bu-py	CF_3CO_2H	p.c.	80	21.9	74
19	$Pd(OAc)_2$	Pyrazine	CF_3CO_2H	p.c.	80	1.3	92
20	$Pd(OAc)_2$	Pyridazine	CF_3CO_2H	p.c.	80	1.0	83
21	$Pd(OAc)_2$	2-NH_2-py	CF_3CO_2H	p.c.	80	0.0	--
22	$Pd(OAc)_2$	2-NMe_2-py	CF_3CO_2H	p.c.	80	0.0	--

23	Pd(OAc)$_2$	2-PhNH-py	CF_3CO_2H	p.c.	80	0.0	--
24	Pd(OAc)$_2$	bpy	CF_3CO_2H	p.c.	80	0.0	--
25	Pd(OAc)$_2$	phen	CF_3CO_2H	p.c.	80	0.3	90
26	Pd(OAc)$_2$	en	CF_3CO_2H	p.c.	80	0.4	76
27	Pd(OAc)$_2$	TMEDA	CF_3CO_2H	p.c.	80	1.7	71
28	Pd(OAc)$_2$	2-F-py (2.5%)	CF_3CO_2H	p.c.	80	33.9[e]	84
29	Pd(OAc)$_2$	2-F-py (3.8%)	CF_3CO_2H	p.c.	80	29.6	87
30	Pd(OAc)$_2$	2-F-py (10%)	CF_3CO_2H	p.c.	80	25.4	91
31	Pd(OAc)$_2$	2-F-py (15%)	CF_3CO_2H	p.c.	80	19.0	92
32	Pd(OAc)$_2$	2-F-py (15%)	CF_3CO_2H	p.c.	80	19.0	92
33	Pd(OAc)$_2$	2-F-py	CF_3CO_2H (1%)	p.c.	80	8.3	79
34	Pd(OAc)$_2$	2-F-py	CF_3CO_2H (2%)	p.c.	80	19.6	85
35	Pd(OAc)$_2$	2-F-py	CF_3CO_2H (4%)	p.c.	80	21.2	87
36	Pd(OAc)$_2$	2-F-py	CF_3CO_2H (8%)	p.c.	80	12.7	72
37	Pd(OAc)$_2$	2-F-py	--	p.c.	80	5.1	65
38	Pd(OAc)$_2$ + Pd(TFA)$_2$ (8:2)	2-F-py	--	p.c.	80	8.5	74
39	Pd(OAc)2 + Pd(TFA)2 (5:5)	2-F-py	--	p.c.	80	20.4	82
40	Pd(OAc)2 + Pd(TFA)2 (2:8)	2-F-py	--	p.c.	80	22.4	81
41	Pd(TFA)$_2$	2-F-py	--	p.c.	80	17.7	78
42	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	p.c.	60	13.1 (18.7)[d]	89
43	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	DMA	80	11.0	72
44	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	DMF	80	9.9	70
45	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	NMP	80	10.0	87
46	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	DMSO	80	1.1	60
47	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	AcOH	80	18.1	72
48	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	$EtCO_2H$	80	9.6	87
49	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	PivOH	80	2.8	85
50	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	d.c.	80	10.9	87
51	Pd(OAc)$_2$	2-F-py	CF_3CO_2H	--	80	23.7	82

52	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / AlCl$_3$	p.c.	80	0	--
53	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / Ag$_2$O	p.c.	80	21.8	87
54	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / AgNO$_3$, KF	p.c.	80	10.2	81
55	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / Tl(TFA)$_3$	p.c.	80	11.9	90
56	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / LiF	p.c.	80	26.4	87
57	Pd(OAc)$_2$	2-F-py	CF$_3$CO$_2$H / AgOTf	p.c.	80	11.1	84

Conditions: **1** (3.8 mmole), 1 atm O$_2$, solvent (0.4 mL), 17 hr., N/Pd = 2. [a]py = pyridine, bpy = 2,2'-dipyridyl, phen = 1,10-phenanthroline, en = ethylene diamine, TMEDA = tetramethyl ethylene diamine. [b]p.c. = propylene carbonate; DMA = *N,N*-dimethylacetamide; *N,N*-dimethylformamide; NMP = *N*-methylpyrrolidinone; PivOH = trimethylacetic acid; d.c. = diethyl carbonate. [c]Determined by GC, internal standard = n-hexadecane. [d]48 hr. [e]Although the highest yield was obtained under these conditions, the regioselectivity was decreased.

NMR spectroscopic studies of $Pd(OAc)_2$ and 2-fluoropyridine in benzene-*d*$_6$.

$Pd(OAc)_2$ (2.8 mg, 12.4 μmol) was added to an NMR tube together with benzene-*d*$_6$ (400 μL). Independently, a solution of 2-fluoropyridine (12.6 mg, 0.13 mmol) was prepared in benzene-*d*$_6$ (1.21 g, 107 mM). ^1H NMR spectra (300 MHz) and ^{19}F NMR spectra of a titration of 2-fluoropyridine against $Pd(OAc)_2$ at room temperature are shown in the stacked plots below. The assignments of 2-fluoropyridine ligand resonances are made on the basis of 2-fluoropyridine reagent in benzene-*d*$_6$.

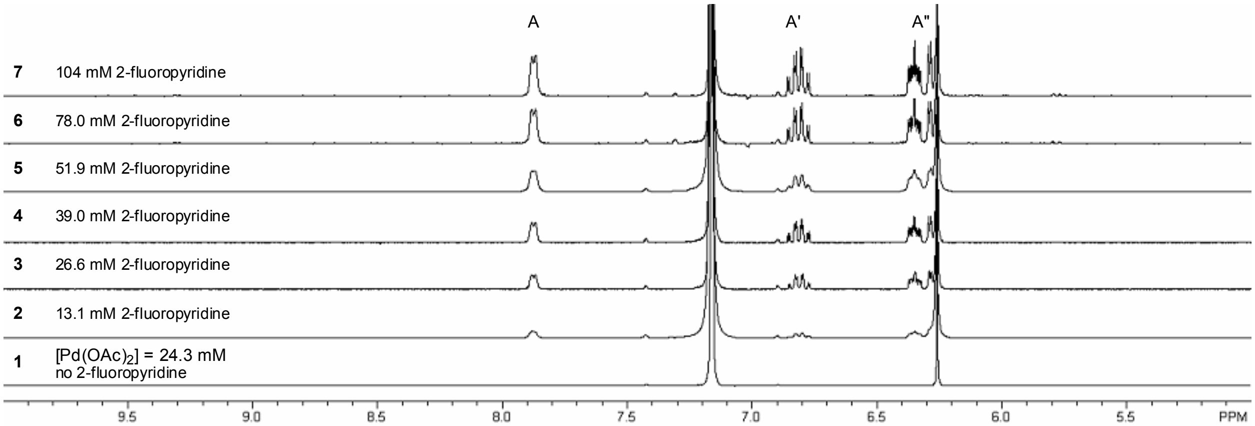


Figure S1. ^1H NMR spectra of a titration of 2-fluoropyridine against $Pd(OAc)_2$. Conditions : $[Pd(OAc)_2]$ = 24.3 mM, [1,3,5-trimethoxybenzene] = 23.4 mM.

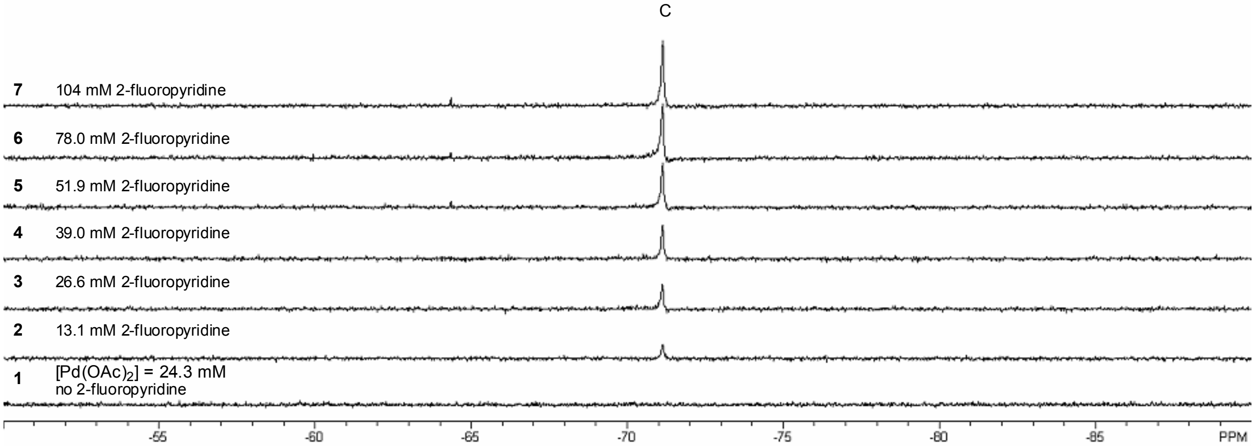
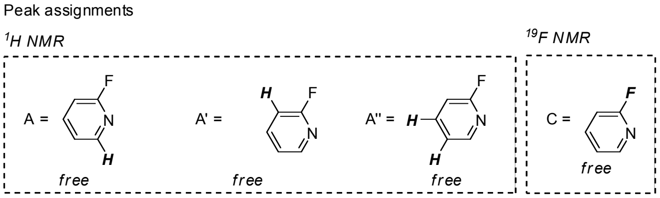


Figure S2. ^{19}F NMR spectra of a titration of 2-fluoropyridine against $Pd(OAc)_2$. Conditions : $[Pd(OAc)_2]$ = 24.3 mM, [hexafluorobenzene] = 24.0 mM.



NMR spectroscopic studies of Pd(TFA)$_2$ and 2-fluoropyridine in benzene-*d*$_6$.

Pd(TFA)$_2$ (2.5 mg, 7.5 μmol) was added to an NMR tube together with benzene-*d*$_6$ (400 μL). Independently, a solution of 2-fluoropyridine (12.6 mg, 0.13 mmol) was prepared in benzene-*d*$_6$ (1.21 g, 107 mM). ^{1}H NMR spectra (300 MHz) and ^{19}F NMR spectra of a titration of 2-fluoropyridine against Pd(TFA)$_2$ at room temperature are shown in the stacked plots below. The assignments of 2-fluoropyridine ligand resonances are made on the basis of the ^{1}H and ^{19}F NMR spectra for the isolated Pd^{II} complex, (^{2F}py)$_2$Pd(TFA)$_2$ (see X-ray crystal structure below) and free 2-fluoropyridine.

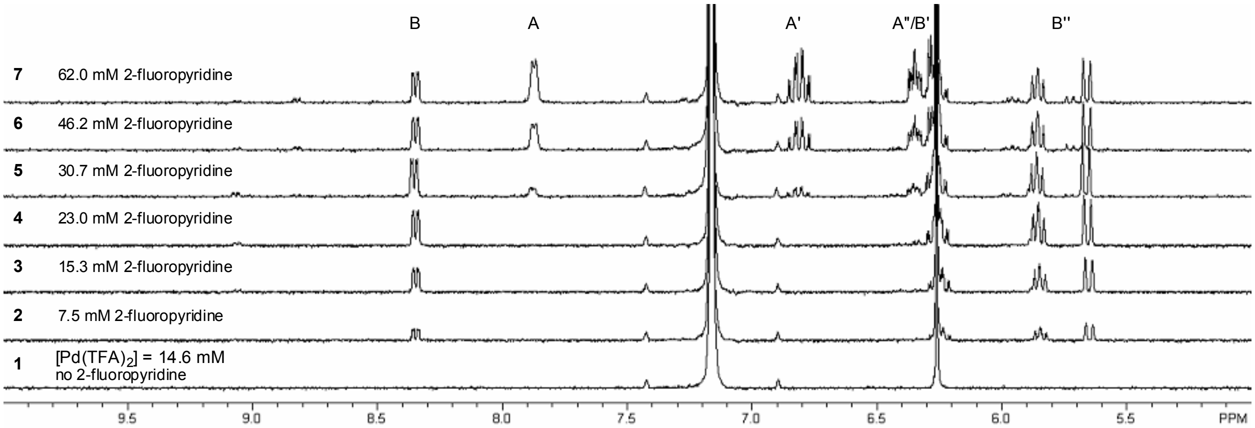


Figure S3. ^{1}H NMR spectra of a titration of 2-fluoropyridine against Pd(TFA)$_2$. Conditions : [Pd(TFA)$_2$] = 14.6 mM, [1,3,5-trimethoxybenzene] = 17.3 mM.

