Electronic Supplementary Material (ESI) for Dalton Transactions

Synthesis and X-ray characterization of novel palladium(II) complexes with tunable chiral anionic counterions

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Supporting Information

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General Methods. All commercially available reagents were used without further purification. All dry solvents were freshly distilled under nitrogen from appropriate drying agents before use. Toluene, tetrahydrofuran, and ethyl ether were distilled from sodium-benzophenone. Dichloromethane was distilled from CaH_2. Column chromatography was performed on silica gel (200-300 mesh). ^1H NMR spectra were recorded on a 400 MHz NMR spectrometer and ^{13}C NMR spectra were recorded on a 100 MHz NMR spectrometer. IR spectra were recorded on a FT-IR spectrometer. Melting points were uncorrected. The dialkylpalladium(II) agents were prepared according to published procedures [for $Pd(CH_2SiMe_3)_2(dppe)$, see: ref. 1; for $Pd(CH_2SiMe_3)_2(cod)$, see: ref. 2; for $PdMe_2(TMEDA)$ and *cis*-$PdMe_2(PPh_3)_2$, see: ref. 3]. The chiral acids were prepared according to published procedures [for **1**, see: ref. 4; for **2a**, see: ref. 5; for **3b**, see: ref. 6; for **4b**, see: ref. 7]. Other starting materials were purchased from commercial suppliers.

Ref :

(1) R. A. Stockland, G. K. Anderson and N. P. Rath, *Organometallics*, 1997, **16**, 5096.

(2) Y. Pan and G. B. Young, *J. Organomet. Chem.*, 1999, **577**, 257.

(3) W. D. Graaf, J. Boersma, W. J. J. Smeets, A. L. Spek and G. V. Koten, *Organometallics*, 1989, **8**, 2907.

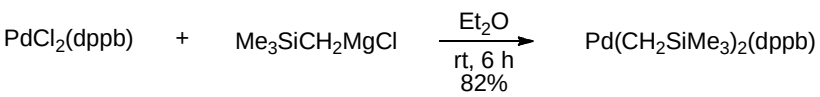
(4) K. Mikami, H. Kakuno and K. Aikawa, *Angew. Chem., Int. Ed.*, 2005, **44**, 7257.

(5) T. Ohta, M. Ito, K. Inagaki and H. Takaya, *Tetrahedron Lett.*, 1993, **34**, 1615.

(6) A. Korostylev, V. I. Tararov, C. Fischer, A. Monsees and A. Börner, *J. Org. Chem.*, 2004, **69**, 3220.

(7) D. Sälinger and R. Brückner, *Chem.-Eur. J.*, 2009, **15**, 6688.

Preparation of $Pd(CH_2SiMe_3)_2(dppb)$



To a suspension of $PdCl_2(dppb)$ (0.604 g, 1.0 mmol) in Et_2O (30 mL) in a two-necked

round bottom flask under N_2 was added Me_3SiCH_2MgCl (1.0 M in Et_2O) (8.0 mL, 8.0 mmol) dropwise at rt. Upon stirring at rt for 6 h, the reaction mixture was quenched with methanol and concentrated. A suspension of the resulting solid in Et_2O was stirred at -78 ^oC for 30 min and quickly filtered to remove the solid. The filtrate was concentrated. A suspension of the resulting solid in hexane was stirred at -78 ^oC for 30 min and quickly filtered. The filter funnel with the cake was moved onto another flask, and the cake was rinsed with CH_2Cl_2 to dissolve the desired compound and leave any solid impurity on the filter paper. The resulting filtrate was concentrated under vacuum to give the title compound as pink solid (0.583 g, 82%). decomp. 127 ^oC; IR (film) 3054, 2942, 1484, 1435, 1235 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62-7.33 (m, 20H), 2.36-2.26 (m, 4H), 1.87-1.72 (m, 4H), 0.36-0.27 (m, 4H), -0.22 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 136.3, 136.2, 133.94, 133.91, 133.88, 129.5, 128.4, 128.35, 128.30, 27.9, 27.8, 27.7, 25.2, 25.13, 25.08, 9.4, 9.3, 8.4, 8.3, 4.2; ^{31}P NMR ($CDCl_3$): 16.13 (s); HRMS (ESI) Calcd for $C_{32}H_{39}P_2PdSi$ (M-CH_2SiMe_3): 619.1338; Found: 619.1336.

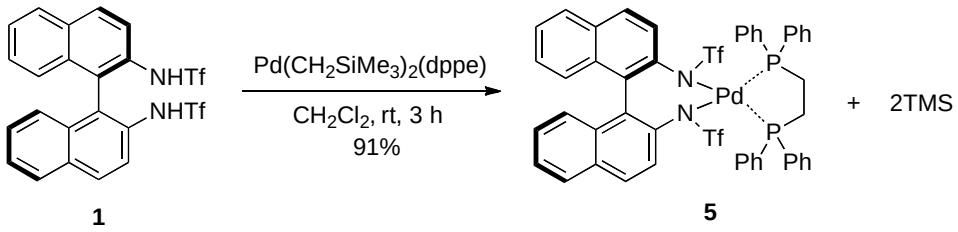
Ref :

(1) A. L. Seligson and W. C. Trogler, *Organometallics*, 1993, **12**, 744.

(2) R. A. Stockland, G. K. Anderson and N. P. Rath, *Organometallics*, 1997, **16**, 5096.

(3) Y. Pan and G. B. Young, *J. Organomet. Chem.*, 1999, **577**, 257.

Preparation of Compound 5

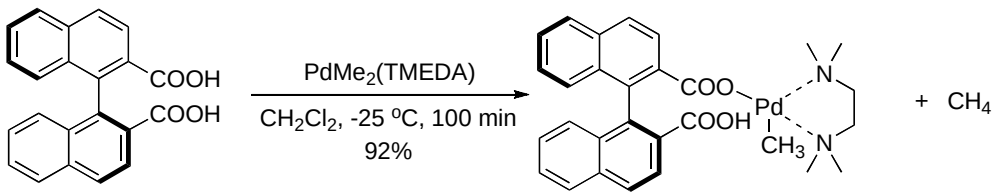


1 **5**

To a solution of $Pd(CH_2SiMe_3)_2(dppe)$ (0.041 g, 0.060 mmol) in CH_2Cl_2 (0.4 mL) in the Schlenk tube under N_2 was added a solution of (*R*)-DABNTf (0.033 g, 0.060 mmol) in CH_2Cl_2 (0.6 mL). After the reaction mixture was stirred at rt for 3 h, hexane was added. The resulting suspension was filtered. The filter cake was washed with hexane and dried

under vacuum to give complex **5** as orange solid (0.058 g, 91%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Hexane solvent at rt). mp. 205-209 ^oC; $[\alpha]^{20}_D$ = +98.1 (*c* 1.06, $CHCl_3$); IR (film) 3056, 1437, 1328, 1170 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.17-8.07 (m, 4H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.68-7.61 (m, 2H), 7.60-7.48 (m, 10H), 7.46-7.38 (m, 4H), 7.37-7.29 (m, 2H), 7.11-7.03 (m, 4H), 6.95 (d, *J* = 8.4 Hz, 2H), 2.51-2.28 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 135.0, 134.4, 134.3, 133.9, 133.8, 132.8, 132.4, 132.3, 130.4, 129.8, 129.7, 129.6, 129.2, 129.0, 128.8, 128.7, 128.6, 128.5, 127.5, 125.1, 125.0, 124.7, 121.5, 118.2, 114.9, 28.5, 28.4, 28.2, 28.1; ^{31}P NMR ($CDCl_3$): 54.73 (s); HRMS (ESI) Calcd for $C_{48}H_{37}F_6N_2O_4P_2PdS_2$ (M+H): 1051.0619; Found: 1051.0616.

Preparation of Compound 6a

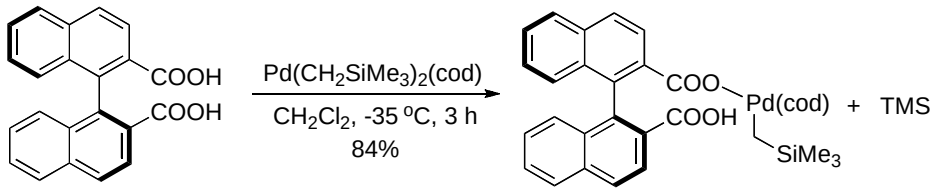


2a **6a**

To a solution of $PdMe_2$(TMEDA) (0.025 g, 0.10 mmol) in CH_2Cl_2 (0.3 mL) in the Schlenk tube under N_2 was added a solution of (*S*)-1,1'-binaphthyl-2,2'-dicarboxylic acid (0.034 g, 0.10 mmol) in CH_2Cl_2 (2.7 mL). After the reaction mixture was stirred at -25 ^oC for 100 min, pentane was added. The resulting suspension was filtered. The filter cake was washed with pentane, dissolved in $CHCl_3$ and concentrated under vacuum to give complex **6a** as white solid (0.054 g, 92%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Pentane solvent at rt). decomp. 210 ^oC; $[\alpha]^{20}_D$ = -185.9 (*c* 0.34, $CHCl_3$); IR (film) 3405, 2879, 1719, 1546, 1419 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 15.39 (s, 1H), 7.95 (d, *J* = 8.8 Hz, 2H), 7.90-7.79 (m, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.46-7.38 (m, 2H), 7.25-7.14 (m, 2H), 7.06-6.96 (m, 2H), 2.63-2.51 (m, 1H), 2.55 (s, 3H), 2.53 (s, 3H), 2.48-2.40 (m, 1H), 2.33-2.24 (m, 1H), 2.19-2.11 (m, 1H), 1.85 (s, 3H), 1.56 (s, 3H), 0.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.7, 171.9, 136.1, 134.7, 134.2, 133.9, 133.7, 133.0,

132.8, 131.9, 128.9, 128.4, 128.12, 128.06, 127.4, 127.3, 127.1, 126.9, 126.82, 126.79, 125.1, 124.3, 63.7, 57.3, 51.7, 51.2, 47.6, 46.7, -2.4; HRMS (ESI) Calcd for $C_{29}H_{33}N_2O_4Pd$ (M+H): 579.1481; Found: 579.1486.

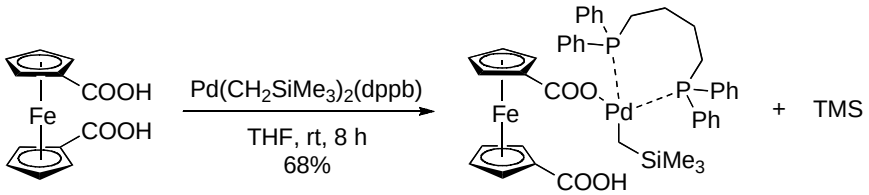
Preparation of Compound 6b



2a **6b**

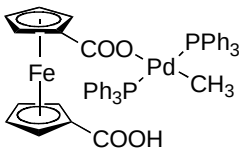
A solution of (*S*)-1,1'-binaphthyl-2,2'-dicarboxylic acid (0.034 g, 0.10 mmol) and $Pd(CH_2SiMe_3)_2(cod)$ (0.039 g, 0.10 mmol) in CH_2Cl_2 (1 mL) in the Schlenk Tube was stirred at -35 °C under N_2 for 3 h. Upon addition of pentane, the reaction mixture was filtered. The filter cake was washed with pentane and dried under vacuum to give complex **6b** as white solid (0.054 g, 84%). decomp. 172 °C; $[\alpha]^{20}_D$ = -184.8 (*c* 0.81, $CHCl_3$); IR (film) 3402, 3058, 2947, 2887, 1723, 1544, 1411 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 14.74 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 2H), 4.90-4.79 (m, 2H), 4.67-4.59 (m, 1H), 4.33-4.24 (m, 1H), 2.50-2.25 (m, 4H), 2.14-1.93 (m, 4H), 1.26 (d, *J* = 10.8 Hz, 1H), 1.07 (d, *J* = 10.8 Hz, 1H), 0.09 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 134.9, 134.1, 133.4, 132.9, 128.8, 128.1, 127.3, 127.03, 126.97, 124.4, 122.4, 122.2, 96.6, 96.4, 31.0, 30.8, 27.16, 27.15, 26.7, -1.6; Anal. Calcd for $C_{34}H_{36}O_4PdSi$: C, 63.49; H, 5.64. Found: C, 63.55; H, 5.79.

Preparation of Compound 6c



2b **6c**

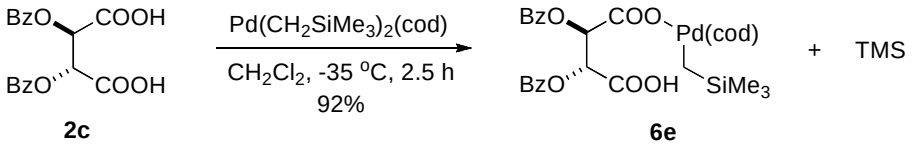
A suspension of $Pd(CH_2SiMe_3)_2(dppb)$ (0.057 g, 0.080 mmol) and 1,1'-ferrocenedicarboxylic acid (0.023 g, 0.080 mmol) in the Schlenk tube was stirred at rt under N_2 for 8 h and then centrifuged. Upon removal of the solvent, the solid was dissolved in $CHCl_3$ and filtered to remove any solid impurity. The filtrate was concentrated to give complex **6c** as yellow solid (0.048 g, 68%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Et_2O solvent at rt). decomp. 179-182 ^oC; IR (film) 3443, 3053, 2925, 1701, 1544, 1466, 1383 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 14.27 (s, 1H), 7.83-7.65 (m, 8H), 7.53-7.32 (m, 12H), 4.32-4.05 (m, 8H), 2.51-2.41 (m, 2H), 2.33-2.22 (m, 2H), 2.01-1.86 (m, 2H), 1.59-1.45 (m, 2H), 0.93-0.84 (m, 2H), -0.30 (s, 9H); ^{31}P NMR ($CDCl_3$): 33.16 (s), 15.74 (s); HRMS (ESI) Calcd for $C_{44}H_{48}FeNaO_4P_2PdSi$ (M+Na): 915.1091; Found: 915.1098.



6d, 69%

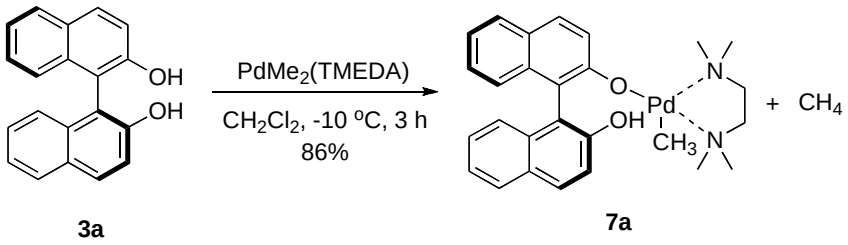
Prepared similarly as compound **6c**. Yellow solid (0.051 g, 69%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Et_2O solvent at rt). decomp. 164-166 ^oC; IR (film) 3423, 2922, 1691, 1435, 1384 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.76-7.66 (m, 12H), 7.44-7.34 (m, 18H), 4.02-3.64 (m, 8H), -0.01--0.08 (m, 3H); ^{31}P NMR ($CDCl_3$): 28.67 (s); HRMS (ESI) Calcd for $C_{49}H_{42}FeNaO_4P_2Pd$ (M+Na): 941.0854; Found: 941.0887.

Preparation of Compound 6e



A solution of $Pd(CH_2SiMe_3)_2(cod)$ (0.058 g, 0.15 mmol) in CH_2Cl_2 (0.3 mL) in the Schlenk Tube under N_2 was added a solution of dibenzoyl-L-tartaric acid (0.054 g, 0.15 mmol) in CH_2Cl_2 (0.7 mL). After the reaction mixture was stirred at -35 °C for 3 h, pentane was added. The resulting suspension was filtered. The filter cake was washed with pentane and dried under vacuum to give complex **6e** as white solid (0.091 g, 92%). mp. 104-106 °C; $[\alpha]^{20}_D$ = +1.89 (*c* 1.32, $CHCl_3$); IR (film) 3434, 2947, 2888, 1719, 1271, 1116 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.12-8.04 (m, 4H), 7.54-7.46 (m, 2H), 7.42-7.33 (m, 4H), 5.95 (s, 2H), 5.82-5.72 (m, 1H), 5.67-5.58 (m, 1H), 5.01-4.93 (m, 1H), 4.91-4.84 (m, 1H), 2.66-2.47 (m, 2H), 2.46-2.29 (m, 4H), 2.28-2.14 (m, 2H), 1.29 (d, *J* = 10.4 Hz, 1H), 1.11 (d, *J* = 10.4 Hz, 1H), 0.03 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 165.5, 133.0, 130.1, 129.6, 128.2, 122.5, 122.4, 96.7, 95.9, 73.0, 30.9, 30.6, 27.4, 27.1, 26.6, 1.4; HRMS (ESI) Calcd for $C_{30}H_{36}NaO_8PdSi$ (M+Na): 681.1118; Found: 681.1115.

