Unexpected [2+2] C-C Bond Coupling Due to Photoisomerization on Orthopalladated (*Z*)–2–Aryl–4–Arylidene–5(4*H*)–Oxazolones

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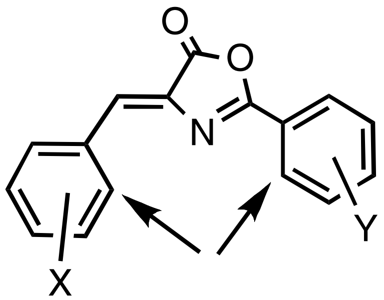
Electronic Supplementary Information

Complete Experimental Section

General Methods. General methods are as published elsewhere.[1,2,3] The starting amides *N*-3-methoxybenzoylglycine and *N*-3,4-dimethoxybenzoylglycine were already synthesized,[4] but only partial spectroscopic characterization is provided and therefore a fully characterization is given here. The oxazolone **1a**[5] was prepared and characterized before. Compound **1c**[6] is mentioned in the literature, but no NMR data nor MS studies are given. $Pd(OAc)_2$[7] and Tlacac[8] have been prepared by reported procedures.

Synthesis of Oxazolones



X=H; Y= H (**1a**), 3-OMe (**1b**), 3,4-$(OMe)_2$ (**1c**); X=Y=3,4-$(OMe)_2$ (**1d**).
X=4-NO_2, Y=3,4-$(OMe)_2$ (**1e**)

(*Z*)-2-(3-methoxyphenyl)-4-benzylidene-5(4*H*)-oxazolone (1b)

Benzaldehyde (0.650 g, 6.125 mmol), *N*-3-methoxybenzoylglycine (1.281 g, 6.125 mmol), anhydrous sodium acetate (0.502 g, 6.125 mmol) and acetic anhydride (1.876 g, 18.375 mmol) were reacted for 1 h at 100 ^{o}C giving **1a** as a yellow solid after recrystallization from EtOH (Yield 1.334 g, 78%). ^{1}H NMR (400 MHz, *$CDCl_3$*) δ ppm: 3.90 (s, 3H, OCH_3), 7.16 (dd, ^{3}J = 8.3 Hz, ^{4}J = 2.3 Hz, 1H, $H_{4'}$), 7.27 (s, 1H, $H_{7''}$), 7.42-7.51 (m, 4H, $H_{5'}$, $H_{3''}$, $H_{4''}$, $H_{5''}$), 7.68 (s, 1H, $H_{2'}$), 7.80 (d, ^{3}J = 7.7 Hz, 1H, $H_{6'}$), 8.20 (d, ^{3}J = 8.0 Hz, 2H, $H_{2''}$, $H_{6''}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 55.55 (1C, OCH_3), 112.69 (1C, $C_{2'}$), 119.84 (1C, $C_{4'}$), 120.96 (1C, $C_{6'}$), 126.75, 133.21, 133.45 (3C, $C_{1'}$, $C_{1''}$, C_2), 128.90 (2C, $C_{3''}$, $C_{5''}$), 130.03, 131.23 (2C, $C_{4''}$, $C_{5'}$), 131.91 (1C, $C_{7''}$), 132.46 (2C, $C_{2''}$, $C_{6''}$), 159.83 (1C, $C_{3'}$), 163.44 (1C,

C_1), 167.62 (1C, C_3). MS (ESI +) m/z: 279.9 $[M]^+$. IR: ν = 1780 cm^{-1} vs (C=O), 1657 cm^{-1} vs (C=N). Anal. Calc. for $C_{17}H_{13}NO_3$ (279.09): C, 73.11; H, 4.69; N, 5.02. Found: C, 73.34; H, 4.91; N, 5.37.

(*Z*)-2-(3,4-dimethoxyphenyl)-4-benzylidene-5(4*H*)-oxazolone (1c)[5]

Benzaldehyde (0.541 g, 5.098 mmol), *N*-3,4-dimethoxybenzoylglycine (1.220 g, 5.098 mmol), anhydrous sodium acetate (0.418 g, 5.098 mmol) and acetic anhydride (1.561 g, 15.294 mmol) were reacted for 2 h at 100 °C giving **1b** as a yellow solid after recrystallization from EtOH (Yield 0.583 g, 37%). ^{1}H NMR (400 MHz, *CDCl₃*) δ ppm: 3.99 (s, 3H, OCH_3), 4.01 (s, 3H, OCH_3), 6.99 (d, ^3J = 8.5 Hz, 1H, $H_{5'}$), 7.20 (s, 1H, $H_{7''}$), 7.41-7.53 (m, 3H, $H_{3''}$, $H_{4''}$, $H_{5''}$), 7.64 (d, ^4J = 1.9 Hz, 1H, $H_{2'}$), 7.84 (dd, ^3J = 8.5 Hz, ^4J = 1.9 Hz, 1H, $H_{6'}$), 8.19-8.23 (d, ^3J = 8.0 Hz, 2H, $H_{2''}$, $H_{6''}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 56.15 (1C, OCH_3), 56.17 (1C, OCH_3), 110.24 (1C, $C_{2'}$), 110.99 (1C, $C_{5'}$), 117.90, 133.48, 133.66 (3C, $C_{1'}$, $C_{1''}$, C_2), 122.92 (1C, $C_{6'}$), 128.87 (2C, $C_{3''}$, $C_{5''}$), 130.41 (1C, $C_{7''}$), 130.90 (1C, $C_{4''}$), 132.23 (2C, $C_{2''}$, $C_{6''}$), 149.24 (1C, $C_{3'}$), 153.67 (1C, $C_{4'}$), 163.27 (1C, C_1), 167.73 (1C, C_3). MS (MALDI +) m/z, (rel. int. %): 309.1 (57.3%) $[M]^+$. IR: ν = 1782, 1740 cm^{-1} vs (C=O), 1650 cm^{-1} vs (C=N). Anal. Calc. for $C_{18}H_{15}NO_4$ (309.10): C, 69.89; H, 4.89; N, 4.53. Found: C, 69.67; H, 4.67; N, 4.38.

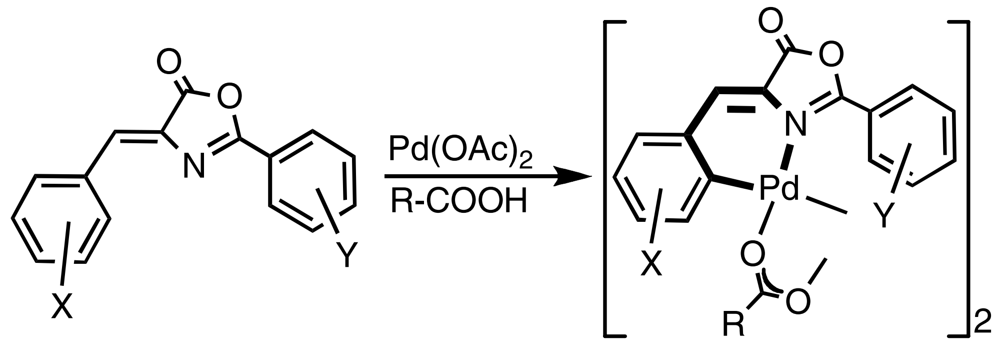
(*Z*)-2-(3,4-dimethoxyphenyl)-4-(3,4-dimethoxybenzylidene)-5(4*H*)-oxazolone (1d)

3,4-dimethoxybenzaldehyde (3.120 g, 18.775 mmol), *N*-3,4-dimethoxybenzoylglycine (4.490 g, 18.775 mmol), anhydrous sodium acetate (1.540 g, 18.775 mmol) and acetic anhydride (5.750 g, 56.327 mmol) were reacted for 2h at 100 °C giving **1c** as an intense yellow solid after recrystallization from EtOH (Yield 5.830 g, 84%). ^{1}H NMR (400 MHz, *$CDCl_3$*) δ ppm: 3.96 (s, 6H, OCH_3), 3.97 (s, 3H, OCH_3), 4.01 (s, 3H, OCH_3), 6.93 (d, ^3J = 8.2 Hz, 1H, $H_{5''}$), 6.98 (d, ^3J = 8.5 Hz, 1H, $H_{5'}$), 7.13 (s, 1H, $H_{7''}$), 7.54 (dd, ^3J = 8.4 Hz, ^4J = 2.0 Hz, 1H, $H_{6''}$), 7.61 (d, ^{4}J = 2.7 Hz, 1H, $H_{2'}$), 7.76 (dd, ^{3}J = 8.4 Hz, ^{4}J = 2.0 Hz, 1H, $H_{6'}$), 8.17 (d, ^{4}J = 1.9 Hz, 1H, $H_{2''}$). ^{13}C NMR (101 MHz, *CDCl₃*) δ ppm: 55.63, 55.89, 55.99, 56.12 (4C, OCH_3), 109.96 (1C, $C_{2'}$), 110.86, 111.02 (2C, $C_{5'}$, $C_{5''}$), 113.81 (1C, $C_{2''}$), 118.12, 127.00, 131.39 (3C, $C_{1'}$, $C_{1''}$, C_2), 122.35 (1C, $C_{6'}$), 127.36 (1C, $C_{6''}$), 130.63 (1C, $C_{7''}$), 149.02, 149.15, 151.76, 153.32 (4C, $C_{3'}$, $C_{4'}$, $C_{3''}$, $C_{4''}$), 162.25 (1C, C_1), 168.00 (1C, C_3). MS (MALDI+) m/z, (rel. int. %): 369.2 (100%) $[M]^+$. IR: ν = 1772 cm^{-1} vs (C=O), 1648 cm^{-1} vs (C=N). Anal. Calc. for $C_{20}H_{19}NO_6$ (369.12): C, 65.03; H, 5.18; N, 3.79. Found: C, 65.34; H, 4.87; N, 3.79.

(*Z*)-2-(3,4-dimethoxyphenyl)-4-(4-nitrobenzylidene)-5(4*H*)-oxazolone (1e)

4-Nitrobenzaldehyde (0.451 g, 2.984 mmol), *N*-3,4-dimethoxybenzylglycine (0.714 g, 2.984 mmol), anhydrous sodium acetate (0.245 g, 2.984 mmol) and acetic anhydride (0.914 g, 8.952 mmol) were reacted for 2 h at 100 °C giving **1d** as a yellow solid after recrystallization from EtOH (Yield 0.782 g, 74%). ^{1}H NMR (400 MHz, *CDCl₃*) δ ppm: 4.01 (s, 3H, OCH_3), 4.02 (s, 3H, OCH_3), 7.02 (d, ^{3}J = 8.5 Hz, 1H, $H_{5'}$), 7.17 (s, 1H, $H_{7''}$), 7.64 (d, ^{4}J = 1.9 Hz, 1H, $H_{2'}$), 7.89 (dd, ^{3}J = 8.5 Hz, ^{4}J = 2.0 Hz, 1H, $H_{6'}$), 8.29-8.38 (m, 4H, $H_{2''}$, $H_{3''}$, $H_{5''}$, $H_{6''}$). ^{13}C NMR (101 MHz, *CDCl₃*) δ ppm: 56.26 (1C, OCH_3), 56.29 (1C, OCH_3), 110.50 (1C, $C_{2'}$), 111.19 (1C, $C_{5'}$), 117.29, 122.06,129.42 (3C, $C_{1'}$, $C_{1''}$, C_2), 123.72 (1C, $C_{6'}$), 123.96 (2C, $C_{3''}$, $C_{5''}$), 126.02 (1C, $C_{7''}$), 132.50 (2C, $C_{2''}$, $C_{6''}$), 148.07, 149.70 (2C, $C_{3'}$, $C_{4'}$), 154.10 (1C, $C_{4''}$), 158.27 (1C, C_1), 168.46 (1C, C_3). MS (MALDI+) m/z, (rel. int. %): 354.2 (100%) $[M]^+$. IR: ν = 1781 cm^{-1} vs (C=O), 1655 cm^{-1} vs (C=N). Anal. Calc. for $C_{18}H_{14}N_2O_6$ (354.09): C, 61.02; H, 3.98; N, 7.91. Found: C, 61.43; H, 4.18; N, 8.12.

Synthesis of orthopalladated complexes. Dependence of the pK_a of the solvent.



(**1a**) - (**1e**) (**2d**) - (**3d**)

R=Me: CH_3CO_2H, 2h (95 °C), X=Y= 3,4-$(OMe)_2$ (**2d**).
R=CF_3: CF_3CO_2H, 5min (rt) to 4h (75 °C) or 2h (95 °C). X=Y=H (**3a**)
X=H, Y=3-OMe (**3b**), 3,4-$(OMe)_2$ (**3c**), X=Y=3,4-$(OMe)_2$ (**3d**).