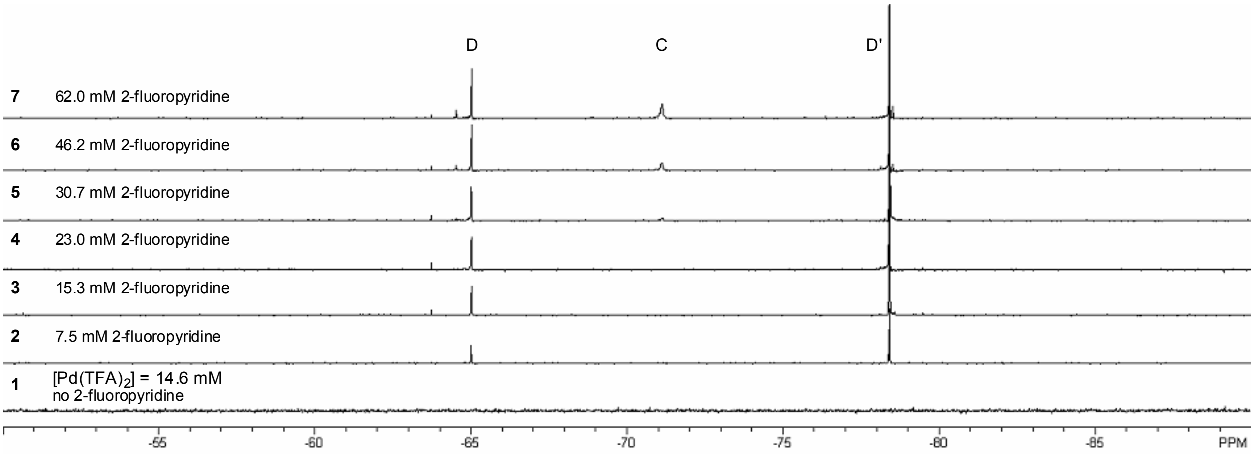
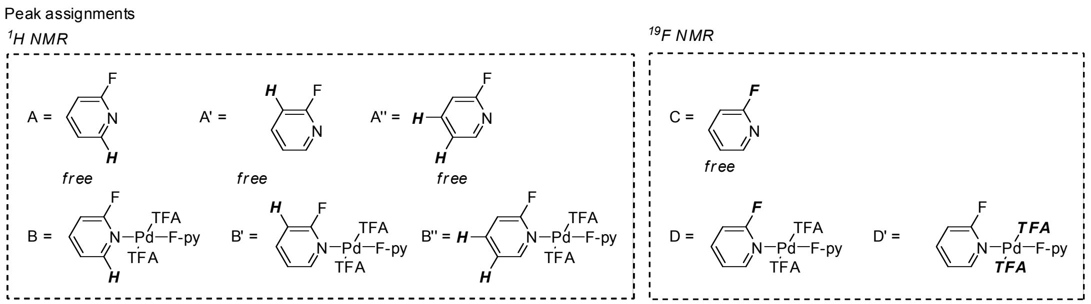


Figure S4. ^{19}F NMR spectra of a titration of 2-fluoropyridine against Pd(TFA)$_2$. Conditions : [Pd(TFA)$_2$] = 14.6 mM, [hexafluorobenzene] = 14.5mM.



NMR spectroscopic studies of $Pd(OAc)_2$, 2-fluoropyridine and trifluoroacetic acid in benzene-d_6.

$Pd(OAc)_2$ (2.4 mg, 10.7 μmol) was added to an NMR tube together with benzene-d_6 (400 μL). Independently, a solution of 2-fluoropyridine (12.6 mg, 0.13 μmol) and a solution of trifluoroacetic acid (26.5mg, 0.23 μmol) were prepared in benzene-d_6 (1.21 g, 107 mM and 0.79 g, 293 mM, respectively). ^1H NMR spectra (300 MHz) and ^{19}F NMR spectra of a titration of 2-fluoropyridine against $Pd(TFA)_2$ at room temperature are shown in the stacked plots below. The assignments of 2-fluoropyridine ligand resonances are made on the basis of the ^1H and ^{19}F NMR spectra for the isolated Pd^{II} complex, $(^{2F}py)_2Pd(TFA)_2$ (see X-ray crystal structure below) and free 2-fluoropyridine.

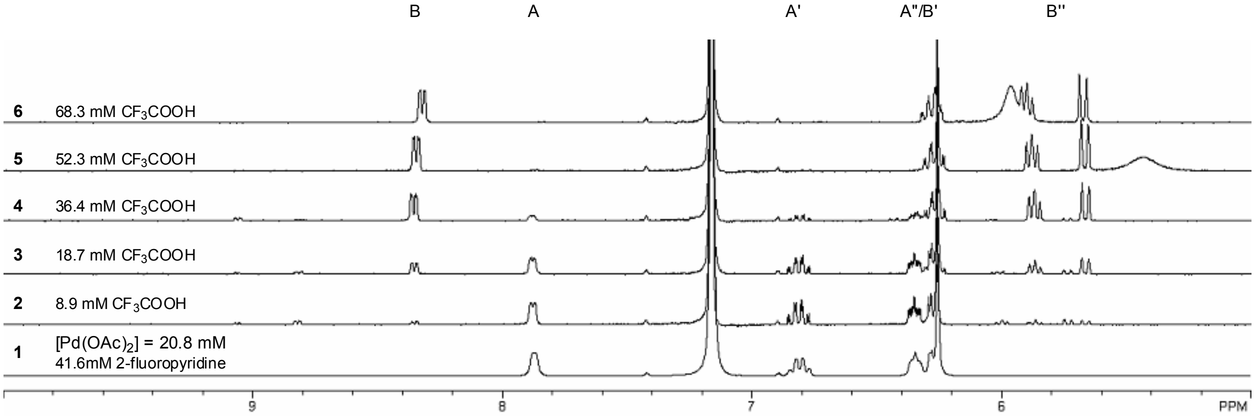


Figure S5. ^1H NMR spectra of a titration of trifluoroacetic acid against $Pd(OAc)_2$ and 2-fluoropyridine. Conditions : $[Pd(OAc)_2]$ = 20.8 mM, [1,3,5-trimethoxybenzene] = 19.8 mM.

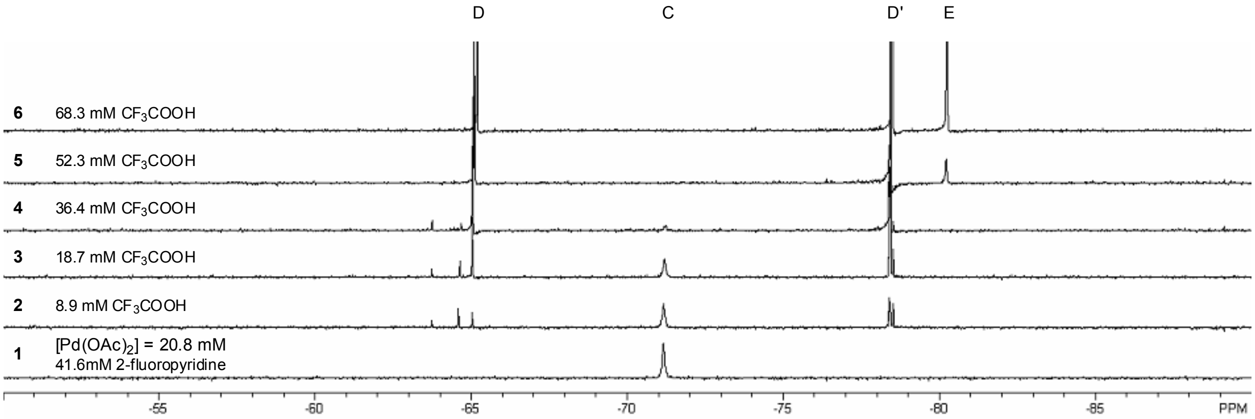
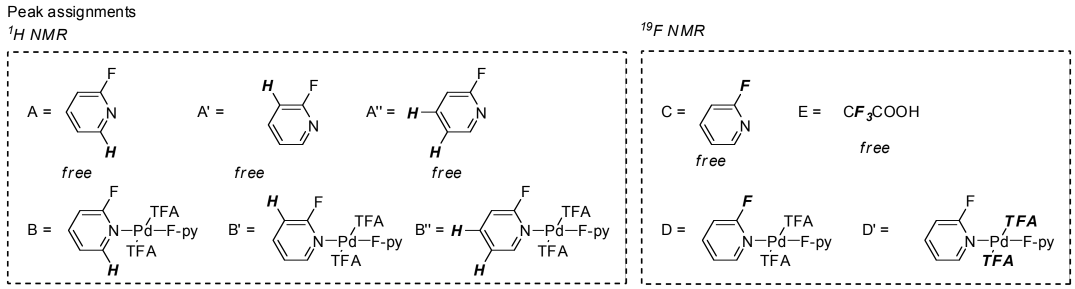


Figure S6. ^{19}F NMR spectra of a titration of trifluoroacetic acid against $Pd(OAc)_2$ and 2-fluoropyridine. Conditions : $[Pd(OAc)_2]$ = 20.8 mM, [hexafluorobenzene] = 19.8 mM.



NMR spectroscopic studies of $Pd(OAc)_2$, $Pd(TFA)_2$ and 2-fluoropyridine in benzene-d_6.

$Pd(OAc)_2$ (0.9 mg, 4.0 μmol) and $Pd(TFA)_2$ (1.4 mg, 4.2 μmol) were added to an NMR tube together with benzene-d_6 (400 μL). Independently, a solution of 2-fluoropyridine (12.5 mg, 0.13 μmol) and a solution of trifluoroacetic acid (26.5mg, 0.23 μmol) were prepared in benzene-d_6 (0.62 g, 207 mM). After adding 2-fluoropyridine solution (194 mg, 21.0 mmol), trifluoroacetic acid was titrated into the mixture. ^1H NMR spectra (300 MHz) and ^{19}F NMR spectra of the titration at room temperature are shown in the stacked plots below. The assignments of 2-fluoropyridine ligand resonances are made on the basis of the ^1H and ^{19}F NMR spectra for the isolated Pd^{II} complex, $(^{2F}py)_2Pd(TFA)_2$ (see X-ray crystal structure below) and free 2-fluoropyridine.

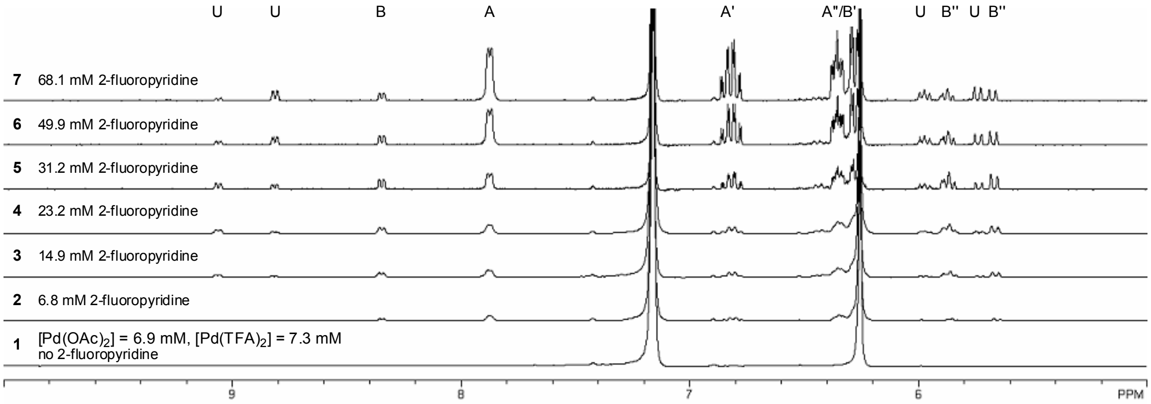


Figure S7. ^1H NMR spectra of a titration of 2-fluoropyridine against $Pd(OAc)_2$ and $Pd(TFA)_2$. Conditions : $[Pd(OAc)_2] = 6.9$ mM , $[Pd(TFA)_2] = 7.3$ mM, [1,3,5-trimethoxybenzene] = 27.8 mM.