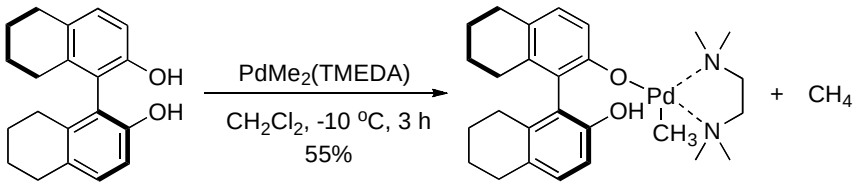
Preparation of Compound 7a



A solution of $PdMe_2(TMEDA)$ (0.051 g, 0.20 mmol) and (*S*)-BINOL (0.057 g, 0.20 mmol) in CH_2Cl_2 (0.8 mL) was stirred in the Schlenk tube at -10 °C under N_2. After the reaction mixture was stirred for 3 h, hexane was added. The resulting suspension was

filtered. The filter cake was washed with hexane and dried under vacuum to give complex **7a** as yellow solid (0.090 g, 86%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Pentane solvent at rt). decomp. 215-217 °C; $[\alpha]^{20}_D$ = +291.8 (*c* 0.77, $CHCl_3$); IR (film) 3385, 2876, 1613, 1591, 1461, 1337 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.68 (s, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.81-7.65 (m, 4H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.24-7.15 (m, 2H), 7.12-6.94 (m, 3H), 6.87 (d, *J* = 8.4 Hz, 1H), 2.60-2.48 (m, 2H), 2.56 (s, 6H), 2.36-2.26 (m, 2H), 2.30 (s, 3H), 2.15 (s, 3H), 0.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 154.1, 135.1, 134.7, 129.3, 128.7, 128.1, 127.9, 127.8, 127.2, 126.9, 126.8, 125.4, 125.3, 125.1, 122.3, 120.53, 120.48, 120.3, 116.4, 63.6, 57.3, 51.3, 51.1, 47.6, 47.4, -2.0; Anal. Calcd for $C_{27}H_{32}N_2O_2Pd$: C, 62.01; H, 6.17; N, 5.36. Found: C, 61.71; H, 6.32; N, 5.24.

Preparation of Compound 7b

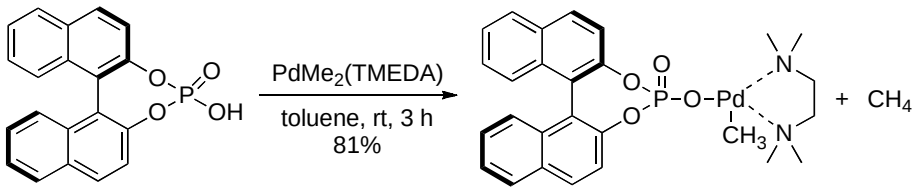


3b **7b**

To a solution of $PdMe_2$(TMEDA) (0.051 g, 0.20 mmol) in CH_2Cl_2 (0.1 mL) in the Schlenk tube under N_2 was added a solution of (*S*)-H_8-BINOL (0.059 g, 0.20 mmol) in CH_2Cl_2 (0.4 mL). After the reaction mixture was stirred at -10 °C for 3 h, hexane was added. The resulting suspension was filtered. The filter cake was washed with hexane and dried under vacuum to give complex **7b** as white solid (0.059 g, 55%) (the crystal for the X-ray structure was obtained from a CH_2Cl_2/Pentane solvent at rt). mp. 134-136 °C; $[\alpha]^{20}_D$ = +106.9 (*c* 0.29, THF); IR (film) 3483, 2921, 1584, 1461, 1278 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.4 Hz, 1H), 6.90-6.83 (m, 2H), 6.71 (d, *J* = 8.0 Hz, 1H), 5.89 (s, 1H), 2.79-2.64 (m, 4H), 2.64-2.55 (m, 2H), 2.61 (s, 3H), 2.58 (s, 3H), 2.46-2.29 (m, 4H), 2.41 (s, 3H), 2.35 (s, 3H), 2.20-2.06 (m, 2H), 1.75-1.52 (m, 8H), 0.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 151.5, 136.7, 136.6, 129.2, 128.6, 127.9, 127.2, 123.1, 122.3, 120.6, 112.6, 63.5, 57.4, 51.2, 51.1, 47.8, 29.7, 29.5, 27.73, 27.69, 23.8, 23.7, 23.53, 23.52, -2.4; HRMS

(ESI) Calcd for $C_{26}H_{37}N_2O_2Pd$ (M-CH_3): 515.1894; Found: 515.1886.

Preparation of Compound 8a

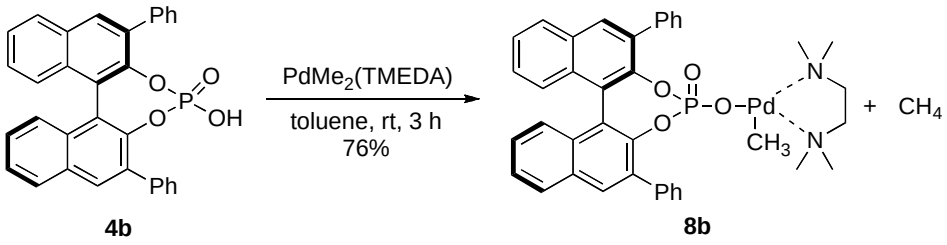


4a **8a**

A solution of (*R*)-BINOL phosphoric acid (0.052 g, 0.15 mmol) and $PdMe_2$(TMEDA) (0.038 g, 0.15 mmol) in toluene (1 mL) was stirred in the Schlenk Tube at rt under N_2. The mixture was filtered after stirring for 3 h. The filter cake was washed with pentane and dried under vacuum to give complex **8a** as white solid (0.071 g, 81%). decomp. 230 ^oC; $[\alpha]^{20}_D$ = -285.7 (*c* 0.88, $CHCl_3$); IR (film) 2883, 1591, 1464, 1270, 1099 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.95-7.85 (m, 4H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.42-7.33 (m, 4H), 7.21 (t, *J* = 8.0 Hz, 2H), 2.60-2.52 (m, 2H), 2.58 (s, 3H), 2.56 (s, 3H), 2.47 (s, 3H), 2.42 (s, 3H), 2.37-2.32 (m, 2H), 0.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 149.4, 132.8, 131.3, 130.2, 128.3, 127.3, 126.0, 124.8, 122.40, 122.38, 122.34, 122.32, 64.0, 57.2, 51.7, 51.6, 47.4, 47.3, -1.5; ^{31}P NMR ($CDCl_3$): 9.73 (s); Anal. Calcd for $C_{27}H_{31}N_2O_4PPd$: C, 55.44; H, 5.34; N, 4.79. Found: C, 55.30; H, 5.25; N, 4.97.

Ref : J. Kanada and M. Tanaka, *Adv. Synth. Catal.*, 2011, **353**, 890.

Preparation of Compound 8b

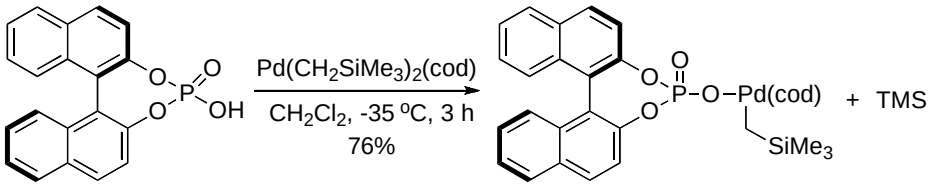


4b **8b**

A solution of (*R*)-3,3'-biphenyl-BINOL phosphoric acid (0.050 g, 0.10 mmol) and

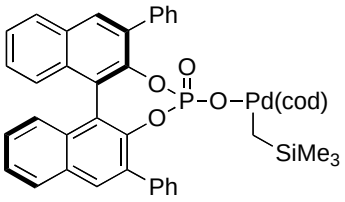
$PdMe_2$(TMEDA) (0.025 g, 0.10 mmol) in toluene (1 mL) was stirred in the Schlenk Tube at rt under N_2. The mixture was filtered after stirring for 3 h. The filter cake was washed with hexane and dried under vacuum to give complex **8b** as white solid (0.056 g, 76%). decomp. 214 °C; $[\alpha]^{20}_D$ = -233.8 (*c* 0.28, CH_2Cl_2); IR (film) 3054, 2883, 1411, 1269, 1099 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.00-7.84 (m, 8H), 7.46-7.35 (m, 6H), 7.34-7.26 (m, 4H), 7.23-7.16 (m, 2H), 2.50-2.36 (m, 2H), 2.43 (s, 3H), 2.42 (s, 3H), 2.27-2.18 (m, 1H), 2.17-2.07 (m, 1H), 1.98 (s, 3H), 1.84 (s, 3H), 0.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 147.0, 138.7, 134.6, 132.8, 131.2, 130.8, 130.6, 128.3, 128.2, 127.3, 127.1, 126.0, 125.1, 123.7, 123.6, 64.0, 57.0, 51.7, 51.4, 47.2, 46.8, -1.9; ^{31}P NMR ($CDCl_3$): 8.11 (s); HRMS (ESI) Calcd for $C_{39}H_{40}N_2O_4PPd$ (M+H): 737.1769; Found: 737.1764.

Preparation of Compound 8c



4a **8c**

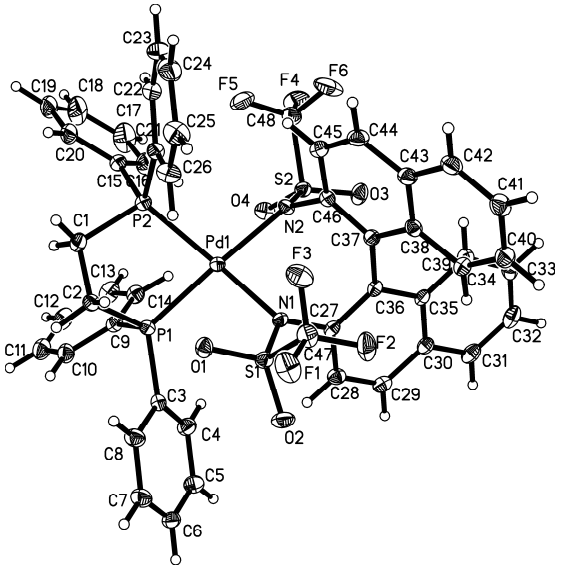
A solution of (*R*)-BINOL phosphoric acid (0.036 g, 0.10 mmol) and $Pd(CH_2SiMe_3)_2$(cod) (0.039 g, 0.10 mmol) was stirred in the Schlenk Tube at -35 °C under N_2. After the reaction mixture was stirred for 3 h, pentane was added. The resulting suspension was filtered. The filter cake was washed with pentane and dried under vacuum to give complex **8c** as white solid (0.050 g, 76%). decomp. 181 °C; $[\alpha]^{20}_D$ = -281.7 (*c* 0.82, $CHCl_3$); IR (film) 2946, 2887, 1507, 1242, 1103 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.98-7.86 (m, 4H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.43-7.35 (m, 4H), 7.27-7.20 (m, 2H), 6.19-6.08 (m, 1H), 5.94-5.83 (m, 1H), 4.93-4.84 (m, 2H), 2.68-2.30 (m, 6H), 2.27-2.15 (m, 2H), 1.43 (d, *J* = 10.0 Hz, 1H), 1.37 (d, *J* = 10.0 Hz, 1H), 0.05 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 149.3, 132.9, 131.4, 130.4, 128.4, 127.4, 126.2, 125.0, 124.31, 124.26, 122.41, 122.39, 122.2, 122.1, 95.0, 94.7, 31.2, 31.0, 30.3, 27.6, 27.3, 1.6; ^{31}P NMR ($CDCl_3$): 6.68 (s); Anal. Calcd for $C_{32}H_{35}O_4PPdSi$: C, 59.21; H, 5.43. Found: C, 59.20; H, 5.46.



8d, 70%

Prepared similarly as compound **8c**. White solid (0.056 g, 70%). decomp. 183 ^{o}C; $[\alpha]^{20}_{D}$ = -216.4 (*c* 0.81, $CHCl_3$); IR (film) 3053, 2947, 2887, 1411, 1270, 1100 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 2H), 7.93-7.86 (m, 6H), 7.46-7.37 (m, 6H), 7.36-7.29 (m, 4H), 7.26-7.19 (m, 2H), 5.52-5.43 (m, 1H), 5.18-5.09 (m, 1H), 4.75-4.62 (m, 2H), 2.48-2.22 (m, 4H), 2.21-2.02 (m, 4H), 1.08 (d, *J* =10.0 Hz, 1H), 1.02 (d, *J* =10.0 Hz, 1H), -0.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.0, 146.9, 138.6, 134.78, 134.76, 132.7, 131.2, 130.8, 130.5, 128.3, 128.2, 127.3, 127.2, 126.0, 125.1, 124.0, 123.48, 123.46, 123.4, 94.7, 94.2, 31.0, 30.8, 29.4, 27.29, 27.28, -1.3; ^{31}P NMR ($CDCl_3$): 5.17 (s); Anal. Calcd for $C_{44}H_{43}O_4PPdSi$: C, 65.95; H, 5.41. Found: C, 65.71; H, 5.43.

The X-ray Structure of Compound 5



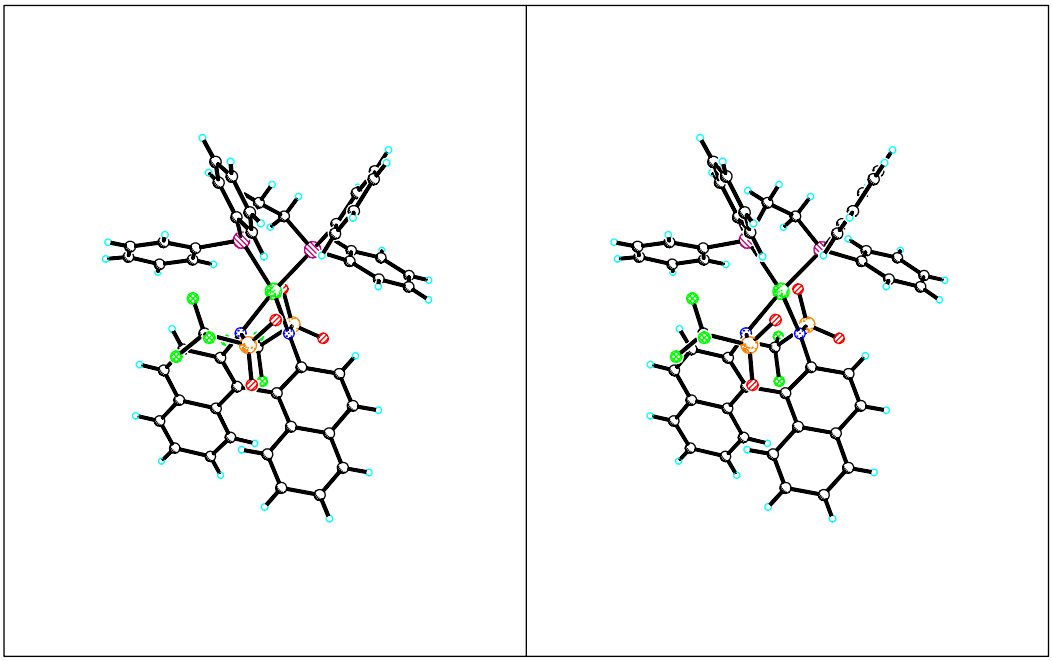


Table 1. Crystal data and structure refinement for **5**.