Preparation of 2d

To a stirred solution of **1d** (0.076 g, 0.206 mmol) in glacial acetic acid (10 mL), palladium acetate (0.046 g, 0.206 mmol) was added and then the solution was refluxed for 2 h at 95 ^{o}C meanwhile the color of the solution changed from yellow to orange-red. After cooling, solution was diluted with water and the product extracted with CH_2Cl_2, washed three times with water, dried over Na_2SO_4 and then concentrated under reduce pressure until 3 mL. To the concentrated solution, hexane was added to afford the precipitation of **2d** as a dark red solid (Yield 0.090 g, 82%). ^{1}H NMR (400 MHz, *$CDCl_3$*) δ ppm: 1.26 (s, 3H, CH_3COO), 3.81 (s, 3H, OCH_3), 3.93 (s, 3H, OCH_3), 3.97 (s, 3H, OCH_3), 4.00 (s, 3H, OCH_3), 6.83 (s, 1H, $H_{6''}$), 6.89 (d, ^3J = 8.6 Hz, 1H, $H_{5'}$), 6.92 (s, 1H, $H_{3''}$), 7.18 (broad s, 1H, $H_{2'}$), 7.39 (s, 1H, $H_{7''}$), 7.74 (broad s, 1H, $H_{6'}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 22.97 (1C, $\underline{C}H_3COO$), 55.75, 56.05, 56.19, 56.30 (4C, 4OCH_3), 109.97 (1C, $C_{5'}$), 112.68 (1C, $C_{2'}$), 114.20 (1C, $C_{6''}$), 115.99 (1C, $C_{3''}$), 115.48, 121.80, 123.23, 133.74 (4C, $C_{1'}$, $C_{1''}$, $C_{2''}$, C_2), 126.79 (1C, $C_{6'}$), 138.12 (1C, $C_{7''}$), 146.93, 147.98, 149.69, 153.78 (4C, 4$\underline{C}OCH_3$), 161.97 (1C, C_1), 165.82 (1C, C_3), 179.58 (1C, CH_3COO). MS (MALDI +) m/z, (rel. int. %): 1009.6 (86.5%) [M–

$CH_3COO^-]^+$, 474.0 (100%) $[M/2–CH_3COO^-]^+$. IR: ν = 1780 cm^{-1} (C=O), 1650 cm^{-1} (C=N). Anal. Calc. for $C_{44}H_{42}N_2O_{16}Pd_2$ (1066.06):C, 49.50; H, 3.97; N, 2.62. Found: C, 49.78; H, 3.62; N, 2.91.

Preparation of 3a

To a stirred solution of **1a** (0.259 g, 1.039 mmol) in TFA (5 mL), palladium acetate (0.233 g, 1.039 mmol) was added. Immediately a precipitate was observed. The suspension was refluxed at 75 °C for 4 h, while the solution color changed slowly to dark yellow. The resulting mixture was then treated with water (5 mL) and the precipitate formed filtered and washed several times with water (3×5 mL) to remove the acid. After complete dryness and recrystallization from dichloromethane/pentane twice, **3a** was obtained as a yellow brown solid (Yield 0.165 g, 34%). ^{1}H NMR (400 MHz, *$CDCl_3$*) δ ppm: 7.06-7.15 (m, 3H, $H_{4''}$, $H_{5''}$, $H_{6''}$), 7.22-7.24 (m, 1H, $H_{3''}$), 7.43 (s, 1H, $H_{7''}$), 7.59 (t, ^3J = 8.0 Hz, 2H, $H_{3'}$, $H_{5'}$), 7.71 (t, ^3J = 7.6 Hz, 1H, $H_{4'}$), 8.39 (d, ^3J = 7.6 Hz, 2H, $H_{2'}$, $H_{6'}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 122.10, 122.29, 123.77, 131.13 (4C, $C_{1'}$, $C_{1''}$, C_2, $C_{2''}$), 126.28 (1C, $C_{6''}$), 128.79 (2C, $C_{3'}$, $C_{5'}$), 130.45 (2C, $C_{2'}$, $C_{6'}$), 130.82, 132.15 (2C, $C_{4''}$, $C_{5''}$), 133.07 (1C, $C_{3''}$), 135.23 (1C, $C_{4'}$), 138.56 (1C, $C_{7''}$), 160.21 (1C, C_1), 168.09 (1C, C_3), 188.03 (1C, $CF_3\underline{C}OO$). ^{19}F NMR (376 MHz, *$CDCl_3$*) δ ppm, -74.64, -73.54. IR: ν = 1796 cm^{-1} vs (C=O), 1647 cm^{-1} vs (C=N). MS (MALDI+) m/z, (rel. int. %): 822.9 (24.1%) $[M-CF_3COO^-]^+$, 353.6 (46.1%) $[M/2 - CH_3COCOO^-]^+$. Anal. Calc. for $C_{36}H_{20}F_6N_2O_8Pd_2$ (933.92): C, 46.23; H, 2.16; N, 2.99. Found: C, 46.45; H, 2.46; N, 3.35.

Preparation of 3b

To a stirred solution of **1b** (0.147 g, 0.526 mmol) in TFA (5 mL), palladium acetate (0.118 g, 0.526 mmol) was added. The suspension was refluxed at 75 °C for 4 hours while the solution color changed slowly from yellow to dark yellow. The mixture was then treated with water (5 mL) and the precipitate formed filtered and washed several times with water (3×5 mL) to remove the acid. After complete dryness, the resulting solid was dissolved in a small quantity of CH_2Cl_2 and precipitated with pentane to afford **3b** as a yellow brown solid (Yield 0.238 g, 91%). ^{1}H NMR (400 MHz, *CD_2Cl_2*) δ ppm: 3.77 (s, 3H, OCH_3), 7.03-7.11 (m, 3H), 7.19 (td, ^3J = 9.2 Hz, ^4J = 2.3 Hz, 1H), 7.24-7.34 (m, 3H), 7.43-7.47 (d, ^3J = 7.6 Hz, 1H), 7.48 (s, 1H, $H_{7''}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 56.06 (1C, OCH_3), 115.75 (1C), 121.29 (1C), 123.22 (1C), 123.58 (1C), 123.80 (1C), 126.78 (1C), 129.98 (1C), 130.02 (1C), 131.47 (1C), 133.88 (1C), 134.15 (1C), 135.98 (1C), 139.10 (1C, $C_{7''}$), 159.78 (1C, $C_{3'}$), 160.92 (1C, C_1), 168.48 (1C, C_2), 188.90 (1C, $CF_3\underline{C}OO$). ^{19}F NMR (376 MHz, *CD_2Cl_2*) δ ppm: -75.12. IR: ν = 1801 cm^{-1} vs (C=O), 1669 cm^{-1} 1658 vs (C=N). MS (MALDI +) m/z, (rel. int. %): 882.9 (72.0%) $[M\text{-}CF_3COO^-]^+$, 383.6 (26.4%) $[M/2\text{-}CF_3COO^-]^+$. Anal. Calc. for $C_{38}H_{24}F_6N_2O_{10}Pd_2$ (993.94): C, 45.85; H, 2.43; N, 2.81. Found: C, 45.75; H, 2.54; N, 2.72.

Preparation of 3c

To a stirred solution of **1c** (0.064 g, 0.207 mmol) in TFA (5 mL), palladium acetate (0.046 g, 0.207 mmol) was added. The suspension was refluxed at 81 °C for 3 hours while the solution color changed slowly from yellow to dark yellow. The mixture was then treated with water and the precipitate formed filtered and washed several times with water to remove the acid. After complete dryness **3c** was obtained as a yellow brown solid (Yield 0.060 g, 55%). ^{1}H NMR (400 MHz, *$CDCl_3$*) δ ppm: 3.95 (s, 3H, OCH_3), 3.96 (s, 3H, OCH_3), 6.93 (d, ^3J = 8.6 Hz, 1H, $H_{5'}$), 7.09-7.32 (m, 4H, $H_{3''}$, $H_{4''}$ $H_{5''}$, $H_{6''}$), 7.40 (broad s, 1H, $H_{2'}$), 7.44 (s, 1H, $H_{7''}$), 7.82 (broad d, ^3J = 7.2 Hz, 1H, $H_{6'}$). ^{19}F NMR (376 MHz, *$CDCl_3$*) δ ppm: -75.23. IR: ν = 1801 cm^{-1} vs (C=O), 1657 cm^{-1} vs (C=N). MS (MALDI +) m/z, (rel. int. %): 942.9 (19.4%) $[M–CF_3COO^- + 2H]^+$. Anal. Calc. for $C_{40}H_{28}F_6N_2O_{12}Pd_2$ (1053.96): C, 45.52; H, 2.67; N, 2.65. Found: C, 45.43; H, 2.82; N, 2.91.

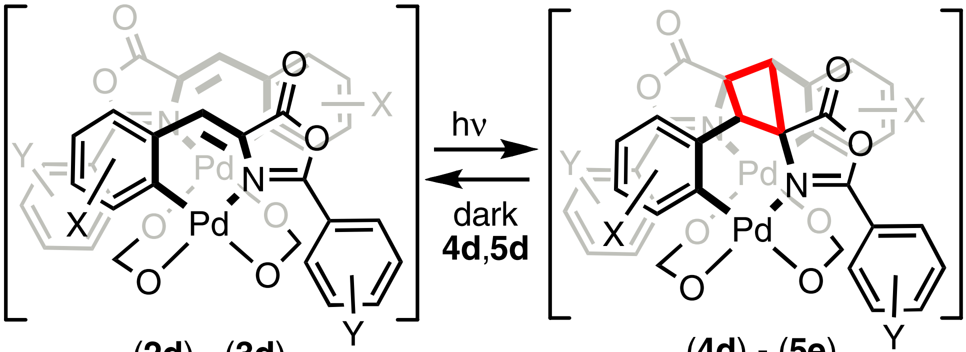
Preparation of 3d

To a stirred solution of **1d** (0.256 g, 0.693 mmol) in TFA (10 mL), palladium acetate (0.156 g, 0.693 mmol) was added and then the solution was refluxed for 2 h at 95 ^{o}C meanwhile the color of the solution changed from pale brown to orange-red. After cooling, solution was diluted with water and the product extracted with CH_2Cl_2, washed three times with water, dried over Na_2SO_4 and then concentrated under reduced pressure until 3 mL. To the concentrated solution, hexane was added to afford the precipitation of **3d** as a dark red solid (Yield 0.338 g, 83%). ^{1}H NMR (400 MHz, *CDCl$_3$*) δ ppm: 3.63, 3.85, 3.89, 3.91 (s, 12H, 4OCH_3), 6.49 (s, 1H, $H_{6''}$), 6.73 (s, 1H, $H_{3''}$), 6.84 (d, ^{3}J = 8.6 Hz, 1H, $H_{5'}$), 7.25 (broad s, 1H, $H_{2'}$), 7.28 (s, 1H, $H_{7''}$), 7.67 (broad d, ^{3}J = 6.5 Hz, 1H, $H_{6'}$). ^{13}C NMR (101 MHz, *CDCl$_3$*) δ ppm: 55.57, 56.04, 56.12, 56.18 (4C, 4OCH_3), 110.54 (1C, $C_{5'}$), 112.33 (1C, $C_{2'}$), 114.00 (1C, $C_{3''}$), 114.99 (1C, $C_{6''}$), 114.03, 121.26, 122.35, 128.86, (4C, $C_{1'}$, $C_{1''}$, C_2, $C_{2''}$), 126.41 (1C, $C_{6'}$), 137.19, (1C, $C_{7''}$), 147.22, 148.41, 149.86, 154.80 (4C, $C_{3'}$, $C_{4'}$, $C_{4''}$, $C_{5''}$), 161.30 (1C, C_1), 166.11 (1C, C_3). ^{19}F NMR (376 MHz, *CDCl$_3$*) δ ppm: -75.85. IR: ν = 1767 cm^{-1} vs (C=O), 1669 cm^{-1}, 1656 vs (C=N). MS (MALDI +) m/z, (rel. int. %): 1061.4 (8.6%) [M–CF_3COO^-]$^+$; 474.0 (100%) [M/2–CF_3COO^-]$^+$. Anal. Calc. for $C_{44}H_{36}F_6N_2O_{16}Pd_2$ (1174.00): C, 44.95; H, 3.09; N, 2.38. Found: C, 44.82; H, 2.97; N, 2.41

Preparation of 3e

Complex 3e could not be prepared in pure form due to fast evolution to **5e** in presence of sunlight. In all attempted cases mixtures **3e**/**5e** were obtained.