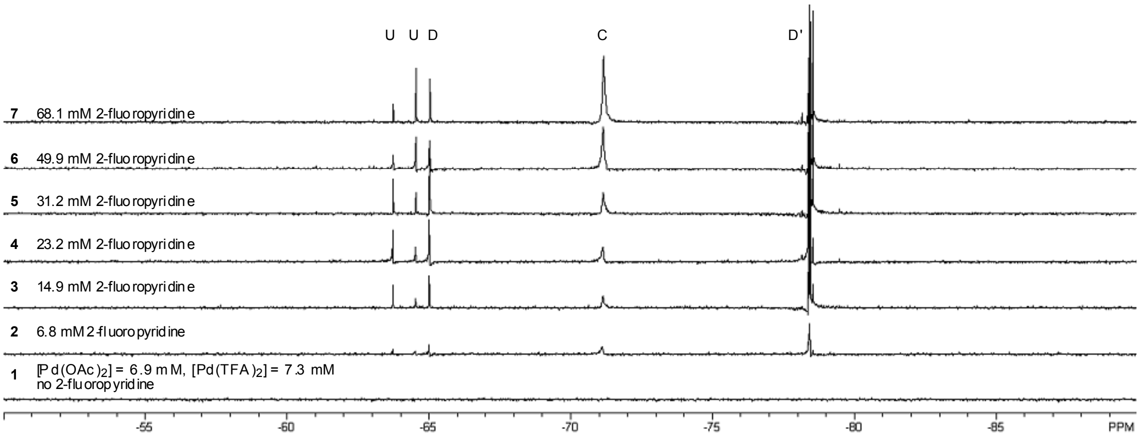
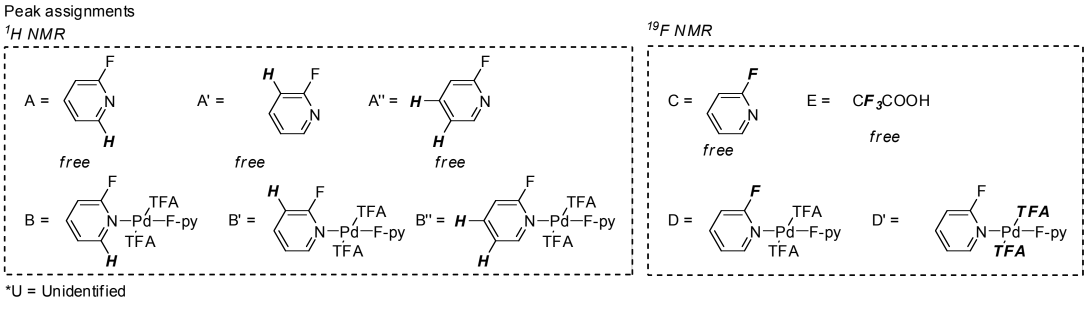


Figure S8. ^{19}F NMR spectra of a titration of 2-fluoropyridine against $Pd(OAc)_2$ and $Pd(TFA)_2$. Conditions : $[Pd(OAc)_2] = 6.9$ mM , $[Pd(TFA)_2] = 7.3$ mM, [hexafluorobenzene] = 23.1 mM.



NMR spectroscopic studies of $Pd(TFA)_2$ and 2,4,6-trifluoropyridine in benzene-d_6.

$Pd(TFA)_2$ (2.4 mg, 7.2 μmol) was added to a NMR tube together with benzene-d_6 (400 μL). Independently, a solution of 2,4,6-trifluoropyridine (10.8 mg, 0.081 mmol) was prepared in benzene-d_6 (0.57 g, 140 mM). ^1H NMR spectra (300 MHz) and ^{19}F NMR spectra of a titration of 2,4,6-trifluoropyridine against $Pd(TFA)_2$ at room temperature are shown in the stacked plots below. The assignments of 2,4,6-trifluoropyridine ligand resonances are made on the basis of free 2,4,6-trifluoropyridine in benzene-d_6.

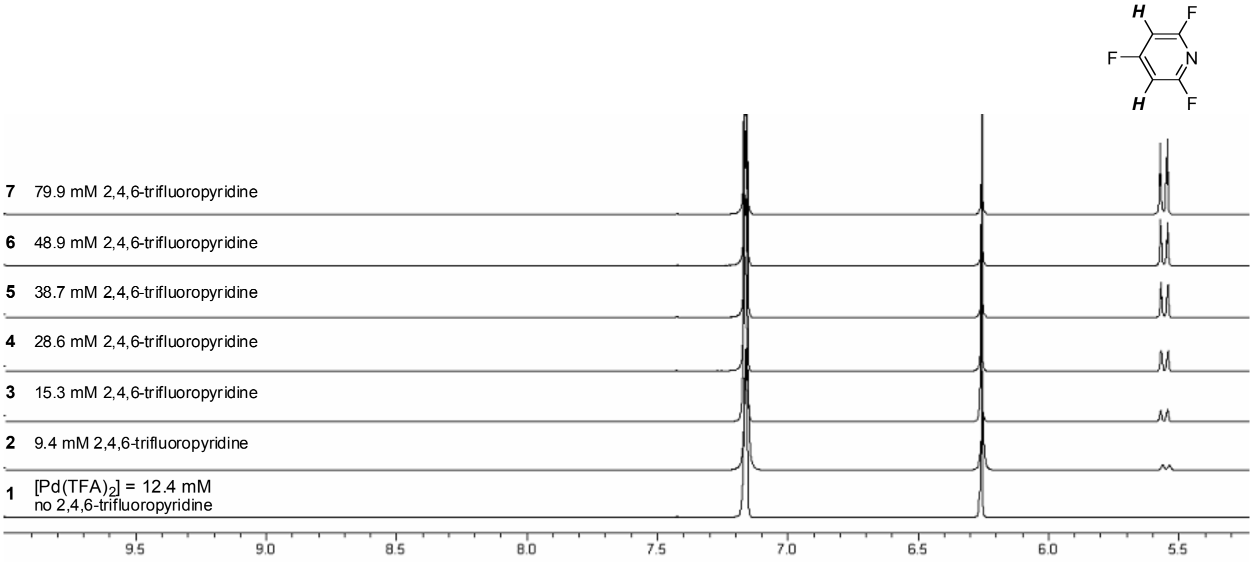


Figure S9. ^1H NMR spectra of a titration of 2,4,6-trifluoropyridine against $Pd(TFA)_2$. Conditions : $[Pd(TFA)_2]$ = 12.4 mM, [1,3,5-trimethoxybenzene] = 24.3 mM.

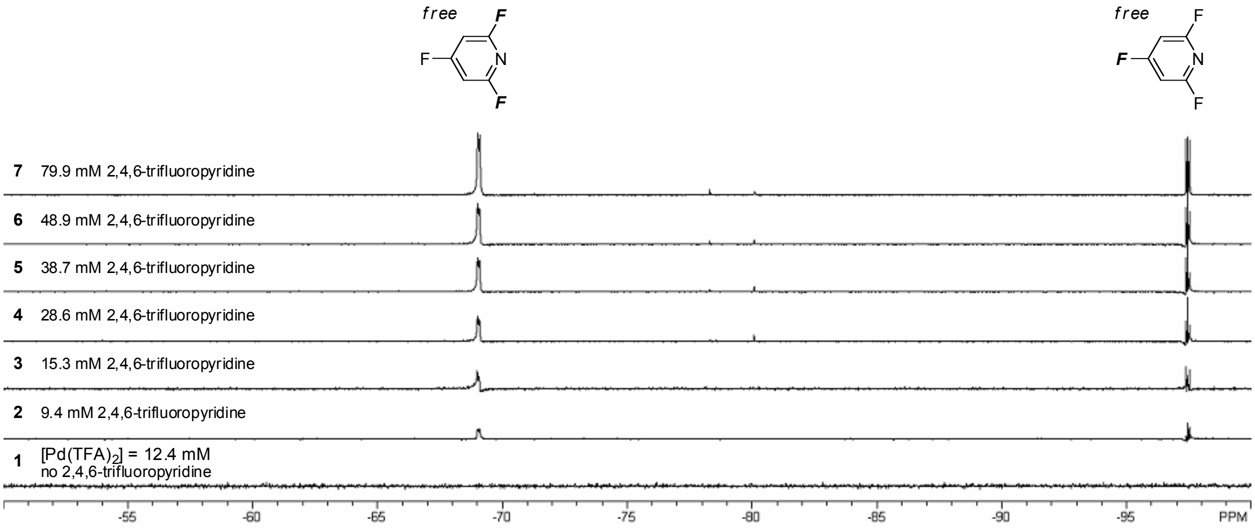


Figure S10. ^{19}F NMR spectra of a titration of 2,4,6-fluoropyridine against $Pd(TFA)_2$. Conditions : $[Pd(TFA)_2]$ = 12.4 mM, [hexafluorobenzene] = 18.9 mM.

NMR spectroscopic studies of $Pd(TFA)_2$ and 2,3,5-trifluoropyridine in benzene-d_6.

$Pd(TFA)_2$ (3.8 mg, 11.4 μmol) was added to a NMR tube, followed by addition of benzene-d_6 (760 μL) and 2,3,5-trifluoropyridine (6.1 mg, 45.7 μmol). The assignments of 2,3,5-trifluoropyridine ligand resonances are made on the basis of 2,3,5-trifluoropyridine reagent in benzene-d_6.

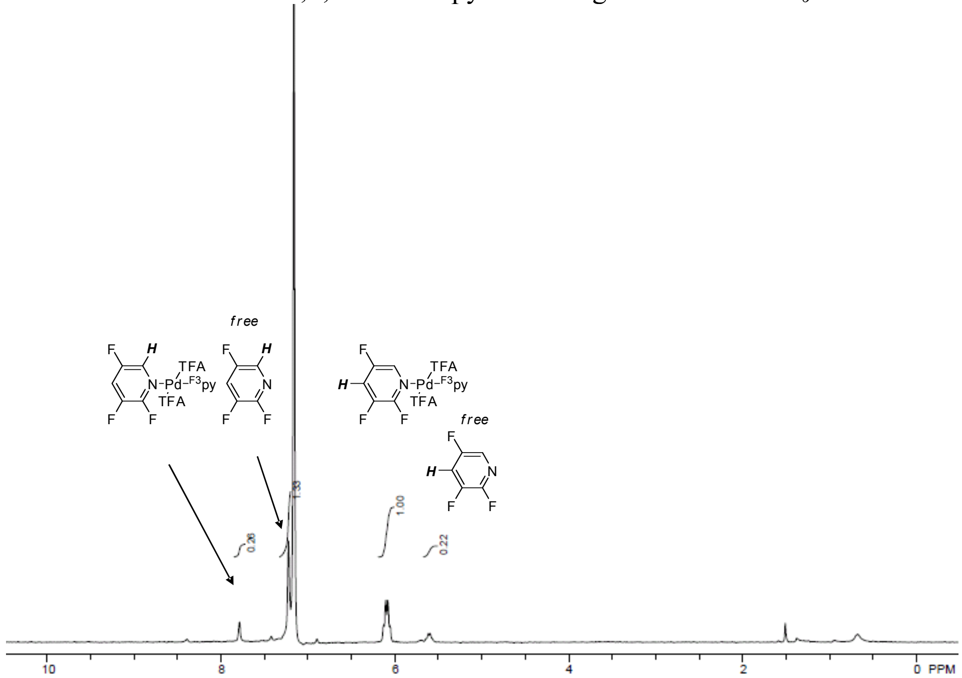


Figure S11. ^1H NMR spectra of a mixture of 2,3,5-trifluoropyridine and $Pd(TFA)_2$. Conditions : $[Pd(TFA)_2]$ = 17.0 mM, 2,3,5-trifluoropyridine = 68.7 mM.