Identification code	sa1575
Empirical formula	C48 H36 F6 N2 O4 P2 Pd S2
Formula weight	1051.25
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 13.8039(17) A alpha = 90 deg.
	b = 14.5782(16) A beta = 90 deg.
	c = 22.466(3) A gamma = 90 deg.
Volume	4521.0(9) A^3
Z, Calculated density	4, 1.544 Mg/m^3
Absorption coefficient	0.646 mm^-1
F(000)	2128
Crystal size	0.32 x 0.31 x 0.13 mm
Theta range for data collection	2.72 to 27.48 deg.
Limiting indices	-13<=h<=17, -16<=k<=18, -14<=l<=29
Reflections collected / unique	28506 / 10315 [R(int) = 0.0519]
Completeness to theta = 27.48	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9208 and 0.8201
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10315 / 0 / 586
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0889
R indices (all data)	R1 = 0.0479, wR2 = 0.0914
Absolute structure parameter	0.01(2)
Largest diff. peak and hole	0.674 and -0.648 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	862(1)	3796(1)	9895(1)	23(1)
S(1)	1500(1)	4032(1)	8530(1)	28(1)
S(2)	-770(1)	5113(1)	10444(1)	27(1)
P(1)	1347(1)	2356(1)	9690(1)	25(1)
P(2)	1708(1)	3532(1)	10753(1)	28(1)
F(1)	2837(2)	4949(2)	7969(1)	53(1)
F(2)	1456(2)	5636(2)	7986(1)	52(1)
F(3)	2347(2)	5608(2)	8774(1)	49(1)
F(4)	-1300(2)	5617(2)	11519(1)	57(1)
F(5)	211(2)	5331(2)	11443(1)	57(1)
F(6)	-365(3)	6574(2)	11082(2)	66(1)
O(1)	2293(2)	3597(2)	8828(1)	31(1)
O(2)	1169(2)	3679(2)	7970(1)	39(1)
O(3)	-1511(2)	5682(2)	10191(1)	40(1)
O(4)	-1023(2)	4196(2)	10622(1)	34(1)
N(1)	681(2)	4236(2)	8992(1)	23(1)
N(2)	207(2)	5092(2)	10107(2)	24(1)
C(1)	2559(3)	2579(3)	10598(2)	33(1)
C(2)	2598(3)	2320(3)	9939(2)	29(1)
C(3)	1201(3)	1835(3)	8969(2)	27(1)
C(4)	268(3)	1601(3)	8796(2)	34(1)
C(5)	103(3)	1146(3)	8263(2)	40(1)
C(6)	885(4)	904(3)	7909(2)	40(1)
C(7)	1812(3)	1122(3)	8084(2)	41(1)
C(8)	1980(3)	1594(3)	8609(2)	35(1)
C(9)	760(3)	1508(2)	10161(2)	29(1)
C(10)	1128(3)	610(3)	10147(2)	37(1)
C(11)	714(4)	-44(3)	10517(2)	44(1)
C(12)	-40(4)	166(3)	10889(2)	47(1)
C(13)	-412(3)	1049(3)	10891(2)	44(1)
C(14)	-13(3)	1718(3)	10525(2)	34(1)
C(15)	1273(3)	3244(3)	11487(2)	34(1)
C(16)	290(4)	3214(3)	11618(2)	45(1)
C(17)	-26(5)	2938(4)	12169(3)	71(2)
C(18)	633(5)	2688(4)	12602(2)	73(2)
C(19)	1619(4)	2734(3)	12484(2)	57(2)

C(20)	1930(4)	3003(3)	11924(2)	41(1)
C(21)	2484(3)	4533(3)	10843(2)	31(1)
C(22)	2564(3)	5007(3)	11383(2)	40(1)
C(23)	3213(4)	5719(3)	11427(3)	50(1)
C(24)	3769(4)	5975(3)	10955(3)	50(1)
C(25)	3668(3)	5534(3)	10403(3)	49(1)
C(26)	3022(3)	4807(3)	10357(2)	43(1)
C(27)	-235(3)	4565(3)	8792(2)	25(1)
C(28)	-860(3)	3958(2)	8480(2)	30(1)
C(29)	-1753(3)	4241(3)	8298(2)	30(1)
C(30)	-2098(3)	5133(3)	8435(2)	27(1)
C(31)	-3024(3)	5436(3)	8249(2)	36(1)
C(32)	-3351(3)	6295(4)	8382(2)	43(1)
C(33)	-2760(3)	6887(3)	8715(2)	38(1)
C(34)	-1868(3)	6613(3)	8912(2)	33(1)
C(35)	-1493(3)	5736(3)	8758(2)	25(1)
C(36)	-530(3)	5456(3)	8930(2)	23(1)
C(37)	157(3)	6101(2)	9225(2)	24(1)
C(38)	503(3)	6911(3)	8927(2)	26(1)
C(39)	187(3)	7167(3)	8352(2)	30(1)
C(40)	531(3)	7936(3)	8077(2)	37(1)
C(41)	1222(3)	8501(3)	8364(2)	39(1)
C(42)	1539(3)	8278(3)	8922(2)	37(1)
C(43)	1200(3)	7484(3)	9216(2)	30(1)
C(44)	1547(3)	7236(3)	9782(2)	34(1)
C(45)	1215(3)	6471(2)	10066(2)	32(1)
C(46)	510(3)	5905(2)	9787(2)	25(1)
C(47)	2058(3)	5125(3)	8303(2)	38(1)
C(48)	-545(3)	5682(3)	11161(2)	37(1)

Table 3. Bond lengths [A] and angles [deg] for **5**.

Pd(1)-N(1)	2.144(3)
Pd(1)-N(2)	2.148(3)
Pd(1)-P(1)	2.2515(10)
Pd(1)-P(2)	2.2850(11)
S(1)-O(1)	1.432(3)
S(1)-O(2)	1.435(3)
S(1)-N(1)	1.562(3)
S(1)-C(47)	1.841(5)
S(2)-O(3)	1.435(3)
S(2)-O(4)	1.437(3)
S(2)-N(2)	1.547(3)
S(2)-C(48)	1.838(5)
P(1)-C(3)	1.800(4)
P(1)-C(2)	1.816(4)
P(1)-C(9)	1.817(4)
P(2)-C(15)	1.804(5)
P(2)-C(21)	1.822(4)
P(2)-C(1)	1.852(4)
F(1)-C(47)	1.338(5)
F(2)-C(47)	1.325(5)
F(3)-C(47)	1.332(5)
F(4)-C(48)	1.320(5)
F(5)-C(48)	1.324(5)
F(6)-C(48)	1.335(5)
N(1)-C(27)	1.426(5)
N(2)-C(46)	1.449(4)
C(1)-C(2)	1.528(6)
C(1)-H(1B)	0.9900
C(1)-H(1A)	0.9900
C(2)-H(2B)	0.9900
C(2)-H(2A)	0.9900
C(3)-C(4)	1.388(6)
C(3)-C(8)	1.391(6)
C(4)-C(5)	1.387(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.375(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.386(6)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500

C(9)-C(14)	1.379(6)
C(9)-C(10)	1.405(5)
C(10)-C(11)	1.388(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.368(7)
C(11)-H(11)	0.9500
C(12)-C(13)	1.385(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.390(6)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(20)	1.382(6)
C(15)-C(16)	1.390(6)
C(16)-C(17)	1.374(7)
C(16)-H(16)	0.9500
C(17)-C(18)	1.380(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.389(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.386(7)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(26)	1.379(6)
C(21)-C(22)	1.401(6)
C(22)-C(23)	1.375(6)
C(22)-H(22)	0.9500
C(23)-C(24)	1.361(8)
C(23)-H(23)	0.9500
C(24)-C(25)	1.404(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.389(6)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(36)	1.395(5)
C(27)-C(28)	1.420(5)
C(28)-C(29)	1.363(6)
C(28)-H(28)	0.9500
C(29)-C(30)	1.420(6)
C(29)-H(29)	0.9500
C(30)-C(35)	1.413(5)
C(30)-C(31)	1.415(5)
C(31)-C(32)	1.364(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.403(7)

C(32)-H(32)	0.9500
C(33)-C(34)	1.369(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.421(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.443(5)
C(36)-C(37)	1.491(5)
C(37)-C(46)	1.384(5)
C(37)-C(38)	1.438(5)
C(38)-C(39)	1.414(5)
C(38)-C(43)	1.431(5)
C(39)-C(40)	1.364(6)
C(39)-H(39)	0.9500
C(40)-C(41)	1.416(6)
C(40)-H(40)	0.9500
C(41)-C(42)	1.366(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.412(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.407(6)
C(44)-C(45)	1.364(5)
C(44)-H(44)	0.9500
C(45)-C(46)	1.421(5)
C(45)-H(45)	0.9500

N(1)-Pd(1)-N(2)	84.13(12)
N(1)-Pd(1)-P(1)	96.88(8)
N(2)-Pd(1)-P(1)	172.23(8)
N(1)-Pd(1)-P(2)	155.26(9)
N(2)-Pd(1)-P(2)	100.19(10)
P(1)-Pd(1)-P(2)	82.13(4)
O(1)-S(1)-O(2)	119.63(18)
O(1)-S(1)-N(1)	109.07(17)
O(2)-S(1)-N(1)	114.86(17)
O(1)-S(1)-C(47)	101.16(19)
O(2)-S(1)-C(47)	101.6(2)
N(1)-S(1)-C(47)	108.75(18)
O(3)-S(2)-O(4)	118.30(19)
O(3)-S(2)-N(2)	115.99(18)
O(4)-S(2)-N(2)	109.24(16)
O(3)-S(2)-C(48)	102.0(2)
O(4)-S(2)-C(48)	102.62(19)
N(2)-S(2)-C(48)	106.9(2)
C(3)-P(1)-C(2)	111.83(18)

C(3)-P(1)-C(9)	100.71(18)
C(2)-P(1)-C(9)	103.03(18)
C(3)-P(1)-Pd(1)	122.98(13)
C(2)-P(1)-Pd(1)	104.28(13)
C(9)-P(1)-Pd(1)	112.50(13)
C(15)-P(2)-C(21)	106.3(2)
C(15)-P(2)-C(1)	102.0(2)
C(21)-P(2)-C(1)	104.40(19)
C(15)-P(2)-Pd(1)	129.75(16)
C(21)-P(2)-Pd(1)	105.00(14)
C(1)-P(2)-Pd(1)	107.02(14)
C(27)-N(1)-S(1)	119.8(3)
C(27)-N(1)-Pd(1)	120.2(2)
S(1)-N(1)-Pd(1)	119.17(17)
C(46)-N(2)-S(2)	118.6(2)
C(46)-N(2)-Pd(1)	119.2(2)
S(2)-N(2)-Pd(1)	119.51(15)
C(2)-C(1)-P(2)	112.9(3)
C(2)-C(1)-H(1B)	109.0
P(2)-C(1)-H(1B)	109.0
C(2)-C(1)-H(1A)	109.0
P(2)-C(1)-H(1A)	109.0
H(1B)-C(1)-H(1A)	107.8
C(1)-C(2)-P(1)	104.9(3)
C(1)-C(2)-H(2B)	110.8
P(1)-C(2)-H(2B)	110.8
C(1)-C(2)-H(2A)	110.8
P(1)-C(2)-H(2A)	110.8
H(2B)-C(2)-H(2A)	108.8
C(4)-C(3)-C(8)	119.4(4)
C(4)-C(3)-P(1)	117.4(3)
C(8)-C(3)-P(1)	122.9(3)
C(5)-C(4)-C(3)	120.9(4)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	119.2(4)
C(4)-C(5)-H(5)	120.4
C(6)-C(5)-H(5)	120.4
C(7)-C(6)-C(5)	120.1(4)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	120.9(4)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5

C(7)-C(8)-C(3)	119.4(4)
C(7)-C(8)-H(8)	120.3
C(3)-C(8)-H(8)	120.3
C(14)-C(9)-C(10)	119.9(4)
C(14)-C(9)-P(1)	122.6(3)
C(10)-C(9)-P(1)	117.5(3)
C(11)-C(10)-C(9)	118.6(4)
C(11)-C(10)-H(10)	120.7
C(9)-C(10)-H(10)	120.7
C(12)-C(11)-C(10)	121.6(4)
C(12)-C(11)-H(11)	119.2
C(10)-C(11)-H(11)	119.2
C(11)-C(12)-C(13)	119.5(4)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(12)-C(13)-C(14)	120.2(4)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(9)-C(14)-C(13)	120.1(4)
C(9)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(20)-C(15)-C(16)	118.8(5)
C(20)-C(15)-P(2)	119.4(4)
C(16)-C(15)-P(2)	121.7(4)
C(17)-C(16)-C(15)	120.7(5)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(18)	120.3(6)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	119.9(5)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(20)-C(19)-C(18)	119.4(5)
C(20)-C(19)-H(19)	120.3
C(18)-C(19)-H(19)	120.3
C(15)-C(20)-C(19)	120.9(5)
C(15)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(26)-C(21)-C(22)	120.1(4)
C(26)-C(21)-P(2)	117.4(3)
C(22)-C(21)-P(2)	122.5(4)
C(23)-C(22)-C(21)	119.1(5)
C(23)-C(22)-H(22)	120.4

C(21)-C(22)-H(22)	120.4
C(24)-C(23)-C(22)	121.2(5)
C(24)-C(23)-H(23)	119.4
C(22)-C(23)-H(23)	119.4
C(23)-C(24)-C(25)	120.4(4)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(26)-C(25)-C(24)	118.7(5)
C(26)-C(25)-H(25)	120.7
C(24)-C(25)-H(25)	120.7
C(21)-C(26)-C(25)	120.4(5)
C(21)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(36)-C(27)-C(28)	120.9(4)
C(36)-C(27)-N(1)	120.1(3)
C(28)-C(27)-N(1)	118.9(3)
C(29)-C(28)-C(27)	120.5(4)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	121.0(4)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(35)-C(30)-C(31)	119.4(4)
C(35)-C(30)-C(29)	118.9(4)
C(31)-C(30)-C(29)	121.7(4)
C(32)-C(31)-C(30)	121.4(4)
C(32)-C(31)-H(31)	119.3
C(30)-C(31)-H(31)	119.3
C(31)-C(32)-C(33)	119.3(4)
C(31)-C(32)-H(32)	120.4
C(33)-C(32)-H(32)	120.4
C(34)-C(33)-C(32)	121.0(4)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	120.8(4)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(30)-C(35)-C(34)	118.0(4)
C(30)-C(35)-C(36)	120.4(4)
C(34)-C(35)-C(36)	121.7(4)
C(27)-C(36)-C(35)	118.2(4)
C(27)-C(36)-C(37)	120.0(3)
C(35)-C(36)-C(37)	121.7(3)
C(46)-C(37)-C(38)	118.5(3)

C(46)-C(37)-C(36)	120.0(3)
C(38)-C(37)-C(36)	121.5(3)
C(39)-C(38)-C(43)	117.8(4)
C(39)-C(38)-C(37)	122.7(4)
C(43)-C(38)-C(37)	119.5(4)
C(40)-C(39)-C(38)	121.6(4)
C(40)-C(39)-H(39)	119.2
C(38)-C(39)-H(39)	119.2
C(39)-C(40)-C(41)	120.4(4)
C(39)-C(40)-H(40)	119.8
C(41)-C(40)-H(40)	119.8
C(42)-C(41)-C(40)	119.6(4)
C(42)-C(41)-H(41)	120.2
C(40)-C(41)-H(41)	120.2
C(41)-C(42)-C(43)	121.3(4)
C(41)-C(42)-H(42)	119.4
C(43)-C(42)-H(42)	119.4
C(44)-C(43)-C(42)	121.4(4)
C(44)-C(43)-C(38)	119.3(4)
C(42)-C(43)-C(38)	119.3(4)
C(45)-C(44)-C(43)	121.2(4)
C(45)-C(44)-H(44)	119.4
C(43)-C(44)-H(44)	119.4
C(44)-C(45)-C(46)	119.9(4)
C(44)-C(45)-H(45)	120.0
C(46)-C(45)-H(45)	120.0
C(37)-C(46)-C(45)	121.6(4)
C(37)-C(46)-N(2)	121.4(3)
C(45)-C(46)-N(2)	117.0(4)
F(2)-C(47)-F(3)	108.6(4)
F(2)-C(47)-F(1)	108.0(4)
F(3)-C(47)-F(1)	107.9(4)
F(2)-C(47)-S(1)	111.9(3)
F(3)-C(47)-S(1)	111.3(3)
F(1)-C(47)-S(1)	109.0(3)
F(4)-C(48)-F(5)	107.7(4)
F(4)-C(48)-F(6)	107.3(4)
F(5)-C(48)-F(6)	107.0(4)
F(4)-C(48)-S(2)	111.6(3)
F(5)-C(48)-S(2)	112.2(3)
F(6)-C(48)-S(2)	110.8(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	25(1)	23(1)	20(1)	-1(1)	0(1)	2(1)
S(1)	29(1)	31(1)	23(1)	-1(1)	2(1)	2(1)
S(2)	28(1)	30(1)	23(1)	-2(1)	1(1)	2(1)
P(1)	26(1)	26(1)	23(1)	-4(1)	1(1)	4(1)
P(2)	32(1)	27(1)	23(1)	-1(1)	-3(1)	2(1)
F(1)	46(2)	52(2)	62(2)	12(2)	28(2)	6(1)
F(2)	59(2)	48(2)	50(2)	20(1)	12(2)	19(1)
F(3)	51(2)	37(1)	59(2)	-6(1)	7(2)	-11(1)
F(4)	55(2)	82(2)	34(2)	-13(2)	18(2)	3(2)
F(5)	55(2)	79(2)	38(2)	-18(2)	-16(2)	10(2)
F(6)	113(3)	39(2)	47(2)	-17(1)	18(2)	-10(2)
O(1)	26(1)	37(2)	32(2)	4(1)	3(1)	6(1)
O(2)	41(2)	52(2)	25(2)	-12(1)	2(1)	2(1)
O(3)	34(2)	54(2)	33(2)	6(2)	3(1)	15(1)
O(4)	37(2)	35(1)	30(2)	0(1)	8(1)	-8(1)
N(1)	26(2)	27(2)	17(2)	-1(1)	0(1)	3(1)
N(2)	29(2)	19(1)	23(2)	-2(1)	5(2)	2(1)
C(1)	30(2)	34(2)	33(2)	1(2)	-7(2)	3(2)
C(2)	27(2)	33(2)	27(2)	-4(2)	1(2)	7(2)
C(3)	30(2)	25(2)	27(2)	0(2)	-1(2)	5(2)
C(4)	32(2)	40(2)	31(2)	-3(2)	-3(2)	0(2)
C(5)	41(2)	38(2)	39(3)	-7(2)	-9(2)	-3(2)
C(6)	68(3)	26(2)	27(2)	-2(2)	-10(3)	4(2)
C(7)	47(3)	44(2)	32(2)	-3(2)	9(2)	9(2)
C(8)	34(2)	39(2)	32(2)	-7(2)	5(2)	2(2)
C(9)	28(2)	32(2)	26(2)	-1(2)	-2(2)	-1(2)
C(10)	39(2)	34(2)	37(2)	5(2)	-2(2)	5(2)
C(11)	48(3)	41(2)	44(3)	10(2)	-7(2)	0(2)
C(12)	51(3)	49(3)	42(3)	19(2)	-6(2)	-13(2)
C(13)	28(2)	62(3)	42(3)	10(2)	3(2)	-7(2)
C(14)	26(2)	39(2)	36(2)	0(2)	-1(2)	-2(2)
C(15)	48(3)	31(2)	24(2)	-1(2)	-5(2)	7(2)
C(16)	54(3)	49(3)	31(3)	9(2)	6(2)	11(2)
C(17)	75(4)	86(4)	52(4)	26(3)	29(3)	23(3)
C(18)	103(5)	83(4)	34(3)	27(3)	21(3)	43(4)
C(19)	89(4)	53(3)	30(3)	8(2)	-4(3)	31(3)
C(20)	58(3)	37(2)	30(3)	6(2)	-3(2)	12(2)
C(21)	30(2)	30(2)	33(2)	-5(2)	-4(2)	5(2)