Photoisomerization and [2+2] C–C coupling reactions



(**2d**) - (**3d**) (**4d**) - (**5e**)

Solvent CD_2Cl_2; CH_3COO bridge: X=Y= 3,4-$(OMe)_2$ (**4d**).
CF_3COO bridge; X=Y=H (**5a**); X=H, Y=3-OMe (**5b**), 3,4-$(OMe)_2$ (**5c**)
X=Y=3,4-$(OMe)_2$ (**5d**); X=4-NO_2, Y=3,4-$(OMe)_2$ (**5e**) (see text)

Preparation of 4d

A red solution of complex **2d** (25.2 mg, 0.022 mmol) in $CDCl_3$ (0.6 mL), placed on a NMR tube, was exposed to sunlight until complete conversion was observed. In case of complex **4d**, 240 h were needed. The resulting red solution was evaporated to dryness allowing the obtention of **4d** as a red-brown solid (Yield of isolated product: 0.0251 g, 99.6 %). ^1H NMR (400 MHz, *$CDCl_3$*): δ = 1.89 (s, 3H, CH_3COO), 3.66 (s, 3H, OCH_3), 3.70 (s, 3H, OCH_3) 3.93 (s, 3H, OCH_3), 4.06 (s, 3H, OCH_3), 4.87 (s, 1H, $H_{7''}$), 6.22 (s, 1H, $H_{3''}$), 6.58 (s, 1H, $H_{6''}$), 6.98 (d, ^3J = 8.8 Hz, 1H, $H_{5'}$), 8.58 (dd, ^3J = 8.6 Hz, ^4J = 2.1 Hz, 1H, $H_{6'}$), 9.00 (d, ^4J = 2.1 Hz, 1H, $H_{2'}$). $^{13}C\{^1H\}$ NMR (101 MHz, *$CDCl_3$*): δ = 24.08 (s, $\underline{C}H_3COO$), 55.74, 55.91, 56.50, 56.85 (4C, 4 OCH_3), 60.71 (1C, $C_{7''}$), 71,67 (1C, C_2), 110.86 (1C, $C_{5'}$), 111.48 (1C, $C_{3''}$), 113.09 (1C, $C_{2'}$), 115.10 (1C, $C_{1'}$), 115.75 (1C, $C_{6''}$), 120.33 (1C, $C_{1''}$), 126.35 (1C, $C_{6'}$), 129.68 (1C, $C_{2''}$), 146.52, 146.71, 149.20, 155.09 (4C, $C_{3'}$, $C_{4'}$, $C_{4''}$, $C_{5''}$), 166.76 (1C, C_1), 175.18 (1C, C_3), 181.82 (1C, $\underline{C}OO$). IR: ν = 1831 vs (C=O) cm^{-1}, 1649 vs (C=N) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 474.2 (56.2%) $[M/2–CH_3COO^-]^+$. Complex **4d** crystallized from CH_2Cl_2/Et_2O, giving crystals of **4d**·$0.75CH_2Cl_2$, which were used for analytic and spectroscopic purposes.

Anal. Calc. for $C_{44}H_{42}N_2O_{16}Pd_2 \cdot 0.75CH_2Cl_2$ (1131.31): C, 47.51; H, 3.88; N, 2.48. Found: C, 47.67 H, 4.33; N, 2.28. In the absence of sunlight, complex **4d** reverts to complex **2d**. After 19 h in the dark, a 1.5/1 molar ratio (**4d**/**2d**) was observed.

Preparation of 5a

A yellow solution of complex **3a** (30.1 mg, 0.032 mmol) in $CDCl_3$ (0.6 mL), placed on a NMR tube, was exposed to sunlight until complete conversion was observed. In case of complex **5a**, 28 h were needed. The resulting solution was evaporated to dryness allowing the obtention of **5a** as a yellow-brown solid (Yield of isolated product: 0.0296 g, 98.3 %). ^{1}H NMR (300 MHz, *CDCl$_3$*): δ = 5.04 (s, 1H, $H_{7''}$), 6.75 (dd, ^3J = 7.1 Hz, ^4J = 2.2 Hz, 1H, $H_{3''}$), 6.84-6.92 (m, 2H, $H_{4''}$, $H_{5''}$), 7.05 (dd, ^3J = 7.4 Hz, ^4J = 1.7 Hz, 1H, $H_{6''}$), 7.60 (t, ^3J = 8.1 Hz, 2H, $H_{3'}$, $H_{5'}$), 7.71 (t, ^3J = 8.1 Hz, 1H, $H_{4'}$), 9.09 (d, 2H, $H_{2'}$, $H_{6'}$). ^{13}C{^{1}H} NMR (75.5 MHz, *CDCl$_3$*): δ = 60.58 (1C, $C_{7''}$), 70.35 (1C, C_2), 122.22 (1C, $C_{1'}$), 125.93, 127.90 (2C, $C_{4''}$,$C_{5''}$), 128.08 (1C, $C_{2''}$), 129.41 (3C, $C_{3''}$,$C_{3'}$,$C_{5'}$), 130.92 (2C, $C_{2'}$,$C_{6'}$), 133.79 (1C, $C_{6''}$), 135.88 (1C, $C_{1''}$), 136.09 (1C, $C_{4'}$), 168.95 (1C, C_1), 173.62 (1C, C_3). ^{19}F NMR (282 MHz, *CDCl$_3$*): δ = -74.80. IR: ν = 1838 (ν_{CO}) cm^{-1}, 1655 (ν_{CN}) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 354.2 (64.2%) [M/2-CF_3COO^-]$^+$. Anal. Calc. for $C_{36}H_{20}F_6N_2O_8Pd_2$ (933.9): C, 46.23; H, 2.16; N, 2.99. Found: C, 46.69; H, 2.67; N, 2.76. In the absence of sunlight, **5a** does not revert.

Preparation of 5b

A yellow solution of complex **3b** (25.0 mg, 0.025 mmol) in $CDCl_3$ (0.6 mL), placed on a NMR tube, was exposed to sunlight until complete conversion was observed. In case of complex **5b**, 50 h were needed. The resulting solution was evaporated to dryness allowing the obtention of **5b** as a deep yellow solid (Yield of isolated product: 0.025 g, quantitative). ^{1}H NMR (400 MHz, *CD$_2$Cl$_2$*): δ = 3.94 (s, 3H, OCH_3), 5.06 (s, 1H, $H_{7''}$), 6.78 (dd, ^3J = 7.2 Hz, ^4J = 1.6 Hz, 1H, $H_{3''}$), 6.82-6.90 (m, 2H, $H_{4''}$, $H_{5''}$), 6.96 (d, ^3J = 7.8 Hz, 1H, $H_{6''}$), 7.28 (dd, ^3J =

8.3 Hz, ^4J = 1.3 Hz, 1H, $H_{4'}$), 7.47 (t, ^3J = 8.0 Hz, 1H, $H_{5'}$), 8.30 (d, ^3J = 7.8 Hz, 1H, $H_{6'}$), 8.96 (s, 1H, $H_{2'}$).$^{13}C\{^1H\}$ NMR (101 MHz, *CD_2Cl_2*): δ = 56.41 (1C, OCH_3), 60.78 (1C, $C_{7''}$), 70,68 (1C, C_2), 113.97 (1C, $C_{2'}$), 123.85 (1C, $C_{6'}$), 123.88 (1C, $C_{1'}$), 124.19 (1C, $C_{4'}$), 126.25 (1C, $C_{4''}$), 128.14 (1C, $C_{5''}$), 128.72 (1C, $C_{2''}$), 130.29 (1C, $C_{3''}$), 130.81 (1C, $C_{5'}$), 133.73 (1C, $C_{6''}$), 136.04 (1C, $C_{1''}$), 160.67 (1C, $C_{3'}$), 169.45 (1C, C_1), 174.12 (1C, C_3).^{19}F NMR (376 MHz, *CD_2Cl_2*): δ = -75.15. IR: ν = 1835 (ν_{CO}) cm^{-1}, 1655 (ν_{CN}) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 384.1 (32.2%) $[M/2–CF_3COO^-]^+$. Anal. Calc. for $C_{38}H_{24}F_6N_2O_{10}Pd_2$ (993.94): C, 45.85; H, 2.43; N, 2.81. Found: C, 46.09; H, 2.58; N, 2.69. In the absence of sunlight, **5b** does not revert.

Preparation of 5c

A yellow solution of complex **3c** (28.3 mg, 0.027 mmol) in $CDCl_3$ (0.6 mL), placed on a NMR tube, was exposed to sunlight until complete conversion was observed. In case of complex **5c**, 50 h were needed. The resulting solution was evaporated to dryness allowing the obtention of **5c** as a deep yellow solid (Yield of isolated product: 0.0271 g, 95.7 %). ^1H NMR (500 MHz, *$CDCl_3$*) δ ppm: 4.00 (s, 3H, OCH_3), 4.15 (s, 3H, OCH_3), 5.09 (s, 1H, $H_{7''}$), 6.81 (dd, ^3J = 7.3 Hz, ^4J = 1.8 Hz, 1H, $H_{3''}$), 6.88-6.98 (m, 2H, $H_{4''}$, $H_{5''}$), 7.00 (d, ^3J = 8.7 Hz, 1H, $H_{5'}$), 7.07 (dd, ^3J = 7.8 Hz, ^4J = 1.2 Hz, 1H, $H_{6''}$), 8.25 (dd, ^3J = 8.7 Hz, ^4J = 2.2 Hz, 1H, $H_{6'}$), 9.33 (d, ^4J = 2.2 Hz, 1H, $H_{2'}$). ^{13}C NMR (101 MHz, *$CDCl_3$*) δ ppm: 56.44, 56.69 (2C, $2OCH_3$), 60.72 (1C, $C_{7''}$), 70.14 (1C, C_2), 114.27, 128.48, 136.00 (3C, $C_{1'}$, $C_{1''}$, $C_{2''}$), 110.87 (1C, $C_{2'}$), 112.23 (1C, $C_{5'}$), 125.82, 126.66, 127.69 (3C, $C_{6'}$, $C_{4''}$, $C_{5''}$), 129.48 (1C, $C_{3''}$), 133.66 (1C, $C_{6''}$), 149.66, 155.81 (2C, $C_{3'}$, $C_{4'}$), 167.99 (1C, C_1), 174.08 (1C, C_3). ^{19}F NMR (376 MHz, *$CDCl_3$*) δ ppm: -75.23. IR: ν = 1801 cm^{-1} vs (C=O), 1657 cm^{-1} vs (C=N). MS (MALDI+) m/z, (rel. int. %): 942.9 (19.4%) $[M-CF_3COO^-]^+$. Anal. Calc. for

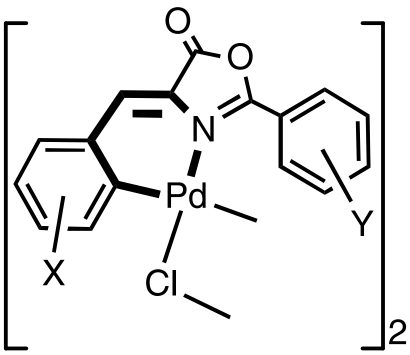
$C_{40}H_{28}F_6N_2O_{12}Pd_2$ (1053.96): C, 45.52; H, 2.67; N, 2.65. Found: C, 45.43; H, 2.82; N, 2.91. In the absence of sunlight, complex **5c** does not revert.

Preparation of 5d

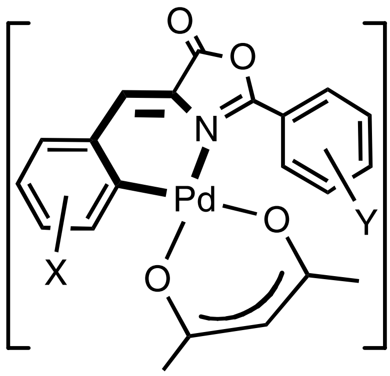
A dark red solution of complex **3d** (28.6 mg, 0.0243 mmol) in $CDCl_3$ (0.6 mL), placed on a NMR tube, was exposed to sunlight until complete conversion was observed. In case of complex **5d**, 240 h were needed. The resulting solution was evaporated to dryness allowing the obtention of **5d** as a red solid (Yield of isolated product: 0.0280 g, 97.9 %). ^{1}H NMR (300 MHz, *CDCl₃*): δ = 3.75 (s, 3H, OCH_3), 3.76 (s, 3H, OCH_3) 4.02 (s, 3H, OCH_3), 4.14 (s, 3H, OCH_3), 4.99 (s, 1H, $H_{7''}$), 6.30 (s, 1H, $H_{3''}$), 6.50 (s, 1H, $H_{6''}$), 7.04 (d, ^{3}J = 8.7 Hz, 1H, $H_{5'}$), 8.33 (dd, ^{3}J = 8.6 Hz, ^{4}J = 2.0 Hz, 1H, $H_{6'}$), 9.19 (d, ^{4}J = 2.0 Hz, 1H, $H_{2'}$). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, *CDCl₃*): δ = 55.91, 55.98, 56.41, 56.73 (4C, 4 OCH_3), 60.50 (1C, $C_{7''}$), 70,95 (1C, C_2), 110.92 (1C, $C_{5'}$), 111.67 (1C, $C_{3''}$), 112.29 (1C, $C_{2'}$), 114.41 (1C, $C_{1'}$), 114.69 (1C, $C_{6''}$), 119.16 (1C, $C_{1''}$), 125.78 (1C, $C_{6'}$), 126.64 (1C, $C_{2''}$), 147.18, 147.29, 149.70, 155.86 (4C, $C_{3'}$, $C_{4'}$, $C_{4''}$, $C_{5''}$), 167.94 (1C, C_1), 174.32 (1C, C_3). ^{19}F NMR (282 MHz, CD_2Cl_2): δ = -74.29. IR: ν = 1836 vs (C=O) cm^{-1}, 1660 vs (C=N) cm^{-1}. MS (MALDI+) m/z, (rel.int.%): 474.2 (40.9%) $[M/2-CF_3COO^-]^+$. Anal. Calc. for $C_{44}H_{36}F_6N_2O_6Pd_2$ (1174.0): C, 45.01; H, 3.09; N, 2.38. Found: C, 45.01; H, 3.17; N, 2.19. In the absence of sunlight, **5d** reverts to **3d**. After 19 h in the dark, a 1.5/1 molar ratio (**5d**/**3d**) was observed.