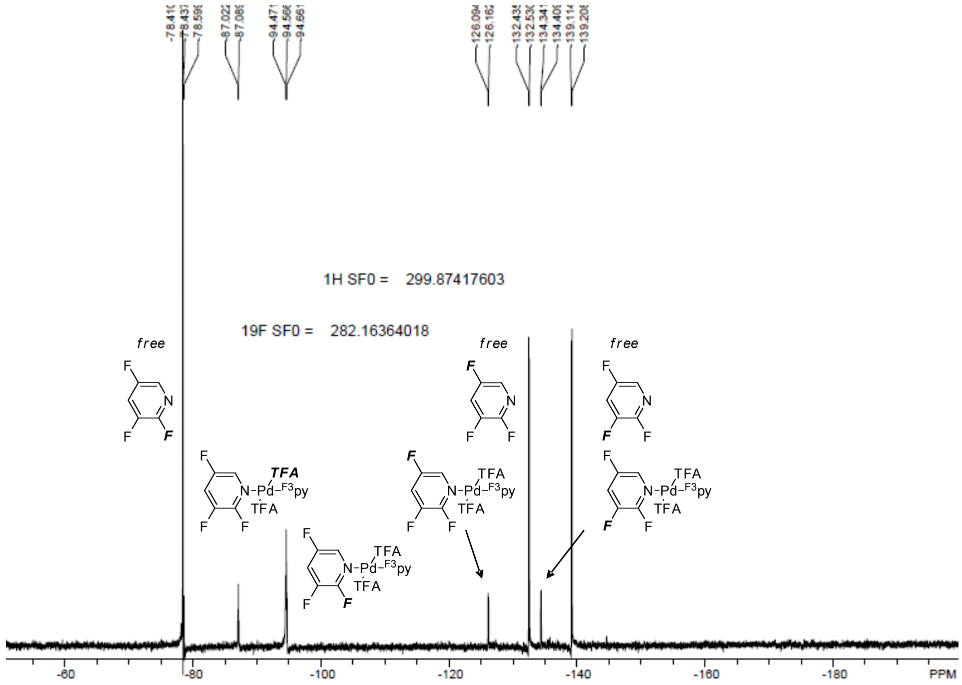


Figure S12. ^{19}F NMR spectra of a mixture of 2,3,5-trifluoropyridine and $Pd(TFA)_2$. Conditions: $[Pd(TFA)_2]$ = 17.0 mM, 2,3,5-trifluoropyridine = 68.7 mM.

NMR spectroscopic studies of Pd(TFA)$_2$ and pentafluoropyridine in benzene-d_6.

Pd(TFA)$_2$ (2.5 mg, 7.5 µmol) was added to a NMR tube, together with benzene-d_6 (600 µL) and pentafluoropyridine (5.2 mg, 30.1 µmol). The assignments of pentafluoropyridine ligand resonances are made on the basis of pentafluoropyridine reagent in benzene-d_6.

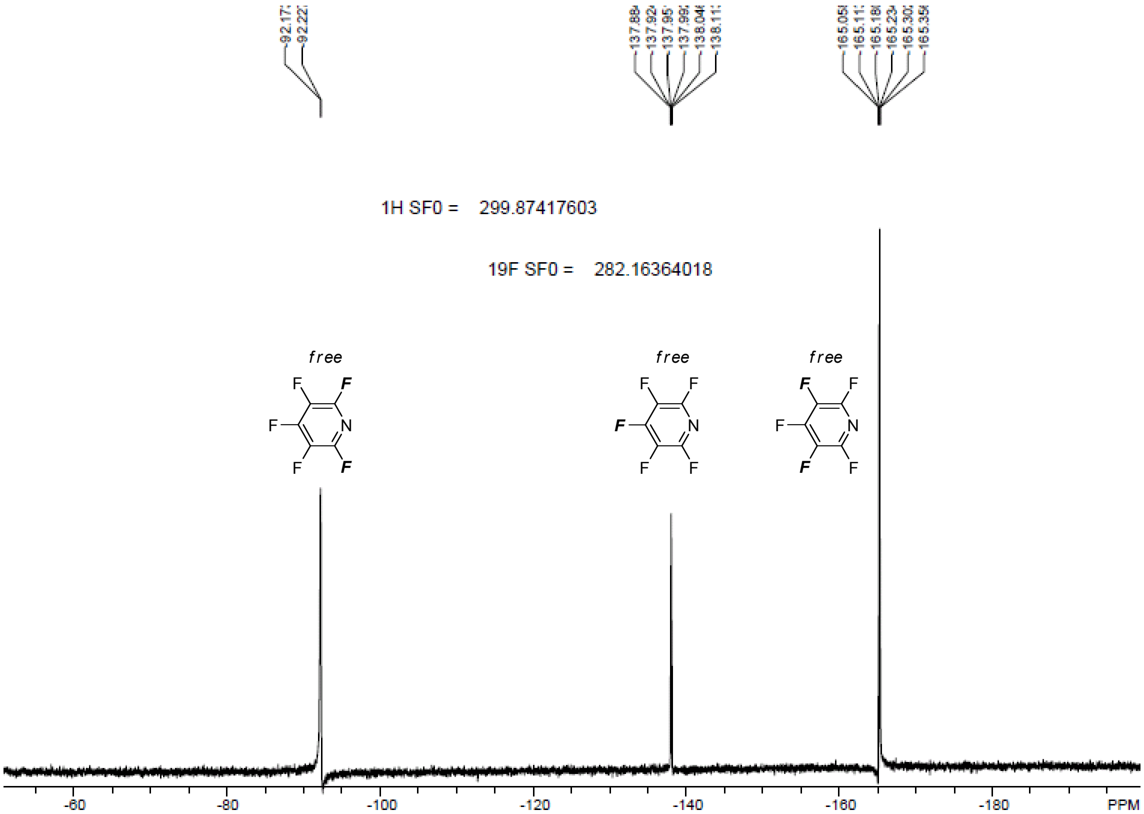


Figure S13. ^{19}F NMR spectra of a mixture of pentafluoropyridine and Pd(TFA)$_2$. Conditions : [Pd(TFA)$_2$] = 14.4 mM, pentafluoropyridine = 57.8 mM.

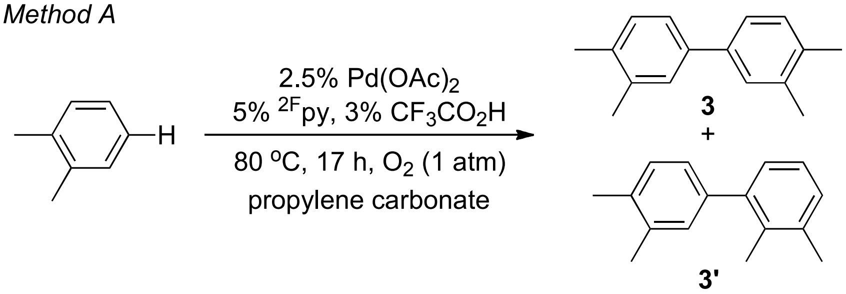
Experimental.

1. General Considerations.

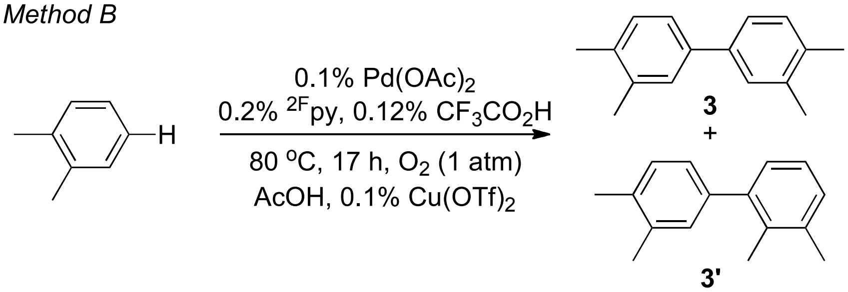
All commercially available compounds were purchased and used as received. Solvents were dried over alumina columns prior to use; however, purification and drying of commercial solvents is not required for the catalytic reactions described here. ^{1}H and ^{19}F NMR spectra were recorded on a Bruker AC-300MHz or Varian Mercury-300 MHz, and $CDCl_3$ and benzene-d_6 were purchased from Aldrich. The chemical shift values were given in parts per million relative to internal TMS (0 ppm for ^{1}H), benzene (7.16 ppm), and ^{19}F was referenced on TMS for ^{1}H spectrum and reference parameters were transferred for the fluorine spectrum. Gas chromatographic analysis of reactions was conducted with a Shimadzu GC-17A gas chromatograph with either a DB-Wax or a RTX-5 column.

2. Representative Procedure for Aerobic Oxidative Coupling of *o*-Xylene.

Method A



Method B



All of the catalytic aerobic oxidation reactions were performed using a custom reaction apparatus

Method A:

In a disposable culture tube, palladium complexes (0.094 mmol), 2-fluoropyridine (0.19 mmol), trifluoroacetic acid (0.113 mmol), *o*-xylene (0.4 g) and propylene carbonate (0.4 g) were combined. The reaction tubes were placed in a 48-well aluminum block mounted on a Large Capacity Mixer (Glas-Col) that enabled several reactions to be performed simultaneously under a constant pressure of (approx 1 atm) with controlled temperature and orbital agitation. The headspace above the tubes was purged with oxygen gas for ca. 5 min. The reactions were vortexed for 17 hr under 1 atm of O_2. After the reactions were stopped, *n*-hexadecane was added to the reaction mixture as an internal standard. Samples were evaluated by GC for the products and remaining starting materials.

Method B:

In a 6 ml vial, palladium complexes (0.02 mmol), 2-fluoropyridine (0.04 mmol), trifluoroacetic acid (0.024 mmol) and acetic acid (2 g) were combined and stirred at room temperature for 30 min. The mixture was used as a stock solution. In a disposable culture tube, copper triflate (0.04 mmol) and *o*-xylene (0.4 g) were combined. Then, the stock solution (0.4 g) was added. Reaction tubes were placed in a 48-well parallel reaction mounted on a Large Capacity Mixer (Glas-Col) that enabled several reactions to be performed simultaneously under a constant pressure of (approx 1 atm) with controlled temperature and orbital agitation. The headspace above the tubes was purged with oxygen gas for ca. 5 min. The reactions were vortexed for 17 hr under 1 atm of O_2. After the reactions were stopped, *n*-hexadecane was added to the reaction mixture as an internal standard. Samples were evaluated by GC for the products and remaining starting materials.

3. Determination of Initial Reaction Rates

In a disposable culture tube, palladium acetate (4.2 mg, 0.019 mmol), ligand (0.038 mmol), trifluoroacetic acid (2.6 mg, 0.023 mmol), copper triflate (6.8 mg, 0.019 mmol), *o*-xylene (0.4 g) and acetic acid (0.4 g) were combined. Reaction tubes were placed in a 48-well aluminum block mounted on a Large Capacity Mixer (Glas-Col) that enabled several reactions to be performed simultaneously under a constant pressure of O_2 (approx 1 atm) with controlled temperature and orbital agitation. The headspace above the tubes was purged with oxygen gas for ca. 5 min. The reactions were vortexed for 6 hr under 1 atm of O_2. The reaction mixture was sampled at 1 h, 2 h, 4 h and 6 h reaction times (20 µL aliquots). After the aliquots were diluted with dioxane (400 mg), *n*-hexadecane (20 mg) was added to the sampled reaction mixture as an internal standard. Samples were evaluated by GC for the products and remaining starting materials. The initial reaction rates were determined according to previously reported methods,[1] involving plotting the rates obtained from each of the four time intervals (0–1 h, 1–2 h, 2–4 h and 4–6 h) vs. reaction time, and extrapolating these points back to t = 0. In nearly all cases, the conversion at 6 h was less than 10% of total substrate.

