Materials and Methods. All reactions involving metal complexes were conducted in oven-dried glassware under a nitrogen atmosphere with freshly distilled solvents using standard glovebox techniques. All commercially obtained reagents were used as received. ICN silica gel (particle size 0.032-0.063 mm) was used for flash column chromatography. Organic reagents were purchased from the Sigma-Aldrich Chemical Company, Milwaukee, WI and metal salts obtained from Strem Chemicals, Newburyport, MA. Palladium complexes $((PEt_3)PdMeCl)_2$ and $((PPh_3)PdMeCl)_2$ were synthesized according to literature procedure.[1] ^1H, ^{13}C and ^{31}P NMR spectra were recorded on a Varian Mercury 300 spectrometer (at 300 MHz, 75 MHz and 121 MHz respectively) and are reported relative to Me_4Si (δ 0.0) for ^1H and ^{13}C, and H_3PO_4 (δ 0.0) for ^{31}P. Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. Data for ^{13}C and ^{31}P NMR spectra are reported in terms of chemical shift. Quantitative analysis was carried out by Desert Analytics Laboratory, Tuscon, AZ. X-ray crystallographic structures were obtained by Mr. Larry M. Henling and Dr. Mike W. Day of the California Institute of Technology Beckman Institute X-Ray Crystallography Laboratory.

N-(Mesityl)-oxanilic acid ethyl ester (1, Ar = Mesityl). 2,4,6-Trimethylaniline (20 mL, 142 mmol, 1.0 equiv.) and triethylamine (20 mL, 143 mmol, 1 equiv.) were dissolved in dry THF (150 mL). This solution was cooled to 0 °C, and ethyl chlorooxoactetate (15.3 mL, 142 mmol, 1.0 equiv.) was added slowly via syringe. Precipitation of a white solid occurred immediately upon addition. It was allowed to stir overnight, warming to room temperature. At this point, the solid was filtered off, and the organic layer was washed with 2 M HCl solution (2x100 mL). The aqueous layer was washed with ethyl acetate, and the combined organic layers were washed with brine (100 mL), and dried over $MgSO_4$. The solvent was then removed under reduced pressure, leaving a yellowish solid. This was recrystallized from hexanes/EtOAc (9:1), producing a white crystalline solid (30.15 g, 128 mmol, 90% yield). ^1H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 6.92 (s, 2H), 4.43 (q, J = 7.2 Hz, 2H), 2.28 (s, 3H), 2.20 (s, 6H), 1.45 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ161.2, 154.9, 138.0, 134.9, 129.7, 129.3, 63.8, 21.2, 18.6, 14.3. Anal. Calcd for $C_{13}H_{17}NO_3$: C, 66.36; H, 7.28; N, 5.95. Found: C, 66.56; H, 7.15; N, 6.04.

N-(2,6-Diisopropylphenyl)-oxanilic acid ethyl ester (1, Ar = 2,6-diisopropylphenyl). 2,6-Diisopropylaniline (90%) (10 mL, 48 mmol, 1.1 equiv.) and triethylamine (7.3 mL, 48 mmol, 1 equiv.) were dissolved in dry THF (150 mL). This solution was cooled to 0 °C, and ethyl chlorooxoactetate (5.12 mL, 48 mmol, 1.0 equiv.) was added slowly via syringe. Precipitation of a white solid occurred immediately upon addition. It was allowed to stir overnight, warming to room temperature. At this point, the solid was filtered off, and the organic layer was washed with 2 M HCl solution (2x100 mL). The aqueous layer was washed with ethyl acetate, and the combined organic layers were washed with brine (100 mL), and dried over $MgSO_4$. The solvent was then removed under reduced pressure, leaving a yellowish solid. This was recrystallized from hexanes/EtOAc (9:1), producing a white crystalline solid (12.15 g, 44 mmol, 92% yield). ^1H NMR (300 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.34 (t, J = 7.1 Hz, 1H), 7.20 (d, J = 7.8 Hz, 2H), 4.45 (q, J = 7.2 Hz, 2H), 3.01 (septet, J = 7.2 Hz, 2H), 1.47 (t, J = 7.2 Hz, 3H), 1.21 (d, J = 6.6 Hz, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 156.1, 146.1, 129.6, 129.2, 124.0, 63.9, 29.1, 23.9, 14.2. Anal. Calcd for $C_{16}H_{23}NO_3$: C, 69.29; H, 8.36; N, 5.05. Found: C, 69.31; H, 8.13; N, 5.10.

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[1] Ladipo, F.T.; Anderson, G.K. *Organometallics* **1994**, *13*, 303-306

N-(Mesityl)-N'-(2-hydroxyphenyl)-oxalamide (2a). N-(Mesityl)-oxanilic acid ethyl ester (**1**, Ar = mesityl) (5.23 g, 24.4 mmol, 1 equiv.) and 2-aminophenol (2.67 g, 24.4 mmol, 1.0 equiv.) were dissolved in toluene (50 mL). To this suspension was added triethylamine (6.8 mL, 50 mmol, 2 equiv.). The suspension was heated to reflux, causing the solids to dissolve. After heating at reflux overnight, the product precipitated. At this point, ethyl acetate was added until the solid redissolved. The solution was washed with 2 M HCl solution (2x100 mL). The aqueous layer was then washed with ethyl acetate, and the combined organic layers were washed with brine (100 mL), and dried over $MgSO_4$. The solvent was then removed under reduced pressure, leaving a yellowish solid. This was recrystallized from toluene, producing a white crystalline solid (5.26 g, 17.7 mmol, 72.4% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.69 (s, 1H), 8.84 (s, 1H), 8.11 (s, 1H), 7.51 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.14 (ddd, *J* = 1.5, 8.1, 7.2 Hz, 1H), 6.92 (m, 3H), 2.30 (s, 3H), 2.22 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.2, 157.9, 148.2, 138.2, 134.9, 129.5, 129.4, 127.7, 124.3, 122.2, 121.1, 118.9, 21.2, 18.6. Anal. Calcd for $C_{17}H_{18}N_2O_3$: C, 68.44; H, 6.08; N, 9.39. Found: C, 68.50; H, 5.96; N, 9.44.

N-(2,6-Diisopropylphenyl)-N'-(2-hydroxyphenyl)-oxalamide (2b). N-(2,6-Diisopropylphenyl)-oxanilic acid ethyl ester (**1**, Ar = 2,6-diisopropylphenyl) (2.78 g, 10 mmol, 1 equiv.) and 2-aminophenol (1.31 g, 12 mmol, 1.2 equiv.) were dissolved in toluene (50 mL). To this suspension was added triethylamine (2.78 mL, 20 mmol, 2 equiv.). The suspension was heated to reflux, causing the solids to dissolve. After heating at reflux overnight, the product precipitated. At this point, ethyl acetate was added until the solid redissolved. The solution was washed with 2 M HCl solution (2x100 mL). The aqueous layer was then washed with ethyl acetate, and the combined organic layers were washed with brine (100 mL), and dried over $MgSO_4$. The solvent was then removed under reduced pressure, leaving a yellowish solid. This was recrystallized from toluene, producing a white crystalline solid (2.9 g, 8.5 mmol, 85% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.67 (s, 1H), 8.84 (s, 1H), 8.12 (s, 1H), 7.50 (dd, *J* = 8.25, 1.8 Hz 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.16 (dt, *J* = 7.7, 1.5 Hz, 1H), 6.95 (comp m, 2H), 3.03 (septet, *J* = 6.6 Hz, 2H), 1.22 (d, *J* = 6.9, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 158.2, 148.2, 146.1, 129.4, 127.9, 124.2, 124.0, 122.3, 121.2, 119.1, 29.2, 23.9. Anal. Calcd for $C_{20}H_{24}N_2O_3$: C, 70.56; H, 7.11; N, 8.23; O, 14.10. Found: C, 34.90; H, 4.64; N, 5.79.

N-(Mesityl)-oxanilic acid (5). N-(Mesityl)-oxanilic acid ethyl ester (**1**, Ar = mesityl) (1.99 g, 8.5 mmol) was dissolved in THF (50 mL). To this solution was added 1M NaOH solution (40 mL), and the mixture was stirred for 2 hours. Diethyl ether (25 mL) was added, and the layers were separated. The organic layer was washed with 1M NaOH solution (40 mL). The aqueous layer was then acidified with 2M HCl until precipitation occurred. This was then extracted with ethyl acetate (2x50 mL). The ethyl acetate was washed with brine (50 mL), and then dried over $MgSO_4$. Removal of the solvent under reduced pressure provided the product as a white solid (1.74 g, 8.4 mmol, 99% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.51 (s, 1H), 6.93 (s, 2H), 2.29 (s,3H), 2.19 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 156.1, 138.6, 134.7, 129.5, 128.9, 21.2, 18.5. Anal. Calcd for $C_{11}H_{13}NO_3$: C, 63.76; H, 6.32; N, 6.76. Found: C, 63.59; H, 6.32; N, 6.79.

2-Amino-4-methyl-6-*tert*-butylphenol (6).[2] 2-*tert*-Butyl-4-methylphenol (20.04 g, 122 mmol, 1.0 equiv.) is dissolved in AcOH (200 mL) and cooled to 0 °C. To this solution was added a

[2] Albert, H. E. *J. Am. Chem. Soc.* **1954**, *76*, 4985–4988.

solution of concentrated nitric acid (7.73 mL, 122 mmol, 1 equiv.) in an equal volume of acetic acid. Upon addition, the solution turned yellow. After addition was complete, it was allowed to stir at 0 °C for 2.5 hours. At this time, some needles of product began to grow. Deionized water (~25 mL) was added, causing a great deal of precipitation. This was filtered, and water was again added to the filtrate, causing more precipitate that was again filtered. More precipitation/filtration cycles did not yield substantial further product. The orange/yellow solid obtained from the filtrations (13.06 g, 62.4 mmol, 51% yield) was dried overnight by vacuum. ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.40 (s, 1H), 7.77 (d, J = 1.5 Hz, 1H), 7.37 (d, J = 2.1 Hz, 1H), 2.31 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.3, 140.4, 136.3, 128.8, 122.5, 35.7, 29.6, 20.0. Anal. Calcd for $C_{11}H_{15}NO_3$: C, 63.14; H, 7.23; N, 6.69. Found: C, 64.52; H, 7.69; N, 5.89. The resulting product, 2-amino-4-methyl-6-*tert*-butylphenol (4.13 g, 20 mmol, 1.0 equiv.) was added to an oven dried, two-necked flask, and Pd (10% on charcoal) (1.051 g, 1 mmol Pd, 0.05 equiv.) was added. The flask was evacuated, and filled with argon, and then dry, degassed methanol (50 mL) was added. A balloon of hydrogen gas was placed over the reaction, and it was allowed to stir for 16 hours. The solution was then filtered through celite, removing the Pd. It should be noted that although the product is stable in inert atmosphere, it rapidly oxidizes in solution when exposed to air. Therefore, the clear Pd/C suspension turns immediately to a red solution upon filtration on the benchtop. The methanol is evaporated under reduced pressure, leaving a dark red solid. This can then be recrystallized from hexane to yield a whitish solid (2.41 g, 13.4 mmol, 68 % yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.67 (d, J = 1.5 Hz, 1H), 6.61 (d, J = 1.8 Hz, 1H), 5.57 (bs, 1H), 3.20 (bs, 2H), 2.22 (s, 3H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.1, 135.5, 133.4, 129.3, 120.7, 119.2, 34.6, 30.0, 21.2.

N-(Mesityl)-N'-(2-hydroxy-3-tert-butyl-5-methylphenyl)-oxalamide (2c). N-(Mesityl)-oxanilic acid (**5**) (2.15 g, 10.4 mmol, 1.0 equiv.) and 1-hydroxybenzotriazole (2.39 g, 15.6 mmol, 1.5 equiv.) were added to an oven dried, two-necked flask. THF (100 mL) was added and the solution was cooled to 0 °C. To this was then added 1,3-dicyclohexylcarbodiimide (1 M in CH_2Cl_2) (12.5 mL, 12.5 mmol, 1.2 equiv.). It was allowed to stir at 0° for one hour. During this time, a white precipitate formed. At this point, 2-amino-4-methyl-6-*tert*-butylphenol (**6**) (1.863 g, 10.4 mmol, 1.0 equiv.) was added to the suspension. It was allowed to stir overnight. The next day, the solvent was removed under reduced pressure, and ethyl acetate was added to make a suspension which was then filtered to remove the solid. The filtrate was washed with 10% citric acid solution (2x50 mL), 5% $NaHCO_3$ (2x50 mL) and brine (50 mL). It was dried over $MgSO_4$, and the solvent was removed under reduced pressure, leaving a solid which was recrystallized from hexane to give the product as a white solid (2.92 g, 7.9 mmol, 76% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.55 (s, 1H), 8.77 (s, 1H), 7.84 (s, 1H), 7.05 (d, J = 1.8 Hz, 1H), 6.92 (m, 3H), 2.30 (s, 3H), 2.28 (s, 3H), 2.22 (s, 6H), 1.45 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.5, 157.4, 146.2, 140.6, 138.1, 134.9, 129.9, 129.6, 129.4, 126.9, 124.9, 121.4, 35.3, 30.0, 21.2, 21.0, 18.5. Anal. Calcd for $C_{22}H_{28}N_2O_3$: C, 71.71; H, 7.66; N, 7.60. Found: C, 72.01; H, 8.03; N, 7.36.