Preparation of 5e

To a stirred solution of **1e** (0.078 g, 0.220 mmol) in TFA (15 mL), palladium acetate (0.049 g, 0.220 mmol) was added. The suspension was refluxed at 75 ^{o}C for 2 hours while the solution color changed slowly from yellow to dark yellow. The mixture was then treated with water and the precipitate formed filtered and washed several times with water to remove the acid. After complete dryness compound **5e** was obtained as a brown yellow solid (Yield 0.072 g, 57%). ^{1}H NMR (400 MHz, *CDCl₃*) δ ppm: 4.03 (s, 3H, OCH_3), 4.14 (s, 3H, OCH_3), 5.20 (s, 1H, $H_{7''}$), 7.05 (d, ^3J = 8.8 Hz, 1H, $H_{4''}$), 7.00 (d, ^3J = 8.3 Hz, 1H, $H_{5''}$), 7.83 (dd, ^3J = 8.2 Hz, ^4J = 2.2 Hz, 1H, $H_{3''}$), 7.92 (d, ^4J = 2.3 Hz, 1H, $H_{6''}$), 8.30 (dd, ^3J = 8.6 Hz, ^4J = 2.2 Hz, 1H, $H_{6'}$), 9.13 (d, ^4J = 2.2 Hz, 1H, $H_{2'}$). ^{19}F NMR (376 MHz, *$CDCl_3$*) δ ppm: -74.47 (s, 3F). MS (MALDI+) m/z, (rel. int. %): 458.1 (23.2%) $[M/2–CF_3COO^-+H]^+$. Anal. Calc. for $C_{40}H_{26}F_6N_4O_{16}Pd_2$ (1143.93): C, 41.94; H, 2.29; N, 4.89. Found: C, 41.76; H, 2.39; N, 4.65.



(**6b**), (**6c**)



(**7b**), (**7c**)

Preparation of 6b

To a solution of **3b** (0.042 g, 0.042 mmol) in MeOH (20 mL), an excess of anhydrous LiCl (0.007 g, 0.176 mmol) was added. After few seconds, a deep yellow precipitate was formed. The mixture was stirred at room temperature for 30 min. After the reaction time, the solid was filtered, washed with cold methanol (5 mL), Et_2O (10 mL) and *n*–pentane (45 mL), dried by suction and identified as **6b** (Yield 0.036 g, 49 %). Anal. Calc. for $C_{34}H_{24}Cl_2N_2O_6Pd_2$ (840.3): C, 48.59; H, 2.88; N, 3.33. Found: C, 48.76; H, 3.03; N, 3.45. IR: ν = 1583 vs (C=O) cm^{-1}, 1583 vs (C=N) cm^{-1} MS (MALDI+) [m/z, (%)]: 548.8 (10%) $[M–Cl]^+$. This complex was not soluble at all in the usual NMR solvents, avoiding its complete characterization.

Preparation of 6c

Complex **6c** was prepared following the same experimental procedure than that described for **6b**. Therefore **3c** (0.092 g, 0.087 mmol) was reacted with an excess of LiCl (0.017 g, 0.398 mmol) in MeOH (20 mL) to give **6c** as a yellow solid (Yield 0.056 g, 71%). Anal. Calc. for $C_{36}H_{28}Cl_2N_2O_8Pd_2$ (900.4): C, 48.02; H, 3.13; N, 3.11. Found: C, 47.94 H, 3.27; N, 2.96. IR: ν = 1583 vs (C=O) cm^{-1}, 1583 vs (C=N) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 548.8 (10%) $[M–Cl]^+$. This complex was not soluble at all in the usual NMR solvents, avoiding its characterization.

Preparation of 7b

To a suspension of **6b** (0.036 g, 0.0428 mmol) in CH_2Cl_2 (10 mL), Tl(acac) (0.027 g, 0.086 mmol) was added. The resulting grey suspension was stirred at room temperature for 30 min, and then filtered though celite. The resulting solution was evaporated to dryness and the oily residue was treated with cold Et_2O (20 mL), allowing the obtention of **7b** as a yellow solid (Yield 0.020 g, 48 %). ^1H NMR (400 MHz, *$CDCl_3$*): δ = 1.20 (s, 3H, CH_3, acac), 1.97 (s, 3H, CH_3, acac) 3.82 (s, 3H, OCH_3), 5.14 (s, 1H, CH, acac), 7.07–7.11 (m, 2H, $H_{4'}$, $H_{3''}$), 7.19–7.24 (m, 2H, $H_{4''}$, $H_{5''}$), 7.33 (t, ^3J = 7.9 Hz, 1H, $H_{5'}$), 7.53 (s, 1H, $H_{7''}$), 7.71 (d, ^3J = 8.0 Hz, 1H, $H_{6''}$), 7.86 (s, 1H, $H_{2'}$), 7.98 (d, 1H, $H_{6'}$). IR: ν = 1792 vs (C=O) cm^{-1}, 1646 vs (C=N) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 384.0 (100%) $[M–acac]^+$. Anal. Calc. for $C_{22}H_{19}NO_5Pd$ (483.8): C, 54.61; H, 3.96; N, 2.89. Found: C, 54.85 H, 4.08; N, 3.01.

Preparation of 7c

Complex **7c** was obtained following the same preparative method than that reported for **7b**. Therefore, **6c** (0.050 g, 0.055 mmol) was reacted with Tl(acac) (0.034 g, 0.108 mmol) in CH_2Cl_2 (20 mL) to give **7c** as yellow solid (Yield 0.048 g 84 %). ^1H NMR (300 MHz, *$CDCl_3$*): δ = 1.36 (s, 3H, CH_3-acac), 2.04 (s, 3H, CH_3-acac) 3.99 (s, 6H, 2 OCH_3), 5.23 (s, 1H, CH-acac), 6.96 (d, ^3J = 8.6 Hz, 1H, $H_{5'}$), 7.16 (t, ^3J = 7.2 Hz, 1H, $H_{4''}$), 7.25–7.31 (m, 2H, $H_{3''}$,

$H_{5''}$), 7.54 (s, 1H, $H_{7''}$), 7.77 (dd, ^3J = 8.8 Hz, ^4J = 1.2 Hz, 1H, $H_{6''}$), 8.08 (d, ^4J = 2.0 Hz, 1H, $H_{2'}$), 8.14 (dd, ^3J = 8.5 Hz, ^4J = 2.0 Hz, 1H, $H_{6'}$). $^{13}C\{^1H\}$ NMR (75.5 MHz, $CDCl_3$): δ = 26.92 (1C, CH_3-acac), 27.55 (1C, CH_3-acac), 56.21 (1C, OCH_3), 56.28 (1C, OCH_3), 99.83 (1C, CH-acac), 60.50 (1C, $C_{7''}$), 110.08 (1C, $C_{5'}$), 112.96 (1C, $C_{2'}$), 114.41 (1C, $C_{1'}$), 123.82 (1C, $C_{2''}$), 125.32, 125.77 (2C, $C_{4''}$, $C_{6'}$),130.68, 132.40 (2C, $C_{3''}$, $C_{5''}$), 132.88 (1C, $C_{1''}$), 134.78 (1C, $C_{6''}$), 139.07 (1C, $C_{7''}$), 144.91 (1C, C_2), 148.17, 154.38 (2C, $C_{3'}$, $C_{4'}$), 159.40 (1C, C_1), 165.62 (1C, C_3), 186.29 (1C, CO-acac), 187.19 (1C, CO-acac). IR: ν = 1784 vs (C=O) cm^{-1}, 1639 vs (C=N) cm^{-1}. MS (MALDI+) m/z, (rel. int. %): 414.0 (100%) $[M–acac]^+$. Anal. Calc. for $C_{23}H_{21}NO_6Pd$ (513.8): C, 53.76; H, 4.12; N, 2.72. Found: C, 53.35 H, 4.48; N, 2.71.

X–ray crystallography: Crystals of **5c·2CH$_2$Cl$_2$** of quality for X-ray measurement were grown by vapour diffusion of Et_2O into CH_2Cl_2 solutions of the crude product at 0 ºC. A single crystal was mounted at the end of a quartz fibber in a random orientation, covered with perfluorinated oil and placed under a cold stream of N_2 gas. A large crystal (dimensions in Table S1) was selected and it was not manipulated due to its fragility. All attempts to cut the crystal resulted in the obtention of fragments of poor crystallinity. Data collection was performed at 150 K on a Oxford Diffraction Xcalibur2 diffractometer using graphite-monocromated Mo-Kα radiation (λ = 0.71073 Å). A hemisphere of data was collected based on ω-scan and ϕ-scan runs. The diffraction frames were integrated using the program CrysAlis RED[9] and the integrated intensities were corrected for absorption with SADABS.[10] The structure was solved and developed by Fourier methods.[11] All non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms were placed at idealized positions and treated as riding atoms. Each H atom was assigned an isotropic displacement parameter equal to 1.2 times the equivalent isotropic displacement parameter of its parent atom. The structures were refined to F_o^2 and all reflections were used in the least-squares calculations.[12] The large ADP parameters shown by the fluorine atoms are probably originated by dinamic disorder, due to the free rotation of the CF_3 groups. Only in one of the fragments we were able to refine the disorder in two separate congeners, improving the overall structure refinement (even though the fluorine's ADP are still too large). The reason could be the presence of a short contact between one of the fluorine atoms of this group (F10) and one of the –OMe groups of a neighbour molecule [F10...C78 (-x+1, -y, -z+1): 3.35(2) Å] that restrict the free rotation of this particular CF_3 group.

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Table S1. Crystal data and structure refinement for **5c·2CH$_2$Cl$_2$**.

Empirical formula	C42 H32 Cl4 F6 N2 O12 Pd2	
Formula weight	1225.30	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.7400(3) Å	α= 88.7425(17)°.
	b = 16.7687(3) Å	β= 74.758(2)°.
	c = 19.4056(4) Å	γ = 80.4262(18)°.
Volume	4562.12(16) Å^3	
Z	4	
Density (calculated)	1.784 Mg/m^3	
Absorption coefficient	1.111 mm^{-1}	
F(000)	2432	
Crystal size	1.11 x 0.74 x 0.21 mm^3	
Theta range for data collection	2.64 to 25.00°.	
Index ranges	-17<=h<=17, -19<=k<=19, -23<=l<=22	
Reflections collected	73418	
Independent reflections	15894 [R(int) = 0.0458]	
Completeness to theta = 25.00°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7919 and 0.7145	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15894 / 3 / 1260	
Goodness-of-fit on F^2	1.116	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1394	
R indices (all data)	R1 = 0.0705, wR2 = 0.1447	
Largest diff. peak and hole	1.228 and -0.680 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5c·2CH$_2$Cl$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	9786(1)	7385(1)	3274(1)	25(1)
Pd(2)	11096(1)	6293(1)	2296(1)	23(1)
N(1)	10480(4)	6474(3)	1480(3)	21(1)
N(2)	9898(3)	8406(3)	2710(3)	21(1)
O(1)	9550(4)	6379(3)	3875(2)	35(1)
O(2)	10123(3)	5507(3)	2939(2)	31(1)
O(3)	11800(3)	6128(3)	3089(2)	32(1)
O(4)	11063(4)	7310(3)	3669(3)	34(1)
O(5)	9777(3)	7627(3)	135(2)	31(1)
O(6)	10305(3)	6340(3)	384(2)	26(1)
O(7)	12483(3)	2810(3)	528(3)	34(1)
O(8)	11898(3)	3391(3)	1807(3)	34(1)
O(9)	9842(3)	9642(3)	1248(2)	27(1)
O(10)	9542(3)	9711(2)	2442(2)	22(1)
O(11)	8335(4)	10333(3)	5763(3)	40(1)
O(12)	8943(4)	8807(3)	5549(3)	42(1)
C(1)	12039(5)	6930(4)	1767(3)	25(2)
C(2)	12996(5)	6669(4)	1728(4)	31(2)
C(3)	13689(5)	7085(5)	1345(4)	36(2)
C(4)	13438(5)	7795(5)	1016(4)	34(2)
C(5)	12500(5)	8060(4)	1046(4)	28(2)
C(6)	11784(4)	7632(4)	1413(3)	22(1)
C(7)	10793(4)	7927(4)	1353(3)	20(1)
C(8)	9954(4)	8409(4)	1945(3)	20(1)
C(9)	9785(4)	9294(4)	1785(4)	22(1)
C(10)	9610(4)	9146(4)	2958(4)	24(2)
C(11)	9334(4)	9462(4)	3673(4)	25(2)
C(12)	9000(5)	10291(4)	3804(4)	28(2)
C(13)	8686(5)	10592(4)	4497(4)	30(2)
C(14)	8661(5)	10100(4)	5065(4)	28(2)
C(15)	8998(5)	9251(4)	4953(4)	31(2)
C(16)	9333(5)	8950(4)	4273(4)	28(2)
C(17)	7987(6)	11173(4)	5912(4)	46(2)
C(18)	9190(7)	7969(5)	5450(4)	47(2)
C(19)	11650(5)	6664(4)	3549(4)	30(2)
C(20)	12314(7)	6500(5)	4053(5)	46(2)
C(21)	8603(5)	7382(4)	2994(4)	26(2)
C(22)	7844(5)	7129(5)	3481(4)	40(2)
C(23)	7014(6)	7074(5)	3308(5)	51(2)
C(24)	6901(5)	7314(5)	2653(5)	49(2)
C(25)	7650(5)	7557(4)	2153(4)	36(2)
C(26)	10050(4)	7166(4)	537(4)	24(2)
C(27)	9282(4)	7884(4)	1747(4)	25(2)
C(28)	10169(4)	7289(4)	1271(3)	16(1)
C(29)	8506(4)	7599(4)	2312(4)	23(2)
C(30)	10580(4)	5979(4)	958(3)	20(1)
C(31)	10997(4)	5138(4)	847(3)	22(1)
C(32)	11247(5)	4795(4)	170(4)	25(2)
C(33)	11734(5)	4012(4)	51(4)	26(2)
C(34)	11967(4)	3562(4)	593(4)	24(2)
C(35)	11665(4)	3887(4)	1302(4)	26(2)