4. Synthesis of *trans*-(^{2F}py)$_2$Pd(TFA)$_2$.[2]

A solution of $Pd(OAc)_2$ (206.1 mg, 0.92 mmol) and 2-fluoropyridine (265.9 mg, 2.7 mmol) in dry benzene (7 ml) was stirred with CF_3CO_2H (293.9mg, 2.6 mmol) at room temperature for 5hr. Dry pentane (15 ml) was added and after 5 min of stirring the pale yellow solid was separated by filtration, washed with dry pentane (5 ml) three times, and dried under vacuum (quantitative yield). Recrystallization of the complex was done from benzene-pentane at 0 °C, and the structure was determined by X-ray crystallography (see below).

^{1}H NMR (300 MHz, C_6D_6) δ 5.65 (d, *J* = 8.6 Hz, 2H), δ 5.85 (m, 2H), δ 6.25 (m, 2H), δ 8.35 (dd, 2H, 5.7 Hz, 2.0 Hz), ; ^{19}F NMR (282 MHz, C_6D_6) δ -78.4, δ -65.0.

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[1] This method is previously used in many references. For example, a) Schuh M. D.; *J. Chem. Educ.* **1988**, *65*, 740-741.; b) Corma, A.; Cid, R.; Agudo, A. L.; *Can. J. Chem. Eng.* **1979**, *57*, 638-642.

[2] A similar procedure was employed in the preparation of [Pd(TFA)$_2$(py)$_2$]: Trend, R. M.; Ramtohul, Y. K., Stoltz, B. M.; *J. Am. Chem. Soc.* **2005**, 17778-17788.

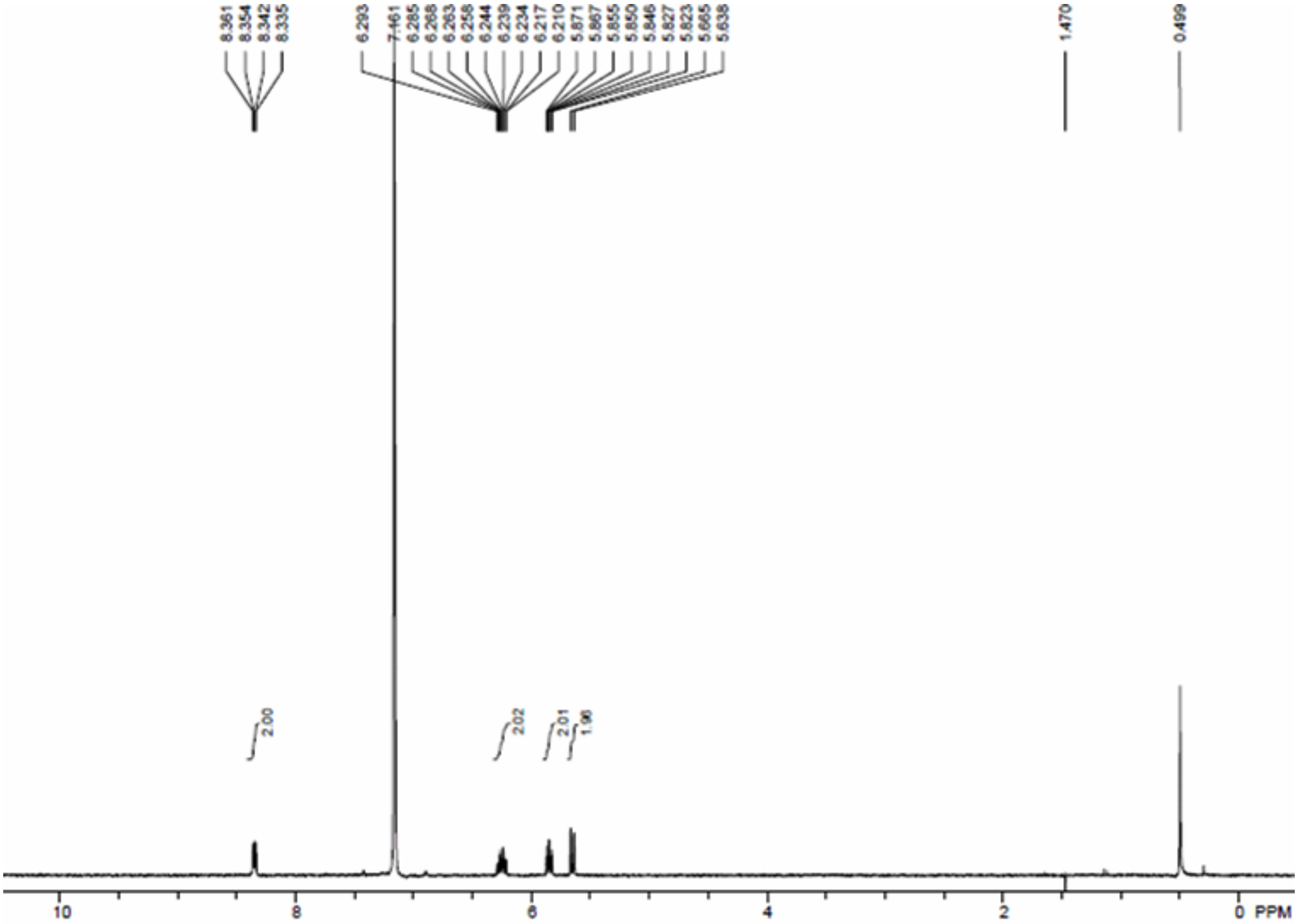

Figure S14. ^{1}H NMR spectrum of *trans*-(^{2F}py)$_2$Pd(TFA)$_2$.

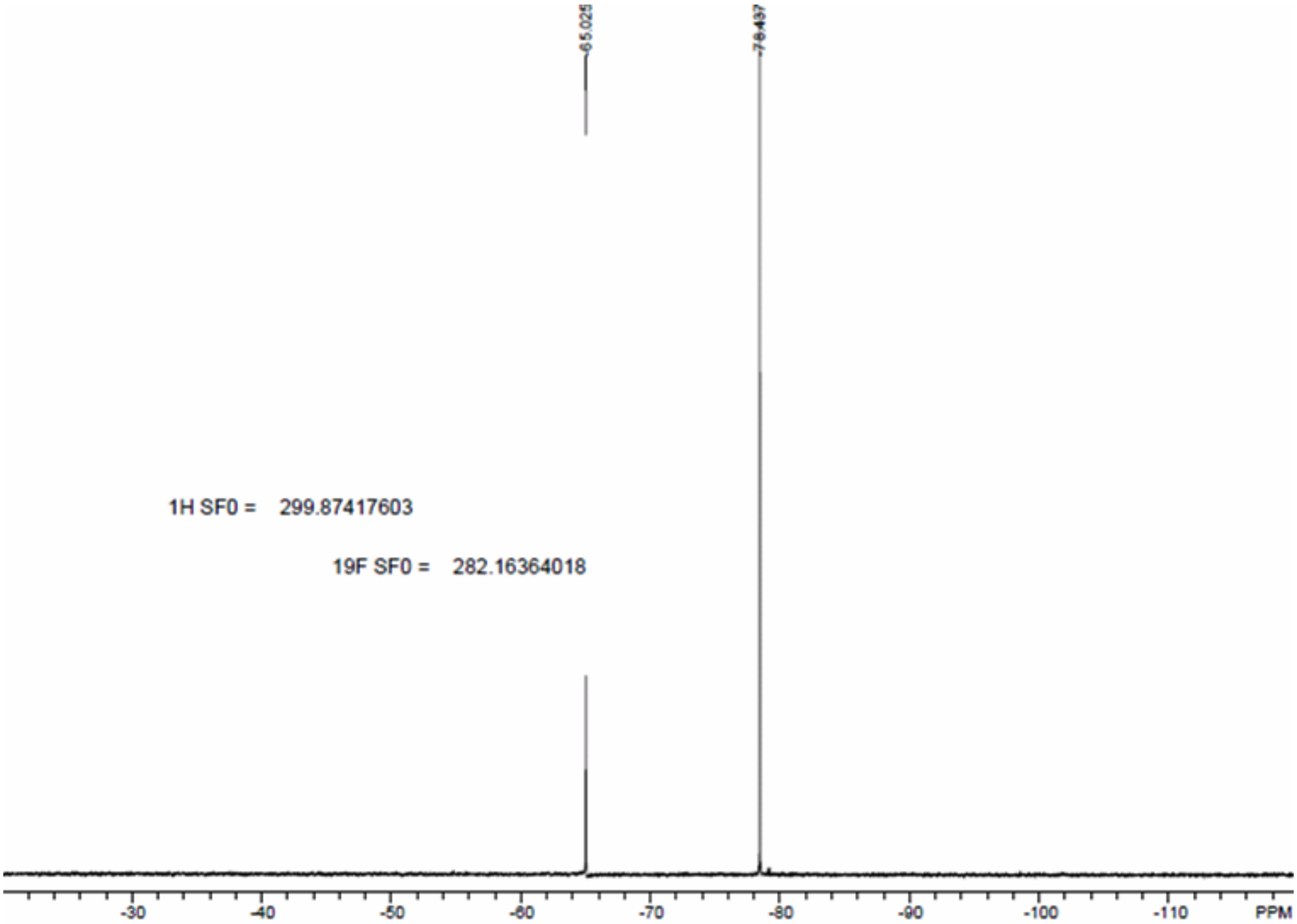

Figure S15. ^{19}F NMR spectrum of *trans*-(^{2F}py)$_2$Pd(TFA)$_2$.

Crystallographic Characterization of *trans*-(^{2F}py)$_2$Pd (TFA)$_2$.

Data Collection

A yellow crystal with approximate dimensions 0.33 x 0.16 x 0.07 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker SMART APEXII diffractometer with Cu K_α (λ = 1.54178 Å) radiation and the diffractometer to crystal distance of 4.03 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 50 frames collected at intervals of 0.5° in a 25° range about ω with the exposure time of 5 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program. The final cell constants were calculated from a set of 9823 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.82 Å. A total of 36697 data were harvested by collecting 18 sets of frames with 0.8° scans in ω with an exposure time 10-20 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement [2-3]. A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There are 1.5 independent Pd complexes in the asymmetric unit. The complex containing atom Pd1 is entirely in the asymmetric unit and the complex containing atom Pd2 lies on a crystallographic inversion center. Atoms F9-F11 are disordered over two positions with a minor component contribution of 22.6(7)% and were refined with restraints. The is one high residual peak (2.083 e/Å3) near the disordered fluorine atoms, but it was not reasonable to split the fluorine atoms over more positions.

The final least-squares refinement of 405 parameters against 4838 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0396 and 0.1083, respectively.

The molecular diagram is drawn with 50% probability ellipsoids.

References

[1] Bruker-AXS. (2000-2007) SADABS, SAINT, and SMART 5.622 Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

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[4] Pennington, W.T. (1999) *J. Appl. Cryst.* **32**(5), 1028-1029.