C(22)	50(3)	34(2)	36(3)	−5(2)	−8(2)	7(2)
C(23)	57(3)	38(3)	54(3)	−14(2)	−22(3)	−2(2)
C(24)	40(3)	35(3)	76(4)	−9(2)	−15(3)	−5(2)
C(25)	40(3)	44(3)	62(4)	−4(2)	7(3)	−9(2)
C(26)	45(3)	39(2)	45(3)	−9(2)	3(2)	−4(2)
C(27)	27(2)	30(2)	18(2)	2(2)	−1(2)	0(2)
C(28)	35(2)	27(2)	27(2)	−1(2)	−1(2)	−7(2)
C(29)	33(2)	33(2)	24(2)	2(2)	−1(2)	−11(2)
C(30)	27(2)	34(2)	21(2)	4(2)	2(2)	−2(2)
C(31)	26(2)	54(3)	29(2)	6(2)	−2(2)	−4(2)
C(32)	31(2)	62(3)	34(3)	13(2)	−2(2)	9(2)
C(33)	34(2)	40(2)	40(3)	7(2)	7(2)	14(2)
C(34)	34(2)	34(2)	31(2)	0(2)	0(2)	7(2)
C(35)	25(2)	31(2)	19(2)	2(2)	−4(2)	2(2)
C(36)	23(2)	26(2)	20(2)	4(2)	−1(2)	−1(2)
C(37)	26(2)	22(2)	25(2)	0(2)	−1(2)	−3(2)
C(38)	28(2)	24(2)	27(2)	−1(2)	4(2)	3(2)
C(39)	33(2)	30(2)	26(2)	2(2)	−1(2)	1(2)
C(40)	44(3)	36(2)	32(2)	4(2)	3(2)	2(2)
C(41)	49(3)	30(2)	38(3)	5(2)	6(2)	−3(2)
C(42)	48(3)	26(2)	36(3)	−4(2)	1(2)	−3(2)
C(43)	31(2)	27(2)	32(2)	−4(2)	−1(2)	−2(2)
C(44)	39(2)	30(2)	33(3)	−6(2)	−4(2)	−9(2)
C(45)	36(2)	32(2)	28(2)	−2(2)	−4(2)	−1(2)
C(46)	29(2)	21(2)	25(2)	0(2)	−1(2)	1(1)
C(47)	39(2)	39(2)	35(3)	6(2)	13(2)	4(2)
C(48)	41(3)	38(2)	32(3)	−4(2)	5(2)	5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(1B)	3216	2759	10731	39
H(1A)	2360	2035	10832	39
H(2B)	2873	1698	9887	35
H(2A)	2999	2763	9714	35
H(4)	-264	1755	9045	41
H(5)	-539	1002	8142	47
H(6)	781	587	7545	48
H(7)	2344	946	7841	49
H(8)	2622	1751	8722	42
H(10)	1649	453	9890	44
H(11)	959	-653	10513	53
H(12)	-305	-289	11143	57
H(13)	-942	1197	11143	52
H(14)	-273	2322	10525	41
H(16)	-169	3386	11323	54
H(17)	-700	2920	12253	85
H(18)	411	2484	12980	88
H(19)	2077	2582	12784	69
H(20)	2604	3021	11839	50
H(22)	2176	4838	11714	48
H(23)	3274	6039	11794	60
H(24)	4228	6455	10999	61
H(25)	4035	5728	10068	58
H(26)	2950	4496	9988	52
H(28)	-653	3349	8398	36
H(29)	-2150	3834	8076	36
H(31)	-3427	5032	8028	44
H(32)	-3971	6491	8250	51
H(33)	-2983	7488	8804	45
H(34)	-1495	7013	9154	40
H(39)	-275	6796	8152	36
H(40)	304	8093	7691	45
H(41)	1465	9032	8170	47
H(42)	1995	8663	9115	44
H(44)	2022	7608	9971	41
H(45)	1455	6316	10449	38

Table 6. Torsion angles [deg] for **5**.

N(1)-Pd(1)-P(1)-C(3)	-15.13(18)
N(2)-Pd(1)-P(1)-C(3)	81.9(7)
P(2)-Pd(1)-P(1)-C(3)	-170.20(17)
N(1)-Pd(1)-P(1)-C(2)	113.38(17)
N(2)-Pd(1)-P(1)-C(2)	-149.6(7)
P(2)-Pd(1)-P(1)-C(2)	-41.69(15)
N(1)-Pd(1)-P(1)-C(9)	-135.69(16)
N(2)-Pd(1)-P(1)-C(9)	-38.7(7)
P(2)-Pd(1)-P(1)-C(9)	69.24(14)
N(1)-Pd(1)-P(2)-C(15)	168.7(3)
N(2)-Pd(1)-P(2)-C(15)	70.6(2)
P(1)-Pd(1)-P(2)-C(15)	-101.91(18)
N(1)-Pd(1)-P(2)-C(21)	41.8(2)
N(2)-Pd(1)-P(2)-C(21)	-56.31(16)
P(1)-Pd(1)-P(2)-C(21)	131.20(14)
N(1)-Pd(1)-P(2)-C(1)	-68.7(2)
N(2)-Pd(1)-P(2)-C(1)	-166.88(16)
P(1)-Pd(1)-P(2)-C(1)	20.63(15)
O(1)-S(1)-N(1)-C(27)	-172.2(3)
O(2)-S(1)-N(1)-C(27)	-34.8(3)
C(47)-S(1)-N(1)-C(27)	78.3(3)
O(1)-S(1)-N(1)-Pd(1)	-2.9(2)
O(2)-S(1)-N(1)-Pd(1)	134.52(19)
C(47)-S(1)-N(1)-Pd(1)	-112.4(2)
N(2)-Pd(1)-N(1)-C(27)	-50.4(3)
P(1)-Pd(1)-N(1)-C(27)	121.9(3)
P(2)-Pd(1)-N(1)-C(27)	-152.0(2)
N(2)-Pd(1)-N(1)-S(1)	140.36(19)
P(1)-Pd(1)-N(1)-S(1)	-47.40(18)
P(2)-Pd(1)-N(1)-S(1)	38.7(3)
O(3)-S(2)-N(2)-C(46)	31.3(4)
O(4)-S(2)-N(2)-C(46)	168.0(3)
C(48)-S(2)-N(2)-C(46)	-81.6(3)
O(3)-S(2)-N(2)-Pd(1)	-130.2(2)
O(4)-S(2)-N(2)-Pd(1)	6.6(3)
C(48)-S(2)-N(2)-Pd(1)	116.9(2)
N(1)-Pd(1)-N(2)-C(46)	-43.3(3)
P(1)-Pd(1)-N(2)-C(46)	-141.2(6)
P(2)-Pd(1)-N(2)-C(46)	112.1(3)
N(1)-Pd(1)-N(2)-S(2)	118.0(2)
P(1)-Pd(1)-N(2)-S(2)	20.1(9)
P(2)-Pd(1)-N(2)-S(2)	-86.6(2)

C(15)-P(2)-C(1)-C(2)	147.3(3)
C(21)-P(2)-C(1)-C(2)	-102.1(3)
Pd(1)-P(2)-C(1)-C(2)	8.8(3)
P(2)-C(1)-C(2)-P(1)	-41.4(3)
C(3)-P(1)-C(2)-C(1)	-167.5(3)
C(9)-P(1)-C(2)-C(1)	-60.1(3)
Pd(1)-P(1)-C(2)-C(1)	57.5(3)
C(2)-P(1)-C(3)-C(4)	163.6(3)
C(9)-P(1)-C(3)-C(4)	54.8(4)
Pd(1)-P(1)-C(3)-C(4)	-71.2(4)
C(2)-P(1)-C(3)-C(8)	-11.0(4)
C(9)-P(1)-C(3)-C(8)	-119.8(4)
Pd(1)-P(1)-C(3)-C(8)	114.2(3)
C(8)-C(3)-C(4)-C(5)	-1.2(7)
P(1)-C(3)-C(4)-C(5)	-176.0(3)
C(3)-C(4)-C(5)-C(6)	1.6(7)
C(4)-C(5)-C(6)-C(7)	-0.6(7)
C(5)-C(6)-C(7)-C(8)	-0.8(7)
C(6)-C(7)-C(8)-C(3)	1.2(7)
C(4)-C(3)-C(8)-C(7)	-0.2(6)
P(1)-C(3)-C(8)-C(7)	174.3(3)
C(3)-P(1)-C(9)-C(14)	-122.1(4)
C(2)-P(1)-C(9)-C(14)	122.2(4)
Pd(1)-P(1)-C(9)-C(14)	10.5(4)
C(3)-P(1)-C(9)-C(10)	58.3(4)
C(2)-P(1)-C(9)-C(10)	-57.3(4)
Pd(1)-P(1)-C(9)-C(10)	-169.0(3)
C(14)-C(9)-C(10)-C(11)	-1.7(6)
P(1)-C(9)-C(10)-C(11)	177.8(3)
C(9)-C(10)-C(11)-C(12)	0.3(7)
C(10)-C(11)-C(12)-C(13)	1.1(7)
C(11)-C(12)-C(13)-C(14)	-1.0(7)
C(10)-C(9)-C(14)-C(13)	1.7(6)
P(1)-C(9)-C(14)-C(13)	-177.7(3)
C(12)-C(13)-C(14)-C(9)	-0.4(7)
C(21)-P(2)-C(15)-C(20)	-61.6(4)
C(1)-P(2)-C(15)-C(20)	47.5(4)
Pd(1)-P(2)-C(15)-C(20)	172.0(3)
C(21)-P(2)-C(15)-C(16)	121.7(4)
C(1)-P(2)-C(15)-C(16)	-129.2(4)
Pd(1)-P(2)-C(15)-C(16)	-4.7(5)
C(20)-C(15)-C(16)-C(17)	-0.8(8)
P(2)-C(15)-C(16)-C(17)	175.9(4)
C(15)-C(16)-C(17)-C(18)	0.1(9)

C(16)-C(17)-C(18)-C(19)	1.4(10)
C(17)-C(18)-C(19)-C(20)	-2.1(9)
C(16)-C(15)-C(20)-C(19)	0.0(7)
P(2)-C(15)-C(20)-C(19)	-176.8(4)
C(18)-C(19)-C(20)-C(15)	1.4(8)
C(15)-P(2)-C(21)-C(26)	170.6(3)
C(1)-P(2)-C(21)-C(26)	63.2(4)
Pd(1)-P(2)-C(21)-C(26)	-49.2(4)
C(15)-P(2)-C(21)-C(22)	-7.9(4)
C(1)-P(2)-C(21)-C(22)	-115.3(4)
Pd(1)-P(2)-C(21)-C(22)	132.3(3)
C(26)-C(21)-C(22)-C(23)	-2.7(7)
P(2)-C(21)-C(22)-C(23)	175.8(3)
C(21)-C(22)-C(23)-C(24)	0.6(7)
C(22)-C(23)-C(24)-C(25)	2.2(8)
C(23)-C(24)-C(25)-C(26)	-2.8(8)
C(22)-C(21)-C(26)-C(25)	2.0(7)
P(2)-C(21)-C(26)-C(25)	-176.5(4)
C(24)-C(25)-C(26)-C(21)	0.7(7)
S(1)-N(1)-C(27)-C(36)	-112.4(4)
Pd(1)-N(1)-C(27)-C(36)	78.4(4)
S(1)-N(1)-C(27)-C(28)	71.0(4)
Pd(1)-N(1)-C(27)-C(28)	-98.2(4)
C(36)-C(27)-C(28)-C(29)	1.4(6)
N(1)-C(27)-C(28)-C(29)	178.0(4)
C(27)-C(28)-C(29)-C(30)	-2.6(6)
C(28)-C(29)-C(30)-C(35)	0.9(6)
C(28)-C(29)-C(30)-C(31)	-179.9(4)
C(35)-C(30)-C(31)-C(32)	-0.7(6)
C(29)-C(30)-C(31)-C(32)	-179.8(4)
C(30)-C(31)-C(32)-C(33)	-0.7(7)
C(31)-C(32)-C(33)-C(34)	-0.5(7)
C(32)-C(33)-C(34)-C(35)	3.3(7)
C(31)-C(30)-C(35)-C(34)	3.4(6)
C(29)-C(30)-C(35)-C(34)	-177.5(4)
C(31)-C(30)-C(35)-C(36)	-177.3(4)
C(29)-C(30)-C(35)-C(36)	1.8(6)
C(33)-C(34)-C(35)-C(30)	-4.7(6)
C(33)-C(34)-C(35)-C(36)	176.0(4)
C(28)-C(27)-C(36)-C(35)	1.3(6)
N(1)-C(27)-C(36)-C(35)	-175.3(3)
C(28)-C(27)-C(36)-C(37)	-176.3(4)
N(1)-C(27)-C(36)-C(37)	7.2(6)
C(30)-C(35)-C(36)-C(27)	-2.9(6)

C(34)-C(35)-C(36)-C(27)	176.4(4)
C(30)-C(35)-C(36)-C(37)	174.6(4)
C(34)-C(35)-C(36)-C(37)	-6.1(6)
C(27)-C(36)-C(37)-C(46)	-62.9(5)
C(35)-C(36)-C(37)-C(46)	119.6(4)
C(27)-C(36)-C(37)-C(38)	114.2(4)
C(35)-C(36)-C(37)-C(38)	-63.3(5)
C(46)-C(37)-C(38)-C(39)	179.9(4)
C(36)-C(37)-C(38)-C(39)	2.7(6)
C(46)-C(37)-C(38)-C(43)	0.3(5)
C(36)-C(37)-C(38)-C(43)	-176.8(3)
C(43)-C(38)-C(39)-C(40)	0.0(6)
C(37)-C(38)-C(39)-C(40)	-179.6(4)
C(38)-C(39)-C(40)-C(41)	0.2(6)
C(39)-C(40)-C(41)-C(42)	-0.7(7)
C(40)-C(41)-C(42)-C(43)	0.9(7)
C(41)-C(42)-C(43)-C(44)	177.9(4)
C(41)-C(42)-C(43)-C(38)	-0.8(6)
C(39)-C(38)-C(43)-C(44)	-178.4(4)
C(37)-C(38)-C(43)-C(44)	1.2(6)
C(39)-C(38)-C(43)-C(42)	0.3(6)
C(37)-C(38)-C(43)-C(42)	179.9(4)
C(42)-C(43)-C(44)-C(45)	179.8(4)
C(38)-C(43)-C(44)-C(45)	-1.5(6)
C(43)-C(44)-C(45)-C(46)	0.4(6)
C(38)-C(37)-C(46)-C(45)	-1.5(6)
C(36)-C(37)-C(46)-C(45)	175.7(3)
C(38)-C(37)-C(46)-N(2)	-178.8(3)
C(36)-C(37)-C(46)-N(2)	-1.6(5)
C(44)-C(45)-C(46)-C(37)	1.1(6)
C(44)-C(45)-C(46)-N(2)	178.6(3)
S(2)-N(2)-C(46)-C(37)	-81.3(4)
Pd(1)-N(2)-C(46)-C(37)	80.2(4)
S(2)-N(2)-C(46)-C(45)	101.2(4)
Pd(1)-N(2)-C(46)-C(45)	-97.3(4)
O(1)-S(1)-C(47)-F(2)	176.8(3)
O(2)-S(1)-C(47)-F(2)	53.1(4)
N(1)-S(1)-C(47)-F(2)	-68.4(4)
O(1)-S(1)-C(47)-F(3)	-61.5(3)
O(2)-S(1)-C(47)-F(3)	174.8(3)
N(1)-S(1)-C(47)-F(3)	53.3(4)
O(1)-S(1)-C(47)-F(1)	57.4(4)
O(2)-S(1)-C(47)-F(1)	-66.3(4)
N(1)-S(1)-C(47)-F(1)	172.2(3)