C(36)	11192(4)	4668(4)	1417(4)	23(1)
C(37)	11648(6)	3718(5)	2519(4)	40(2)
C(38)	12847(6)	2448(5)	-160(4)	43(2)
C(39)	9715(5)	5702(4)	3569(4)	31(2)
C(40)	9360(6)	5015(5)	4045(4)	45(2)
F(1)	13041(6)	6842(6)	3807(5)	153(4)
F(2)	11929(6)	6823(6)	4679(4)	148(4)
F(3)	12595(6)	5769(3)	4135(4)	111(3)
F(4)	8778(5)	5259(3)	4656(3)	86(2)
F(5)	8963(5)	4555(3)	3726(3)	80(2)
F(6)	10093(5)	4521(4)	4174(4)	91(2)
Pd(3)	5853(1)	3100(1)	2376(1)	21(1)
Pd(4)	6448(1)	2225(1)	3465(1)	23(1)
N(4)	6676(3)	1100(3)	3034(3)	18(1)
N(3)	7012(3)	2736(3)	1557(3)	18(1)
O(13)	6433(3)	4004(3)	2887(2)	29(1)
O(14)	6294(3)	3350(3)	3917(2)	29(1)
O(15)	8546(3)	1289(3)	339(2)	27(1)
O(16)	7890(3)	2609(3)	415(2)	23(1)
O(17)	5671(3)	6117(3)	188(2)	32(1)
O(18)	5670(3)	5893(3)	1502(3)	35(1)
O(19)	7101(3)	-255(3)	2918(2)	26(1)
O(20)	7796(3)	-408(3)	1737(2)	26(1)
O(21)	4885(3)	2410(3)	3890(2)	30(1)
O(22)	4620(3)	3444(3)	3172(2)	27(1)
O(23)	5448(4)	1302(3)	5856(3)	42(1)
O(24)	5822(4)	-136(3)	6285(3)	38(1)
C(41)	5230(4)	2345(4)	1982(3)	19(1)
C(42)	5703(4)	1581(4)	1710(3)	21(1)
C(43)	5206(5)	1067(4)	1433(3)	26(2)
C(44)	4268(5)	1310(4)	1419(4)	31(2)
C(45)	3815(5)	2088(4)	1695(4)	33(2)
C(46)	4283(4)	2580(4)	1973(3)	21(1)
C(47)	6733(4)	1291(4)	1650(3)	19(1)
C(48)	7434(4)	1886(4)	1452(3)	17(1)
C(49)	8039(4)	1842(4)	683(4)	25(2)
C(50)	7245(4)	3093(4)	960(4)	22(2)
C(51)	6901(4)	3882(4)	742(3)	21(1)
C(52)	6914(4)	4025(4)	29(3)	24(2)
C(53)	6502(4)	4755(4)	-169(4)	25(2)
C(54)	6085(4)	5378(4)	328(4)	23(2)
C(55)	6078(4)	5253(4)	1059(4)	25(2)
C(56)	6479(4)	4510(4)	1258(3)	22(1)
C(57)	5600(5)	6279(5)	-523(4)	36(2)
C(58)	5514(6)	5755(5)	2243(4)	41(2)
C(59)	6349(5)	3955(4)	3539(4)	27(2)
C(60)	6314(7)	4746(5)	3928(4)	46(2)
C(61)	7821(5)	2194(4)	3140(3)	24(2)
C(62)	8375(4)	1864(4)	2475(4)	23(2)
C(63)	9330(5)	1946(4)	2250(4)	32(2)
C(64)	9748(6)	2332(5)	2666(5)	45(2)
C(65)	9223(6)	2623(5)	3331(5)	45(2)
C(66)	8269(5)	2560(4)	3558(4)	35(2)
C(67)	7994(4)	1424(4)	1979(3)	21(1)
C(68)	7161(4)	944(4)	2278(3)	21(1)
C(69)	7422(4)	40(4)	2233(3)	21(1)
C(70)	6699(4)	418(4)	3357(3)	21(1)
C(71)	6435(4)	240(4)	4109(3)	23(2)

C(72)	6639(5)	-534(4)	4339(3)	25(2)
C(73)	6450(5)	-689(4)	5067(4)	31(2)
C(74)	6039(5)	-60(4)	5568(4)	29(2)
C(75)	5823(5)	726(4)	5335(3)	26(2)
C(76)	6007(5)	874(4)	4619(4)	31(2)
C(77)	5335(7)	2119(5)	5626(4)	51(2)
C(78)	6093(7)	-937(5)	6546(4)	54(2)
C(79)	4411(5)	3027(4)	3703(4)	27(2)
F(7)	5489(5)	5211(4)	3985(4)	100(2)
F(8)	6413(6)	4649(3)	4573(3)	90(2)
F(9)	6957(5)	5159(3)	3570(3)	84(2)
C(80)	3411(6)	3308(5)	4195(5)	44(2)
F(10)	2877(15)	2792(19)	4120(30)	161(16)
F(11)	3005(16)	3973(11)	4078(14)	88(9)
F(12)	3380(20)	3250(30)	4849(8)	172(17)
F(10B)	2789(15)	3540(30)	3890(12)	118(12)
F(11B)	3455(17)	3860(20)	4640(20)	133(14)
F(12B)	3080(19)	2781(11)	4615(17)	80(10)
C(201)	8715(6)	4365(5)	2068(4)	47(2)
Cl(1)	8382(2)	5387(1)	1887(1)	54(1)
Cl(2)	9185(1)	3756(1)	1299(1)	40(1)
C(202)	8306(7)	-459(6)	-221(5)	63(3)
Cl(3)	7102(2)	-29(2)	11(1)	66(1)
Cl(4)	8550(2)	-1168(2)	-902(1)	70(1)
C(203)	8677(6)	9513(5)	7233(5)	47(2)
Cl(5)	8128(2)	10446(1)	7711(1)	60(1)
Cl(6)	7916(2)	8804(2)	7410(1)	65(1)
C(204)	5277(12)	1078(7)	7588(6)	111(5)
Cl(7)	5784(2)	1949(2)	7368(2)	72(1)
Cl(8)	4414(2)	1172(2)	8389(2)	97(1)

Table S3. Bond lengths [Å] and angles [°] for **5c·2CH₂Cl₂**.

Pd(1)-C(21)	1.958(7)
Pd(1)-N(2)	2.018(5)
Pd(1)-O(1)	2.055(5)
Pd(1)-O(4)	2.195(5)
Pd(1)-Pd(2)	2.7815(7)
Pd(2)-C(1)	1.955(7)
Pd(2)-N(1)	2.016(5)
Pd(2)-O(3)	2.060(4)
Pd(2)-O(2)	2.228(5)
N(1)-C(30)	1.286(8)
N(1)-C(28)	1.452(7)
N(2)-C(10)	1.303(8)
N(2)-C(8)	1.465(8)
O(1)-C(39)	1.250(8)
O(2)-C(39)	1.237(8)
O(3)-C(19)	1.234(8)
O(4)-C(19)	1.253(8)
O(5)-C(26)	1.185(8)
O(6)-C(30)	1.378(7)
O(6)-C(26)	1.391(8)
O(7)-C(34)	1.350(7)
O(7)-C(38)	1.411(8)
O(8)-C(35)	1.349(8)
O(8)-C(37)	1.429(8)
O(9)-C(9)	1.174(8)
O(10)-C(10)	1.375(8)
O(10)-C(9)	1.399(8)
O(11)-C(14)	1.354(8)
O(11)-C(17)	1.425(9)
O(12)-C(15)	1.355(8)
O(12)-C(18)	1.395(9)
C(1)-C(2)	1.389(9)
C(1)-C(6)	1.396(9)
C(2)-C(3)	1.378(10)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.381(10)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.367(9)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.405(9)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.498(8)
C(7)-C(28)	1.558(8)
C(7)-C(8)	1.568(8)
C(7)-H(7A)	0.9800
C(8)-C(9)	1.504(9)
C(8)-C(27)	1.551(9)
C(10)-C(11)	1.425(9)
C(11)-C(12)	1.401(9)
C(11)-C(16)	1.432(9)
C(12)-C(13)	1.378(9)
C(12)-H(12A)	0.9300
C(13)-C(14)	1.360(10)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.430(10)

C(15)-C(16)	1.358(9)
C(16)-H(16A)	0.9300
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-C(20)	1.545(10)
C(20)-F(3)	1.247(9)
C(20)-F(1)	1.277(11)
C(20)-F(2)	1.288(10)
C(21)-C(22)	1.382(10)
C(21)-C(29)	1.403(9)
C(22)-C(23)	1.368(12)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.369(12)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.377(10)
C(24)-H(24A)	0.9300
C(25)-C(29)	1.387(9)
C(25)-H(25A)	0.9300
C(26)-C(28)	1.504(9)
C(27)-C(29)	1.497(9)
C(27)-C(28)	1.590(8)
C(27)-H(27A)	0.9800
C(30)-C(31)	1.439(9)
C(31)-C(32)	1.377(9)
C(31)-C(36)	1.407(9)
C(32)-C(33)	1.381(9)
C(32)-H(32A)	0.9300
C(33)-C(34)	1.365(9)
C(33)-H(33A)	0.9300
C(34)-C(35)	1.421(9)
C(35)-C(36)	1.370(9)
C(36)-H(36A)	0.9300
C(37)-H(37A)	0.9600
C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-C(40)	1.534(11)
C(40)-F(4)	1.295(9)
C(40)-F(5)	1.298(10)
C(40)-F(6)	1.323(10)
Pd(3)-C(41)	1.956(6)
Pd(3)-N(3)	2.021(5)
Pd(3)-O(22)	2.059(4)
Pd(3)-O(13)	2.225(5)
Pd(3)-Pd(4)	2.7926(7)
Pd(4)-C(61)	1.947(7)
Pd(4)-N(4)	2.021(5)
Pd(4)-O(14)	2.050(5)
Pd(4)-O(21)	2.205(4)
N(4)-C(70)	1.292(8)
N(4)-C(68)	1.461(8)
N(3)-C(50)	1.285(8)