N-(2,6-Diisopropylphenyl)-N'-(2-hydroxy-5-methylphenyl)-oxalamide (7). N-(2,6-Diisopropylphenyl)-oxanilic acid ethyl ester (**1**, Ar = 2,6-diisopropylphenyl) (5.14 g, 18.5 mmol, 1.0 equiv.) and 2-amino-5-methylphenol (2.28 g, 18.5 mmol, 1 equiv.) were dissolved in toluene (50 mL). To this suspension was added triethylamine (2.6 mL, 18.5 mmol, 1 equiv.). The suspension was heated to reflux, causing the solids to dissolve. After heating at reflux

overnight, the product precipitated. At this point, ethyl acetate was added until the solid redissolved. The solution was washed with 2 M HCl solution (2x100 mL). The aqueous layer was then washed with ethyl acetate, and the combined organic layers were washed with brine (100 mL), and dried over $MgSO_4$. The solvent was then removed under reduced pressure, leaving a yellowish solid. This was recrystallized from toluene, producing a white crystalline solid (5.90 g, 16.6 mmol, 90% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.58 (s, 1H), 8.81 (s, 1H), 7.92 (s, 1H), 7.37 (t, *J* = 7.8 Hz 1H), 7.27 (d, *J* = 0.9 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 6.97 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.90 (d, *J* = 8.1 Hz, 1H), 3.02 (septet, *J* = 6.6, 2H), 2.29 (s, 3H), 1.22 (d, *J* = 7.2, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 158.2, 146.0, 130.7, 129.4, 128.7, 124.0, 123.8, 122.6, 119.1, 29.2, 23.9, 20.7. Anal. Calcd for $C_{21}H_{26}N_2O_3$: C, 71.16; H, 7.39; N, 7.90. Found: C, 70.85; H, 7.68; N, 7.73.

N-(2,6-Diisopropylphenyl)-N'-(2-hydroxy-3-(adamant-1-yl)-5-methylphenyl)-oxalamide (2d). N-(2,6-Diisopropylphenyl)-N'-(2-hydroxy-5-methylphenyl)-oxalamide (**7**) (5.59 g, 15.5 mmol, 1.0 equiv.) and 1-adamantol (2.83 g, 18.6 mmol, 1.2 equiv.) were dissolved in CH_2Cl_2 (150 mL). To this suspension was added conc. H_2SO_4 (1 mL). After addition of the acid, the solids eventually went into solution. After stirring at room temperature for 24 hours, the TLC (9:1 hexanes:ethyl acetate, visualized by UV) showed that most of the starting material had gone to product. At this point, the solvent was removed under reduced pressure, and the resulting solids were redissolved in ethyl acetate (100 mL). This solution was washed with sat. $NaHCO_3$ (3x50 mL, gas is evolved), and brine, then dried over $MgSO_4$. The solvent was removed under reduced pressure, and the resulting solid was purified via column chromatography to give a light yellow solid (3.68 g, 7.5 mmol, 48 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.77 (s, 1H), 7.84 (s, 1H), 7.37 (t, *J* = 7.2 Hz 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.00 (d, *J* = 2.1 Hz, 1H), 6.94 (d, *J* = 1.8 Hz, 1H), 3.01 (septet, *J* = 6.9, 2H), 2.29 (s, 3H), 2.18 (bs, 6H), 2.10 (bs, 3H), 1.80 (bs, 6H), 1.22 (d, *J* = 6.9, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.3, 158.2, 146.2, 145.8, 140.6, 129.9, 129.2, 129.2, 126.8,, 124.7, 123.8, 120.9, 40.7, 37.3, 37.1, 29.1, 29.0, 23.6, 20.8. Anal. Calcd for $C_{31}H_{40}N_2O_3$: C, 76.19; H, 8.25; N, 5.73. Found: C, 75.89; H, 8.42; N, 5.37.

1-(Mesityl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolium chloride (4a) N-(Mesityl)-N'-(2-hydroxyphenyl)-oxalamide (**2a**) (1.47g, 4.9 mmol, 1 equiv.) was weighed into an oven-dried round-bottom flask. To this was added BH_3–THF (1M in THF) (39 mL, 39.2 mmol, 8 equiv.). A great deal of bubbling resulted, as the solution turned bright orange. It was allowed to reflux overnight. The next day, the solution had turned clear. It was allowed to cool to room temperature, and then methanol was added very slowly, until all bubbling ceased. Conc. HCl solution (1.5 mL) was then added, and the solvent was removed under reduced pressure. The resulting solid was dissolved in methanol, and then the solvent was again removed under reduced pressure. This process was repeated twice more. In this way, the remaining boron was removed as $B(OMe)_3$. The resulting solid material was the dihydrochloride salt of the diimine (**3b**). This was not isolated or characterized. To this solid was added triethylorthoformate (15 mL). The resulting suspension was heated to 100 °C. As it heated, the solid slowly went into solution. After aprx. one minute at high temperature, a white solid precipitated. It was allowed to stir for five more minutes, and was then filtered. The resulting solid was washed with ether, to provide the desired product as a white powder (.854 g, 2.7 mmol, 55% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.43 (s, 1H), 8.84 (s, 1H), 7.54 (dd, *J* = 8.25, 1.2 Hz, 1H), 7.05 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.92 (m, 2H), 6.73 (dt, *J* = 7.7, 0.9 Hz 1H), 4.80 (t, *J* = 11.4 Hz, 2H), 4.37 (t, *J* = 11.7 Hz,

2H), 2.33 (s, 3H), 2.29 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.4, 150.0, 141.0, 135.3, 130.7, 130.3, 128.8, 122.8, 120.4, 119.9, 118.8, 51.0, 50.4, 21.3, 18.2. Anal. Calcd for $C_{18}H_{21}ClN_2O$: C, 68.24; H, 6.68; N, 8.84. Found: C, 67.86; H, 6.92; N, 8.52.

1-(2,6-Diisopropylphenyl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolium chloride (4b) N-(2,6-Diisopropylphenyl)-N'-(2-hydroxyphenyl)-oxalamide (**2b**) (.7356 g, 2.2 mmol, 1 equiv.) was treated in a fashion similar to that for **4a** to yield **4b** (.657 g, 1.83 mmol, 85% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (s, 1H), 7.57 (dd, *J* = 8.9, 1.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 6.6 Hz, 1H), 6.97 (dt, *J* = 7.8, 1.8 Hz, 1H), 6.78 (dt, *J* = 8.3, 0.9 Hz, 1H), 4.88 (t, *J* = 11.4 Hz, 2H), 4.44 (t, *J* = 11.1, 2H), 2.95 (septet, *J* = 6.6 Hz, 2H), 1.25 (d, *J* = 7.2 Hz, 6H), 1.16 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.0, 149.8, 146.6, 131.6, 130.0, 128.7, 125.1, 122.6, 120.3, 120.0, 118.6, 52.7, 51.1, 28.9, 25.0, 24.3. Anal. Calcd for $C_{21}H_{27}ClN_2O$: C, 70.28; H, 7.58; N, 7.81. Found: C, 70.32; H, 7.76; N, 7.63.

1-(Mesityl)-3-(2-hydroxy-3-*tert*-butyl-5-methylphenyl)-4,5-dihydro-imidazolium chloride (4c) N-(Mesityl)-N'-(2-hydroxy-3-*tert*-butyl-5-methylphenyl)-oxalamide (**2c**) (2.385 g, 6.5 mmol, 1 equiv.) was treated in a fashion similar to that for **4a** to yield **4c** (.884 g, 2.28 mmol, 35% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.10 (d, *J* = 1.5 Hz, 1H), 6.96 (s, 2H), 6.80 (s, 1H), 4.79 (t, *J* = 11.1 Hz, 2H), 4.43 (t, *J* = 9.6 Hz, 2H), 2.47 (s, 6H), 2.30 (s, 3H), 2.27 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.7, 148.1, 144.2, 140.7, 135.8, 130.8, 130.6, 130.3, 128.9, 127.5, 121.6, 52.3, 51.6, 35.6, 30.1, 21.2, 21.1, 18.6. Anal. Calcd for $C_{23}H_{31}ClN_2O$: C, 71.39; H, 8.07; N, 7.24. Found: C, 72.01; H, 8.03; N, 7.36.

1-(2,6-Diisopropylphenyl)-3-(2-hydroxy-3-(adamant-1-yl)-5-methylphenyl)-4,5-dihydro-imidazolium chloride (4d) N-(2,6-Diisopropylphenyl)-N'-(2-hydroxy-3-(adamant-1-yl)-5-methylphenyl)-oxalamide (**2d**) (1.83 g, 3.7 mmol, 1 equiv.) was treated in a fashion similar to that for **4a** to yield **4d** (1.19 g, 2.3 mmol, 63% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.45 (t, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.1 2H), 7.04 (s, 1H), 6.80 (s, 1H), 4.88 (t, *J* = 10.8 Hz, 2H), 4.45 (t, *J* = 11.7 Hz, 2H), 3.41 (septet, *J* = 6.6 Hz 2H), 2.28 (s, 3H), 2.13 (bs, 6H), 2.04 (bs, 3H), 1.74 (m, 6H), 1.34 (d, *J* = 6.9 Hz, 6H), 1.29 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.4, 148.3, 147.3, 144.4, 131.4, 130.8, 130.2, 128.8, 127.8, 125.2, 121.1, 54.0, 52.4, 40.8, 37.8, 37.2, 29.2, 28.8, 25.5, 24.4, 21.1. Anal. Calcd for $C_{32}H_{43}ClN_2O$: C, 75.78; H, 8.55; N, 5.52. Found: C, 74.78; H, 8.64; N, 5.44.

1-(Mesityl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolyl methyl triethylphosphine palladium(II) (8a) 1-(Mesityl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolium chloride (**4a**) (75.3 mg, 0.24 mmol, 1 equiv.) and potassium hexamethyldisilazide (99.4 mg, 0.50 mmol, 2.1 equiv.) were weighed together in a vial in the glovebox. THF (5 mL) was added to the mixture of solids, providing a light yellow solution with a light precipitate. This was added to a round-bottomed flask and allowed to stir for ten minutes. At this point, a suspension of $((PEt_3)PdMeCl)_2$ (65.4 mg, 0.12 mmol, 0.5 equiv.) in THF (5 mL) was added. The resulting yellow suspension quickly turned to a light yellow solution with a light precipitate. It was allowed to stir at room temperature for one hour, then filtered through celite. The solvent was then removed under reduced pressure until ca. 1 mL remained. To this was added pentane, and the resulting suspension was allowed to sit at -40 °C overnight. The next day, the product, a beige solid, was collected by filtration (39 mg, 0.08 mmol, 32% yield). Crystals suitable for X-

ray crystallographic analysis were obtained by layering pentane over a saturated methylene chloride solution of **8a** and storing this solution at -40 °C. ^{1}H NMR (300 MHz, C_7D_8) δ 7.12 (m, 2H), 6.78 (s, 2H), 6.64 (m, 2H), 3.31 (t, *J* = 10.2 Hz, 2H), 3.02 (t, *J* = 10.2, 2H), 2.44 (s, 6H), 2.12 (s, 3H), 1.41 (apparent quintet, *J* = 8.1 Hz, 6H), 0.93 (ddd, *J* = 15.3, 7.8 Hz, 9H), -0.50 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (75 MHz, C_7D_8) δ 197.7, 162.7, 137.2, 136.3, 129.4, 126.0, 120.9, 118.8, 111.4, 51.3, 51.2, 19.0, 13.8, 13.5, 8.2, -17.4, -17.6; ^{31}P NMR (121 MHz, C_7D_8) δ 18.29.

1-(2,6-diisopropylphenyl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolyl methyl triphenylphosphine palladium(II) (8b) This complex was synthesized in a manner analogous to that for **8a**, using 1-(2,6-diisopropylphenyl)-3-(2-hydroxyphenyl)-4,5-dihydro-imidazolium chloride (**4b**) (73.7 mg, 0.2 mmol, 1 equiv.) and $((PPh_3)_2PdMeCl)_2$ (86 mg, 0.1 mmol, 0.5 equiv.) (Yield: 78.9 mg, 0.13 mmol, 63%). ^{1}H NMR (300 MHz, C_6D_6) δ 7.74 (m, 6H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 1H), 7.01 (bs, 9H), 6.92 (t, *J* = 7.8 Hz, 1H), 6.80 (dd, *J* = 1.8, 7.8 Hz 1H), 6.9 (t, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 8.1 Hz, 1H), 3.47 (septet, *J* = 6.9 Hz, 2H), 3.38 (t, *J* = 9 Hz, 2H), 3.25 (t, *J* = 9.3, 2H), 1.57 (d, *J* = 6.6, 6H), 1.12 (d, *J* = 6.9, 6H), -0.32 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, C_6D_6) δ 147.6, 135.6, 135.5, 130.1, 130.1, 129.3, 128.6, 128.5, 126.6, 124.9, 122.3, 119.2, 112.1, 54.6, 49.1, 29.1, 26.7, 25.0, 3.0, -9.6, -9.7; ^{31}P NMR (121 MHz, C_6D_6) δ 26.27.