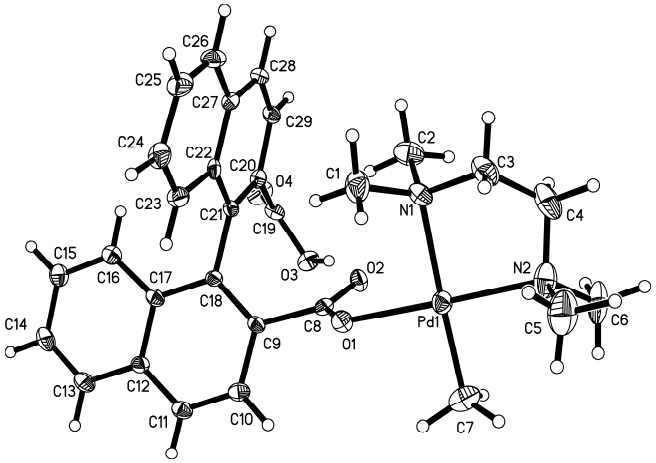
O(3)-S(2)-C(48)-F(4)	67.0(4)
O(4)-S(2)-C(48)-F(4)	-56.0(4)
N(2)-S(2)-C(48)-F(4)	-170.9(3)
O(3)-S(2)-C(48)-F(5)	-172.1(3)
O(4)-S(2)-C(48)-F(5)	64.9(4)
N(2)-S(2)-C(48)-F(5)	-50.0(4)
O(3)-S(2)-C(48)-F(6)	-52.5(4)
O(4)-S(2)-C(48)-F(6)	-175.5(3)
N(2)-S(2)-C(48)-F(6)	69.6(4)

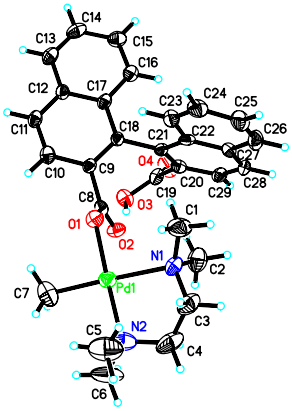
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **5** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

The X-ray structure of compound 6a





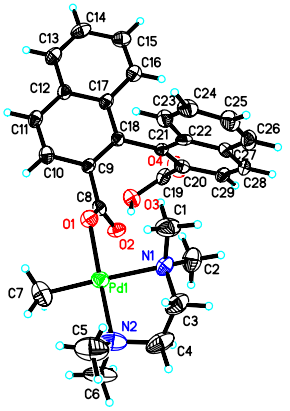


Table 1. Crystal data and structure refinement for **6a**.

Identification code	a
Empirical formula	C29 H32 N2 O4 Pd
Formula weight	578.97
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 9.5931(19) A alpha = 90 deg.
	b = 12.862(3) A beta = 113.40(3) deg.
	c = 11.787(2) A gamma = 90 deg.
Volume	1334.8(5) A^3
Z, Calculated density	2, 1.441 Mg/m^3
Absorption coefficient	0.732 mm^-1
F(000)	596
Crystal size	0.17 x 0.15 x 0.10 mm
Theta range for data collection	1.88 to 27.47 deg.
Limiting indices	-12<=h<=12, -16<=k<=16, -15<=l<=15
Reflections collected / unique	9952 / 5613 [R(int) = 0.0439]
Completeness to theta = 27.47	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.7825
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5613 / 1 / 330
Goodness-of-fit on F^2	1.102
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.0900
R indices (all data)	R1 = 0.0567, wR2 = 0.0933
Absolute structure parameter	0.03(3)
Largest diff. peak and hole	0.650 and -0.547 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	6069(1)	979(1)	1510(1)	31(1)
O(1)	6725(4)	208(3)	3171(3)	31(1)
O(2)	6276(4)	1597(3)	4103(4)	31(1)
O(3)	6340(3)	2280(3)	6156(3)	32(1)
O(4)	7896(5)	3051(4)	7844(4)	45(1)
N(1)	8341(5)	1623(3)	1948(4)	34(1)
N(2)	5527(6)	1708(5)	-191(4)	52(1)
C(1)	9554(6)	849(7)	2462(5)	51(2)
C(2)	8658(7)	2477(4)	2844(6)	49(2)
C(3)	8276(7)	1992(5)	753(6)	51(2)
C(4)	6790(8)	2464(5)	30(6)	59(2)
C(5)	5530(7)	922(10)	-1111(5)	74(2)
C(6)	4087(7)	2288(6)	-679(6)	70(2)
C(7)	3953(6)	405(5)	1054(6)	56(2)
C(8)	6664(5)	671(4)	4095(5)	25(1)
C(9)	7076(5)	46(3)	5251(4)	22(1)
C(10)	6154(5)	-835(4)	5221(5)	29(1)
C(11)	6374(5)	-1363(4)	6282(5)	27(1)
C(12)	7519(6)	-1068(4)	7424(5)	25(1)
C(13)	7752(6)	-1594(4)	8535(5)	32(1)
C(14)	8892(6)	-1329(4)	9611(5)	38(1)
C(15)	9893(6)	-510(4)	9645(5)	33(1)
C(16)	9693(5)	39(4)	8607(4)	28(1)
C(17)	8509(5)	-214(4)	7455(5)	24(1)
C(18)	8244(5)	343(3)	6345(4)	22(1)
C(19)	7722(6)	2546(4)	6946(5)	28(1)
C(20)	9035(5)	2226(4)	6631(4)	24(1)
C(21)	9263(5)	1228(3)	6346(4)	22(1)
C(22)	10582(4)	1022(6)	6085(3)	23(1)
C(23)	10961(6)	-17(4)	5843(5)	30(1)
C(24)	12218(6)	-190(5)	5609(5)	36(1)
C(25)	13118(6)	633(5)	5544(6)	41(2)
C(26)	12833(6)	1608(5)	5786(5)	35(1)
C(27)	11547(5)	1830(4)	6059(5)	25(1)
C(28)	11248(5)	2846(4)	6368(4)	30(1)
C(29)	10034(5)	3035(4)	6660(4)	27(1)

Table 3. Bond lengths [A] and angles [deg] for **6a**.

Pd(1)-C(7)	2.022(6)
Pd(1)-O(1)	2.057(3)
Pd(1)-N(2)	2.084(5)
Pd(1)-N(1)	2.193(4)
O(1)-C(8)	1.262(6)
O(2)-C(8)	1.249(6)
O(3)-C(19)	1.327(6)
O(3)-H(3)	0.8400
O(4)-C(19)	1.195(6)
N(1)-C(3)	1.464(7)
N(1)-C(1)	1.467(7)
N(1)-C(2)	1.470(7)
N(2)-C(6)	1.471(7)
N(2)-C(5)	1.483(10)
N(2)-C(4)	1.494(8)
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(1)-H(1A)	0.9800
C(2)-H(2A)	0.9800
C(2)-H(2C)	0.9800
C(2)-H(2B)	0.9800
C(3)-C(4)	1.470(8)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4B)	0.9900
C(4)-H(4A)	0.9900
C(5)-H(5A)	0.9800
C(5)-H(5C)	0.9800
C(5)-H(5B)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6C)	0.9800
C(6)-H(6B)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7C)	0.9800
C(7)-H(7B)	0.9800
C(8)-C(9)	1.494(7)
C(9)-C(18)	1.384(6)
C(9)-C(10)	1.430(6)
C(10)-C(11)	1.364(7)
C(10)-H(10)	0.9500
C(11)-C(12)	1.410(7)
C(11)-H(11)	0.9500

C(12)-C(13)	1.410(8)
C(12)-C(17)	1.444(7)
C(13)-C(14)	1.349(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.415(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.359(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.420(7)
C(16)-H(16)	0.9500
C(17)-C(18)	1.423(7)
C(18)-C(21)	1.500(6)
C(19)-C(20)	1.505(6)
C(20)-C(21)	1.366(6)
C(20)-C(29)	1.406(6)
C(21)-C(22)	1.440(5)
C(22)-C(27)	1.400(8)
C(22)-C(23)	1.443(9)
C(23)-C(24)	1.357(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.387(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.339(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.422(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.417(7)
C(28)-C(29)	1.361(7)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500

C(7)-Pd(1)-O(1)	88.4(2)
C(7)-Pd(1)-N(2)	93.9(2)
O(1)-Pd(1)-N(2)	176.06(18)
C(7)-Pd(1)-N(1)	178.2(2)
O(1)-Pd(1)-N(1)	93.37(15)
N(2)-Pd(1)-N(1)	84.33(19)
C(8)-O(1)-Pd(1)	119.5(3)
C(19)-O(3)-H(3)	108.9
C(3)-N(1)-C(1)	110.0(4)
C(3)-N(1)-C(2)	111.5(5)
C(1)-N(1)-C(2)	107.8(5)
C(3)-N(1)-Pd(1)	103.7(3)
C(1)-N(1)-Pd(1)	113.1(4)

C(2)-N(1)-Pd(1)	110.7(3)
C(6)-N(2)-C(5)	109.5(5)
C(6)-N(2)-C(4)	107.9(6)
C(5)-N(2)-C(4)	109.5(5)
C(6)-N(2)-Pd(1)	116.2(4)
C(5)-N(2)-Pd(1)	108.9(5)
C(4)-N(2)-Pd(1)	104.5(4)
N(1)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(1)-H(1A)	109.5
H(1B)-C(1)-H(1A)	109.5
H(1C)-C(1)-H(1A)	109.5
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
H(2C)-C(2)-H(2B)	109.5
N(1)-C(3)-C(4)	110.7(5)
N(1)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
N(1)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(3)-C(4)-N(2)	111.4(5)
C(3)-C(4)-H(4B)	109.4
N(2)-C(4)-H(4B)	109.4
C(3)-C(4)-H(4A)	109.4
N(2)-C(4)-H(4A)	109.4
H(4B)-C(4)-H(4A)	108.0
N(2)-C(5)-H(5A)	109.5
N(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
N(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
H(5C)-C(5)-H(5B)	109.5
N(2)-C(6)-H(6A)	109.5
N(2)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
N(2)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
H(6C)-C(6)-H(6B)	109.5
Pd(1)-C(7)-H(7A)	109.5

Pd(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
Pd(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
H(7C)-C(7)-H(7B)	109.5
O(2)-C(8)-O(1)	124.9(6)
O(2)-C(8)-C(9)	118.5(6)
O(1)-C(8)-C(9)	116.6(4)
C(18)-C(9)-C(10)	120.4(4)
C(18)-C(9)-C(8)	121.6(4)
C(10)-C(9)-C(8)	117.8(4)
C(11)-C(10)-C(9)	120.2(5)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	121.3(5)
C(10)-C(11)-H(11)	119.3
C(12)-C(11)-H(11)	119.3
C(11)-C(12)-C(13)	122.3(5)
C(11)-C(12)-C(17)	118.9(5)
C(13)-C(12)-C(17)	118.8(5)
C(14)-C(13)-C(12)	121.5(5)
C(14)-C(13)-H(13)	119.2
C(12)-C(13)-H(13)	119.2
C(13)-C(14)-C(15)	120.1(5)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	120.6(5)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(15)-C(16)-C(17)	121.1(5)
C(15)-C(16)-H(16)	119.5
C(17)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	123.2(4)
C(16)-C(17)-C(12)	117.8(4)
C(18)-C(17)-C(12)	119.0(4)
C(9)-C(18)-C(17)	120.0(4)
C(9)-C(18)-C(21)	119.8(4)
C(17)-C(18)-C(21)	120.2(4)
O(4)-C(19)-O(3)	120.8(5)
O(4)-C(19)-C(20)	122.0(5)
O(3)-C(19)-C(20)	117.2(4)
C(21)-C(20)-C(29)	121.8(4)
C(21)-C(20)-C(19)	123.3(4)
C(29)-C(20)-C(19)	114.9(4)

C(20)-C(21)-C(22)	117.8(5)
C(20)-C(21)-C(18)	123.0(4)
C(22)-C(21)-C(18)	119.2(4)
C(27)-C(22)-C(21)	120.8(6)
C(27)-C(22)-C(23)	117.5(4)
C(21)-C(22)-C(23)	121.6(5)
C(24)-C(23)-C(22)	120.4(5)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	120.5(6)
C(23)-C(24)-H(24)	119.7
C(25)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	121.3(5)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(25)-C(26)-C(27)	120.3(5)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(22)-C(27)-C(28)	118.4(5)
C(22)-C(27)-C(26)	119.8(5)
C(28)-C(27)-C(26)	121.7(5)
C(29)-C(28)-C(27)	120.7(4)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(20)	120.4(4)
C(28)-C(29)-H(29)	119.8
C(20)-C(29)-H(29)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	35(1)	32(1)	23(1)	0(1)	11(1)	-1(1)
O(1)	36(2)	29(2)	29(2)	-1(2)	14(2)	0(2)
O(2)	39(2)	24(2)	28(2)	4(2)	11(2)	6(2)
O(3)	25(2)	37(2)	37(2)	-6(2)	15(2)	4(2)
O(4)	40(2)	57(3)	42(3)	-15(2)	19(2)	-1(2)
N(1)	40(2)	31(2)	38(3)	4(2)	22(2)	-3(2)
N(2)	57(3)	69(4)	31(3)	7(3)	20(2)	21(3)
C(1)	40(3)	58(5)	55(3)	19(4)	20(2)	18(4)
C(2)	54(4)	37(3)	62(4)	-9(3)	29(3)	-7(3)
C(3)	56(4)	49(4)	59(4)	18(3)	36(3)	6(3)
C(4)	78(5)	57(4)	61(4)	24(4)	50(4)	16(4)
C(5)	100(5)	83(5)	39(3)	-3(6)	28(3)	22(7)
C(6)	61(4)	102(6)	45(4)	35(4)	18(3)	42(4)
C(7)	40(3)	60(4)	60(4)	-13(3)	12(3)	-7(3)
C(8)	17(2)	28(3)	27(3)	-1(2)	7(2)	-3(2)
C(9)	22(2)	18(2)	27(3)	2(2)	12(2)	1(2)
C(10)	29(2)	27(3)	31(3)	-6(2)	14(2)	-3(2)
C(11)	26(2)	25(3)	36(3)	0(2)	18(2)	-2(2)
C(12)	22(2)	25(3)	29(3)	1(2)	11(2)	-2(2)
C(13)	38(3)	31(3)	35(3)	5(2)	23(2)	-3(2)
C(14)	49(3)	36(3)	34(3)	13(3)	22(3)	5(3)
C(15)	38(3)	37(3)	27(3)	3(2)	15(2)	4(2)
C(16)	29(2)	29(3)	29(3)	0(2)	16(2)	0(2)
C(17)	28(2)	18(2)	30(3)	-1(2)	15(2)	0(2)
C(18)	18(2)	20(2)	30(3)	2(2)	9(2)	1(2)
C(19)	32(3)	23(3)	35(3)	1(2)	19(2)	-3(2)
C(20)	23(2)	27(3)	20(2)	1(2)	8(2)	3(2)
C(21)	25(2)	22(3)	17(2)	2(2)	6(2)	-3(2)
C(22)	21(2)	25(2)	22(2)	9(3)	8(1)	9(3)
C(23)	27(3)	30(3)	33(3)	-2(2)	12(2)	-1(2)
C(24)	31(3)	38(3)	42(3)	3(3)	16(3)	11(2)
C(25)	27(3)	56(4)	45(4)	5(3)	20(2)	2(2)
C(26)	30(3)	41(4)	40(3)	0(3)	19(3)	-8(3)
C(27)	22(3)	27(3)	22(3)	0(2)	4(2)	-3(2)
C(28)	26(2)	25(3)	34(3)	7(2)	7(2)	-8(2)
C(29)	32(2)	15(2)	30(3)	0(2)	9(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6a**.

	x	y	z	U(eq)
H(3)	6356	2185	5456	38
H(1B)	9609	621	3272	76
H(1C)	10526	1159	2553	76
H(1A)	9336	250	1904	76
H(2A)	7883	3019	2508	74
H(2C)	9661	2771	3005	74
H(2B)	8640	2212	3618	74
H(3A)	8451	1402	287	61
H(3B)	9087	2512	888	61
H(4B)	6769	2707	-774	70
H(4A)	6640	3076	478	70
H(5A)	4756	394	-1204	111
H(5C)	6531	591	-829	111
H(5B)	5304	1262	-1909	111
H(6A)	3237	1804	-857	106
H(6C)	3987	2649	-1440	106
H(6B)	4078	2799	-64	106
H(7A)	3303	943	1177	84
H(7C)	3996	-195	1579	84
H(7B)	3533	189	185	84
H(10)	5386	-1054	4459	34
H(11)	5743	-1941	6251	33
H(13)	7092	-2148	8525	39
H(14)	9024	-1694	10348	46
H(15)	10712	-342	10402	40
H(16)	10356	601	8654	33
H(23)	10328	-583	5848	36
H(24)	12483	-881	5489	44
H(25)	13953	501	5323	49
H(26)	13493	2155	5775	42
H(28)	11902	3402	6371	36
H(29)	9862	3717	6886	32

Table 6. Torsion angles [deg] for **6a**.