N(3)-C(48)	1.453(7)
O(13)-C(59)	1.241(8)
O(14)-C(59)	1.240(8)
O(15)-C(49)	1.182(8)
O(16)-C(49)	1.382(8)
O(16)-C(50)	1.390(7)
O(17)-C(54)	1.343(7)
O(17)-C(57)	1.428(8)
O(18)-C(55)	1.344(8)
O(18)-C(58)	1.414(9)
O(19)-C(70)	1.380(7)
O(19)-C(69)	1.397(8)
O(20)-C(69)	1.189(7)
O(21)-C(79)	1.252(8)
O(22)-C(79)	1.232(8)
O(23)-C(75)	1.353(8)
O(23)-C(77)	1.430(9)
O(24)-C(74)	1.351(8)
O(24)-C(78)	1.455(9)
C(41)-C(46)	1.392(8)
C(41)-C(42)	1.395(9)
C(42)-C(43)	1.416(9)
C(42)-C(47)	1.491(8)
C(43)-C(44)	1.383(9)
C(43)-H(43A)	0.9300
C(44)-C(45)	1.411(10)
C(44)-H(44A)	0.9300
C(45)-C(46)	1.361(10)
C(45)-H(45A)	0.9300
C(46)-H(46A)	0.9300
C(47)-C(48)	1.526(9)
C(47)-C(68)	1.572(8)
C(47)-H(47A)	0.9800
C(48)-C(49)	1.520(9)
C(48)-C(67)	1.590(8)
C(50)-C(51)	1.432(9)
C(51)-C(52)	1.394(9)
C(51)-C(56)	1.414(9)
C(52)-C(53)	1.367(9)
C(52)-H(52A)	0.9300
C(53)-C(54)	1.385(9)
C(53)-H(53A)	0.9300
C(54)-C(55)	1.428(9)
C(55)-C(56)	1.379(9)
C(56)-H(56A)	0.9300
C(57)-H(57A)	0.9600
C(57)-H(57B)	0.9600
C(57)-H(57C)	0.9600
C(58)-H(58A)	0.9600
C(58)-H(58B)	0.9600
C(58)-H(58C)	0.9600
C(59)-C(60)	1.527(10)
C(60)-F(8)	1.302(9)
C(60)-F(7)	1.309(10)
C(60)-F(9)	1.308(10)
C(61)-C(66)	1.382(10)
C(61)-C(62)	1.402(9)
C(62)-C(63)	1.390(9)

C(62)-C(67)	1.497(9)
C(63)-C(64)	1.365(10)
C(63)-H(63A)	0.9300
C(64)-C(65)	1.371(12)
C(64)-H(64A)	0.9300
C(65)-C(66)	1.380(11)
C(65)-H(65A)	0.9300
C(66)-H(66A)	0.9300
C(67)-C(68)	1.556(9)
C(67)-H(67A)	0.9800
C(68)-C(69)	1.500(9)
C(70)-C(71)	1.447(9)
C(71)-C(72)	1.374(9)
C(71)-C(76)	1.415(9)
C(72)-C(73)	1.394(9)
C(72)-H(72A)	0.9300
C(73)-C(74)	1.395(10)
C(73)-H(73A)	0.9300
C(74)-C(75)	1.397(10)
C(75)-C(76)	1.370(9)
C(76)-H(76A)	0.9300
C(77)-H(77A)	0.9600
C(77)-H(77B)	0.9600
C(77)-H(77C)	0.9600
C(78)-H(78A)	0.9600
C(78)-H(78B)	0.9600
C(78)-H(78C)	0.9600
C(79)-C(80)	1.535(10)
C(80)-F(11)	1.221(14)
C(80)-F(10B)	1.223(19)
C(80)-F(12)	1.260(19)
C(80)-F(12B)	1.260(18)
C(80)-F(11B)	1.291(18)
C(80)-F(10)	1.294(19)
C(201)-Cl(2)	1.742(8)
C(201)-Cl(1)	1.757(9)
C(201)-H(20A)	0.9700
C(201)-H(20B)	0.9700
C(202)-Cl(4)	1.724(9)
C(202)-Cl(3)	1.745(10)
C(202)-H(20C)	0.9700
C(202)-H(20D)	0.9700
C(203)-Cl(6)	1.736(8)
C(203)-Cl(5)	1.792(9)
C(203)-H(20E)	0.9700
C(203)-H(20F)	0.9700
C(204)-Cl(8)	1.721(12)
C(204)-Cl(7)	1.745(12)
C(204)-H(20G)	0.9700
C(204)-H(20H)	0.9700

C(21)-Pd(1)-N(2)	86.2(2)
C(21)-Pd(1)-O(1)	89.9(2)
N(2)-Pd(1)-O(1)	175.1(2)
C(21)-Pd(1)-O(4)	174.5(2)
N(2)-Pd(1)-O(4)	98.94(19)
O(1)-Pd(1)-O(4)	84.84(19)
C(21)-Pd(1)-Pd(2)	102.54(19)

N(2)-Pd(1)-Pd(2)	99.30(14)
O(1)-Pd(1)-Pd(2)	84.40(13)
O(4)-Pd(1)-Pd(2)	78.47(12)
C(1)-Pd(2)-N(1)	86.8(2)
C(1)-Pd(2)-O(3)	89.8(2)
N(1)-Pd(2)-O(3)	176.5(2)
C(1)-Pd(2)-O(2)	174.9(2)
N(1)-Pd(2)-O(2)	97.57(19)
O(3)-Pd(2)-O(2)	85.72(19)
C(1)-Pd(2)-Pd(1)	104.65(18)
N(1)-Pd(2)-Pd(1)	97.85(14)
O(3)-Pd(2)-Pd(1)	83.95(13)
O(2)-Pd(2)-Pd(1)	77.34(12)
C(30)-N(1)-C(28)	109.1(5)
C(30)-N(1)-Pd(2)	126.8(4)
C(28)-N(1)-Pd(2)	120.4(4)
C(10)-N(2)-C(8)	108.1(5)
C(10)-N(2)-Pd(1)	126.7(5)
C(8)-N(2)-Pd(1)	121.1(4)
C(39)-O(1)-Pd(1)	119.3(4)
C(39)-O(2)-Pd(2)	118.8(4)
C(19)-O(3)-Pd(2)	119.3(4)
C(19)-O(4)-Pd(1)	117.6(4)
C(30)-O(6)-C(26)	107.5(5)
C(34)-O(7)-C(38)	118.4(6)
C(35)-O(8)-C(37)	116.8(5)
C(10)-O(10)-C(9)	107.5(5)
C(14)-O(11)-C(17)	116.7(6)
C(15)-O(12)-C(18)	116.7(6)
C(2)-C(1)-C(6)	118.7(6)
C(2)-C(1)-Pd(2)	119.1(5)
C(6)-C(1)-Pd(2)	122.2(5)
C(3)-C(2)-C(1)	121.2(7)
C(3)-C(2)-H(2A)	119.4
C(1)-C(2)-H(2A)	119.4
C(2)-C(3)-C(4)	120.3(6)
C(2)-C(3)-H(3A)	119.9
C(4)-C(3)-H(3A)	119.9
C(5)-C(4)-C(3)	119.3(7)
C(5)-C(4)-H(4A)	120.3
C(3)-C(4)-H(4A)	120.3
C(4)-C(5)-C(6)	121.3(7)
C(4)-C(5)-H(5A)	119.3
C(6)-C(5)-H(5A)	119.3
C(1)-C(6)-C(5)	119.1(6)
C(1)-C(6)-C(7)	123.7(6)
C(5)-C(6)-C(7)	117.1(6)
C(6)-C(7)-C(28)	118.3(5)
C(6)-C(7)-C(8)	126.0(5)
C(28)-C(7)-C(8)	91.6(4)
C(6)-C(7)-H(7A)	106.3
C(28)-C(7)-H(7A)	106.3
C(8)-C(7)-H(7A)	106.3
N(2)-C(8)-C(9)	103.4(5)
N(2)-C(8)-C(27)	112.8(5)
C(9)-C(8)-C(27)	116.7(5)
N(2)-C(8)-C(7)	124.8(5)
C(9)-C(8)-C(7)	111.6(5)

C(27)-C(8)-C(7)	88.1(5)
O(9)-C(9)-O(10)	121.2(6)
O(9)-C(9)-C(8)	132.4(6)
O(10)-C(9)-C(8)	106.5(5)
N(2)-C(10)-O(10)	114.0(6)
N(2)-C(10)-C(11)	130.8(6)
O(10)-C(10)-C(11)	115.2(5)
C(12)-C(11)-C(10)	119.7(6)
C(12)-C(11)-C(16)	118.2(6)
C(10)-C(11)-C(16)	122.0(6)
C(13)-C(12)-C(11)	119.9(6)
C(13)-C(12)-H(12A)	120.1
C(11)-C(12)-H(12A)	120.1
C(14)-C(13)-C(12)	121.7(6)
C(14)-C(13)-H(13A)	119.1
C(12)-C(13)-H(13A)	119.1
O(11)-C(14)-C(13)	126.2(6)
O(11)-C(14)-C(15)	113.9(6)
C(13)-C(14)-C(15)	120.0(6)
O(12)-C(15)-C(16)	125.1(7)
O(12)-C(15)-C(14)	116.0(6)
C(16)-C(15)-C(14)	118.9(7)
C(15)-C(16)-C(11)	121.3(6)
C(15)-C(16)-H(16A)	119.3
C(11)-C(16)-H(16A)	119.3
O(11)-C(17)-H(17A)	109.5
O(11)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(11)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(12)-C(18)-H(18A)	109.5
O(12)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(12)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(3)-C(19)-O(4)	130.8(7)
O(3)-C(19)-C(20)	113.3(6)
O(4)-C(19)-C(20)	115.9(6)
F(3)-C(20)-F(1)	108.6(9)
F(3)-C(20)-F(2)	107.2(8)
F(1)-C(20)-F(2)	104.5(9)
F(3)-C(20)-C(19)	114.6(7)
F(1)-C(20)-C(19)	108.8(7)
F(2)-C(20)-C(19)	112.7(7)
C(22)-C(21)-C(29)	118.6(7)
C(22)-C(21)-Pd(1)	118.7(5)
C(29)-C(21)-Pd(1)	122.7(5)
C(23)-C(22)-C(21)	121.7(8)
C(23)-C(22)-H(22A)	119.2
C(21)-C(22)-H(22A)	119.2
C(22)-C(23)-C(24)	120.0(8)
C(22)-C(23)-H(23A)	120.0
C(24)-C(23)-H(23A)	120.0
C(23)-C(24)-C(25)	119.5(8)
C(23)-C(24)-H(24A)	120.2
C(25)-C(24)-H(24A)	120.2

C(24)-C(25)-C(29)	121.2(8)
C(24)-C(25)-H(25A)	119.4
C(29)-C(25)-H(25A)	119.4
O(5)-C(26)-O(6)	122.1(6)
O(5)-C(26)-C(28)	131.5(6)
O(6)-C(26)-C(28)	106.4(5)
C(29)-C(27)-C(8)	120.9(5)
C(29)-C(27)-C(28)	123.2(5)
C(8)-C(27)-C(28)	91.1(4)
C(29)-C(27)-H(27A)	106.6
C(8)-C(27)-H(27A)	106.6
C(28)-C(27)-H(27A)	106.6
N(1)-C(28)-C(26)	103.3(5)
N(1)-C(28)-C(7)	115.8(5)
C(26)-C(28)-C(7)	116.8(5)
N(1)-C(28)-C(27)	123.2(5)
C(26)-C(28)-C(27)	111.2(5)
C(7)-C(28)-C(27)	87.1(4)
C(25)-C(29)-C(21)	118.9(6)
C(25)-C(29)-C(27)	118.3(6)
C(21)-C(29)-C(27)	122.9(6)
N(1)-C(30)-O(6)	113.6(5)
N(1)-C(30)-C(31)	131.3(6)
O(6)-C(30)-C(31)	114.8(5)
C(32)-C(31)-C(36)	119.5(6)
C(32)-C(31)-C(30)	119.8(6)
C(36)-C(31)-C(30)	120.7(6)
C(31)-C(32)-C(33)	119.8(6)
C(31)-C(32)-H(32A)	120.1
C(33)-C(32)-H(32A)	120.1
C(34)-C(33)-C(32)	121.3(6)
C(34)-C(33)-H(33A)	119.3
C(32)-C(33)-H(33A)	119.3
O(7)-C(34)-C(33)	126.1(6)
O(7)-C(34)-C(35)	114.2(6)
C(33)-C(34)-C(35)	119.7(6)
O(8)-C(35)-C(36)	125.6(6)
O(8)-C(35)-C(34)	115.7(6)
C(36)-C(35)-C(34)	118.7(6)
C(35)-C(36)-C(31)	120.9(6)
C(35)-C(36)-H(36A)	119.6
C(31)-C(36)-H(36A)	119.6
O(8)-C(37)-H(37A)	109.5
O(8)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
O(8)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
O(7)-C(38)-H(38A)	109.5
O(7)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
O(7)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
O(2)-C(39)-O(1)	129.3(7)
O(2)-C(39)-C(40)	115.5(6)
O(1)-C(39)-C(40)	115.2(6)
F(4)-C(40)-F(5)	108.9(8)