1-(mesityl)-3-(2-hydroxy-3-*tert*-butyl-5-methylphenyl)-4,5-dihydro-imidazolyl methyl triphenylphosphine palladium(II) (8c) This complex was synthesized in a manner analogous to that for **8a**, using 1-(mesityl)-3-(2-hydroxy-3-*tert*-butyl-5-methylphenyl)-4,5-dihydro-imidazolium chloride (**4c**) (102.2 mg, 0.26 mmol, 1 equiv.) and $((PPh_3)_2PdMeCl)_2$ (110.7 mg, 0.13 mmol, 0.5 equiv.) (Yield: 112.4 mg, 0.15 mmol, 58%). ^{1}H NMR (300 MHz, C_6D_6) δ 7.80 (m, 6H), 7.02 (s, 9H), 6.64 (m, 4H), 3.39 (t, *J* = 10.8 Hz, 2H), 3.02 (t, *J* = 10.5 Hz, 2H), 2.49 (s, 6H), 2.47 (s, 3H), 2.11 (s, 3H), 1.42, (s, 9H), -0.36 (d, *J* = 8.1 Hz, 6H); ^{13}C NMR (75 MHz, C_6D_6) δ 199.2, 197.4, 159.2, 140.1, 137.8, 136.8, 136.3, 135.4, 135.2, 133.6, 133.1, 132.9, 129.7, 129.3., 128.1, 124.1, 118.6, 118.3, 51.0, 50.9, 49.8,49.8, 35.5, 29.9, 29.8, 21.3, 20.9, 19.0, -9.4, -9.6; ^{31}P NMR (121 MHz, C_6D_6) δ 24.90.

1-(2,6-diisopropylphenyl)-3-(2-hydroxy-3-(adamant-1-yl)-5-methylphenyl)-4,5-dihydro-imidazolyl methyl triphenylphosphine palladium(II) (8d) This complex was synthesized in a manner analogous to that for **8a**, using 1-(2,6-diisopropylphenyl)-3-(2-hydroxy-3-(adamant-1-yl)-5-methylphenyl)-4,5-dihydro-imidazolium chloride (**4d**) (179.4 mg, 0.35 mmol, 1 equiv.) and $((PPh_3)_2PdMeCl)_2$ (148 mg, 0.16 mmol, 0.5 equiv.) (Yield: 138.9 mg, 0.16 mmol, 46%). Crystals suitable for X-ray crystallographic analysis were obtained by layering pentane over a saturated THF solution of **8d** and storing this solution at -40 °C. ^{1}H NMR (300 MHz, C_6D_6) δ 7.80 (m, 6H), 7.11 (m, 2H), 7.01 (m, 11H), 6.67 (d, *J* = 1.8 Hz, 1H), 3.51 (m, 6H), 3.22 (t, *J* = 10.2 Hz, 2H), 2.53 (s, 3H), 2.14 (s, 6H), 1.67 (bs, 3H), 1.54 (d, *J* = 6.9 Hz, 6H), 1.43 (m, 6H), 1.09 (d, *J* = 6.6, 6H), -0.44 (d, *J* = 7.8, 3H); ^{13}C NMR (75 MHz, C_6D_6) δ 197.4, 149.5, 147.5, 136.2, 136.1, 134.0, 133.5, 132.8, 130.3, 124.9, 124.7, 118.7, 54.2, 41.2, 38.2, 37.8, 30.5, 30.2, 29.0, 26.8, 25.1, 23.1, 21.9, 14.6; ^{31}P NMR (121 MHz, C_6D_6) δ 27.01.

Table 1. Crystal data and structure refinement for 8a (CCDC 235932).

Empirical formula	$C_{25}H_{37}N_2OPPd \cdot CH_2Cl_2$
Formula weight	603.88
Crystallization Solvent	Dichloromethane/pentane
Crystal Habit	Block
Crystal size	0.24 x 0.17 x 0.16 mm^3
Crystal color	Colorless

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 9026 reflections used in lattice determination	2.15 to 21.67°	
Unit cell dimensions	a = 10.3128(9) Å b = 11.2919(10) Å c = 12.7707(11) Å	α= 104.5880(10)° β= 99.9120(10)° γ = 97.6740(10)°
Volume	1393.1(2) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.425 Mg/m^3	
F(000)	624	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.69 to 21.68°	
Completeness to θ = 21.68°	79.5 %	
Index ranges	$-9 \le h \le 10$, $-10 \le k \le 11$, $-12 \le l \le 13$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v6.022	
Reflections collected	10961	
Independent reflections	2611 [R_{int}= 0.0428]	
Absorption coefficient	0.936 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.8646 and 0.8065	

Table 1 (cont.)

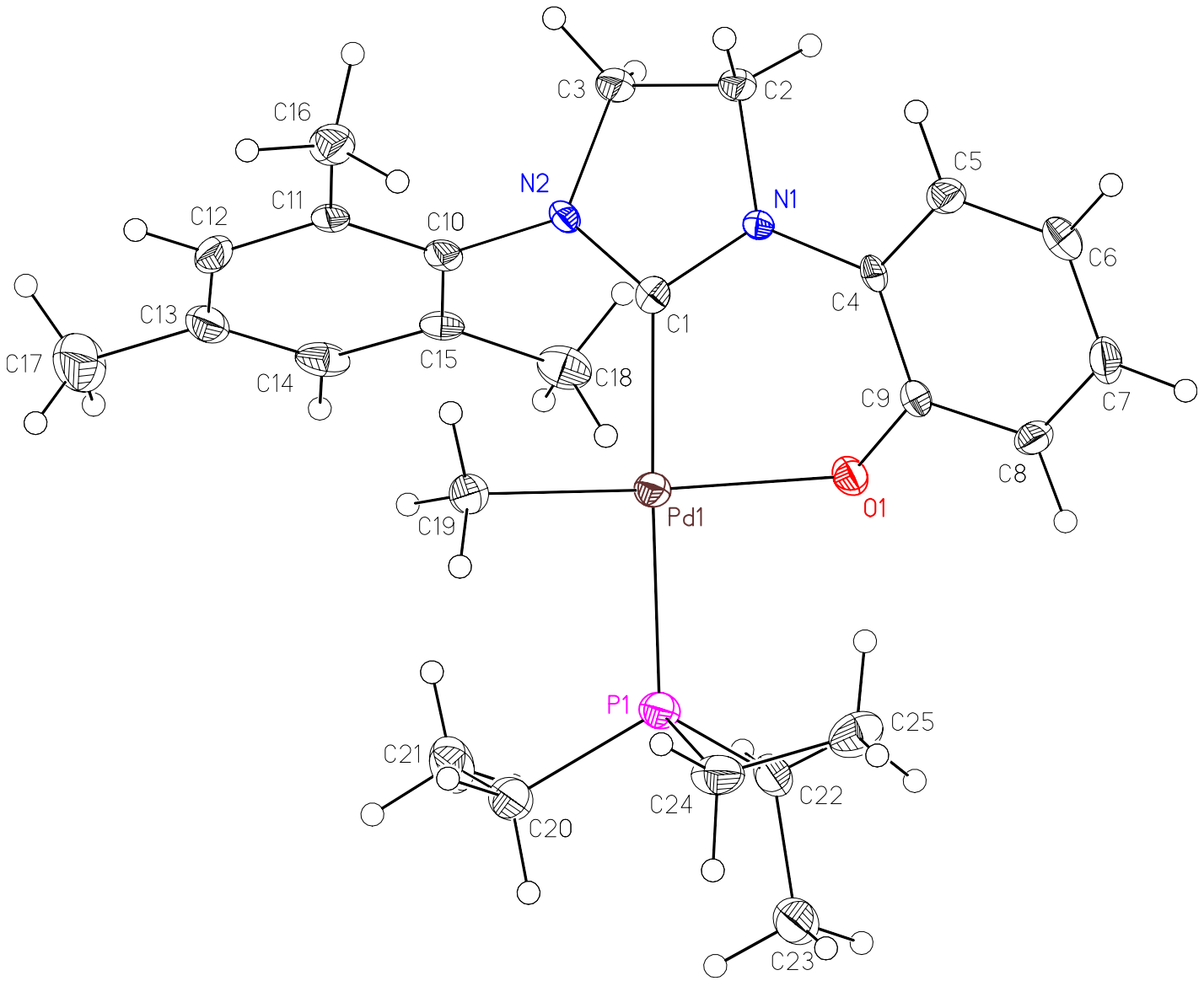
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	2611 / 0 / 305
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.114
Final R indices [$I>2\sigma(I)$, 2452 reflections]	R1 = 0.0217, *w*R2 = 0.0514
R indices (all data)	R1 = 0.0235, *w*R2 = 0.0518
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.006
Average shift/error	0.000
Largest diff. peak and hole	0.281 and -0.270 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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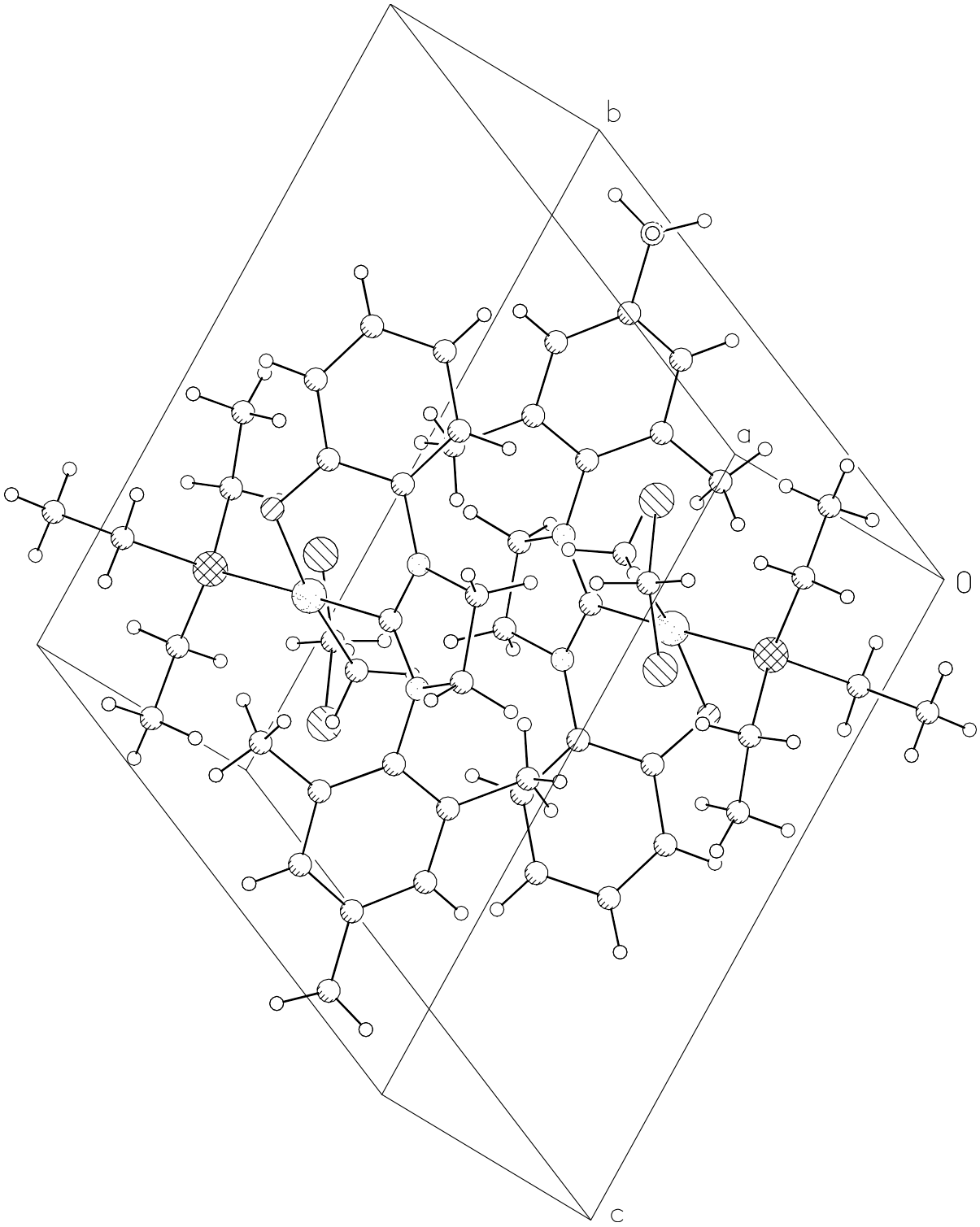
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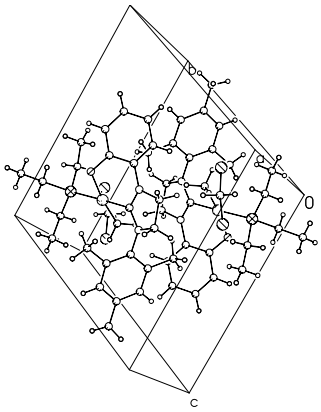

O
O
C

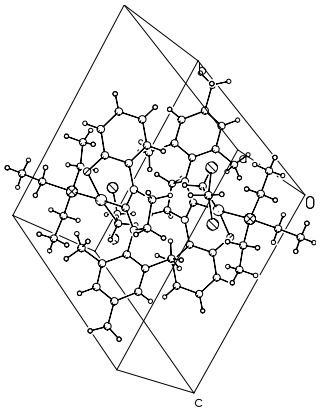

O
C

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 8a (CCDC 235932). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	7238(1)	7160(1)	6702(1)	15(1)
P(1)	7114(1)	9136(1)	7648(1)	19(1)
O(1)	8931(2)	7795(2)	6123(2)	18(1)
N(1)	8025(2)	5234(2)	5016(2)	12(1)
N(2)	7403(2)	4395(2)	6243(2)	13(1)
C(1)	7509(3)	5436(3)	5926(3)	12(1)
C(2)	8138(3)	3913(3)	4591(2)	16(1)
C(3)	8001(3)	3427(3)	5577(2)	18(1)
C(4)	8305(3)	6119(3)	4438(3)	11(1)
C(5)	8162(3)	5731(3)	3300(3)	17(1)
C(6)	8472(3)	6568(3)	2708(3)	20(1)
C(7)	8945(3)	7804(3)	3279(3)	21(1)
C(8)	9086(3)	8195(3)	4411(3)	19(1)
C(9)	8772(3)	7381(3)	5029(3)	14(1)
C(10)	7047(3)	4256(3)	7252(3)	14(1)
C(11)	5835(3)	3500(3)	7177(3)	14(1)
C(12)	5512(3)	3356(3)	8160(3)	21(1)
C(13)	6346(4)	3928(3)	9180(3)	24(1)
C(14)	7541(3)	4675(3)	9212(3)	22(1)
C(15)	7924(3)	4849(3)	8263(3)	16(1)
C(16)	4877(3)	2881(3)	6089(3)	22(1)
C(17)	5962(4)	3760(3)	10227(3)	41(1)
C(18)	9229(3)	5681(3)	8346(3)	25(1)
C(19)	5473(3)	6497(3)	7055(3)	19(1)
C(20)	6338(3)	9332(3)	8842(3)	28(1)
C(21)	7032(3)	8778(3)	9708(3)	38(1)
C(22)	8771(3)	10126(3)	8182(3)	21(1)
C(23)	8835(3)	11503(3)	8753(3)	32(1)
C(24)	6213(3)	9959(3)	6786(3)	26(1)
C(25)	6901(3)	10143(3)	5862(3)	27(1)
Cl(1)	2721(1)	9469(1)	6794(1)	44(1)
Cl(2)	2350(1)	8010(1)	8338(1)	38(1)
C(31)	1648(3)	8968(3)	7581(3)	32(1)

Table 3. Selected bond lengths [Å] and angles [°] for 8a (CCDC 235932).