C(7)-Pd(1)-O(1)-C(8)	-92.0(4)
N(2)-Pd(1)-O(1)-C(8)	142(3)
N(1)-Pd(1)-O(1)-C(8)	88.1(3)
C(7)-Pd(1)-N(1)-C(3)	-12(8)
O(1)-Pd(1)-N(1)-C(3)	165.3(3)
N(2)-Pd(1)-N(1)-C(3)	-11.5(4)
C(7)-Pd(1)-N(1)-C(1)	-131(7)
O(1)-Pd(1)-N(1)-C(1)	46.2(4)
N(2)-Pd(1)-N(1)-C(1)	-130.6(4)
C(7)-Pd(1)-N(1)-C(2)	108(8)
O(1)-Pd(1)-N(1)-C(2)	-74.9(4)
N(2)-Pd(1)-N(1)-C(2)	108.3(4)
C(7)-Pd(1)-N(2)-C(6)	44.7(6)
O(1)-Pd(1)-N(2)-C(6)	170(3)
N(1)-Pd(1)-N(2)-C(6)	-135.3(5)
C(7)-Pd(1)-N(2)-C(5)	-79.5(4)
O(1)-Pd(1)-N(2)-C(5)	46(3)
N(1)-Pd(1)-N(2)-C(5)	100.5(4)
C(7)-Pd(1)-N(2)-C(4)	163.5(4)
O(1)-Pd(1)-N(2)-C(4)	-71(3)
N(1)-Pd(1)-N(2)-C(4)	-16.5(4)
C(1)-N(1)-C(3)-C(4)	160.0(6)
C(2)-N(1)-C(3)-C(4)	-80.4(6)
Pd(1)-N(1)-C(3)-C(4)	38.8(6)
N(1)-C(3)-C(4)-N(2)	-58.9(7)
C(6)-N(2)-C(4)-C(3)	168.2(5)
C(5)-N(2)-C(4)-C(3)	-72.6(7)
Pd(1)-N(2)-C(4)-C(3)	44.0(6)
Pd(1)-O(1)-C(8)-O(2)	-2.5(7)
Pd(1)-O(1)-C(8)-C(9)	176.8(3)
O(2)-C(8)-C(9)-C(18)	-58.9(7)
O(1)-C(8)-C(9)-C(18)	121.8(5)
O(2)-C(8)-C(9)-C(10)	116.8(5)
O(1)-C(8)-C(9)-C(10)	-62.5(6)
C(18)-C(9)-C(10)-C(11)	3.1(7)
C(8)-C(9)-C(10)-C(11)	-172.7(4)
C(9)-C(10)-C(11)-C(12)	-1.0(7)
C(10)-C(11)-C(12)-C(13)	179.2(5)
C(10)-C(11)-C(12)-C(17)	-2.3(7)
C(11)-C(12)-C(13)-C(14)	177.2(5)
C(17)-C(12)-C(13)-C(14)	-1.3(8)
C(12)-C(13)-C(14)-C(15)	-0.3(8)

C(13)-C(14)-C(15)-C(16)	2.0(8)
C(14)-C(15)-C(16)-C(17)	-2.0(8)
C(15)-C(16)-C(17)-C(18)	179.4(5)
C(15)-C(16)-C(17)-C(12)	0.4(7)
C(11)-C(12)-C(17)-C(16)	-177.4(5)
C(13)-C(12)-C(17)-C(16)	1.2(7)
C(11)-C(12)-C(17)-C(18)	3.6(7)
C(13)-C(12)-C(17)-C(18)	-177.8(5)
C(10)-C(9)-C(18)-C(17)	-1.7(7)
C(8)-C(9)-C(18)-C(17)	173.9(4)
C(10)-C(9)-C(18)-C(21)	176.2(4)
C(8)-C(9)-C(18)-C(21)	-8.2(7)
C(16)-C(17)-C(18)-C(9)	179.4(4)
C(12)-C(17)-C(18)-C(9)	-1.7(7)
C(16)-C(17)-C(18)-C(21)	1.6(7)
C(12)-C(17)-C(18)-C(21)	-179.5(4)
O(4)-C(19)-C(20)-C(21)	130.1(6)
O(3)-C(19)-C(20)-C(21)	-52.4(7)
O(4)-C(19)-C(20)-C(29)	-49.4(7)
O(3)-C(19)-C(20)-C(29)	128.1(5)
C(29)-C(20)-C(21)-C(22)	0.6(7)
C(19)-C(20)-C(21)-C(22)	-178.9(4)
C(29)-C(20)-C(21)-C(18)	178.1(4)
C(19)-C(20)-C(21)-C(18)	-1.4(7)
C(9)-C(18)-C(21)-C(20)	95.3(5)
C(17)-C(18)-C(21)-C(20)	-86.9(6)
C(9)-C(18)-C(21)-C(22)	-87.2(5)
C(17)-C(18)-C(21)-C(22)	90.6(5)
C(20)-C(21)-C(22)-C(27)	-3.4(6)
C(18)-C(21)-C(22)-C(27)	179.0(4)
C(20)-C(21)-C(22)-C(23)	176.5(4)
C(18)-C(21)-C(22)-C(23)	-1.1(6)
C(27)-C(22)-C(23)-C(24)	0.4(7)
C(21)-C(22)-C(23)-C(24)	-179.5(5)
C(22)-C(23)-C(24)-C(25)	-2.9(9)
C(23)-C(24)-C(25)-C(26)	4.3(10)
C(24)-C(25)-C(26)-C(27)	-3.1(11)
C(21)-C(22)-C(27)-C(28)	3.7(7)
C(23)-C(22)-C(27)-C(28)	-176.2(5)
C(21)-C(22)-C(27)-C(26)	-179.3(5)
C(23)-C(22)-C(27)-C(26)	0.7(7)
C(25)-C(26)-C(27)-C(22)	0.6(9)
C(25)-C(26)-C(27)-C(28)	177.4(6)
C(22)-C(27)-C(28)-C(29)	-1.2(7)

C(26)-C(27)-C(28)-C(29)	-178.1(5)
C(27)-C(28)-C(29)-C(20)	-1.6(8)
C(21)-C(20)-C(29)-C(28)	1.9(7)
C(19)-C(20)-C(29)-C(28)	-178.6(4)

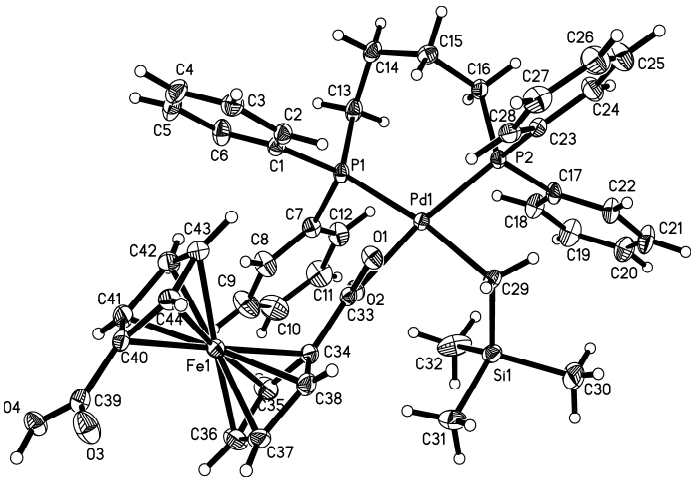
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **6a** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(2)	0.84	1.74	2.552(5)	162.2

Symmetry transformations used to generate equivalent atoms:

The X-ray structure of compound 6c



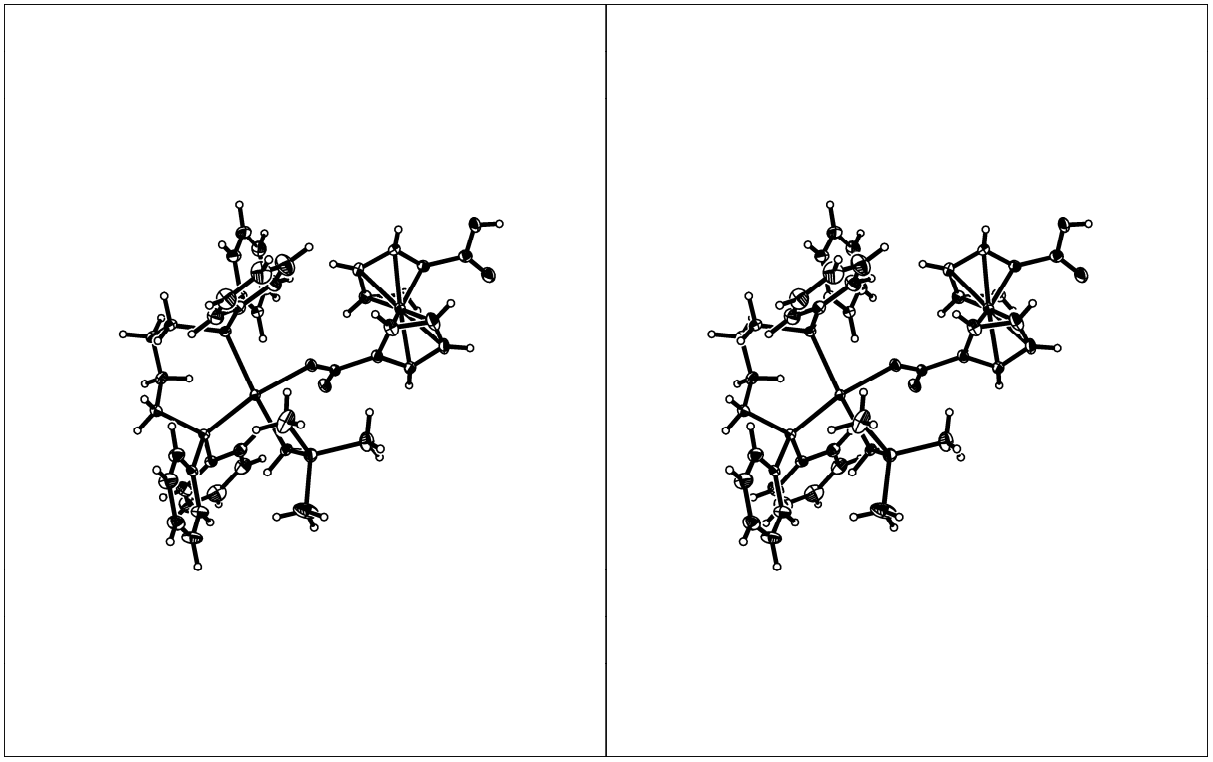


Table 1. Crystal data and structure refinement for **6c**.

Identification code	a
Empirical formula	C45 H50 Cl2 Fe O4 P2 Pd Si
Formula weight	978.03
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 12.5186(13) A alpha = 90 deg.
	b = 17.3401(18) A beta = 90 deg.
	c = 20.879(2) A gamma = 90 deg.
Volume	4532.2(8) A^3
Z, Calculated density	4, 1.433 Mg/m^3
Absorption coefficient	0.972 mm^-1
F(000)	2008
Crystal size	0.23 x 0.19 x 0.14 mm
Theta range for data collection	1.95 to 27.49 deg.
Limiting indices	-14<=h<=16, -13<=k<=22, -27<=l<=27
Reflections collected / unique	20337 / 10348 [R(int) = 0.0339]
Completeness to theta = 27.49	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.6506
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10348 / 0 / 508
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.0921
R indices (all data)	R1 = 0.0449, wR2 = 0.0944
Absolute structure parameter	-0.014(17)
Largest diff. peak and hole	0.778 and -0.528 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6c**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	5903(1)	3886(1)	7874(1)	22(1)
Fe(1)	8121(1)	2863(1)	5556(1)	28(1)
Cl(1)	1200(2)	4203(2)	6275(2)	184(2)
Cl(2)	2185(2)	4720(2)	5124(1)	134(1)
P(1)	6179(1)	5127(1)	7469(1)	26(1)
P(2)	4512(1)	4036(1)	8506(1)	25(1)
Si(1)	7204(1)	2570(1)	8662(1)	32(1)
O(1)	5976(2)	2859(2)	6743(1)	31(1)
O(2)	7194(2)	3533(2)	7278(1)	27(1)
O(3)	8888(3)	1882(2)	4027(2)	49(1)
O(4)	9986(2)	2900(2)	4104(1)	37(1)
C(1)	6011(3)	5258(2)	6610(2)	30(1)
C(2)	5404(3)	4732(2)	6270(2)	31(1)
C(3)	5182(3)	4853(3)	5625(2)	37(1)
C(4)	5584(4)	5491(3)	5318(2)	45(1)
C(5)	6213(4)	6014(3)	5645(2)	52(1)
C(6)	6420(4)	5908(2)	6293(2)	42(1)
C(7)	7561(3)	5377(2)	7642(2)	33(1)
C(8)	8375(3)	5237(3)	7215(2)	45(1)
C(9)	9437(4)	5409(4)	7367(3)	65(2)
C(10)	9679(4)	5713(3)	7957(3)	65(2)
C(11)	8872(4)	5835(3)	8398(2)	57(1)
C(12)	7822(4)	5670(3)	8246(2)	43(1)
C(13)	5450(3)	5966(2)	7779(2)	35(1)
C(14)	4253(3)	5975(2)	7625(2)	36(1)
C(15)	3636(3)	5256(2)	7819(2)	35(1)
C(16)	3865(3)	4986(2)	8507(2)	33(1)
C(17)	4807(3)	3867(2)	9349(2)	29(1)
C(18)	5491(4)	4388(3)	9646(2)	40(1)
C(19)	5807(4)	4282(3)	10275(2)	50(1)
C(20)	5465(4)	3653(3)	10608(2)	47(1)
C(21)	4806(4)	3126(3)	10318(2)	51(1)
C(22)	4467(4)	3231(3)	9687(2)	40(1)
C(23)	3384(3)	3437(2)	8274(2)	31(1)
C(24)	2452(3)	3406(3)	8646(2)	45(1)
C(25)	1571(4)	3014(3)	8422(3)	60(1)
C(26)	1576(4)	2658(3)	7839(3)	58(1)

C(27)	2489(4)	2689(3)	7460(2)	48(1)
C(28)	3388(3)	3078(2)	7682(2)	34(1)
C(29)	5905(3)	2770(2)	8265(2)	26(1)
C(30)	6913(4)	2002(4)	9399(3)	77(2)
C(31)	8111(4)	1984(3)	8144(2)	46(1)
C(32)	7937(4)	3460(3)	8884(3)	59(2)
C(33)	6926(3)	3040(2)	6859(2)	23(1)
C(34)	7807(3)	2661(2)	6498(2)	28(1)
C(35)	8862(3)	2951(3)	6431(2)	40(1)
C(36)	9431(4)	2440(3)	6033(2)	46(1)
C(37)	8739(4)	1835(3)	5850(2)	42(1)
C(38)	7734(4)	1968(2)	6132(2)	35(1)
C(39)	9085(3)	2529(2)	4217(2)	32(1)
C(40)	8326(3)	2987(2)	4596(2)	31(1)
C(41)	8522(3)	3696(2)	4915(2)	36(1)
C(42)	7570(3)	3910(2)	5240(2)	37(1)
C(43)	6787(3)	3329(2)	5127(2)	36(1)
C(44)	7253(3)	2759(2)	4736(2)	34(1)
C(45)	2326(5)	4586(4)	5937(3)	77(2)

Table 3. Bond lengths [A] and angles [deg] for **6c**.