F(4)-C(40)-F(6)	107.6(7)
F(5)-C(40)-F(6)	103.9(7)
F(4)-C(40)-C(39)	114.0(7)
F(5)-C(40)-C(39)	111.9(7)
F(6)-C(40)-C(39)	109.9(7)
C(41)-Pd(3)-N(3)	86.4(2)
C(41)-Pd(3)-O(22)	90.1(2)
N(3)-Pd(3)-O(22)	176.3(2)
C(41)-Pd(3)-O(13)	174.8(2)
N(3)-Pd(3)-O(13)	98.62(18)
O(22)-Pd(3)-O(13)	84.81(18)
C(41)-Pd(3)-Pd(4)	103.16(18)
N(3)-Pd(3)-Pd(4)	98.81(14)
O(22)-Pd(3)-Pd(4)	83.24(13)
O(13)-Pd(3)-Pd(4)	77.22(12)
C(61)-Pd(4)-N(4)	87.2(2)
C(61)-Pd(4)-O(14)	90.0(2)
N(4)-Pd(4)-O(14)	176.55(19)
C(61)-Pd(4)-O(21)	172.9(2)
N(4)-Pd(4)-O(21)	99.96(19)
O(14)-Pd(4)-O(21)	82.92(18)
C(61)-Pd(4)-Pd(3)	100.72(18)
N(4)-Pd(4)-Pd(3)	98.87(14)
O(14)-Pd(4)-Pd(3)	83.52(12)
O(21)-Pd(4)-Pd(3)	78.51(12)
C(70)-N(4)-C(68)	108.4(5)
C(70)-N(4)-Pd(4)	128.2(4)
C(68)-N(4)-Pd(4)	120.5(4)
C(50)-N(3)-C(48)	108.6(5)
C(50)-N(3)-Pd(3)	126.1(4)
C(48)-N(3)-Pd(3)	120.5(4)
C(59)-O(13)-Pd(3)	117.5(4)
C(59)-O(14)-Pd(4)	120.5(4)
C(49)-O(16)-C(50)	107.0(5)
C(54)-O(17)-C(57)	118.5(5)
C(55)-O(18)-C(58)	116.9(5)
C(70)-O(19)-C(69)	105.8(5)
C(79)-O(21)-Pd(4)	117.7(4)
C(79)-O(22)-Pd(3)	120.9(4)
C(75)-O(23)-C(77)	116.2(5)
C(74)-O(24)-C(78)	116.3(6)
C(46)-C(41)-C(42)	118.9(6)
C(46)-C(41)-Pd(3)	118.8(5)
C(42)-C(41)-Pd(3)	122.3(5)
C(41)-C(42)-C(43)	119.2(6)
C(41)-C(42)-C(47)	123.2(6)
C(43)-C(42)-C(47)	117.5(6)
C(44)-C(43)-C(42)	121.4(6)
C(44)-C(43)-H(43A)	119.3
C(42)-C(43)-H(43A)	119.3
C(43)-C(44)-C(45)	117.8(7)
C(43)-C(44)-H(44A)	121.1
C(45)-C(44)-H(44A)	121.1
C(46)-C(45)-C(44)	121.1(6)
C(46)-C(45)-H(45A)	119.4
C(44)-C(45)-H(45A)	119.4
C(45)-C(46)-C(41)	121.6(6)
C(45)-C(46)-H(46A)	119.2

C(41)-C(46)-H(46A)	119.2
C(42)-C(47)-C(48)	119.3(5)
C(42)-C(47)-C(68)	125.4(5)
C(48)-C(47)-C(68)	92.2(5)
C(42)-C(47)-H(47A)	106.0
C(48)-C(47)-H(47A)	106.0
C(68)-C(47)-H(47A)	106.0
N(3)-C(48)-C(49)	103.1(5)
N(3)-C(48)-C(47)	115.5(5)
C(49)-C(48)-C(47)	116.3(5)
N(3)-C(48)-C(67)	122.1(5)
C(49)-C(48)-C(67)	112.4(5)
C(47)-C(48)-C(67)	87.9(4)
O(15)-C(49)-O(16)	122.9(6)
O(15)-C(49)-C(48)	130.5(6)
O(16)-C(49)-C(48)	106.6(5)
N(3)-C(50)-O(16)	114.3(5)
N(3)-C(50)-C(51)	131.1(6)
O(16)-C(50)-C(51)	114.4(6)
C(52)-C(51)-C(56)	119.1(6)
C(52)-C(51)-C(50)	120.6(6)
C(56)-C(51)-C(50)	120.1(6)
C(53)-C(52)-C(51)	120.7(6)
C(53)-C(52)-H(52A)	119.6
C(51)-C(52)-H(52A)	119.6
C(52)-C(53)-C(54)	121.0(6)
C(52)-C(53)-H(53A)	119.5
C(54)-C(53)-H(53A)	119.5
O(17)-C(54)-C(53)	125.7(6)
O(17)-C(54)-C(55)	114.8(6)
C(53)-C(54)-C(55)	119.5(6)
O(18)-C(55)-C(56)	125.3(6)
O(18)-C(55)-C(54)	115.4(6)
C(56)-C(55)-C(54)	119.2(6)
C(55)-C(56)-C(51)	120.5(6)
C(55)-C(56)-H(56A)	119.8
C(51)-C(56)-H(56A)	119.8
O(17)-C(57)-H(57A)	109.5
O(17)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
O(17)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
O(18)-C(58)-H(58A)	109.5
O(18)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
O(18)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
O(13)-C(59)-O(14)	128.8(6)
O(13)-C(59)-C(60)	115.6(6)
O(14)-C(59)-C(60)	115.6(6)
F(8)-C(60)-F(7)	106.6(8)
F(8)-C(60)-F(9)	108.6(8)
F(7)-C(60)-F(9)	105.9(8)
F(8)-C(60)-C(59)	113.7(7)
F(7)-C(60)-C(59)	109.9(7)
F(9)-C(60)-C(59)	111.6(7)

C(66)-C(61)-C(62)	117.7(6)
C(66)-C(61)-Pd(4)	119.0(5)
C(62)-C(61)-Pd(4)	123.1(5)
C(63)-C(62)-C(61)	119.4(6)
C(63)-C(62)-C(67)	117.1(6)
C(61)-C(62)-C(67)	123.5(6)
C(64)-C(63)-C(62)	121.6(7)
C(64)-C(63)-H(63A)	119.2
C(62)-C(63)-H(63A)	119.2
C(65)-C(64)-C(63)	119.4(7)
C(65)-C(64)-H(64A)	120.3
C(63)-C(64)-H(64A)	120.3
C(64)-C(65)-C(66)	119.8(7)
C(64)-C(65)-H(65A)	120.1
C(66)-C(65)-H(65A)	120.1
C(65)-C(66)-C(61)	122.0(7)
C(65)-C(66)-H(66A)	119.0
C(61)-C(66)-H(66A)	119.0
C(62)-C(67)-C(68)	120.6(5)
C(62)-C(67)-C(48)	122.1(5)
C(68)-C(67)-C(48)	90.5(4)
C(62)-C(67)-H(67A)	107.4
C(68)-C(67)-H(67A)	107.4
C(48)-C(67)-H(67A)	107.4
N(4)-C(68)-C(69)	102.8(5)
N(4)-C(68)-C(67)	114.9(5)
C(69)-C(68)-C(67)	116.0(5)
N(4)-C(68)-C(47)	124.0(5)
C(69)-C(68)-C(47)	112.2(5)
C(67)-C(68)-C(47)	87.5(5)
O(20)-C(69)-O(19)	121.0(6)
O(20)-C(69)-C(68)	131.1(6)
O(19)-C(69)-C(68)	107.9(5)
N(4)-C(70)-O(19)	115.0(5)
N(4)-C(70)-C(71)	130.9(6)
O(19)-C(70)-C(71)	113.9(5)
C(72)-C(71)-C(76)	119.4(6)
C(72)-C(71)-C(70)	120.7(6)
C(76)-C(71)-C(70)	119.8(6)
C(71)-C(72)-C(73)	120.3(6)
C(71)-C(72)-H(72A)	119.9
C(73)-C(72)-H(72A)	119.9
C(72)-C(73)-C(74)	120.2(6)
C(72)-C(73)-H(73A)	119.9
C(74)-C(73)-H(73A)	119.9
O(24)-C(74)-C(73)	125.5(6)
O(24)-C(74)-C(75)	114.9(6)
C(73)-C(74)-C(75)	119.6(6)
O(23)-C(75)-C(76)	124.3(6)
O(23)-C(75)-C(74)	115.7(6)
C(76)-C(75)-C(74)	120.0(6)
C(75)-C(76)-C(71)	120.5(6)
C(75)-C(76)-H(76A)	119.7
C(71)-C(76)-H(76A)	119.7
O(23)-C(77)-H(77A)	109.5
O(23)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	109.5
O(23)-C(77)-H(77C)	109.5

H(77A)-C(77)-H(77C)	109.5
H(77B)-C(77)-H(77C)	109.5
O(24)-C(78)-H(78A)	109.5
O(24)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
O(24)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
O(22)-C(79)-O(21)	129.7(6)
O(22)-C(79)-C(80)	114.2(6)
O(21)-C(79)-C(80)	116.1(6)
F(11)-C(80)-F(12)	110.1(17)
F(10B)-C(80)-F(12B)	104.0(19)
F(10B)-C(80)-F(11B)	111.2(19)
F(12B)-C(80)-F(11B)	101.6(17)
F(11)-C(80)-F(10)	106.7(18)
F(12)-C(80)-F(10)	101.3(19)
F(11)-C(80)-C(79)	116.3(10)
F(10B)-C(80)-C(79)	115.3(13)
F(12)-C(80)-C(79)	113.3(12)
F(12B)-C(80)-C(79)	114.8(11)
F(11B)-C(80)-C(79)	109.1(11)
F(10)-C(80)-C(79)	107.8(12)
Cl(2)-C(201)-Cl(1)	113.2(4)
Cl(2)-C(201)-H(20A)	108.9
Cl(1)-C(201)-H(20A)	108.9
Cl(2)-C(201)-H(20B)	108.9
Cl(1)-C(201)-H(20B)	108.9
H(20A)-C(201)-H(20B)	107.7
Cl(4)-C(202)-Cl(3)	110.8(6)
Cl(4)-C(202)-H(20C)	109.5
Cl(3)-C(202)-H(20C)	109.5
Cl(4)-C(202)-H(20D)	109.5
Cl(3)-C(202)-H(20D)	109.5
H(20C)-C(202)-H(20D)	108.1
Cl(6)-C(203)-Cl(5)	111.2(4)
Cl(6)-C(203)-H(20E)	109.4
Cl(5)-C(203)-H(20E)	109.4
Cl(6)-C(203)-H(20F)	109.4
Cl(5)-C(203)-H(20F)	109.4
H(20E)-C(203)-H(20F)	108.0
Cl(8)-C(204)-Cl(7)	113.1(6)
Cl(8)-C(204)-H(20G)	109.0
Cl(7)-C(204)-H(20G)	109.0
Cl(8)-C(204)-H(20H)	109.0
Cl(7)-C(204)-H(20H)	109.0
H(20G)-C(204)-H(20H)	107.8

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) for **5c·2CH$_2$Cl$_2$**. 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)	37(1)	18(1)	18(1)	1(1)	-5(1)	-1(1)
Pd(2)	32(1)	20(1)	18(1)	1(1)	-9(1)	1(1)
N(1)	23(3)	22(3)	19(3)	0(2)	-7(2)	-1(2)
N(2)	22(3)	12(3)	27(3)	-1(2)	-1(2)	-1(2)
O(1)	59(3)	22(3)	20(3)	7(2)	-7(2)	-4(2)
O(2)	48(3)	21(3)	21(3)	1(2)	-4(2)	-6(2)
O(3)	48(3)	23(3)	25(3)	0(2)	-17(2)	1(2)
O(4)	51(3)	22(3)	33(3)	-4(2)	-19(2)	0(2)
O(5)	42(3)	28(3)	23(3)	1(2)	-15(2)	4(2)
O(6)	32(3)	21(2)	24(3)	-1(2)	-12(2)	1(2)
O(7)	38(3)	24(3)	35(3)	-9(2)	-9(2)	6(2)
O(8)	44(3)	26(3)	31(3)	3(2)	-14(2)	7(2)
O(9)	30(3)	26(3)	23(3)	8(2)	-5(2)	1(2)
O(10)	30(2)	15(2)	20(2)	2(2)	-6(2)	-1(2)
O(11)	52(3)	36(3)	27(3)	-13(2)	-5(2)	3(2)
O(12)	66(4)	29(3)	25(3)	-1(2)	-8(3)	-1(3)
C(1)	26(3)	29(4)	20(4)	-11(3)	-6(3)	1(3)
C(2)	37(4)	28(4)	30(4)	-3(3)	-20(3)	7(3)
C(3)	23(4)	46(5)	38(5)	-10(4)	-13(3)	5(3)
C(4)	22(4)	42(5)	36(5)	-2(4)	-1(3)	-6(3)
C(5)	27(4)	32(4)	24(4)	-5(3)	-5(3)	-2(3)
C(6)	22(3)	21(3)	21(4)	-2(3)	-4(3)	4(3)
C(7)	18(3)	21(3)	19(4)	2(3)	-4(3)	1(3)
C(8)	21(3)	21(3)	16(3)	2(3)	-4(3)	0(3)
C(9)	15(3)	25(4)	23(4)	0(3)	-1(3)	2(3)
C(10)	18(3)	25(4)	26(4)	2(3)	-5(3)	-3(3)
C(11)	22(3)	26(4)	25(4)	1(3)	-4(3)	-5(3)
C(12)	32(4)	24(4)	25(4)	2(3)	-2(3)	-1(3)
C(13)	35(4)	20(4)	31(4)	-5(3)	-9(3)	0(3)
C(14)	30(4)	27(4)	28(4)	-10(3)	-7(3)	-1(3)
C(15)	34(4)	36(4)	22(4)	2(3)	-6(3)	-6(3)
C(16)	30(4)	28(4)	23(4)	-5(3)	-4(3)	0(3)
C(17)	67(6)	29(4)	37(5)	-11(4)	-13(4)	8(4)
C(18)	76(6)	32(5)	30(5)	10(4)	-15(4)	1(4)
C(19)	45(4)	28(4)	21(4)	0(3)	-13(3)	-6(3)
C(20)	64(6)	30(5)	53(6)	-1(4)	-39(5)	4(4)
C(21)	27(4)	19(3)	27(4)	4(3)	-1(3)	-1(3)
C(22)	33(4)	35(4)	40(5)	12(4)	6(4)	0(3)
C(23)	41(5)	45(5)	55(6)	17(4)	9(4)	-12(4)
C(24)	24(4)	42(5)	75(7)	12(5)	-2(4)	-9(3)
C(25)	27(4)	30(4)	48(5)	6(4)	-7(4)	-7(3)
C(26)	20(3)	22(4)	26(4)	-4(3)	-2(3)	-1(3)
C(27)	22(3)	28(4)	23(4)	0(3)	-5(3)	-1(3)
C(28)	19(3)	16(3)	15(3)	6(3)	-6(3)	-2(2)
C(29)	24(3)	12(3)	27(4)	1(3)	0(3)	0(3)
C(30)	17(3)	25(4)	19(4)	4(3)	-7(3)	-5(3)
C(31)	20(3)	22(3)	23(4)	0(3)	-6(3)	-5(3)
C(32)	30(4)	27(4)	20(4)	2(3)	-10(3)	-2(3)
C(33)	30(4)	25(4)	22(4)	-7(3)	-6(3)	-3(3)
C(34)	25(3)	19(3)	27(4)	-4(3)	-6(3)	-2(3)
C(35)	21(3)	29(4)	27(4)	-1(3)	-7(3)	-1(3)