Pd(1)-C(1)	2.030(3)	C(1)-Pd(1)-C(19)	93.37(12)
Pd(1)-C(19)	2.041(3)	C(1)-Pd(1)-O(1)	84.61(10)
Pd(1)-O(1)	2.1182(19)	C(19)-Pd(1)-O(1)	172.65(10)
Pd(1)-P(1)	2.2858(9)	C(1)-Pd(1)-P(1)	175.26(8)
		C(19)-Pd(1)-P(1)	90.02(9)
		O(1)-Pd(1)-P(1)	92.44(6)

Table 4. Bond lengths [Å] and angles [°] for 8a (CCDC 235932).

Pd(1)-C(1)	2.030(3)	C(16)-H(16A)	0.9800
Pd(1)-C(19)	2.041(3)	C(16)-H(16B)	0.9800
Pd(1)-O(1)	2.1182(19)	C(16)-H(16C)	0.9800
Pd(1)-P(1)	2.2858(9)	C(17)-H(17A)	0.9800
P(1)-C(20)	1.820(3)	C(17)-H(17B)	0.9800
P(1)-C(24)	1.826(3)	C(17)-H(17C)	0.9800
P(1)-C(22)	1.827(3)	C(18)-H(18A)	0.9800
O(1)-C(9)	1.329(4)	C(18)-H(18B)	0.9800
N(1)-C(1)	1.340(3)	C(18)-H(18C)	0.9800
N(1)-C(4)	1.413(4)	C(19)-H(19A)	0.9800
N(1)-C(2)	1.481(3)	C(19)-H(19B)	0.9800
N(2)-C(1)	1.334(3)	C(19)-H(19C)	0.9800
N(2)-C(10)	1.438(4)	C(20)-C(21)	1.524(4)
N(2)-C(3)	1.480(3)	C(20)-H(20A)	0.9900
C(2)-C(3)	1.515(4)	C(20)-H(20B)	0.9900
C(2)-H(2A)	0.9900	C(21)-H(21A)	0.9800
C(2)-H(2B)	0.9900	C(21)-H(21B)	0.9800
C(3)-H(3A)	0.9900	C(21)-H(21C)	0.9800
C(3)-H(3B)	0.9900	C(22)-C(23)	1.529(4)
C(4)-C(5)	1.383(4)	C(22)-H(22A)	0.9900
C(4)-C(9)	1.408(4)	C(22)-H(22B)	0.9900
C(5)-C(6)	1.390(4)	C(23)-H(23A)	0.9800
C(5)-H(5)	0.9500	C(23)-H(23B)	0.9800
C(6)-C(7)	1.378(4)	C(23)-H(23C)	0.9800
C(6)-H(6)	0.9500	C(24)-C(25)	1.520(4)
C(7)-C(8)	1.377(4)	C(24)-H(24A)	0.9900
C(7)-H(7)	0.9500	C(24)-H(24B)	0.9900
C(8)-C(9)	1.395(4)	C(25)-H(25A)	0.9800
C(8)-H(8)	0.9500	C(25)-H(25B)	0.9800
C(10)-C(11)	1.390(4)	C(25)-H(25C)	0.9800
C(10)-C(15)	1.390(4)	Cl(1)-C(31)	1.747(3)
C(11)-C(12)	1.395(4)	Cl(2)-C(31)	1.768(3)
C(11)-C(16)	1.500(4)	C(31)-H(31A)	0.9900
C(12)-C(13)	1.377(4)	C(31)-H(31B)	0.9900
C(12)-H(12)	0.9500		
C(13)-C(14)	1.385(4)	C(1)-Pd(1)-C(19)	93.37(12)
C(13)-C(17)	1.507(4)	C(1)-Pd(1)-O(1)	84.61(10)
C(14)-C(15)	1.389(4)	C(19)-Pd(1)-O(1)	172.65(10)
C(14)-H(14)	0.9500	C(1)-Pd(1)-P(1)	175.26(8)
C(15)-C(18)	1.507(4)	C(19)-Pd(1)-P(1)	90.02(9)

O(1)-Pd(1)-P(1)	92.44(6)	C(13)-C(12)-H(12)	118.8
C(20)-P(1)-C(24)	104.05(15)	C(11)-C(12)-H(12)	118.8
C(20)-P(1)-C(22)	104.50(15)	C(12)-C(13)-C(14)	117.8(3)
C(24)-P(1)-C(22)	103.70(14)	C(12)-C(13)-C(17)	121.0(3)
C(20)-P(1)-Pd(1)	118.05(11)	C(14)-C(13)-C(17)	121.2(3)
C(24)-P(1)-Pd(1)	113.40(11)	C(13)-C(14)-C(15)	122.5(3)
C(22)-P(1)-Pd(1)	111.75(10)	C(13)-C(14)-H(14)	118.7
C(9)-O(1)-Pd(1)	112.98(17)	C(15)-C(14)-H(14)	118.7
C(1)-N(1)-C(4)	125.4(3)	C(14)-C(15)-C(10)	117.6(3)
C(1)-N(1)-C(2)	112.2(2)	C(14)-C(15)-C(18)	120.3(3)
C(4)-N(1)-C(2)	122.1(3)	C(10)-C(15)-C(18)	122.0(3)
C(1)-N(2)-C(10)	126.3(3)	C(11)-C(16)-H(16A)	109.5
C(1)-N(2)-C(3)	112.5(2)	C(11)-C(16)-H(16B)	109.5
C(10)-N(2)-C(3)	119.9(2)	H(16A)-C(16)-H(16B)	109.5
N(2)-C(1)-N(1)	108.3(3)	C(11)-C(16)-H(16C)	109.5
N(2)-C(1)-Pd(1)	130.0(2)	H(16A)-C(16)-H(16C)	109.5
N(1)-C(1)-Pd(1)	121.3(2)	H(16B)-C(16)-H(16C)	109.5
N(1)-C(2)-C(3)	101.8(2)	C(13)-C(17)-H(17A)	109.5
N(1)-C(2)-H(2A)	111.4	C(13)-C(17)-H(17B)	109.5
C(3)-C(2)-H(2A)	111.4	H(17A)-C(17)-H(17B)	109.5
N(1)-C(2)-H(2B)	111.4	C(13)-C(17)-H(17C)	109.5
C(3)-C(2)-H(2B)	111.4	H(17A)-C(17)-H(17C)	109.5
H(2A)-C(2)-H(2B)	109.3	H(17B)-C(17)-H(17C)	109.5
N(2)-C(3)-C(2)	101.8(2)	C(15)-C(18)-H(18A)	109.5
N(2)-C(3)-H(3A)	111.4	C(15)-C(18)-H(18B)	109.5
C(2)-C(3)-H(3A)	111.4	H(18A)-C(18)-H(18B)	109.5
N(2)-C(3)-H(3B)	111.4	C(15)-C(18)-H(18C)	109.5
C(2)-C(3)-H(3B)	111.4	H(18A)-C(18)-H(18C)	109.5
H(3A)-C(3)-H(3B)	109.3	H(18B)-C(18)-H(18C)	109.5
C(5)-C(4)-C(9)	120.7(3)	Pd(1)-C(19)-H(19A)	109.5
C(5)-C(4)-N(1)	119.6(3)	Pd(1)-C(19)-H(19B)	109.5
C(9)-C(4)-N(1)	119.7(3)	H(19A)-C(19)-H(19B)	109.5
C(4)-C(5)-C(6)	121.2(3)	Pd(1)-C(19)-H(19C)	109.5
C(4)-C(5)-H(5)	119.4	H(19A)-C(19)-H(19C)	109.5
C(6)-C(5)-H(5)	119.4	H(19B)-C(19)-H(19C)	109.5
C(7)-C(6)-C(5)	118.7(3)	C(21)-C(20)-P(1)	111.8(2)
C(7)-C(6)-H(6)	120.7	C(21)-C(20)-H(20A)	109.3
C(5)-C(6)-H(6)	120.7	P(1)-C(20)-H(20A)	109.3
C(6)-C(7)-C(8)	120.2(3)	C(21)-C(20)-H(20B)	109.3
C(6)-C(7)-H(7)	119.9	P(1)-C(20)-H(20B)	109.3
C(8)-C(7)-H(7)	119.9	H(20A)-C(20)-H(20B)	107.9
C(7)-C(8)-C(9)	122.6(3)	C(20)-C(21)-H(21A)	109.5
C(7)-C(8)-H(8)	118.7	C(20)-C(21)-H(21B)	109.5
C(9)-C(8)-H(8)	118.7	H(21A)-C(21)-H(21B)	109.5
O(1)-C(9)-C(8)	120.7(3)	C(20)-C(21)-H(21C)	109.5
O(1)-C(9)-C(4)	122.7(3)	H(21A)-C(21)-H(21C)	109.5
C(8)-C(9)-C(4)	116.6(3)	H(21B)-C(21)-H(21C)	109.5
C(11)-C(10)-C(15)	122.0(3)	C(23)-C(22)-P(1)	117.5(2)
C(11)-C(10)-N(2)	118.2(3)	C(23)-C(22)-H(22A)	107.9
C(15)-C(10)-N(2)	119.8(3)	P(1)-C(22)-H(22A)	107.9
C(10)-C(11)-C(12)	117.7(3)	C(23)-C(22)-H(22B)	107.9
C(10)-C(11)-C(16)	122.0(3)	P(1)-C(22)-H(22B)	107.9
C(12)-C(11)-C(16)	120.3(3)	H(22A)-C(22)-H(22B)	107.2
C(13)-C(12)-C(11)	122.4(3)	C(22)-C(23)-H(23A)	109.5

C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-P(1)	112.2(2)
C(25)-C(24)-H(24A)	109.2
P(1)-C(24)-H(24A)	109.2
C(25)-C(24)-H(24B)	109.2
P(1)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Cl(1)-C(31)-Cl(2)	111.80(17)
Cl(1)-C(31)-H(31A)	109.3
Cl(2)-C(31)-H(31A)	109.3
Cl(1)-C(31)-H(31B)	109.3
Cl(2)-C(31)-H(31B)	109.3
H(31A)-C(31)-H(31B)	107.9

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for 8a (CCDC 235932). 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)	145(2)	139(2)	165(2)	30(1)	42(1)	31(1)
P(1)	173(5)	163(6)	210(6)	17(5)	59(4)	29(4)
O(1)	153(13)	188(13)	159(16)	5(12)	58(11)	-6(10)
N(1)	135(15)	98(18)	142(18)	38(15)	63(14)	42(12)
N(2)	158(16)	134(17)	103(17)	32(14)	64(13)	42(13)
C(1)	58(18)	150(20)	140(20)	42(18)	-12(17)	13(15)
C(2)	156(19)	130(20)	200(20)	37(17)	58(16)	49(15)
C(3)	180(20)	150(20)	230(20)	35(18)	83(17)	52(16)
C(4)	73(19)	160(20)	130(20)	60(20)	47(16)	40(16)
C(5)	140(20)	140(20)	240(30)	40(20)	58(17)	35(15)
C(6)	220(20)	260(30)	140(20)	50(20)	70(17)	64(18)
C(7)	220(20)	240(30)	250(30)	140(20)	135(18)	84(18)
C(8)	170(20)	110(20)	270(30)	20(20)	81(17)	8(15)
C(9)	53(18)	160(20)	210(30)	50(20)	60(17)	34(16)
C(10)	170(20)	130(20)	170(30)	64(18)	60(20)	98(18)
C(11)	170(20)	100(20)	190(20)	52(18)	70(19)	90(17)
C(12)	220(20)	130(20)	340(30)	100(20)	130(20)	55(16)
C(13)	370(30)	190(20)	220(30)	90(20)	160(20)	138(19)
C(14)	320(30)	190(20)	120(20)	10(18)	3(19)	117(19)
C(15)	170(20)	120(20)	180(20)	21(18)	30(20)	84(17)
C(16)	190(20)	190(20)	290(20)	58(18)	59(18)	54(16)
C(17)	620(30)	410(30)	320(30)	200(20)	230(20)	180(20)
C(18)	240(20)	270(20)	190(20)	8(17)	6(17)	75(18)
C(19)	170(20)	180(20)	220(20)	48(17)	60(16)	31(16)
C(20)	230(20)	230(20)	320(20)	-37(19)	116(18)	-47(17)
C(21)	460(30)	390(30)	220(20)	-10(20)	160(20)	-90(20)
C(22)	200(20)	230(20)	190(20)	29(18)	81(16)	24(16)
C(23)	290(20)	280(20)	330(20)	-40(20)	150(19)	-54(17)
C(24)	230(20)	200(20)	320(20)	9(18)	52(18)	56(16)
C(25)	330(20)	200(20)	290(20)	107(18)	18(19)	73(17)
Cl(1)	458(7)	371(6)	562(7)	182(5)	211(5)	142(5)
Cl(2)	434(6)	397(6)	255(6)	43(5)	56(5)	40(5)
C(31)	180(20)	420(20)	280(20)	-48(19)	9(18)	129(17)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 8a (CCDC 235932).