[5] Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. "OLEX2: a complete structure solution, refinement and analysis program". *J. Appl. Cryst.* (2009) **42**, *339-341.*

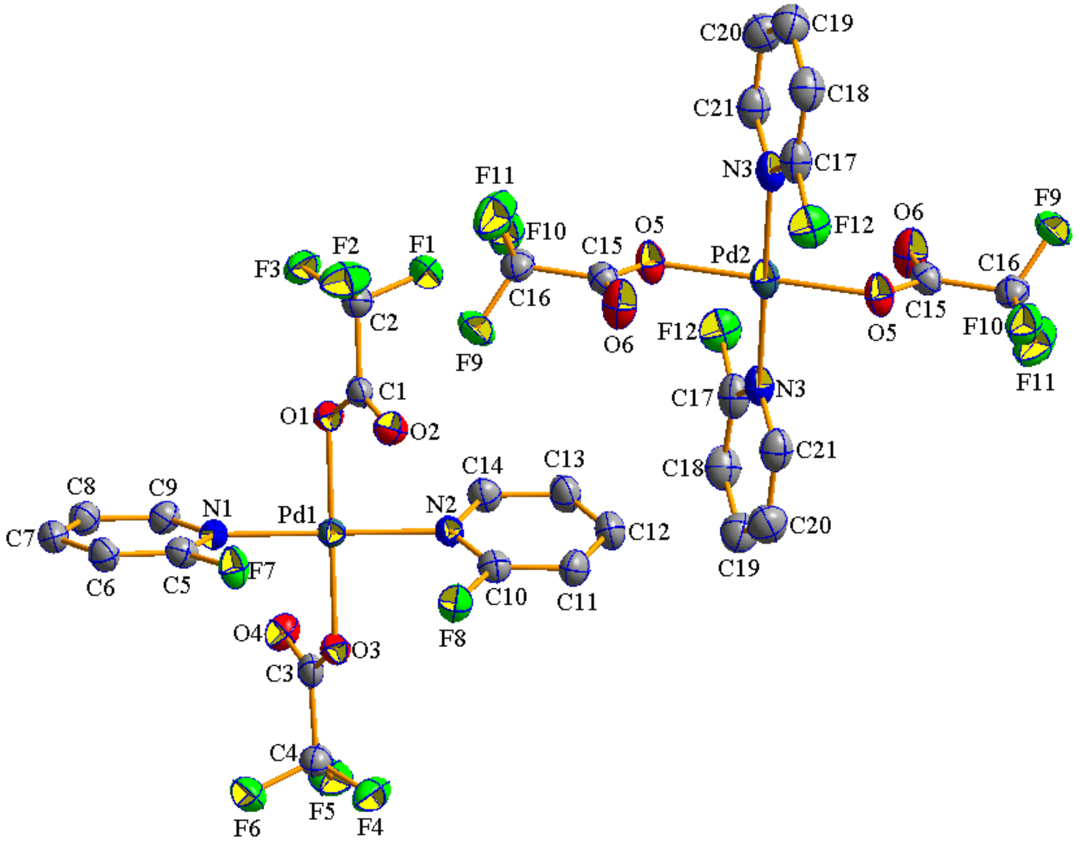

Figure S16. A molecular drawing of stahl89 [4]. All hydrogen atoms and the minor components of disordered atoms were omitted for clarity. The complex containing Pd2 lies on a crystallographic inversion center.

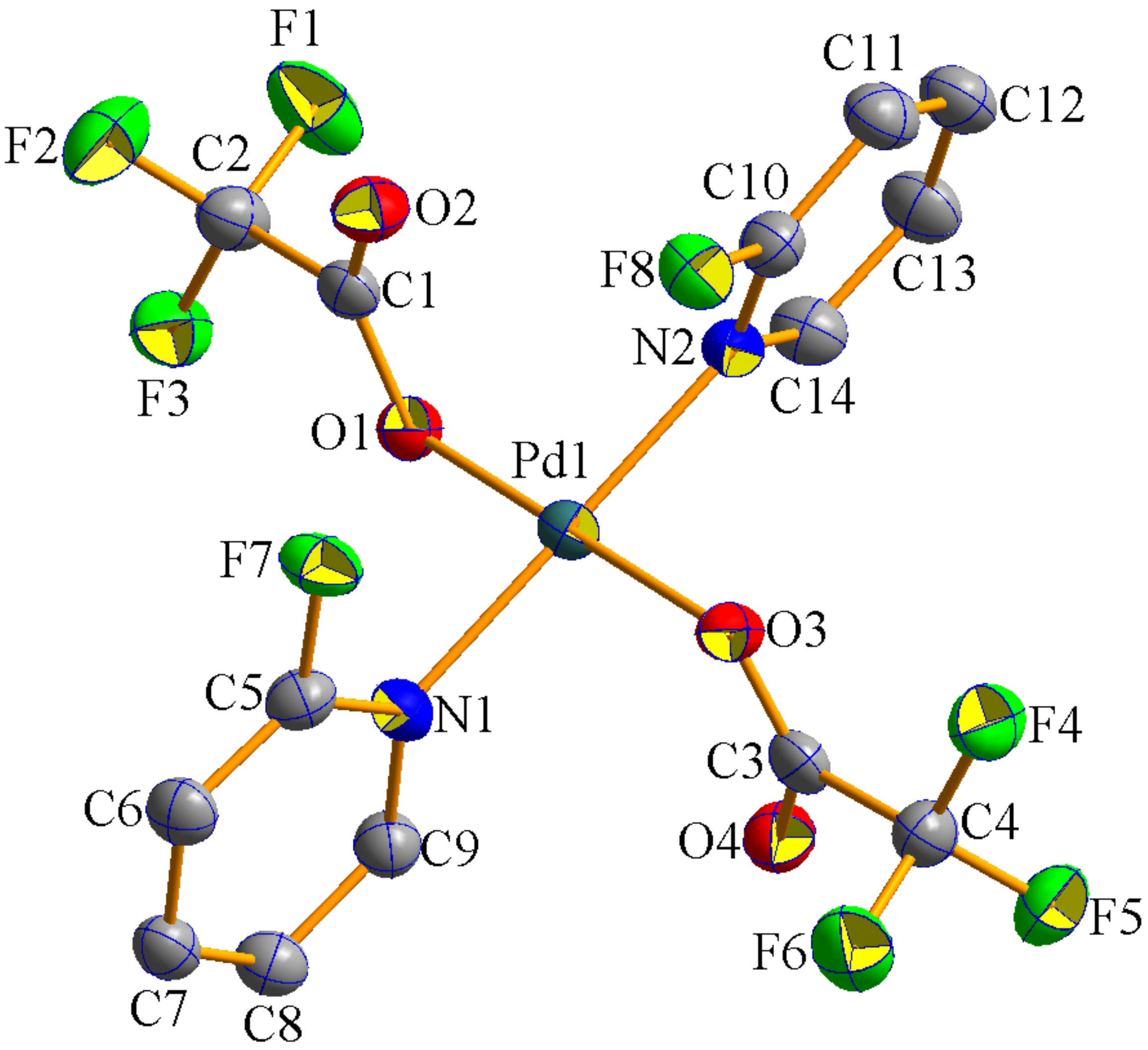

Figure S17. A drawing of the complex containing Pd1 [4]. All hydrogen were omitted for clarity.

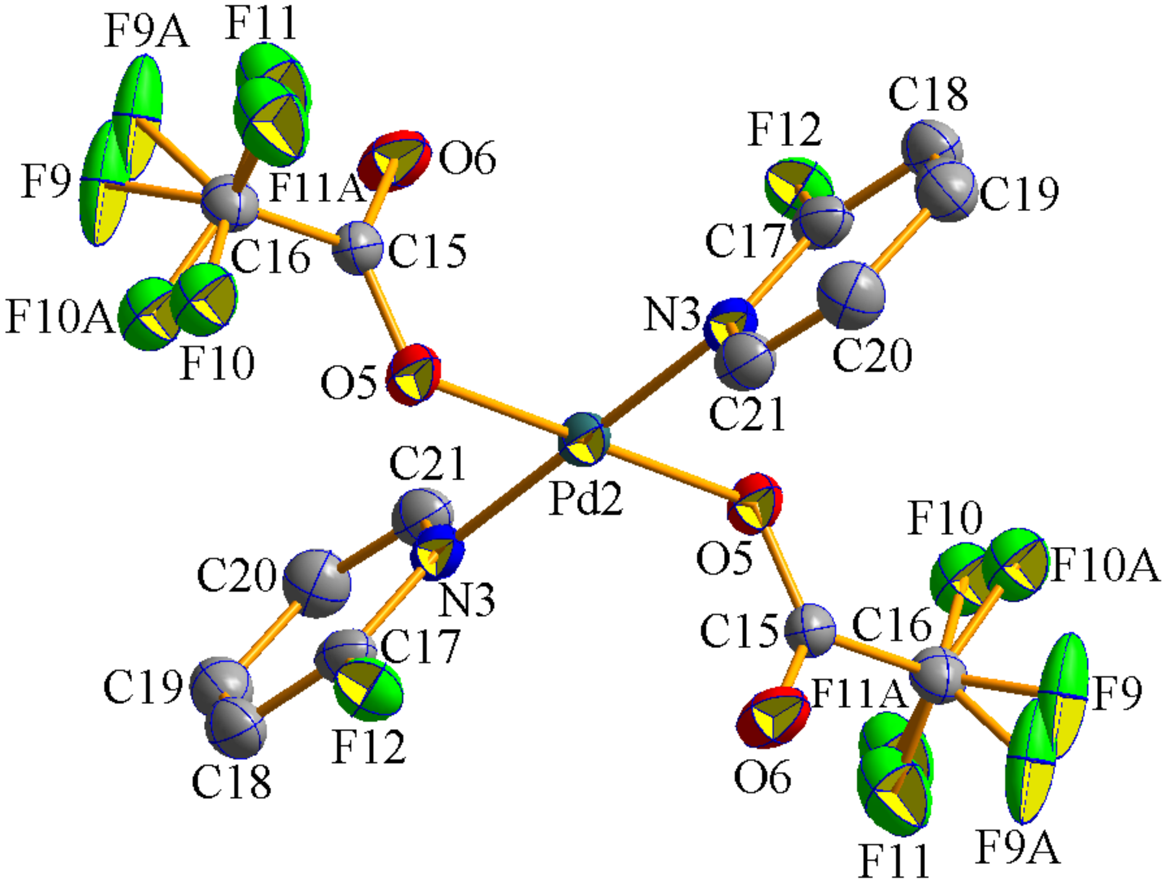

Figure S18. A drawing of the complex containing Pd2 [4]. All hydrogen atoms were omitted for clarity. The complex containing Pd2 lies on a crystallographic inversion center. Atoms F9-F11 are disordered over two positions.

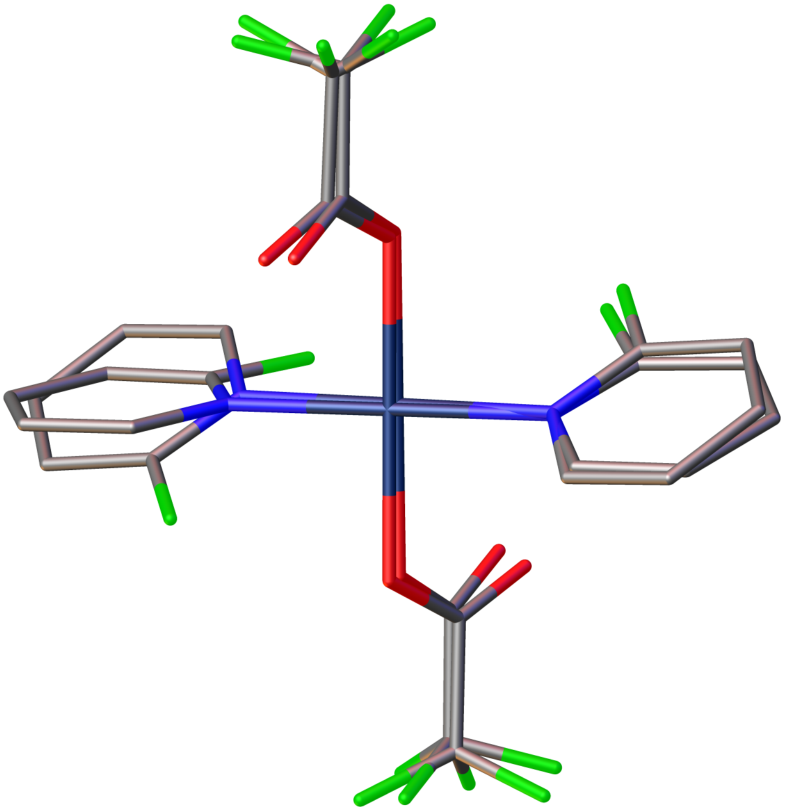

Figure S19. An overlap diagram of the two Pd complexes [5]. All hydrogen atoms and minor components of the disordered atoms were omitted for clarity.