C(36)	29(4)	16(3)	22(4)	-3(3)	-8(3)	-1(3)
C(37)	57(5)	32(4)	26(4)	2(3)	-13(4)	10(4)
C(38)	54(5)	27(4)	41(5)	-10(4)	-6(4)	5(4)
C(39)	44(4)	20(4)	27(4)	3(3)	-10(3)	-2(3)
C(40)	68(6)	39(5)	26(5)	7(4)	-7(4)	-14(4)
F(1)	124(6)	223(10)	181(9)	103(8)	-124(7)	-105(7)
F(2)	183(8)	189(8)	64(4)	-62(5)	-91(5)	96(7)
F(3)	197(8)	45(4)	134(6)	-4(4)	-139(6)	13(4)
F(4)	143(6)	40(3)	44(3)	-4(3)	36(3)	-30(3)
F(5)	141(6)	67(4)	50(3)	13(3)	-25(4)	-66(4)
F(6)	105(5)	64(4)	98(5)	56(4)	-28(4)	-3(3)
Pd(3)	24(1)	18(1)	16(1)	1(1)	-1(1)	2(1)
Pd(4)	31(1)	19(1)	17(1)	1(1)	-4(1)	2(1)
N(4)	23(3)	17(3)	11(3)	4(2)	0(2)	0(2)
N(3)	23(3)	17(3)	12(3)	5(2)	-4(2)	-1(2)
O(13)	37(3)	25(3)	22(3)	-1(2)	-4(2)	-2(2)
O(14)	45(3)	24(3)	16(3)	2(2)	-7(2)	1(2)
O(15)	33(3)	20(2)	19(3)	-2(2)	3(2)	4(2)
O(16)	25(2)	22(2)	17(2)	2(2)	1(2)	-1(2)
O(17)	36(3)	27(3)	28(3)	12(2)	-8(2)	3(2)
O(18)	47(3)	25(3)	30(3)	-1(2)	-13(2)	9(2)
O(19)	34(3)	20(2)	19(3)	3(2)	-4(2)	2(2)
O(20)	29(2)	21(2)	25(3)	1(2)	-3(2)	3(2)
O(21)	32(3)	30(3)	21(3)	6(2)	0(2)	1(2)
O(22)	31(3)	21(2)	20(3)	3(2)	4(2)	4(2)
O(23)	54(3)	40(3)	22(3)	3(2)	-1(2)	6(3)
O(24)	60(3)	33(3)	21(3)	12(2)	-9(2)	-12(2)
C(41)	25(3)	18(3)	13(3)	3(3)	-3(3)	-3(3)
C(42)	21(3)	27(4)	15(3)	4(3)	-3(3)	-4(3)
C(43)	29(4)	25(4)	21(4)	10(3)	-4(3)	-2(3)
C(44)	25(4)	41(4)	29(4)	3(3)	-7(3)	-8(3)
C(45)	23(4)	36(4)	37(4)	17(3)	-9(3)	1(3)
C(46)	22(3)	20(3)	17(3)	7(3)	-1(3)	0(3)
C(47)	24(3)	18(3)	14(3)	3(3)	-5(3)	1(3)
C(48)	25(3)	14(3)	8(3)	-2(2)	4(3)	-3(2)
C(49)	20(3)	29(4)	26(4)	9(3)	-7(3)	-5(3)
C(50)	17(3)	23(3)	24(4)	-6(3)	-3(3)	0(3)
C(51)	19(3)	23(3)	22(4)	5(3)	-4(3)	-6(3)
C(52)	24(3)	30(4)	16(4)	-1(3)	-2(3)	-2(3)
C(53)	27(4)	26(4)	21(4)	5(3)	-4(3)	-4(3)
C(54)	18(3)	23(4)	28(4)	11(3)	-5(3)	-3(3)
C(55)	23(3)	25(4)	23(4)	1(3)	-3(3)	1(3)
C(56)	25(3)	23(4)	16(3)	2(3)	-4(3)	-3(3)
C(57)	31(4)	35(4)	38(5)	18(4)	-10(3)	-1(3)
C(58)	59(5)	27(4)	34(5)	-4(3)	-14(4)	7(4)
C(59)	34(4)	27(4)	18(4)	-4(3)	-2(3)	-4(3)
C(60)	71(6)	37(5)	30(5)	1(4)	-13(4)	-11(4)
C(61)	38(4)	12(3)	23(4)	7(3)	-13(3)	2(3)
C(62)	25(3)	15(3)	31(4)	6(3)	-12(3)	3(3)
C(63)	35(4)	30(4)	33(4)	6(3)	-12(3)	-7(3)
C(64)	36(4)	31(4)	72(6)	4(4)	-22(4)	-7(3)
C(65)	49(5)	40(5)	57(6)	-3(4)	-31(4)	-7(4)
C(66)	46(5)	30(4)	32(4)	2(3)	-20(4)	-2(3)
C(67)	14(3)	24(3)	22(4)	3(3)	-2(3)	3(3)
C(68)	18(3)	24(3)	17(3)	1(3)	-2(3)	2(3)
C(69)	21(3)	18(3)	22(4)	2(3)	-5(3)	0(3)
C(70)	14(3)	24(4)	23(4)	5(3)	-3(3)	0(3)
C(71)	19(3)	30(4)	19(4)	6(3)	-4(3)	-5(3)

C(72)	35(4)	22(4)	19(4)	6(3)	-4(3)	-11(3)
C(73)	43(4)	21(4)	30(4)	10(3)	-11(3)	-10(3)
C(74)	33(4)	37(4)	22(4)	10(3)	-8(3)	-16(3)
C(75)	29(4)	33(4)	13(4)	3(3)	-1(3)	-3(3)
C(76)	32(4)	25(4)	31(4)	7(3)	-6(3)	0(3)
C(77)	76(6)	37(5)	30(5)	-7(4)	-8(4)	14(4)
C(78)	94(7)	33(5)	30(5)	13(4)	-12(5)	-7(4)
C(79)	29(4)	24(4)	23(4)	-4(3)	4(3)	-4(3)
F(7)	101(5)	60(4)	128(6)	-54(4)	-38(4)	37(3)
F(8)	196(7)	50(3)	41(3)	-2(3)	-53(4)	-33(4)
F(9)	133(5)	59(4)	61(4)	-7(3)	-4(4)	-57(4)
C(80)	36(5)	42(5)	41(6)	9(4)	6(4)	0(4)
F(10)	52(10)	120(20)	270(40)	-100(20)	52(19)	-31(12)
F(11)	65(15)	42(8)	95(19)	33(9)	55(11)	38(8)
F(12)	110(20)	300(40)	29(9)	40(20)	22(10)	110(30)
F(10B)	32(9)	250(40)	48(10)	20(20)	-3(7)	30(20)
F(11B)	70(15)	140(20)	160(30)	-130(20)	61(18)	-45(17)
F(12B)	75(16)	34(9)	82(19)	17(10)	59(14)	-2(8)
C(201)	42(5)	72(6)	26(4)	7(4)	-10(4)	-7(4)
Cl(1)	49(1)	53(1)	54(1)	-6(1)	-5(1)	-5(1)
Cl(2)	44(1)	45(1)	34(1)	5(1)	-11(1)	-11(1)
C(202)	66(6)	49(6)	68(7)	-10(5)	-7(5)	-10(5)
Cl(3)	57(1)	65(2)	63(2)	-24(1)	12(1)	-13(1)
Cl(4)	80(2)	61(2)	54(2)	-14(1)	1(1)	4(1)
C(203)	38(5)	59(6)	45(5)	-2(4)	-8(4)	-15(4)
Cl(5)	56(1)	55(1)	62(2)	-6(1)	-13(1)	4(1)
Cl(6)	59(1)	80(2)	62(2)	2(1)	-11(1)	-38(1)
C(204)	223(16)	45(7)	42(7)	-7(5)	3(8)	-17(8)
Cl(7)	78(2)	69(2)	69(2)	-16(1)	-20(1)	-9(1)
Cl(8)	107(2)	71(2)	83(2)	18(2)	5(2)	16(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5c$\cdot$2CH$_2$Cl$_2$**.

	x	y	z	U(eq)
H(2A)	13173	6205	1965	37
H(3A)	14329	6887	1308	43
H(4A)	13903	8090	776	41
H(5A)	12332	8534	818	34
H(7A)	10857	8255	924	24
H(12A)	8989	10638	3425	34
H(13A)	8487	11146	4577	35
H(16A)	9568	8400	4195	33
H(17A)	7791	11269	6420	69
H(17B)	7452	11337	5717	69
H(17C)	8482	11478	5701	69
H(18A)	9062	7715	5906	70
H(18B)	9857	7833	5213	70
H(18C)	8823	7784	5163	70
H(22A)	7898	6992	3937	48
H(23A)	6527	6874	3636	61
H(24A)	6322	7313	2546	59
H(25A)	7582	7695	1701	43
H(27A)	8973	8200	1415	30
H(32A)	11088	5091	-205	30
H(33A)	11907	3787	-408	31
H(36A)	10998	4891	1877	27
H(37A)	11872	3322	2826	60
H(37B)	10967	3863	2685	60
H(37C)	11935	4191	2523	60
H(38A)	13224	1930	-130	65
H(38B)	13237	2789	-465	65
H(38C)	12328	2380	-354	65
H(43A)	5518	555	1257	31
H(44A)	3946	971	1233	38
H(45A)	3187	2269	1686	39
H(46A)	3961	3086	2161	25
H(47A)	6943	870	1273	23
H(52A)	7205	3620	-315	29
H(53A)	6503	4835	-645	30
H(56A)	6471	4422	1734	26
H(57A)	5242	6810	-536	53
H(57B)	5283	5885	-673	53
H(57C)	6228	6251	-839	53
H(58A)	5188	6244	2505	62
H(58B)	6116	5592	2352	62
H(58C)	5132	5337	2373	62
H(63A)	9694	1733	1806	38
H(64A)	10383	2396	2499	54
H(65A)	9509	2863	3628	55
H(66A)	7917	2769	4006	42
H(67A)	8529	1044	1689	26
H(72A)	6904	-956	4007	30
H(73A)	6598	-1212	5219	37
H(76A)	5848	1396	4466	37
H(77A)	5168	2481	6033	77

H(77B)	4840	2208	5382	77
H(77C)	5923	2218	5307	77
H(78A)	5931	-918	7058	80
H(78B)	6767	-1109	6363	80
H(78C)	5758	-1311	6388	80
H(20A)	9185	4323	2340	57
H(20B)	8161	4165	2360	57
H(20C)	8691	-38	-371	76
H(20D)	8473	-713	193	76
H(20E)	8848	9612	6725	57
H(20F)	9257	9302	7370	57
H(20G)	4997	952	7212	133
H(20H)	5775	629	7613	133