	x	y	z	U_{iso}
H(2A)	9016	3838	4392	19
H(2B)	7413	3470	3938	19
H(3A)	7403	2603	5347	22
H(3B)	8883	3366	5989	22
H(5)	7846	4875	2916	21
H(6)	8360	6294	1926	24
H(7)	9175	8388	2889	25
H(8)	9410	9052	4786	23
H(12)	4686	2844	8125	26
H(14)	8122	5083	9911	26
H(16A)	4813	3471	5644	33
H(16B)	3991	2610	6221	33
H(16C)	5200	2156	5691	33
H(17A)	5172	4132	10336	61
H(17B)	6708	4168	10860	61
H(17C)	5755	2869	10167	61
H(18A)	9050	6455	8185	37
H(18B)	9711	5255	7810	37
H(18C)	9777	5874	9096	37
H(19A)	5034	5720	6488	29
H(19B)	4887	7113	7064	29
H(19C)	5650	6340	7782	29
H(20A)	6376	10230	9180	34
H(20B)	5383	8923	8595	34
H(21A)	6975	7884	9382	57
H(21B)	6592	8907	10339	57
H(21C)	7975	9188	9961	57
H(22A)	9290	9772	8716	25
H(22B)	9230	10075	7557	25
H(23A)	8320	11874	8242	49
H(23B)	9770	11937	8969	49
H(23C)	8455	11580	9415	49
H(24A)	5293	9480	6457	31
H(24B)	6144	10782	7255	31
H(25A)	7724	10769	6177	41
H(25B)	6300	10426	5333	41
H(25C)	7124	9353	5481	41
H(31A)	789	8500	7083	38
H(31B)	1457	9703	8101	38

Table 1. Crystal data and structure refinement for 8d (CCDC 235931).

Empirical formula	$C_{51}H_{59}N_2OPPd$
Formula weight	853.37
Crystallization Solvent	Pentane/THF
Crystal Habit	Fragment
Crystal size	0.32 x 0.25 x 0.07 mm^3
Crystal color	Yellow

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 18959 reflections used in lattice determination	2.19 to 27.64°	
Unit cell dimensions	a = 15.1511(9) Å b = 17.8042(11) Å c = 21.5514(13) Å	α= 100.3810(10)° β= 102.6620(10)° γ = 105.9370(10)°
Volume	5272.1(6) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.075 Mg/m^3	
F(000)	1792	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.52 to 28.52°	
Completeness to θ = 28.52°	90.5 %	
Index ranges	$-20 \le h \le 20$, $-23 \le k \le 22$, $-28 \le l \le 27$	
Data collection scan type	ω scans at 5 ϕ settings	
Data reduction program	Bruker SAINT v6.45	
Reflections collected	79175	
Independent reflections	24246 [R_{int}= 0.0847]	
Absorption coefficient	0.415 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9716 and 0.8788	

Table 1 (cont.)

Structure solution and Refinement

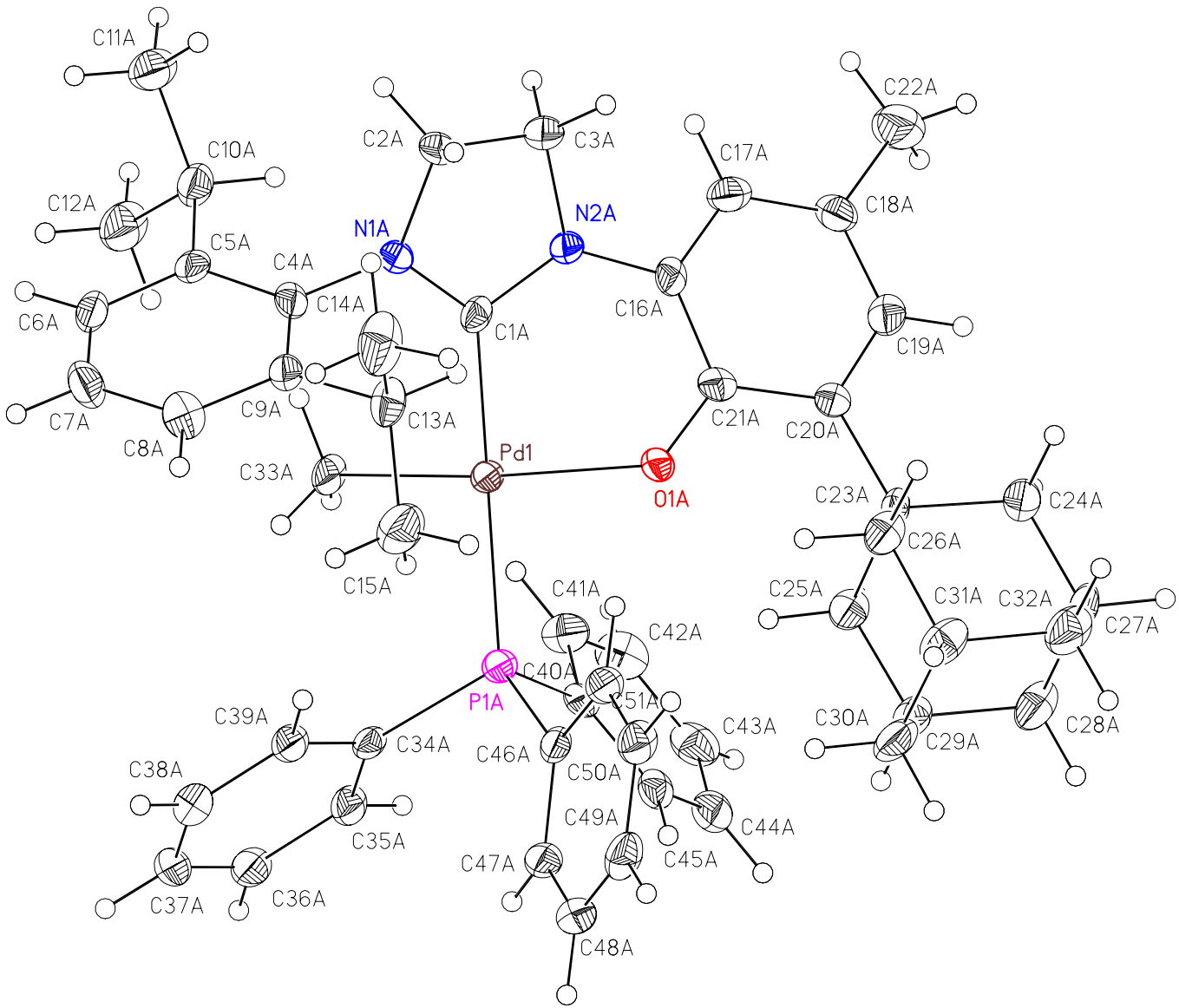
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	24246 / 0 / 1009
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.066
Final R indices [$I>2\sigma(I)$, 14224 reflections]	R1 = 0.0462, *w*R2 = 0.0758
R indices (all data)	R1 = 0.0829, *w*R2 = 0.0799
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.151 and -0.890 e.Å^{-3}

Special Refinement Details

A large portion of the crystal (1474.9Å^3 or approx. 28% of the total volume) is occupied by disordered solvent. The crystals were cloudy, perhaps as result of solvent loss. Difference electron density maps suggest the presence of a combination of dichloromethane, pentane and perhaps THF. It was not possible to model the solvent adequately therefore solvent flattening was applied as implemented in PLATON.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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Pd1
O1A
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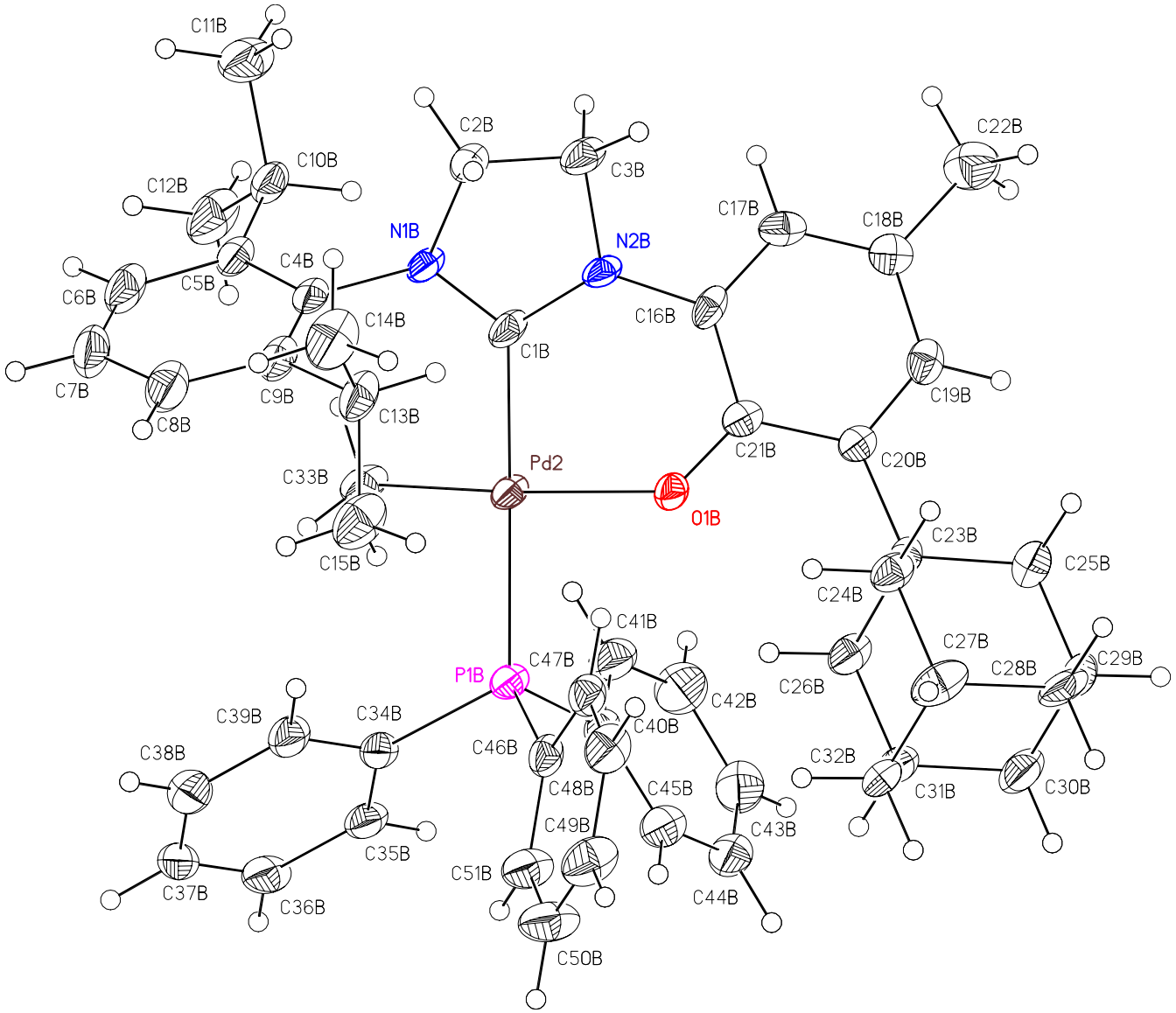
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C32B
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C51B
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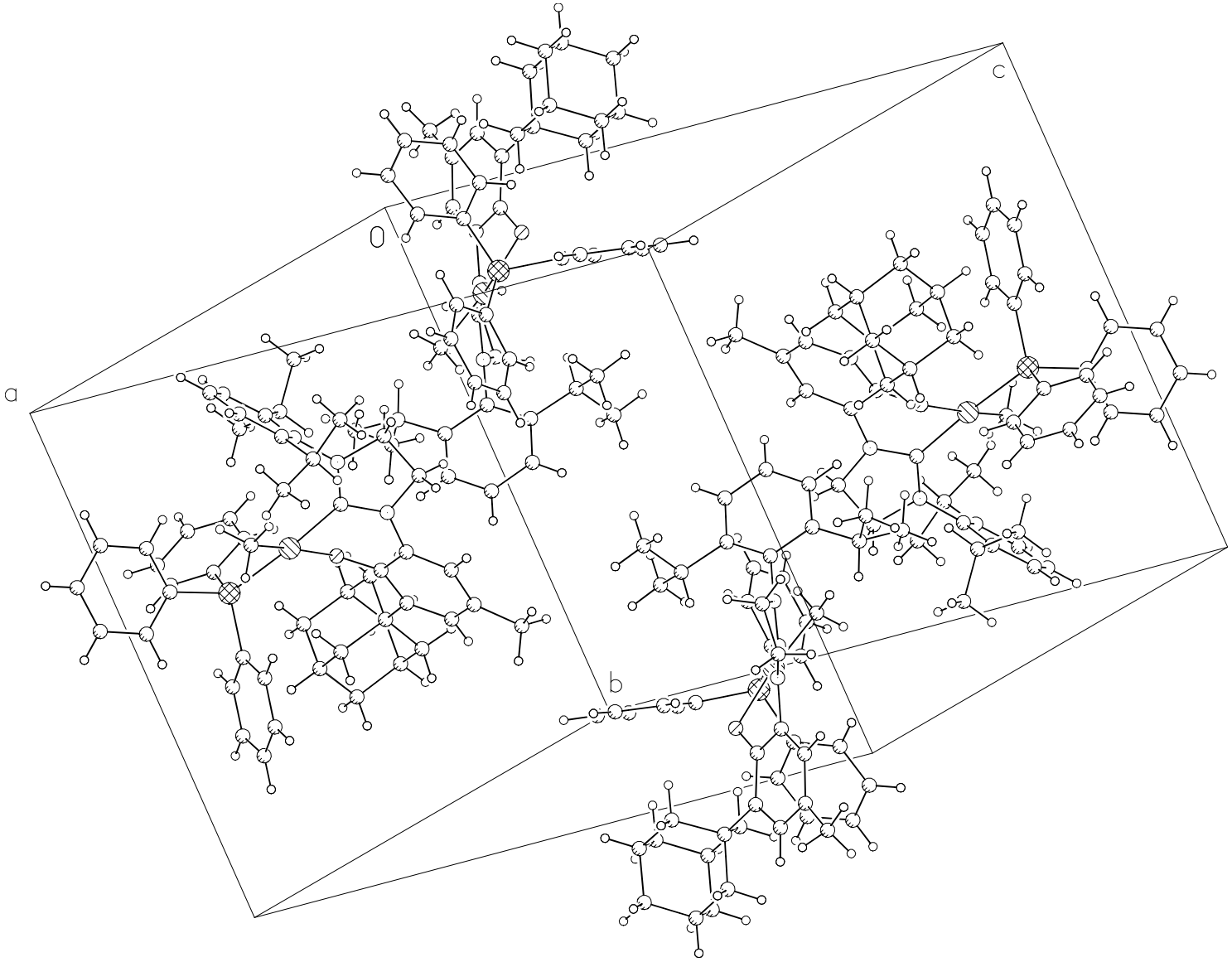
C37B
C36B
C50B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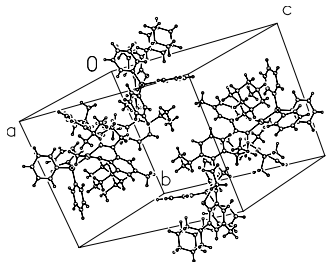
c
b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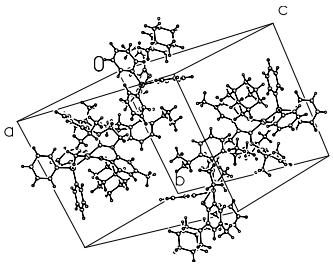
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a
b