Pd(1)-C(29)	2.100(3)
Pd(1)-O(2)	2.129(2)
Pd(1)-P(2)	2.2003(9)
Pd(1)-P(1)	2.3381(10)
Fe(1)-C(38)	2.023(4)
Fe(1)-C(40)	2.031(3)
Fe(1)-C(41)	2.031(4)
Fe(1)-C(44)	2.035(4)
Fe(1)-C(34)	2.036(3)
Fe(1)-C(37)	2.038(4)
Fe(1)-C(42)	2.052(4)
Fe(1)-C(36)	2.055(4)
Fe(1)-C(35)	2.056(4)
Fe(1)-C(43)	2.060(4)
Cl(1)-C(45)	1.711(7)
Cl(2)-C(45)	1.723(7)
P(1)-C(7)	1.820(4)
P(1)-C(1)	1.821(4)
P(1)-C(13)	1.835(4)
P(2)-C(23)	1.820(4)
P(2)-C(17)	1.822(4)
P(2)-C(16)	1.836(4)
Si(1)-C(32)	1.856(5)
Si(1)-C(29)	1.858(4)
Si(1)-C(30)	1.864(5)
Si(1)-C(31)	1.868(4)
O(1)-C(33)	1.253(4)
O(2)-C(33)	1.269(4)
O(3)-C(39)	1.216(5)
O(4)-C(39)	1.319(5)
O(4)-H(4)	0.8399
C(1)-C(2)	1.384(5)
C(1)-C(6)	1.403(5)
C(2)-C(3)	1.392(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.374(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(7)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.391(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500

C(7)-C(8)	1.376(6)
C(7)-C(12)	1.397(6)
C(8)-C(9)	1.399(7)
C(8)-H(8)	0.9500
C(9)-C(10)	1.374(8)
C(9)-H(9)	0.9500
C(10)-C(11)	1.381(8)
C(10)-H(10)	0.9500
C(11)-C(12)	1.383(7)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.533(6)
C(13)-H(13B)	0.9900
C(13)-H(13A)	0.9900
C(14)-C(15)	1.522(5)
C(14)-H(14B)	0.9900
C(14)-H(14A)	0.9900
C(15)-C(16)	1.537(5)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(22)	1.378(5)
C(17)-C(18)	1.390(6)
C(18)-C(19)	1.384(6)
C(18)-H(18)	0.9500
C(19)-C(20)	1.362(6)
C(19)-H(19)	0.9500
C(20)-C(21)	1.371(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.396(6)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(28)	1.383(5)
C(23)-C(24)	1.402(6)
C(24)-C(25)	1.378(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.365(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.391(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.392(6)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500

C(29)-H(29B)	0.9900
C(29)-H(29A)	0.9900
C(30)-H(30C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32C)	0.9800
C(32)-H(32B)	0.9800
C(33)-C(34)	1.489(5)
C(34)-C(35)	1.419(6)
C(34)-C(38)	1.427(5)
C(35)-C(36)	1.410(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.413(7)
C(36)-H(36)	0.9500
C(37)-C(38)	1.409(6)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(40)	1.470(5)
C(40)-C(41)	1.419(5)
C(40)-C(44)	1.430(5)
C(41)-C(42)	1.421(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.425(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.408(6)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900

C(29)-Pd(1)-O(2)	87.80(12)
C(29)-Pd(1)-P(2)	82.95(11)
O(2)-Pd(1)-P(2)	170.09(7)
C(29)-Pd(1)-P(1)	171.35(11)
O(2)-Pd(1)-P(1)	86.61(7)
P(2)-Pd(1)-P(1)	102.98(3)
C(38)-Fe(1)-C(40)	134.35(16)
C(38)-Fe(1)-C(41)	175.16(16)
C(40)-Fe(1)-C(41)	40.88(16)
C(38)-Fe(1)-C(44)	107.78(17)

C(40)-Fe(1)-C(44)	41.17(16)
C(41)-Fe(1)-C(44)	68.96(17)
C(38)-Fe(1)-C(34)	41.17(15)
C(40)-Fe(1)-C(34)	174.55(17)
C(41)-Fe(1)-C(34)	143.65(16)
C(44)-Fe(1)-C(34)	134.00(16)
C(38)-Fe(1)-C(37)	40.60(17)
C(40)-Fe(1)-C(37)	110.04(16)
C(41)-Fe(1)-C(37)	136.59(17)
C(44)-Fe(1)-C(37)	112.29(18)
C(34)-Fe(1)-C(37)	68.41(15)
C(38)-Fe(1)-C(42)	142.17(16)
C(40)-Fe(1)-C(42)	68.36(16)
C(41)-Fe(1)-C(42)	40.72(15)
C(44)-Fe(1)-C(42)	68.18(17)
C(34)-Fe(1)-C(42)	113.41(15)
C(37)-Fe(1)-C(42)	177.19(18)
C(38)-Fe(1)-C(36)	68.21(19)
C(40)-Fe(1)-C(36)	114.54(16)
C(41)-Fe(1)-C(36)	112.06(19)
C(44)-Fe(1)-C(36)	143.37(17)
C(34)-Fe(1)-C(36)	67.93(16)
C(37)-Fe(1)-C(36)	40.39(19)
C(42)-Fe(1)-C(36)	137.8(2)
C(38)-Fe(1)-C(35)	68.63(18)
C(40)-Fe(1)-C(35)	144.32(17)
C(41)-Fe(1)-C(35)	114.89(19)
C(44)-Fe(1)-C(35)	174.46(16)
C(34)-Fe(1)-C(35)	40.57(16)
C(37)-Fe(1)-C(35)	68.01(19)
C(42)-Fe(1)-C(35)	111.81(18)
C(36)-Fe(1)-C(35)	40.11(17)
C(38)-Fe(1)-C(43)	111.46(18)
C(40)-Fe(1)-C(43)	68.39(16)
C(41)-Fe(1)-C(43)	68.60(17)
C(44)-Fe(1)-C(43)	40.21(16)
C(34)-Fe(1)-C(43)	109.34(16)
C(37)-Fe(1)-C(43)	141.47(19)
C(42)-Fe(1)-C(43)	40.56(17)
C(36)-Fe(1)-C(43)	176.42(18)
C(35)-Fe(1)-C(43)	136.31(17)
C(7)-P(1)-C(1)	105.97(19)
C(7)-P(1)-C(13)	102.36(19)
C(1)-P(1)-C(13)	101.03(18)

C(7)-P(1)-Pd(1)	106.73(13)
C(1)-P(1)-Pd(1)	117.01(12)
C(13)-P(1)-Pd(1)	121.93(13)
C(23)-P(2)-C(17)	108.85(17)
C(23)-P(2)-C(16)	99.79(19)
C(17)-P(2)-C(16)	103.48(17)
C(23)-P(2)-Pd(1)	112.79(13)
C(17)-P(2)-Pd(1)	113.54(13)
C(16)-P(2)-Pd(1)	117.13(12)
C(32)-Si(1)-C(29)	112.88(19)
C(32)-Si(1)-C(30)	109.2(3)
C(29)-Si(1)-C(30)	107.2(2)
C(32)-Si(1)-C(31)	107.2(2)
C(29)-Si(1)-C(31)	112.05(18)
C(30)-Si(1)-C(31)	108.1(3)
C(33)-O(2)-Pd(1)	113.4(2)
C(39)-O(4)-H(4)	99.7
C(2)-C(1)-C(6)	119.3(4)
C(2)-C(1)-P(1)	119.1(3)
C(6)-C(1)-P(1)	121.5(3)
C(1)-C(2)-C(3)	120.4(4)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	120.0(4)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	120.5(4)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
C(4)-C(5)-C(6)	120.1(4)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	119.7(4)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
C(8)-C(7)-C(12)	118.4(4)
C(8)-C(7)-P(1)	122.2(3)
C(12)-C(7)-P(1)	119.2(3)
C(7)-C(8)-C(9)	121.2(4)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(10)-C(9)-C(8)	119.7(5)
C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2

C(9)-C(10)-C(11)	119.6(5)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	120.7(5)
C(10)-C(11)-H(11)	119.6
C(12)-C(11)-H(11)	119.6
C(11)-C(12)-C(7)	120.3(4)
C(11)-C(12)-H(12)	119.9
C(7)-C(12)-H(12)	119.9
C(14)-C(13)-P(1)	114.8(3)
C(14)-C(13)-H(13B)	108.6
P(1)-C(13)-H(13B)	108.6
C(14)-C(13)-H(13A)	108.6
P(1)-C(13)-H(13A)	108.6
H(13B)-C(13)-H(13A)	107.5
C(15)-C(14)-C(13)	115.6(3)
C(15)-C(14)-H(14B)	108.4
C(13)-C(14)-H(14B)	108.4
C(15)-C(14)-H(14A)	108.4
C(13)-C(14)-H(14A)	108.4
H(14B)-C(14)-H(14A)	107.4
C(14)-C(15)-C(16)	113.8(3)
C(14)-C(15)-H(15A)	108.8
C(16)-C(15)-H(15A)	108.8
C(14)-C(15)-H(15B)	108.8
C(16)-C(15)-H(15B)	108.8
H(15A)-C(15)-H(15B)	107.7
C(15)-C(16)-P(2)	110.8(3)
C(15)-C(16)-H(16A)	109.5
P(2)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
P(2)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	108.1
C(22)-C(17)-C(18)	118.8(4)
C(22)-C(17)-P(2)	124.2(3)
C(18)-C(17)-P(2)	116.9(3)
C(19)-C(18)-C(17)	120.9(4)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	120.1(4)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(19)-C(20)-C(21)	119.9(4)
C(19)-C(20)-H(20)	120.1

C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	120.7(4)
C(20)-C(21)-H(21)	119.6
C(22)-C(21)-H(21)	119.6
C(17)-C(22)-C(21)	119.7(4)
C(17)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
C(28)-C(23)-C(24)	118.8(4)
C(28)-C(23)-P(2)	119.5(3)
C(24)-C(23)-P(2)	121.3(3)
C(25)-C(24)-C(23)	119.8(5)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(26)-C(25)-C(24)	121.4(5)
C(26)-C(25)-H(25)	119.3
C(24)-C(25)-H(25)	119.3
C(25)-C(26)-C(27)	119.6(4)
C(25)-C(26)-H(26)	120.2
C(27)-C(26)-H(26)	120.2
C(26)-C(27)-C(28)	119.6(5)
C(26)-C(27)-H(27)	120.2
C(28)-C(27)-H(27)	120.2
C(23)-C(28)-C(27)	120.8(4)
C(23)-C(28)-H(28)	119.6
C(27)-C(28)-H(28)	119.6
Si(1)-C(29)-Pd(1)	110.28(18)
Si(1)-C(29)-H(29B)	109.6
Pd(1)-C(29)-H(29B)	109.6
Si(1)-C(29)-H(29A)	109.6
Pd(1)-C(29)-H(29A)	109.6
H(29B)-C(29)-H(29A)	108.1
Si(1)-C(30)-H(30C)	109.5
Si(1)-C(30)-H(30A)	109.5
H(30C)-C(30)-H(30A)	109.5
Si(1)-C(30)-H(30B)	109.5
H(30C)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(1)-C(31)-H(31B)	109.5
Si(1)-C(31)-H(31A)	109.5
H(31B)-C(31)-H(31A)	109.5
Si(1)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
Si(1)-C(32)-H(32A)	109.5

Si(1)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
Si(1)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
H(32C)-C(32)-H(32B)	109.5
O(1)-C(33)-O(2)	123.5(3)
O(1)-C(33)-C(34)	119.7(3)
O(2)-C(33)-C(34)	116.8(3)
C(35)-C(34)-C(38)	107.8(3)
C(35)-C(34)-C(33)	125.7(4)
C(38)-C(34)-C(33)	126.5(4)
C(35)-C(34)-Fe(1)	70.5(2)
C(38)-C(34)-Fe(1)	68.9(2)
C(33)-C(34)-Fe(1)	123.8(2)
C(36)-C(35)-C(34)	107.8(4)
C(36)-C(35)-Fe(1)	69.9(2)
C(34)-C(35)-Fe(1)	69.0(2)
C(36)-C(35)-H(35)	126.1
C(34)-C(35)-H(35)	126.1
Fe(1)-C(35)-H(35)	126.6
C(35)-C(36)-C(37)	108.4(4)
C(35)-C(36)-Fe(1)	70.0(2)
C(37)-C(36)-Fe(1)	69.2(2)
C(35)-C(36)-H(36)	125.8
C(37)-C(36)-H(36)	125.8
Fe(1)-C(36)-H(36)	126.6
C(38)-C(37)-C(36)	108.3(4)
C(38)-C(37)-Fe(1)	69.1(2)
C(36)-C(37)-Fe(1)	70.4(3)
C(38)-C(37)-H(37)	125.9
C(36)-C(37)-H(37)	125.9
Fe(1)-C(37)-H(37)	126.1
C(37)-C(38)-C(34)	107.7(4)
C(37)-C(38)-Fe(1)	70.3(2)
C(34)-C(38)-Fe(1)	69.9(2)
C(37)-C(38)-H(38)	126.1
C(34)-C(38)-H(38)	126.1
Fe(1)-C(38)-H(38)	125.3
O(3)-C(39)-O(4)	124.4(4)
O(3)-C(39)-C(40)	122.9(4)
O(4)-C(39)-C(40)	112.7(3)
C(41)-C(40)-C(44)	107.9(3)
C(41)-C(40)-C(39)	127.5(4)
C(44)-C(40)-C(39)	124.6(4)

C(41)-C(40)-Fe(1)	69.6(2)
C(44)-C(40)-Fe(1)	69.6(2)
C(39)-C(40)-Fe(1)	123.8(3)
C(40)-C(41)-C(42)	107.8(4)
C(40)-C(41)-Fe(1)	69.5(2)
C(42)-C(41)-Fe(1)	70.4(2)
C(40)-C(41)-H(41)	126.1
C(42)-C(41)-H(41)	126.1
Fe(1)-C(41)-H(41)	125.5
C(41)-C(42)-C(43)	108.2(4)
C(41)-C(42)-Fe(1)	68.9(2)
C(43)-C(42)-Fe(1)	70.0(2)
C(41)-C(42)-H(42)	125.9
C(43)-C(42)-H(42)	125.9
Fe(1)-C(42)-H(42)	126.8
C(44)-C(43)-C(42)	107.9(4)
C(44)-C(43)-Fe(1)	68.9(2)
C(42)-C(43)-Fe(1)	69.4(2)
C(44)-C(43)-H(43)	126.1
C(42)-C(43)-H(43)	126.1
Fe(1)-C(43)-H(43)	127.2
C(43)-C(44)-C(40)	108.2(4)
C(43)-C(44)-Fe(1)	70.8(2)
C(40)-C(44)-Fe(1)	69.2(2)
C(43)-C(44)-H(44)	125.9
C(40)-C(44)-H(44)	125.9
Fe(1)-C(44)-H(44)	125.6
Cl(1)-C(45)-Cl(2)	112.0(4)
Cl(1)-C(45)-H(45A)	109.2
Cl(2)-C(45)-H(45A)	109.2
Cl(1)-C(45)-H(45B)	109.2
Cl(2)-C(45)-H(45B)	109.2
H(45A)-C(45)-H(45B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6c**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	26(1)	19(1)	19(1)	-1(1)	2(1)	0(1)
Fe(1)	30(1)	28(1)	25(1)	0(1)	5(1)	6(1)
Cl(1)	134(2)	127(2)	293(4)	58(2)	130(3)	35(2)
Cl(2)	150(2)	165(2)	86(1)	12(1)	-33(1)	59(2)
P(1)	35(1)	20(1)	24(1)	-1(1)	6(1)	-4(1)
P(2)	31(1)	23(1)	23(1)	1(1)	6(1)	0(1)
Si(1)	35(1)	33(1)	27(1)	2(1)	-2(1)	6(1)
O(1)	29(1)	39(1)	24(1)	-8(1)	0(1)	-3(1)
O(2)	29(1)	29(1)	23(1)	-5(1)	4(1)	-1(1)
O(3)	55(2)	41(2)	51(2)	-16(1)	19(2)	-9(2)
O(4)	40(2)	37(2)	34(1)	-10(1)	9(1)	4(1)
C(1)	38(2)	24(2)	28(2)	2(1)	3(2)	2(2)
C(2)	35(2)	25(2)	31(2)	3(2)	5(2)	0(2)
C(3)	38(2)	43(2)	31(2)	-2(2)	-2(2)	5(2)
C(4)	60(3)	50(3)	25(2)	5(2)	-2(2)	14(2)
C(5)	79(3)	37(2)	39(2)	13(2)	14(2)	5(2)
C(6)	60(3)	31(2)	37(2)	1(2)	12(2)	-7(2)
C(7)	35(2)	28(2)	35(2)	-3(2)	3(2)	-4(2)
C(8)	43(2)	51(3)	42(2)	-12(2)	5(2)	-10(2)
C(9)	41(3)	85(4)	69(4)	-13(3)	7(2)	-8(3)
C(10)	38(2)	76(4)	80(4)	-13(3)	-12(3)	-10(3)
C(11)	57(3)	63(3)	52(3)	-16(2)	-12(2)	-13(3)
C(12)	48(3)	46(3)	37(2)	-7(2)	0(2)	-8(2)
C(13)	49(2)	23(2)	33(2)	2(2)	8(2)	-2(2)
C(14)	50(2)	23(2)	35(2)	6(2)	7(2)	7(2)
C(15)	37(2)	26(2)	43(2)	4(2)	3(2)	7(2)
C(16)	38(2)	31(2)	30(2)	5(2)	10(2)	4(2)
C(17)	39(2)	26(2)	21(2)	-2(2)	10(1)	-1(2)
C(18)	57(3)	32(2)	31(2)	-1(2)	-2(2)	-9(2)
C(19)	71(3)	42(2)	37(2)	-3(2)	-10(2)	-17(3)
C(20)	60(3)	52(3)	27(2)	5(2)	-3(2)	-3(2)
C(21)	65(3)	58(3)	31(2)	18(2)	0(2)	-16(3)
C(22)	46(2)	42(2)	30(2)	7(2)	-1(2)	-15(2)
C(23)	33(2)	28(2)	31(2)	7(2)	4(2)	3(2)
C(24)	33(2)	58(3)	42(2)	2(2)	6(2)	-4(2)
C(25)	39(3)	67(4)	75(4)	7(3)	9(3)	-9(2)
C(26)	41(2)	58(3)	75(3)	4(3)	-13(3)	-15(2)
C(27)	49(3)	41(2)	54(3)	-4(2)	-14(2)	-6(2)