Table S2. Crystal data and structure refinement for stahl89.

Identification code	stahl89	
Empirical formula	$C_{14}H_8F_8N_2O_4Pd$	
Formula weight	526.62	
Temperature	100(1) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.9376(2) Å	α= 90°.
	b = 31.0376(7) Å	β= 97.4790(10)°.
	c = 9.5220(2) Å	γ = 90°.
Volume	2618.95(10) Å^3	
Z	6	
Density (calculated)	2.003 Mg/m^3	
Absorption coefficient	9.624 mm^{-1}	
F(000)	1536	
Crystal size	0.33 x 0.16 x 0.07 mm^3	
Theta range for data collection	2.85 to 69.44°.	
Index ranges	-10<=h<=10, -37<=k<=35, -11<=l<=11	
Reflections collected	36697	
Independent reflections	4838 [R(int) = 0.0357]	
Completeness to theta = 67.00°	99.6 %	
Absorption correction	Analytical with SADABS	
Max. and min. transmission	0.5523 and 0.1434	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4838 / 21 / 405	
Goodness-of-fit on F^2	1.228	
Final R indices [I>2sigma(I)]	R1 = 0.0396, wR2 = 0.1063	
R indices (all data)	R1 = 0.0423, wR2 = 0.1083	
Largest diff. peak and hole	2.083 and -1.731 e.Å^{-3}	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for stahl89. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	1680(1)	3353(1)	7902(1)	26(1)
F(1)	5308(4)	4004(1)	5144(3)	61(1)
F(2)	6891(3)	3570(1)	6286(4)	58(1)
F(3)	6042(3)	4102(1)	7357(3)	46(1)
F(4)	-2824(3)	2659(1)	8283(3)	48(1)
F(5)	-3645(3)	3210(1)	9305(3)	48(1)
F(6)	-2189(3)	2754(1)	10510(3)	51(1)
F(7)	3488(3)	2652(1)	9298(3)	39(1)
F(8)	952(3)	2692(1)	5667(3)	40(1)
O(1)	3495(3)	3692(1)	7501(3)	30(1)
O(2)	4202(4)	3167(1)	6092(3)	36(1)
O(3)	-159(3)	3021(1)	8298(3)	30(1)
O(4)	-902(4)	3578(1)	9545(3)	37(1)
N(1)	2655(4)	3290(1)	9931(4)	28(1)
N(2)	723(4)	3408(1)	5869(4)	29(1)
C(1)	4326(5)	3512(1)	6670(4)	28(1)
C(2)	5661(5)	3803(2)	6382(5)	36(1)
C(3)	-1031(5)	3222(1)	9019(4)	31(1)
C(4)	-2445(5)	2957(2)	9265(5)	35(1)
C(5)	3431(5)	2937(1)	10328(5)	30(1)
C(6)	4155(5)	2859(1)	11658(5)	33(1)
C(7)	4064(5)	3177(2)	12670(5)	33(1)
C(8)	3252(5)	3549(2)	12293(5)	34(1)
C(9)	2559(5)	3601(1)	10928(5)	32(1)
C(10)	508(5)	3065(1)	5040(5)	32(1)
C(11)	-123(5)	3071(2)	3646(5)	39(1)
C(12)	-589(6)	3469(2)	3098(5)	40(1)
C(13)	-398(6)	3832(2)	3935(5)	40(1)
C(14)	260(5)	3792(1)	5325(5)	36(1)
Pd(2)	0	5000	0	34(1)
F(9)	1598(8)	4749(2)	5168(4)	80(2)
F(10)	1845(5)	5393(1)	4554(4)	50(1)
F(11)	3512(2)	4966(2)	4319(5)	72(2)
F(9A)	2195(19)	4646(3)	5038(12)	80(2)
F(10A)	1260(7)	5253(2)	4791(12)	50(1)
F(11A)	3487(4)	5135(4)	4400(12)	72(2)
F(12)	2239(3)	4506(1)	-1474(3)	48(1)
O(5)	790(4)	5151(1)	2020(3)	40(1)
O(6)	1821(5)	4499(1)	2322(4)	51(1)
N(3)	1989(4)	5172(1)	-626(4)	36(1)
C(15)	1537(5)	4861(1)	2724(4)	32(1)
C(16)	2119(4)	4989(1)	4241(4)	37(1)
C(17)	2780(6)	4907(2)	-1334(5)	40(1)
C(18)	4076(6)	5016(2)	-1884(6)	45(1)
C(19)	4568(6)	5433(2)	-1675(6)	48(1)

C(20)	3787(6)	5717(2)	-917(6)	48(1)
C(21)	2506(6)	5578(2)	-415(5)	41(1)

Table S4. Bond lengths [Å] and angles [°] for stahl89.

Pd(1)-O(1)	2.011(3)	C(11)-C(12)	1.384(7)
Pd(1)-O(3)	2.015(3)	C(11)-H(11)	0.9500
Pd(1)-N(2)	2.019(4)	C(12)-C(13)	1.377(7)
Pd(1)-N(1)	2.023(4)	C(12)-H(12)	0.9500
F(1)-C(2)	1.333(5)	C(13)-C(14)	1.382(6)
F(2)-C(2)	1.329(6)	C(13)-H(13)	0.9500
F(3)-C(2)	1.323(5)	C(14)-H(14)	0.9500
F(4)-C(4)	1.327(5)	Pd(2)-O(5)#1	2.016(3)
F(5)-C(4)	1.333(5)	Pd(2)-O(5)	2.016(3)
F(6)-C(4)	1.337(5)	Pd(2)-N(3)#1	2.019(4)
F(7)-C(5)	1.327(5)	Pd(2)-N(3)	2.019(4)
F(8)-C(10)	1.340(5)	F(9)-C(16)	1.288(4)
O(1)-C(1)	1.281(5)	F(10)-C(16)	1.321(4)
O(2)-C(1)	1.203(5)	F(11)-C(16)	1.240(4)
O(3)-C(3)	1.267(5)	F(9A)-C(16)	1.304(5)
O(4)-C(3)	1.212(5)	F(10A)-C(16)	1.281(5)
N(1)-C(5)	1.325(6)	F(11A)-C(16)	1.295(5)
N(1)-C(9)	1.365(6)	F(12)-C(17)	1.335(6)
N(2)-C(10)	1.323(6)	O(5)-C(15)	1.259(5)
N(2)-C(14)	1.345(6)	O(6)-C(15)	1.224(5)
C(1)-C(2)	1.550(6)	N(3)-C(17)	1.325(6)
C(3)-C(4)	1.550(6)	N(3)-C(21)	1.348(6)
C(5)-C(6)	1.367(6)	C(15)-C(16)	1.522(5)
C(6)-C(7)	1.389(6)	C(17)-C(18)	1.375(8)
C(6)-H(6)	0.9500	C(18)-C(19)	1.374(8)
C(7)-C(8)	1.387(6)	C(18)-H(18)	0.9500
C(7)-H(7)	0.9500	C(19)-C(20)	1.383(8)
C(8)-C(9)	1.374(6)	C(19)-H(19)	0.9500
C(8)-H(8)	0.9500	C(20)-C(21)	1.367(8)
C(9)-H(9)	0.9500	C(20)-H(20)	0.9500
C(10)-C(11)	1.373(6)	C(21)-H(21)	0.9500

O(1)-Pd(1)-O(3)	179.10(12)	F(3)-C(2)-F(2)	106.9(4)
O(1)-Pd(1)-N(2)	91.42(13)	F(3)-C(2)-F(1)	107.7(4)
O(3)-Pd(1)-N(2)	88.22(13)	F(2)-C(2)-F(1)	107.2(4)
O(1)-Pd(1)-N(1)	88.50(13)	F(3)-C(2)-C(1)	114.7(4)
O(3)-Pd(1)-N(1)	91.87(13)	F(2)-C(2)-C(1)	110.9(4)
N(2)-Pd(1)-N(1)	179.18(14)	F(1)-C(2)-C(1)	109.2(4)
C(1)-O(1)-Pd(1)	115.9(3)	O(4)-C(3)-O(3)	129.7(4)
C(3)-O(3)-Pd(1)	115.2(3)	O(4)-C(3)-C(4)	117.1(4)
C(5)-N(1)-C(9)	117.7(4)	O(3)-C(3)-C(4)	113.1(4)
C(5)-N(1)-Pd(1)	119.7(3)	F(4)-C(4)-F(5)	107.4(4)
C(9)-N(1)-Pd(1)	122.6(3)	F(4)-C(4)-F(6)	107.1(4)
C(10)-N(2)-C(14)	118.0(4)	F(5)-C(4)-F(6)	107.3(4)
C(10)-N(2)-Pd(1)	120.9(3)	F(4)-C(4)-C(3)	113.7(4)
C(14)-N(2)-Pd(1)	121.0(3)	F(5)-C(4)-C(3)	111.5(4)
O(2)-C(1)-O(1)	130.0(4)	F(6)-C(4)-C(3)	109.6(4)
O(2)-C(1)-C(2)	117.8(4)	N(1)-C(5)-F(7)	114.2(4)
O(1)-C(1)-C(2)	112.2(4)	N(1)-C(5)-C(6)	125.3(4)

F(7)-C(5)-C(6)	120.5(4)
C(5)-C(6)-C(7)	116.9(4)
C(5)-C(6)-H(6)	121.5
C(7)-C(6)-H(6)	121.5
C(8)-C(7)-C(6)	119.3(4)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(9)-C(8)-C(7)	119.8(4)
C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1
N(1)-C(9)-C(8)	121.0(4)
N(1)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
N(2)-C(10)-F(8)	114.7(4)
N(2)-C(10)-C(11)	125.1(4)
F(8)-C(10)-C(11)	120.2(4)
C(10)-C(11)-C(12)	116.2(4)
C(10)-C(11)-H(11)	121.9
C(12)-C(11)-H(11)	121.9
C(13)-C(12)-C(11)	120.2(4)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(12)-C(13)-C(14)	119.1(4)
C(12)-C(13)-H(13)	120.4
C(14)-C(13)-H(13)	120.4
N(2)-C(14)-C(13)	121.3(4)
N(2)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
O(5)#1-Pd(2)-O(5)	180.00(18)
O(5)#1-Pd(2)-N(3)#1	90.46(15)
O(5)-Pd(2)-N(3)#1	89.54(15)
O(5)#1-Pd(2)-N(3)	89.54(15)
O(5)-Pd(2)-N(3)	90.46(15)
N(3)#1-Pd(2)-N(3)	180.0(2)
C(15)-O(5)-Pd(2)	116.0(3)
C(17)-N(3)-C(21)	117.5(4)
C(17)-N(3)-Pd(2)	122.3(3)
C(21)-N(3)-Pd(2)	120.1(3)
O(6)-C(15)-O(5)	127.3(4)
O(6)-C(15)-C(16)	118.5(4)
O(5)-C(15)-C(16)	114.3(4)
F(10A)-C(16)-F(11A)	109.5(6)
F(9)-C(16)-F(11)	112.0(5)
F(10A)-C(16)-F(9A)	105.8(7)
F(11A)-C(16)-F(9A)	104.0(7)
F(9)-C(16)-F(10)	107.6(4)
F(11)-C(16)-F(10)	104.8(4)
F(9)-C(16)-C(15)	113.0(4)
F(10A)-C(16)-C(15)	114.0(6)
F(11A)-C(16)-C(15)	113.8(6)
F(11)-C(16)-C(15)	105.0(3)
F(9A)-C(16)-C(15)	109.0(6)
F(10)-C(16)-C(15)	114.2(3)
N(3)-C(17)-F(12)	114.8(5)
N(3)-C(17)-C(18)	124.9(5)
F(12)-C(17)-C(18)	120.3(4)
C(19)-C(18)-C(17)	116.5(5)
C(19)-C(18)-H(18)	121.7
C(17)-C(18)-H(18)	121.7
C(18)-C(19)-C(20)	120.1(5)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(21)-C(20)-C(19)	119.0(5)
C(21)-C(20)-H(20)	120.5
C(19)-C(20)-H(20)	120.5
N(3)-C(21)-C(20)	121.9(5)
N(3)-C(21)-H(21)	119.0
C(20)-C(21)-H(21)	119.0