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 8d (CCDC 235931). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pd(1)	1208(1)	6143(1)	7893(1)	18(1)
P(1A)	745(1)	5722(1)	8755(1)	19(1)
O(1A)	2282(1)	5574(1)	7957(1)	19(1)
N(1A)	1880(2)	7311(2)	7079(1)	20(1)
N(2A)	2080(2)	6144(1)	6813(1)	20(1)
C(1A)	1717(2)	6583(2)	7200(1)	18(1)
C(2A)	2515(2)	7435(2)	6649(2)	28(1)
C(3A)	2450(2)	6579(2)	6355(2)	28(1)
C(4A)	1692(2)	7986(2)	7430(2)	21(1)
C(5A)	927(2)	8217(2)	7106(2)	21(1)
C(6A)	741(2)	8859(2)	7459(2)	27(1)
C(7A)	1278(2)	9264(2)	8089(2)	32(1)
C(8A)	2028(2)	9034(2)	8391(2)	31(1)
C(9A)	2255(2)	8408(2)	8065(2)	21(1)
C(10A)	329(2)	7791(2)	6410(2)	26(1)
C(11A)	595(2)	8306(2)	5939(2)	33(1)
C(12A)	-752(2)	7598(2)	6338(2)	37(1)
C(13A)	3144(2)	8232(2)	8405(2)	27(1)
C(14A)	4045(2)	8916(2)	8447(2)	42(1)
C(15A)	3129(2)	8121(2)	9090(2)	40(1)
C(16A)	2093(2)	5352(2)	6801(2)	19(1)
C(17A)	1992(2)	4841(2)	6201(2)	26(1)
C(18A)	2107(2)	4099(2)	6169(2)	25(1)
C(19A)	2378(2)	3893(2)	6761(2)	24(1)
C(20A)	2477(2)	4371(2)	7370(2)	17(1)
C(21A)	2269(2)	5114(2)	7398(1)	18(1)
C(22A)	1957(3)	3525(2)	5519(2)	44(1)
C(23A)	2809(2)	4113(2)	8000(2)	20(1)
C(24A)	3122(2)	3359(2)	7862(2)	30(1)
C(25A)	2001(2)	3909(2)	8331(2)	24(1)
C(26A)	3671(2)	4786(2)	8498(2)	26(1)
C(27A)	3476(2)	3124(2)	8497(2)	33(1)
C(28A)	2638(2)	2909(2)	8801(2)	33(1)
C(29A)	2333(2)	3647(2)	8956(2)	28(1)
C(30A)	3170(2)	4348(2)	9446(2)	32(1)
C(31A)	3995(2)	4548(2)	9138(2)	32(1)
C(32A)	4303(2)	3806(2)	8979(2)	37(1)
C(33A)	106(2)	6600(2)	7720(2)	25(1)
C(34A)	-36(2)	6179(2)	9100(1)	20(1)
C(35A)	-929(2)	5720(2)	9135(2)	25(1)
C(36A)	-1471(2)	6093(2)	9436(2)	30(1)
C(37A)	-1152(2)	6914(2)	9695(2)	33(1)
C(38A)	-256(2)	7375(2)	9663(2)	31(1)
C(39A)	275(2)	7000(2)	9361(2)	27(1)
C(40A)	97(2)	4650(2)	8551(2)	20(1)
C(41A)	-574(2)	4313(2)	7938(2)	29(1)
C(42A)	-1121(2)	3506(2)	7751(2)	34(1)

C(43A)	-1003(2)	3023(2)	8170(2)	32(1)
C(44A)	-337(2)	3344(2)	8780(2)	29(1)
C(45A)	210(2)	4154(2)	8967(2)	22(1)
C(46A)	1743(2)	5972(2)	9493(1)	19(1)
C(47A)	1609(2)	5968(2)	10109(2)	22(1)
C(48A)	2375(2)	6238(2)	10667(2)	27(1)
C(49A)	3303(2)	6514(2)	10614(2)	28(1)
C(50A)	3437(2)	6507(2)	10005(2)	26(1)
C(51A)	2682(2)	6245(2)	9444(2)	23(1)
Pd(2)	6740(1)	8655(1)	7015(1)	23(1)
P(1B)	6013(1)	9127(1)	6190(1)	24(1)
O(1B)	8142(1)	9282(1)	6982(1)	23(1)
N(1B)	7173(2)	7400(2)	7727(1)	27(1)
N(2B)	8315(2)	8547(2)	8025(1)	23(1)
C(1B)	7415(2)	8161(2)	7663(2)	25(1)
C(2B)	8015(2)	7224(2)	8085(2)	30(1)
C(3B)	8691(2)	8059(2)	8429(2)	32(1)
C(4B)	6282(2)	6755(2)	7391(2)	26(1)
C(5B)	5613(2)	6572(2)	7752(2)	29(1)
C(6B)	4751(2)	5967(2)	7423(2)	38(1)
C(7B)	4580(2)	5541(2)	6784(2)	41(1)
C(8B)	5263(2)	5720(2)	6448(2)	38(1)
C(9B)	6130(2)	6334(2)	6752(2)	29(1)
C(10B)	5801(2)	7006(2)	8464(2)	30(1)
C(11B)	6133(2)	6523(2)	8932(2)	45(1)
C(12B)	4926(2)	7189(2)	8590(2)	44(1)
C(13B)	6873(2)	6507(2)	6378(2)	32(1)
C(14B)	7239(2)	5787(2)	6241(2)	46(1)
C(15B)	6484(2)	6712(2)	5742(2)	43(1)
C(16B)	8860(2)	9364(2)	8099(2)	23(1)
C(17B)	9519(2)	9785(2)	8702(2)	25(1)
C(18B)	10135(2)	10545(2)	8793(2)	25(1)
C(19B)	10091(2)	10864(2)	8247(2)	25(1)
C(20B)	9462(2)	10468(2)	7629(2)	20(1)
C(21B)	8779(2)	9693(2)	7545(2)	21(1)
C(22B)	10903(2)	10976(2)	9437(2)	41(1)
C(23B)	9541(2)	10830(2)	7041(2)	21(1)
C(24B)	9792(2)	10278(2)	6529(2)	26(1)
C(25B)	10331(2)	11663(2)	7243(2)	33(1)
C(26B)	8601(2)	10951(2)	6704(2)	28(1)
C(27B)	9879(2)	10614(2)	5933(2)	35(1)
C(28B)	10661(2)	11438(2)	6161(2)	38(1)
C(29B)	10416(2)	12007(2)	6655(2)	35(1)
C(30B)	9470(2)	12120(2)	6329(2)	36(1)
C(31B)	8691(2)	11295(2)	6113(2)	32(1)
C(32B)	8935(2)	10729(2)	5616(2)	35(1)
C(33B)	5444(2)	8151(2)	7151(2)	31(1)
C(34B)	4724(2)	8668(2)	5816(2)	25(1)
C(35B)	4092(2)	9105(2)	5772(2)	30(1)
C(36B)	3128(2)	8720(2)	5449(2)	36(1)
C(37B)	2777(2)	7900(2)	5160(2)	35(1)
C(38B)	3394(2)	7460(2)	5203(2)	35(1)
C(39B)	4359(2)	7837(2)	5530(2)	32(1)
C(40B)	6161(2)	10190(2)	6452(2)	24(1)

C(41B)	6172(2)	10485(2)	7098(2)	36(1)
C(42B)	6276(2)	11289(2)	7341(2)	41(1)
C(43B)	6370(2)	11812(2)	6938(2)	38(1)
C(44B)	6368(2)	11532(2)	6301(2)	34(1)
C(45B)	6268(2)	10733(2)	6058(2)	32(1)
C(46B)	6436(2)	8974(2)	5464(2)	24(1)
C(47B)	7236(2)	8716(2)	5498(2)	26(1)
C(48B)	7524(2)	8541(2)	4941(2)	32(1)
C(49B)	7042(2)	8620(2)	4347(2)	40(1)
C(50B)	6248(2)	8875(2)	4308(2)	41(1)
C(51B)	5952(2)	9048(2)	4864(2)	34(1)

Table 3. Selected bond lengths [Å] and angles [°] for 8d (CCDC 235931).

Pd(1)-C(1A)	2.009(3)	Pd(2)-C(1B)	2.018(3)
Pd(1)-C(33A)	2.042(3)	Pd(2)-C(33B)	2.031(3)
Pd(1)-O(1A)	2.1332(18)	Pd(2)-O(1B)	2.1352(18)
Pd(1)-P(1A)	2.2987(8)	Pd(2)-P(1B)	2.2952(8)
C(1A)-Pd(1)-C(33A)	91.65(11	C(1B)-Pd(2)-C(33B)	93.19(12)
C(1A)-Pd(1)-O(1A)	85.47(9)	C(1B)-Pd(2)-O(1B)	85.16(9)
C(33A)-Pd(1)-O(1A)	173.07(11)	C(33B)-Pd(2)-O(1B)	173.34(12)
C(1A)-Pd(1)-P(1A)	174.92(8)	C(1B)-Pd(2)-P(1B)	173.58(9)
C(33A)-Pd(1)-P(1A)	90.26(9)	C(33B)-Pd(2)-P(1B)	89.45(9)
O(1A)-Pd(1)-P(1A)	93.14(5)	O(1B)-Pd(2)-P(1B)	92.87(6)

Table 4. Bond lengths [Å] and angles [°] for 8d (CCDC 235931).

Pd(1)-C(1A)	2.009(3)	C(6A)-C(7A)	1.366(4)
Pd(1)-C(33A)	2.042(3)	C(7A)-C(8A)	1.384(4)
Pd(1)-O(1A)	2.1332(18)	C(8A)-C(9A)	1.375(4)
Pd(1)-P(1A)	2.2987(8)	C(9A)-C(13A)	1.526(4)
P(1A)-C(46A)	1.826(3)	C(10A)-C(11A)	1.530(4)
P(1A)-C(34A)	1.821(3)	C(10A)-C(12A)	1.545(4)
P(1A)-C(40A)	1.811(3)	C(13A)-C(15A)	1.527(4)
O(1A)-C(21A)	1.322(3)	C(13A)-C(14A)	1.533(4)
N(1A)-C(1A)	1.336(3)	C(16A)-C(17A)	1.392(4)
N(1A)-C(4A)	1.432(4)	C(16A)-C(21A)	1.419(4)
N(1A)-C(2A)	1.478(3)	C(17A)-C(18A)	1.371(4)
N(2A)-C(1A)	1.345(3)	C(18A)-C(19A)	1.397(4)
N(2A)-C(16A)	1.411(3)	C(18A)-C(22A)	1.508(4)
N(2A)-C(3A)	1.473(3)	C(19A)-C(20A)	1.383(4)
C(2A)-C(3A)	1.508(4)	C(20A)-C(21A)	1.436(4)
C(4A)-C(9A)	1.390(4)	C(20A)-C(23A)	1.534(4)
C(4A)-C(5A)	1.417(4)	C(23A)-C(24A)	1.544(4)
C(5A)-C(6A)	1.386(4)	C(23A)-C(25A)	1.540(4)
C(5A)-C(10A)	1.505(4)	C(23A)-C(26A)	1.536(4)

C(24A)-C(27A)	1.530(4)	C(16B)-C(17B)	1.385(4)
C(25A)-C(29A)	1.531(4)	C(16B)-C(21B)	1.417(4)
C(26A)-C(31A)	1.532(4)	C(17B)-C(18B)	1.368(4)
C(27A)-C(32A)	1.504(4)	C(18B)-C(19B)	1.391(4)
C(27A)-C(28A)	1.541(4)	C(18B)-C(22B)	1.511(4)
C(28A)-C(29A)	1.514(4)	C(19B)-C(20B)	1.385(4)
C(29A)-C(30A)	1.533(4)	C(20B)-C(21B)	1.432(4)
C(30A)-C(31A)	1.529(4)	C(20B)-C(23B)	1.535(4)
C(31A)-C(32A)	1.524(4)	C(23B)-C(24B)	1.524(4)
C(34A)-C(39A)	1.373(4)	C(23B)-C(26B)	1.541(4)
C(34A)-C(35A)	1.400(4)	C(23B)-C(25B)	1.544(4)
C(35A)-C(36A)	1.384(4)	C(24B)-C(27B)	1.529(4)
C(36A)-C(37A)	1.371(4)	C(25B)-C(29B)	1.519(4)
C(37A)-C(38A)	1.404(4)	C(26B)-C(31B)	1.526(4)
C(38A)-C(39A)	1.374(4)	C(27B)-C(32B)	1.529(4)
C(40A)-C(45A)	1.385(4)	C(27B)-C(28B)	1.526(4)
C(40A)-C(41A)	1.389(4)	C(28B)-C(29B)	1.512(5)
C(41A)-C(42A)	1.380(4)	C(29B)-C(30B)	1.534(4)
C(42A)-C(43A)	1.373(4)	C(30B)-C(31B)	1.525(4)
C(43A)-C(44A)	1.379(4)	C(31B)-C(32B)	1.514(5)
C(44A)-C(45A)	1.384(4)	C(34B)-C(39B)	1.394(4)
C(46A)-C(47A)	1.389(4)	C(34B)-C(35B)	1.389(4)
C(46A)-C(51A)	1.405(4)	C(35B)-C(36B)	1.386(4)
C(47A)-C(48A)	1.377(4)	C(36B)-C(37B)	1.379(5)
C(48A)-C(49A)	1.394(4)	C(37B)-C(38B)	1.375(4)
C(49A)-C(50A)	1.370(4)	C(38B)-C(39B)	1.387(4)
C(50A)-C(51A)	1.372(4)	C(40B)-C(41B)	1.390(4)
Pd(2)-C(1B)	2.018(3)	C(40B)-C(45B)	1.397(4)
Pd(2)-C(33B)	2.031(3)	C(41B)-C(42B)	1.385(4)
Pd(2)-O(1B)	2.1352(18)	C(42B)-C(43B)	1.383(5)
Pd(2)-P(1B)	2.2952(8)	C(43B)-C(44B)	1.373(5)
P(1B)-C(40B)	1.811(3)	C(44B)-C(45B)	1.378(4)
P(1B)-C(34B)	1.825(3)	C(46B)-C(51B)	1.388(4)
P(1B)-C(46B)	1.821(3)	C(46B)-C(47B)	1.402(4)
O(1B)-C(21B)	1.311(3)	C(47B)-C(48B)	1.377(4)
N(1B)-C(1B)	1.344(4)	C(48B)-C(49B)	1.380(4)
N(1B)-C(4B)	1.444(4)	C(49B)-C(50B)	1.389(4)
N(1B)-C(2B)	1.483(3)	C(50B)-C(51B)	1.381(4)
N(2B)-C(1B)	1.330(3)		
N(2B)-C(16B)	1.422(4)	C(1A)-Pd(1)-C(33A)	91.65(11)
N(2B)-C(3B)	1.472(3)	C(1A)-Pd(1)-O(1A)	85.47(9)
C(2B)-C(3B)	1.497(4)	C(33A)-Pd(1)-O(1A)	173.07(11)
C(4B)-C(5B)	1.411(4)	C(1A)-Pd(1)-P(1A)	174.92(8)
C(4B)-C(9B)	1.381(4)	C(33A)-Pd(1)-P(1A)	90.26(9)
C(5B)-C(6B)	1.383(4)	O(1A)-Pd(1)-P(1A)	93.14(5)
C(5B)-C(10B)	1.515(5)	C(46A)-P(1A)-C(34A)	99.76(13)
C(6B)-C(7B)	1.378(5)	C(46A)-P(1A)-C(40A)	108.53(14)
C(7B)-C(8B)	1.388(4)	C(34A)-P(1A)-C(40A)	103.10(13)
C(8B)-C(9B)	1.387(4)	C(46A)-P(1A)-Pd(1)	113.15(10)
C(9B)-C(13B)	1.520(4)	C(34A)-P(1A)-Pd(1)	117.64(10)
C(10B)-C(12B)	1.517(4)	C(40A)-P(1A)-Pd(1)	113.33(10)
C(10B)-C(11B)	1.530(4)	C(21A)-O(1A)-Pd(1)	115.76(16)
C(13B)-C(15B)	1.518(4)	C(1A)-N(1A)-C(4A)	126.4(2)
C(13B)-C(14B)	1.536(4)	C(1A)-N(1A)-C(2A)	112.0(2)

C(4A)-N(1A)-C(2A)	120.0(2)	C(28A)-C(29A)-C(30A)	110.1(2)
C(1A)-N(2A)-C(16A)	127.0(2)	C(28A)-C(29A)-C(25A)	110.9(3)
C(1A)-N(2A)-C(3A)	111.5(2)	C(30A)-C(29A)-C(25A)	108.9(2)
C(16A)-N(2A)-C(3A)	121.4(2)	C(29A)-C(30A)-C(31A)	108.8(3)
N(2A)-C(1A)-N(1A)	108.5(2)	C(32A)-C(31A)-C(30A)	109.3(3)
N(2A)-C(1A)-Pd(1)	119.6(2)	C(32A)-C(31A)-C(26A)	108.7(3)
N(1A)-C(1A)-Pd(1)	131.4(2)	C(30A)-C(31A)-C(26A)	110.0(2)
N(1A)-C(2A)-C(3A)	101.7(2)	C(31A)-C(32A)-C(27A)	109.5(3)
N(2A)-C(3A)-C(2A)	102.5(2)	C(39A)-C(34A)-C(35A)	118.5(3)
C(9A)-C(4A)-C(5A)	121.2(3)	C(39A)-C(34A)-P(1A)	118.9(2)
C(9A)-C(4A)-N(1A)	120.7(3)	C(35A)-C(34A)-P(1A)	122.5(2)
C(5A)-C(4A)-N(1A)	118.1(3)	C(36A)-C(35A)-C(34A)	120.1(3)
C(6A)-C(5A)-C(4A)	117.2(3)	C(35A)-C(36A)-C(37A)	120.8(3)
C(6A)-C(5A)-C(10A)	120.4(3)	C(36A)-C(37A)-C(38A)	119.2(3)
C(4A)-C(5A)-C(10A)	122.4(3)	C(37A)-C(38A)-C(39A)	119.5(3)
C(5A)-C(6A)-C(7A)	121.9(3)	C(34A)-C(39A)-C(38A)	121.8(3)
C(8A)-C(7A)-C(6A)	119.9(3)	C(45A)-C(40A)-C(41A)	118.3(3)
C(7A)-C(8A)-C(9A)	121.1(3)	C(45A)-C(40A)-P(1A)	124.6(2)
C(4A)-C(9A)-C(8A)	118.7(3)	C(41A)-C(40A)-P(1A)	117.1(2)
C(4A)-C(9A)-C(13A)	122.9(3)	C(40A)-C(41A)-C(42A)	120.9(3)
C(8A)-C(9A)-C(13A)	118.4(3)	C(43A)-C(42A)-C(41A)	120.0(3)
C(5A)-C(10A)-C(11A)	110.7(3)	C(42A)-C(43A)-C(44A)	120.0(3)
C(5A)-C(10A)-C(12A)	111.9(3)	C(43A)-C(44A)-C(45A)	119.8(3)
C(11A)-C(10A)-C(12A)	108.7(2)	C(40A)-C(45A)-C(44A)	120.9(3)
C(9A)-C(13A)-C(15A)	111.8(3)	C(47A)-C(46A)-C(51A)	118.7(3)
C(9A)-C(13A)-C(14A)	109.6(3)	C(47A)-C(46A)-P(1A)	122.3(2)
C(15A)-C(13A)-C(14A)	110.5(3)	C(51A)-C(46A)-P(1A)	118.7(2)
C(17A)-C(16A)-N(2A)	118.3(3)	C(48A)-C(47A)-C(46A)	121.1(3)
C(17A)-C(16A)-C(21A)	121.7(3)	C(49A)-C(48A)-C(47A)	119.7(3)
N(2A)-C(16A)-C(21A)	119.9(3)	C(50A)-C(49A)-C(48A)	119.2(3)
C(18A)-C(17A)-C(16A)	121.0(3)	C(49A)-C(50A)-C(51A)	121.9(3)
C(17A)-C(18A)-C(19A)	117.7(3)	C(50A)-C(51A)-C(46A)	119.3(3)
C(17A)-C(18A)-C(22A)	121.5(3)	C(1B)-Pd(2)-C(33B)	93.19(12)
C(19A)-C(18A)-C(22A)	120.9(3)	C(1B)-Pd(2)-O(1B)	85.16(9)
C(20A)-C(19A)-C(18A)	123.9(3)	C(33B)-Pd(2)-O(1B)	173.34(12)
C(19A)-C(20A)-C(21A)	118.3(3)	C(1B)-Pd(2)-P(1B)	173.58(9)
C(19A)-C(20A)-C(23A)	120.6(3)	C(33B)-Pd(2)-P(1B)	89.45(9)
C(21A)-C(20A)-C(23A)	121.1(3)	O(1B)-Pd(2)-P(1B)	92.87(6)
O(1A)-C(21A)-C(20A)	121.9(3)	C(40B)-P(1B)-C(34B)	102.83(14)
O(1A)-C(21A)-C(16A)	121.3(3)	C(40B)-P(1B)-C(46B)	107.93(14)
C(20A)-C(21A)-C(16A)	116.8(3)	C(34B)-P(1B)-C(46B)	100.33(14)
C(20A)-C(23A)-C(24A)	112.1(2)	C(40B)-P(1B)-Pd(2)	112.70(11)
C(20A)-C(23A)-C(25A)	111.1(2)	C(34B)-P(1B)-Pd(2)	118.59(10)
C(24A)-C(23A)-C(25A)	107.3(2)	C(46B)-P(1B)-Pd(2)	113.14(10)
C(20A)-C(23A)-C(26A)	111.3(2)	C(21B)-O(1B)-Pd(2)	117.01(17)
C(24A)-C(23A)-C(26A)	106.8(2)	C(1B)-N(1B)-C(4B)	127.0(2)
C(25A)-C(23A)-C(26A)	108.1(2)	C(1B)-N(1B)-C(2B)	111.4(2)
C(27A)-C(24A)-C(23A)	111.5(3)	C(4B)-N(1B)-C(2B)	120.4(2)
C(29A)-C(25A)-C(23A)	110.9(2)	C(1B)-N(2B)-C(16B)	126.9(2)
C(31A)-C(26A)-C(23A)	112.0(2)	C(1B)-N(2B)-C(3B)	112.1(2)
C(24A)-C(27A)-C(32A)	111.2(3)	C(16B)-N(2B)-C(3B)	120.7(2)
C(24A)-C(27A)-C(28A)	108.1(2)	N(2B)-C(1B)-N(1B)	107.9(2)
C(32A)-C(27A)-C(28A)	109.7(3)	N(2B)-C(1B)-Pd(2)	120.8(2)
C(29A)-C(28A)-C(27A)	108.5(2)	N(1B)-C(1B)-Pd(2)	130.0(2)