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

Table S5. Anisotropic displacement parameters ($Å^2$x 10^3) for stahl89. 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}
Pd(1)	28(1)	26(1)	24(1)	-1(1)	3(1)	0(1)
F(1)	71(2)	68(2)	39(2)	18(2)	-7(1)	-33(2)
F(2)	42(2)	59(2)	75(2)	-10(2)	23(2)	-4(1)
F(3)	46(2)	50(2)	43(2)	-11(1)	8(1)	-17(1)
F(4)	39(2)	58(2)	48(2)	-16(1)	8(1)	-13(1)
F(5)	34(1)	56(2)	56(2)	1(1)	14(1)	4(1)
F(6)	49(2)	61(2)	43(2)	18(1)	4(1)	-9(1)
F(7)	54(2)	33(1)	28(1)	-5(1)	4(1)	9(1)
F(8)	46(2)	35(1)	37(1)	-1(1)	-1(1)	2(1)
O(1)	30(1)	31(2)	30(2)	-2(1)	5(1)	-3(1)
O(2)	41(2)	33(2)	36(2)	-4(1)	10(1)	-2(1)
O(3)	33(2)	33(2)	27(2)	-2(1)	7(1)	-2(1)
O(4)	36(2)	36(2)	40(2)	-8(1)	5(1)	2(1)
N(1)	30(2)	30(2)	25(2)	1(1)	0(1)	-3(1)
N(2)	28(2)	34(2)	23(2)	-1(1)	4(1)	-1(1)
C(1)	30(2)	32(2)	22(2)	4(2)	1(2)	1(2)
C(2)	39(2)	37(2)	30(2)	-2(2)	6(2)	-8(2)
C(3)	32(2)	37(2)	22(2)	3(2)	-2(2)	2(2)
C(4)	31(2)	42(2)	32(2)	-2(2)	5(2)	-3(2)
C(5)	33(2)	27(2)	32(2)	-1(2)	9(2)	0(2)
C(6)	38(2)	31(2)	31(2)	4(2)	4(2)	2(2)
C(7)	34(2)	36(2)	27(2)	2(2)	3(2)	-4(2)
C(8)	39(2)	33(2)	31(2)	-3(2)	4(2)	-1(2)
C(9)	32(2)	30(2)	32(2)	-3(2)	3(2)	1(2)
C(10)	31(2)	34(2)	32(2)	0(2)	5(2)	3(2)
C(11)	43(2)	42(3)	31(2)	-6(2)	3(2)	-6(2)
C(12)	47(3)	47(3)	27(2)	3(2)	2(2)	-2(2)
C(13)	49(3)	39(2)	32(2)	6(2)	2(2)	2(2)
C(14)	44(2)	30(2)	33(2)	0(2)	4(2)	1(2)
Pd(2)	43(1)	32(1)	27(1)	-3(1)	3(1)	7(1)
F(9)	125(6)	85(3)	31(2)	-3(2)	18(2)	-64(4)
F(10)	62(3)	43(2)	43(2)	-9(2)	0(2)	-2(2)
F(11)	61(2)	97(5)	57(2)	-32(3)	8(2)	-10(2)
F(9A)	125(6)	85(3)	31(2)	-3(2)	18(2)	-64(4)
F(10A)	62(3)	43(2)	43(2)	-9(2)	0(2)	-2(2)
F(11A)	61(2)	97(5)	57(2)	-32(3)	8(2)	-10(2)
F(12)	58(2)	35(2)	52(2)	-9(1)	10(1)	8(1)
O(5)	55(2)	38(2)	27(2)	-4(1)	2(1)	9(2)
O(6)	69(2)	39(2)	42(2)	-5(2)	-8(2)	15(2)
N(3)	44(2)	36(2)	26(2)	-2(2)	1(2)	6(2)
C(15)	31(2)	36(2)	31(2)	4(2)	7(2)	3(2)
C(16)	29(2)	45(3)	36(2)	-1(2)	4(2)	-2(2)
C(17)	49(3)	38(2)	33(2)	-3(2)	-1(2)	13(2)
C(18)	49(3)	47(3)	39(3)	-7(2)	7(2)	9(2)
C(19)	43(3)	56(3)	44(3)	-3(2)	6(2)	2(2)

C(20)	54(3)	42(3)	49(3)	-4(2)	6(2)	-2(2)
C(21)	49(3)	38(2)	36(2)	-5(2)	1(2)	7(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for stahl89.

	x	y	z	U(eq)
H(6)	4696	2599	11881	40
H(7)	4552	3140	13609	39
H(8)	3176	3769	12976	41
H(9)	2004	3856	10676	38
H(11)	-234	2817	3089	46
H(12)	-1041	3492	2141	48
H(13)	-715	4106	3562	48
H(14)	387	4042	5907	43
H(18)	4605	4814	-2384	54
H(19)	5446	5527	-2051	57
H(20)	4136	6003	-748	58
H(21)	1963	5773	97	50

Table S7. Torsion angles [°] for stahl89.

O(3)-Pd(1)-O(1)-C(1)	-133(7)
N(2)-Pd(1)-O(1)-C(1)	-66.5(3)
N(1)-Pd(1)-O(1)-C(1)	112.7(3)
O(1)-Pd(1)-O(3)-C(3)	-41(7)
N(2)-Pd(1)-O(3)-C(3)	-107.8(3)
N(1)-Pd(1)-O(3)-C(3)	73.0(3)
O(1)-Pd(1)-N(1)-C(5)	-96.3(3)
O(3)-Pd(1)-N(1)-C(5)	84.6(3)
N(2)-Pd(1)-N(1)-C(5)	-12(11)
O(1)-Pd(1)-N(1)-C(9)	83.3(3)
O(3)-Pd(1)-N(1)-C(9)	-95.9(3)
N(2)-Pd(1)-N(1)-C(9)	168(17)
O(1)-Pd(1)-N(2)-C(10)	114.3(3)
O(3)-Pd(1)-N(2)-C(10)	-66.5(3)
N(1)-Pd(1)-N(2)-C(10)	30(11)
O(1)-Pd(1)-N(2)-C(14)	-67.0(3)
O(3)-Pd(1)-N(2)-C(14)	112.2(3)
N(1)-Pd(1)-N(2)-C(14)	-151(11)
Pd(1)-O(1)-C(1)-O(2)	-0.8(6)
Pd(1)-O(1)-C(1)-C(2)	178.0(3)
O(2)-C(1)-C(2)-F(3)	-158.7(4)
O(1)-C(1)-C(2)-F(3)	22.4(5)
O(2)-C(1)-C(2)-F(2)	-37.5(5)
O(1)-C(1)-C(2)-F(2)	143.5(4)
O(2)-C(1)-C(2)-F(1)	80.4(5)
O(1)-C(1)-C(2)-F(1)	-98.5(4)
Pd(1)-O(3)-C(3)-O(4)	-2.7(6)
Pd(1)-O(3)-C(3)-C(4)	178.7(3)
O(4)-C(3)-C(4)-F(4)	156.1(4)
O(3)-C(3)-C(4)-F(4)	-25.1(5)
O(4)-C(3)-C(4)-F(5)	34.5(5)
O(3)-C(3)-C(4)-F(5)	-146.6(4)
O(4)-C(3)-C(4)-F(6)	-84.2(5)
O(3)-C(3)-C(4)-F(6)	94.7(4)
C(9)-N(1)-C(5)-F(7)	-179.3(4)
Pd(1)-N(1)-C(5)-F(7)	0.3(5)
C(9)-N(1)-C(5)-C(6)	-0.4(6)
Pd(1)-N(1)-C(5)-C(6)	179.1(3)
N(1)-C(5)-C(6)-C(7)	0.0(7)
F(7)-C(5)-C(6)-C(7)	178.8(4)
C(5)-C(6)-C(7)-C(8)	0.4(6)
C(6)-C(7)-C(8)-C(9)	-0.4(7)
C(5)-N(1)-C(9)-C(8)	0.4(6)
Pd(1)-N(1)-C(9)-C(8)	-179.1(3)
C(7)-C(8)-C(9)-N(1)	0.0(7)
C(14)-N(2)-C(10)-F(8)	-177.9(4)
Pd(1)-N(2)-C(10)-F(8)	0.9(5)
C(14)-N(2)-C(10)-C(11)	1.6(7)
Pd(1)-N(2)-C(10)-C(11)	-179.6(4)
N(2)-C(10)-C(11)-C(12)	-1.3(7)
F(8)-C(10)-C(11)-C(12)	178.1(4)
C(10)-C(11)-C(12)-C(13)	0.5(7)
C(11)-C(12)-C(13)-C(14)	-0.1(8)
C(10)-N(2)-C(14)-C(13)	-1.1(7)
Pd(1)-N(2)-C(14)-C(13)	-179.9(4)
C(12)-C(13)-C(14)-N(2)	0.4(7)
O(5)#1-Pd(2)-O(5)-C(15)	114(100)
N(3)#1-Pd(2)-O(5)-C(15)	95.3(3)
N(3)-Pd(2)-O(5)-C(15)	-84.7(3)
O(5)#1-Pd(2)-N(3)-C(17)	-55.3(4)
O(5)-Pd(2)-N(3)-C(17)	124.7(4)
N(3)#1-Pd(2)-N(3)-C(17)	0(100)
O(5)#1-Pd(2)-N(3)-C(21)	120.1(3)
O(5)-Pd(2)-N(3)-C(21)	-59.9(3)
N(3)#1-Pd(2)-N(3)-C(21)	0(100)
Pd(2)-O(5)-C(15)-O(6)	-0.8(6)
Pd(2)-O(5)-C(15)-C(16)	179.7(2)
O(6)-C(15)-C(16)-F(9)	-60.8(6)
O(5)-C(15)-C(16)-F(9)	118.7(5)
O(6)-C(15)-C(16)-F(10A)	-148.0(4)
O(5)-C(15)-C(16)-F(10A)	31.5(5)
O(6)-C(15)-C(16)-F(11A)	85.4(7)
O(5)-C(15)-C(16)-F(11A)	-95.0(6)
O(6)-C(15)-C(16)-F(11)	61.6(6)
O(5)-C(15)-C(16)-F(11)	-118.9(5)
O(6)-C(15)-C(16)-F(9A)	-30.1(9)
O(5)-C(15)-C(16)-F(9A)	149.4(8)
O(6)-C(15)-C(16)-F(10)	175.8(4)
O(5)-C(15)-C(16)-F(10)	-4.7(5)
C(21)-N(3)-C(17)-F(12)	178.1(4)
Pd(2)-N(3)-C(17)-F(12)	-6.4(6)
C(21)-N(3)-C(17)-C(18)	-0.9(7)
Pd(2)-N(3)-C(17)-C(18)	174.6(4)
N(3)-C(17)-C(18)-C(19)	0.0(8)
F(12)-C(17)-C(18)-C(19)	-179.1(4)
C(17)-C(18)-C(19)-C(20)	1.3(8)
C(18)-C(19)-C(20)-C(21)	-1.6(8)
C(17)-N(3)-C(21)-C(20)	0.6(7)
Pd(2)-N(3)-C(21)-C(20)	-175.0(4)
C(19)-C(20)-C(21)-N(3)	0.6(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z