N(1B)-C(2B)-C(3B)	101.3(2)	C(31B)-C(32B)-C(27B)	109.9(3)
N(2B)-C(3B)-C(2B)	101.9(2)	C(39B)-C(34B)-C(35B)	118.2(3)
C(5B)-C(4B)-C(9B)	123.1(3)	C(39B)-C(34B)-P(1B)	118.1(2)
C(5B)-C(4B)-N(1B)	117.1(3)	C(35B)-C(34B)-P(1B)	123.6(3)
C(9B)-C(4B)-N(1B)	119.8(3)	C(34B)-C(35B)-C(36B)	120.3(3)
C(4B)-C(5B)-C(6B)	116.9(3)	C(35B)-C(36B)-C(37B)	121.1(3)
C(4B)-C(5B)-C(10B)	123.1(3)	C(38B)-C(37B)-C(36B)	119.1(3)
C(6B)-C(5B)-C(10B)	120.1(3)	C(37B)-C(38B)-C(39B)	120.3(3)
C(7B)-C(6B)-C(5B)	121.1(3)	C(34B)-C(39B)-C(38B)	121.0(3)
C(6B)-C(7B)-C(8B)	120.7(3)	C(41B)-C(40B)-C(45B)	117.9(3)
C(7B)-C(8B)-C(9B)	120.3(4)	C(41B)-C(40B)-P(1B)	117.0(2)
C(4B)-C(9B)-C(8B)	117.9(3)	C(45B)-C(40B)-P(1B)	125.1(3)
C(4B)-C(9B)-C(13B)	122.8(3)	C(40B)-C(41B)-C(42B)	121.1(3)
C(8B)-C(9B)-C(13B)	119.3(3)	C(43B)-C(42B)-C(41B)	119.9(4)
C(5B)-C(10B)-C(12B)	111.7(3)	C(44B)-C(43B)-C(42B)	119.7(3)
C(5B)-C(10B)-C(11B)	111.6(3)	C(43B)-C(44B)-C(45B)	120.6(3)
C(12B)-C(10B)-C(11B)	109.7(3)	C(44B)-C(45B)-C(40B)	120.8(3)
C(9B)-C(13B)-C(15B)	111.7(3)	C(51B)-C(46B)-C(47B)	118.7(3)
C(9B)-C(13B)-C(14B)	110.6(3)	C(51B)-C(46B)-P(1B)	122.2(2)
C(15B)-C(13B)-C(14B)	110.6(3)	C(47B)-C(46B)-P(1B)	119.0(2)
C(17B)-C(16B)-N(2B)	117.9(3)	C(48B)-C(47B)-C(46B)	119.8(3)
C(17B)-C(16B)-C(21B)	122.3(3)	C(49B)-C(48B)-C(47B)	121.1(3)
N(2B)-C(16B)-C(21B)	119.5(3)	C(48B)-C(49B)-C(50B)	119.5(3)
C(18B)-C(17B)-C(16B)	121.4(3)	C(51B)-C(50B)-C(49B)	119.7(3)
C(17B)-C(18B)-C(19B)	117.0(3)	C(50B)-C(51B)-C(46B)	121.2(3)
C(17B)-C(18B)-C(22B)	121.1(3)		
C(19B)-C(18B)-C(22B)	121.5(3)		
C(20B)-C(19B)-C(18B)	124.4(3)		
C(19B)-C(20B)-C(21B)	118.5(3)		
C(19B)-C(20B)-C(23B)	120.4(3)		
C(21B)-C(20B)-C(23B)	121.0(3)		
O(1B)-C(21B)-C(16B)	120.9(3)		
O(1B)-C(21B)-C(20B)	122.7(3)		
C(16B)-C(21B)-C(20B)	116.3(3)		
C(24B)-C(23B)-C(26B)	108.1(2)		
C(24B)-C(23B)-C(20B)	110.4(2)		
C(26B)-C(23B)-C(20B)	112.1(2)		
C(24B)-C(23B)-C(25B)	107.1(2)		
C(26B)-C(23B)-C(25B)	106.8(2)		
C(20B)-C(23B)-C(25B)	112.2(2)		
C(23B)-C(24B)-C(27B)	112.3(3)		
C(29B)-C(25B)-C(23B)	111.7(3)		
C(31B)-C(26B)-C(23B)	111.1(2)		
C(32B)-C(27B)-C(28B)	108.1(3)		
C(32B)-C(27B)-C(24B)	109.4(2)		
C(28B)-C(27B)-C(24B)	109.0(3)		
C(29B)-C(28B)-C(27B)	109.9(3)		
C(25B)-C(29B)-C(28B)	109.6(3)		
C(25B)-C(29B)-C(30B)	110.2(3)		
C(28B)-C(29B)-C(30B)	109.5(3)		
C(29B)-C(30B)-C(31B)	107.8(3)		
C(32B)-C(31B)-C(26B)	110.1(3)		
C(32B)-C(31B)-C(30B)	109.2(3)		
C(26B)-C(31B)-C(30B)	110.5(3)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 8d (CCDC 235931). 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)	151(1)	240(2)	211(2)	117(1)	88(1)	96(1)
P(1A)	160(4)	256(5)	207(5)	109(4)	78(4)	95(4)
O(1A)	183(10)	263(12)	180(12)	76(10)	74(9)	122(9)
N(1A)	209(13)	241(15)	243(15)	123(12)	137(12)	118(12)
N(2A)	220(13)	210(15)	231(15)	122(12)	123(12)	103(12)
C(1A)	149(15)	207(18)	210(18)	89(15)	32(13)	84(13)
C(2A)	384(19)	300(20)	340(20)	193(17)	277(17)	193(16)
C(3A)	341(18)	320(20)	300(20)	186(17)	205(16)	169(16)
C(4A)	204(16)	213(18)	320(20)	134(16)	176(15)	101(14)
C(5A)	219(16)	245(19)	266(19)	160(16)	135(15)	108(14)
C(6A)	275(18)	300(20)	420(20)	235(18)	207(17)	186(16)
C(7A)	321(19)	320(20)	400(20)	93(18)	197(18)	179(17)
C(8A)	300(19)	290(20)	330(20)	48(17)	93(16)	107(16)
C(9A)	230(16)	229(18)	253(19)	109(15)	115(15)	117(15)
C(10A)	250(17)	275(19)	300(20)	120(16)	76(15)	134(15)
C(11A)	307(19)	420(20)	340(20)	199(18)	123(17)	141(17)
C(12A)	254(18)	500(20)	440(20)	240(20)	107(17)	172(17)
C(13A)	203(16)	234(19)	360(20)	93(16)	46(15)	97(14)
C(14A)	211(18)	380(20)	720(30)	220(20)	140(19)	120(17)
C(15A)	400(20)	460(20)	390(20)	195(19)	86(18)	211(18)
C(16A)	117(14)	228(18)	290(19)	111(15)	97(14)	86(13)
C(17A)	257(17)	330(20)	230(19)	128(17)	96(15)	96(16)
C(18A)	301(18)	232(19)	250(19)	57(16)	146(15)	77(15)
C(19A)	221(16)	197(18)	340(20)	119(16)	133(15)	61(14)
C(20A)	115(14)	184(17)	233(18)	80(15)	87(13)	25(13)
C(21A)	102(14)	239(18)	201(18)	70(15)	62(13)	30(13)
C(22A)	680(30)	380(20)	330(20)	90(19)	220(20)	210(20)
C(23A)	157(15)	201(18)	290(19)	118(15)	85(14)	103(13)
C(24A)	345(19)	310(20)	380(20)	176(17)	188(17)	190(16)
C(25A)	169(15)	265(19)	310(20)	134(16)	96(14)	65(14)
C(26A)	176(16)	284(19)	350(20)	159(17)	84(15)	74(14)
C(27A)	400(20)	330(20)	460(20)	235(19)	192(18)	266(17)
C(28A)	288(18)	310(20)	430(20)	209(18)	89(17)	110(16)
C(29A)	244(17)	320(20)	390(20)	223(17)	162(16)	134(16)
C(30A)	350(20)	380(20)	300(20)	200(18)	62(17)	174(17)
C(31A)	228(17)	350(20)	370(20)	186(18)	26(16)	67(16)
C(32A)	249(18)	510(20)	440(20)	260(20)	95(17)	189(18)
C(33A)	166(15)	380(20)	350(20)	219(17)	125(15)	177(15)
C(34A)	167(15)	280(19)	221(18)	150(15)	80(14)	122(14)
C(35A)	209(16)	310(20)	320(20)	165(16)	124(15)	138(15)
C(36A)	248(18)	430(20)	400(20)	264(19)	201(16)	195(17)
C(37A)	350(20)	510(30)	360(20)	250(19)	238(17)	311(18)
C(38A)	390(20)	330(20)	320(20)	154(17)	137(17)	200(17)
C(39A)	237(17)	370(20)	330(20)	209(17)	160(15)	180(16)
C(40A)	135(15)	290(19)	233(18)	97(15)	115(14)	100(14)
C(41A)	331(19)	300(20)	250(20)	93(17)	98(16)	82(16)
C(42A)	272(18)	370(20)	330(20)	44(18)	77(16)	39(17)

C(43A)	308(19)	280(20)	370(20)	66(18)	193(17)	44(16)
C(44A)	280(18)	320(20)	350(20)	131(17)	178(17)	141(16)
C(45A)	179(16)	229(19)	283(19)	75(16)	111(14)	82(14)
C(46A)	199(16)	183(17)	207(18)	78(14)	49(14)	94(13)
C(47A)	197(16)	266(19)	262(19)	132(15)	117(15)	94(14)
C(48A)	324(19)	340(20)	220(19)	121(16)	97(16)	169(16)
C(49A)	269(18)	300(20)	270(20)	83(16)	-14(15)	143(15)
C(50A)	180(16)	330(20)	300(20)	117(17)	50(15)	109(15)
C(51A)	197(16)	289(18)	260(20)	127(16)	93(15)	107(14)
Pd(2)	153(1)	282(2)	358(2)	216(1)	115(1)	112(1)
P(1B)	155(4)	315(5)	343(5)	207(4)	105(4)	116(4)
O(1B)	151(10)	267(13)	307(13)	154(11)	83(10)	55(9)
N(1B)	149(13)	335(17)	448(18)	299(15)	120(13)	110(12)
N(2B)	175(13)	289(16)	334(16)	222(13)	105(12)	124(12)
C(1B)	192(16)	310(20)	380(20)	235(17)	163(15)	112(15)
C(2B)	144(15)	340(20)	510(20)	286(18)	104(16)	120(15)
C(3B)	229(17)	410(20)	460(20)	305(19)	154(16)	169(16)
C(4B)	152(16)	243(19)	450(20)	231(18)	72(16)	105(14)
C(5B)	157(16)	320(20)	510(20)	281(19)	122(16)	114(15)
C(6B)	225(18)	420(20)	620(30)	320(20)	217(19)	113(17)
C(7B)	222(18)	350(20)	640(30)	240(20)	105(19)	28(16)
C(8B)	340(20)	300(20)	530(30)	181(19)	152(19)	93(17)
C(9B)	207(17)	270(20)	500(20)	218(18)	155(17)	110(15)
C(10B)	232(17)	330(20)	390(20)	214(18)	125(16)	59(15)
C(11B)	310(20)	630(30)	600(30)	400(20)	191(19)	251(19)
C(12B)	370(20)	520(30)	650(30)	350(20)	340(20)	213(19)
C(13B)	277(18)	280(20)	480(20)	174(18)	205(17)	87(16)
C(14B)	390(20)	410(20)	730(30)	240(20)	290(20)	222(19)
C(15B)	440(20)	450(20)	580(30)	250(20)	310(20)	205(19)
C(16B)	181(16)	207(18)	400(20)	164(16)	172(16)	105(14)
C(17B)	256(17)	370(20)	228(19)	146(16)	125(15)	182(16)
C(18B)	244(17)	310(20)	241(19)	75(16)	113(15)	136(15)
C(19B)	196(16)	228(18)	350(20)	85(16)	125(16)	83(14)
C(20B)	175(15)	237(18)	265(19)	113(15)	109(14)	117(14)
C(21B)	184(16)	278(19)	278(19)	139(16)	130(15)	142(14)
C(22B)	510(20)	400(20)	340(20)	102(19)	109(19)	173(19)
C(23B)	154(15)	179(17)	316(19)	108(15)	78(14)	69(13)
C(24B)	257(17)	290(20)	310(20)	155(16)	147(15)	138(15)
C(25B)	305(19)	290(20)	390(20)	148(17)	107(17)	38(16)
C(26B)	221(17)	340(20)	430(20)	236(18)	179(16)	159(15)
C(27B)	470(20)	410(20)	390(20)	232(19)	310(18)	275(19)
C(28B)	277(18)	560(30)	530(20)	450(20)	232(18)	191(18)
C(29B)	246(18)	340(20)	450(20)	233(19)	89(17)	18(16)
C(30B)	380(20)	290(20)	470(20)	234(19)	162(18)	113(17)
C(31B)	209(17)	390(20)	450(20)	289(19)	105(16)	109(16)
C(32B)	324(19)	360(20)	330(20)	230(18)	58(17)	0(17)
C(33B)	237(17)	400(20)	480(20)	311(19)	172(16)	207(16)
C(34B)	159(16)	370(20)	281(19)	183(17)	104(14)	84(15)
C(35B)	221(17)	380(20)	400(20)	262(18)	120(16)	136(16)
C(36B)	191(17)	590(30)	450(20)	340(20)	140(17)	193(18)
C(37B)	159(17)	560(30)	350(20)	290(20)	67(16)	55(17)
C(38B)	304(19)	430(20)	340(20)	173(18)	104(17)	77(17)
C(39B)	211(17)	390(20)	440(20)	247(19)	123(16)	106(16)

C(40B)	132(15)	292(19)	370(20)	193(17)	102(15)	91(14)
C(41B)	340(20)	380(20)	460(20)	240(20)	125(18)	156(17)
C(42B)	450(20)	380(20)	420(20)	120(20)	150(19)	156(19)
C(43B)	320(20)	290(20)	550(30)	130(20)	105(19)	160(17)
C(44B)	220(18)	360(20)	540(30)	260(20)	99(18)	146(17)
C(45B)	212(17)	440(20)	430(20)	250(20)	150(17)	164(17)
C(46B)	175(16)	236(19)	350(20)	124(16)	109(15)	64(14)
C(47B)	195(15)	252(18)	360(20)	120(16)	83(15)	77(13)
C(48B)	254(18)	360(20)	470(20)	172(19)	198(17)	170(16)
C(49B)	430(20)	510(20)	450(20)	250(20)	284(19)	247(19)
C(50B)	410(20)	650(30)	370(20)	300(20)	198(19)	300(20)
C(51B)	276(18)	500(20)	390(20)	263(19)	175(17)	224(17)