C(28)	31(2)	31(2)	40(2)	3(2)	−4(2)	1(2)
C(29)	37(2)	19(2)	22(2)	−1(1)	−2(2)	0(2)
C(30)	51(3)	119(5)	60(3)	56(4)	2(3)	13(3)
C(31)	39(2)	55(3)	44(2)	−7(2)	−9(2)	15(2)
C(32)	60(3)	46(3)	72(3)	−17(3)	−38(3)	9(2)
C(33)	30(2)	24(2)	16(1)	−1(1)	1(1)	2(2)
C(34)	35(2)	32(2)	19(2)	−1(1)	3(2)	6(2)
C(35)	33(2)	55(3)	32(2)	−7(2)	−4(2)	3(2)
C(36)	36(2)	70(3)	32(2)	0(2)	4(2)	19(2)
C(37)	55(3)	42(2)	29(2)	4(2)	10(2)	27(2)
C(38)	49(2)	28(2)	27(2)	3(2)	9(2)	7(2)
C(39)	37(2)	34(2)	24(2)	3(2)	−1(2)	−1(2)
C(40)	40(2)	32(2)	21(2)	6(2)	6(2)	6(2)
C(41)	43(2)	23(2)	41(2)	5(2)	13(2)	3(2)
C(42)	45(2)	24(2)	43(2)	1(2)	12(2)	8(2)
C(43)	32(2)	39(2)	37(2)	9(2)	3(2)	10(2)
C(44)	30(2)	40(2)	32(2)	4(2)	−1(2)	4(2)
C(45)	69(4)	76(4)	86(4)	2(4)	0(4)	6(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6c**.

	x	y	z	U(eq)
H(4)	10310	2562	3890	44
H(2)	5136	4285	6479	37
H(3)	4754	4494	5396	45
H(4A)	5428	5573	4878	54
H(5)	6504	6446	5426	62
H(6)	6837	6275	6521	51
H(8)	8213	5018	6809	55
H(9)	9988	5316	7064	78
H(10)	10396	5838	8062	78
H(11)	9041	6034	8809	69
H(12)	7275	5755	8553	52
H(13B)	5538	5984	8250	42
H(13A)	5778	6440	7601	42
H(14B)	3926	6425	7841	43
H(14A)	4166	6050	7157	43
H(15A)	3817	4833	7519	42
H(15B)	2862	5361	7776	42
H(16A)	3186	4957	8749	40
H(16B)	4334	5365	8722	40
H(18)	5745	4822	9414	48
H(19)	6263	4647	10475	60
H(20)	5682	3580	11039	56
H(21)	4577	2684	10550	61
H(22)	4005	2866	9492	47
H(24)	2429	3655	9051	54
H(25)	945	2992	8679	72
H(26)	961	2390	7694	69
H(27)	2498	2446	7052	58
H(28)	4013	3097	7424	41
H(29B)	5319	2722	8581	31
H(29A)	5781	2388	7921	31
H(30C)	7579	1787	9569	115
H(30A)	6419	1582	9296	115
H(30B)	6588	2339	9721	115
H(31B)	8342	2295	7777	69
H(31A)	7730	1527	7990	69
H(31C)	8737	1824	8392	69
H(32A)	8061	3773	8500	89
H(32C)	8625	3322	9077	89

H(32B)	7514	3756	9193	89
H(35)	9135	3408	6622	48
H(36)	10157	2493	5908	55
H(37)	8921	1411	5583	50
H(38)	7118	1652	6088	42
H(41)	9174	3976	4912	43
H(42)	7472	4363	5489	45
H(43)	6077	3327	5286	43
H(44)	6914	2302	4590	41
H(45A)	2937	4236	6017	93
H(45B)	2486	5087	6142	93

Table 6. Torsion angles [deg] for **6c**.

C(29)-Pd(1)-P(1)-C(7)	-7.2(6)
O(2)-Pd(1)-P(1)-C(7)	-57.07(15)
P(2)-Pd(1)-P(1)-C(7)	125.44(13)
C(29)-Pd(1)-P(1)-C(1)	111.2(6)
O(2)-Pd(1)-P(1)-C(1)	61.34(17)
P(2)-Pd(1)-P(1)-C(1)	-116.16(15)
C(29)-Pd(1)-P(1)-C(13)	-124.0(6)
O(2)-Pd(1)-P(1)-C(13)	-173.86(18)
P(2)-Pd(1)-P(1)-C(13)	8.64(17)
C(29)-Pd(1)-P(2)-C(23)	-65.82(16)
O(2)-Pd(1)-P(2)-C(23)	-44.7(4)
P(1)-Pd(1)-P(2)-C(23)	120.58(13)
C(29)-Pd(1)-P(2)-C(17)	58.59(17)
O(2)-Pd(1)-P(2)-C(17)	79.7(4)
P(1)-Pd(1)-P(2)-C(17)	-115.01(14)
C(29)-Pd(1)-P(2)-C(16)	179.18(18)
O(2)-Pd(1)-P(2)-C(16)	-159.7(4)
P(1)-Pd(1)-P(2)-C(16)	5.58(16)
C(29)-Pd(1)-O(2)-C(33)	68.4(2)
P(2)-Pd(1)-O(2)-C(33)	47.4(5)
P(1)-Pd(1)-O(2)-C(33)	-118.2(2)
C(7)-P(1)-C(1)-C(2)	140.4(3)
C(13)-P(1)-C(1)-C(2)	-113.1(3)
Pd(1)-P(1)-C(1)-C(2)	21.6(4)
C(7)-P(1)-C(1)-C(6)	-44.1(4)
C(13)-P(1)-C(1)-C(6)	62.3(4)
Pd(1)-P(1)-C(1)-C(6)	-162.9(3)
C(6)-C(1)-C(2)-C(3)	-1.2(6)
P(1)-C(1)-C(2)-C(3)	174.3(3)
C(1)-C(2)-C(3)-C(4)	1.1(6)
C(2)-C(3)-C(4)-C(5)	0.4(7)
C(3)-C(4)-C(5)-C(6)	-1.8(7)
C(4)-C(5)-C(6)-C(1)	1.7(7)
C(2)-C(1)-C(6)-C(5)	-0.2(6)
P(1)-C(1)-C(6)-C(5)	-175.6(4)
C(1)-P(1)-C(7)-C(8)	-33.5(4)
C(13)-P(1)-C(7)-C(8)	-139.0(4)
Pd(1)-P(1)-C(7)-C(8)	91.9(4)
C(1)-P(1)-C(7)-C(12)	151.3(3)
C(13)-P(1)-C(7)-C(12)	45.9(4)
Pd(1)-P(1)-C(7)-C(12)	-83.3(3)
C(12)-C(7)-C(8)-C(9)	-2.6(7)

P(1)-C(7)-C(8)-C(9)	-177.7(4)
C(7)-C(8)-C(9)-C(10)	1.1(9)
C(8)-C(9)-C(10)-C(11)	0.9(10)
C(9)-C(10)-C(11)-C(12)	-1.4(9)
C(10)-C(11)-C(12)-C(7)	-0.1(8)
C(8)-C(7)-C(12)-C(11)	2.1(7)
P(1)-C(7)-C(12)-C(11)	177.4(4)
C(7)-P(1)-C(13)-C(14)	172.5(3)
C(1)-P(1)-C(13)-C(14)	63.2(3)
Pd(1)-P(1)-C(13)-C(14)	-68.6(3)
P(1)-C(13)-C(14)-C(15)	53.7(4)
C(13)-C(14)-C(15)-C(16)	47.6(5)
C(14)-C(15)-C(16)-P(2)	-115.5(3)
C(23)-P(2)-C(16)-C(15)	-72.3(3)
C(17)-P(2)-C(16)-C(15)	175.5(3)
Pd(1)-P(2)-C(16)-C(15)	49.7(3)
C(23)-P(2)-C(17)-C(22)	18.6(4)
C(16)-P(2)-C(17)-C(22)	124.1(4)
Pd(1)-P(2)-C(17)-C(22)	-107.9(3)
C(23)-P(2)-C(17)-C(18)	-166.8(3)
C(16)-P(2)-C(17)-C(18)	-61.3(4)
Pd(1)-P(2)-C(17)-C(18)	66.7(3)
C(22)-C(17)-C(18)-C(19)	-1.5(7)
P(2)-C(17)-C(18)-C(19)	-176.4(4)
C(17)-C(18)-C(19)-C(20)	1.3(8)
C(18)-C(19)-C(20)-C(21)	0.0(8)
C(19)-C(20)-C(21)-C(22)	-0.9(8)
C(18)-C(17)-C(22)-C(21)	0.6(7)
P(2)-C(17)-C(22)-C(21)	175.0(4)
C(20)-C(21)-C(22)-C(17)	0.7(8)
C(17)-P(2)-C(23)-C(28)	-139.9(3)
C(16)-P(2)-C(23)-C(28)	112.1(3)
Pd(1)-P(2)-C(23)-C(28)	-13.0(3)
C(17)-P(2)-C(23)-C(24)	48.1(4)
C(16)-P(2)-C(23)-C(24)	-59.9(4)
Pd(1)-P(2)-C(23)-C(24)	175.0(3)
C(28)-C(23)-C(24)-C(25)	0.9(7)
P(2)-C(23)-C(24)-C(25)	172.9(4)
C(23)-C(24)-C(25)-C(26)	-0.7(8)
C(24)-C(25)-C(26)-C(27)	-0.1(9)
C(25)-C(26)-C(27)-C(28)	0.5(8)
C(24)-C(23)-C(28)-C(27)	-0.4(6)
P(2)-C(23)-C(28)-C(27)	-172.6(3)
C(26)-C(27)-C(28)-C(23)	-0.3(7)

C(32)-Si(1)-C(29)-Pd(1)	21.5(3)
C(30)-Si(1)-C(29)-Pd(1)	141.8(3)
C(31)-Si(1)-C(29)-Pd(1)	-99.7(2)
O(2)-Pd(1)-C(29)-Si(1)	61.77(16)
P(2)-Pd(1)-C(29)-Si(1)	-121.78(16)
P(1)-Pd(1)-C(29)-Si(1)	12.0(7)
Pd(1)-O(2)-C(33)-O(1)	9.7(4)
Pd(1)-O(2)-C(33)-C(34)	-169.7(2)
O(1)-C(33)-C(34)-C(35)	160.1(4)
O(2)-C(33)-C(34)-C(35)	-20.5(5)
O(1)-C(33)-C(34)-C(38)	-16.6(5)
O(2)-C(33)-C(34)-C(38)	162.8(3)
O(1)-C(33)-C(34)-Fe(1)	71.0(4)
O(2)-C(33)-C(34)-Fe(1)	-109.6(3)
C(38)-Fe(1)-C(34)-C(35)	119.0(3)
C(40)-Fe(1)-C(34)-C(35)	155.4(16)
C(41)-Fe(1)-C(34)-C(35)	-60.3(4)
C(44)-Fe(1)-C(34)-C(35)	-178.4(3)
C(37)-Fe(1)-C(34)-C(35)	81.0(3)
C(42)-Fe(1)-C(34)-C(35)	-96.7(3)
C(36)-Fe(1)-C(34)-C(35)	37.3(3)
C(43)-Fe(1)-C(34)-C(35)	-140.2(3)
C(40)-Fe(1)-C(34)-C(38)	36.4(17)
C(41)-Fe(1)-C(34)-C(38)	-179.3(3)
C(44)-Fe(1)-C(34)-C(38)	62.7(3)
C(37)-Fe(1)-C(34)-C(38)	-38.0(3)
C(42)-Fe(1)-C(34)-C(38)	144.3(3)
C(36)-Fe(1)-C(34)-C(38)	-81.7(3)
C(35)-Fe(1)-C(34)-C(38)	-119.0(3)
C(43)-Fe(1)-C(34)-C(38)	100.8(3)
C(38)-Fe(1)-C(34)-C(33)	-120.6(4)
C(40)-Fe(1)-C(34)-C(33)	-84.1(17)
C(41)-Fe(1)-C(34)-C(33)	60.1(4)
C(44)-Fe(1)-C(34)-C(33)	-57.9(4)
C(37)-Fe(1)-C(34)-C(33)	-158.6(4)
C(42)-Fe(1)-C(34)-C(33)	23.8(4)
C(36)-Fe(1)-C(34)-C(33)	157.8(4)
C(35)-Fe(1)-C(34)-C(33)	120.5(4)
C(43)-Fe(1)-C(34)-C(33)	-19.7(4)
C(38)-C(34)-C(35)-C(36)	-0.3(4)
C(33)-C(34)-C(35)-C(36)	-177.5(4)
Fe(1)-C(34)-C(35)-C(36)	-59.3(3)
C(38)-C(34)-C(35)-Fe(1)	59.0(3)
C(33)-C(34)-C(35)-Fe(1)	-118.2(4)

C(38)-Fe(1)-C(35)-C(36)	81.1(3)
C(40)-Fe(1)-C(35)-C(36)	-56.8(4)
C(41)-Fe(1)-C(35)-C(36)	-95.3(3)
C(44)-Fe(1)-C(35)-C(36)	131.5(18)
C(34)-Fe(1)-C(35)-C(36)	119.3(4)
C(37)-Fe(1)-C(35)-C(36)	37.3(3)
C(42)-Fe(1)-C(35)-C(36)	-139.7(3)
C(43)-Fe(1)-C(35)-C(36)	-179.7(3)
C(38)-Fe(1)-C(35)-C(34)	-38.2(2)
C(40)-Fe(1)-C(35)-C(34)	-176.1(3)
C(41)-Fe(1)-C(35)-C(34)	145.4(2)
C(44)-Fe(1)-C(35)-C(34)	12(2)
C(37)-Fe(1)-C(35)-C(34)	-82.0(3)
C(42)-Fe(1)-C(35)-C(34)	101.0(3)
C(36)-Fe(1)-C(35)-C(34)	-119.3(4)
C(43)-Fe(1)-C(35)-C(34)	61.0(3)
C(34)-C(35)-C(36)-C(37)	0.1(5)
Fe(1)-C(35)-C(36)-C(37)	-58.7(3)
C(34)-C(35)-C(36)-Fe(1)	58.7(3)
C(38)-Fe(1)-C(36)-C(35)	-82.3(3)
C(40)-Fe(1)-C(36)-C(35)	147.6(3)
C(41)-Fe(1)-C(36)-C(35)	102.9(3)
C(44)-Fe(1)-C(36)-C(35)	-173.0(3)
C(34)-Fe(1)-C(36)-C(35)	-37.7(3)
C(37)-Fe(1)-C(36)-C(35)	-119.9(4)
C(42)-Fe(1)-C(36)-C(35)	63.3(4)
C(43)-Fe(1)-C(36)-C(35)	3(3)
C(38)-Fe(1)-C(36)-C(37)	37.6(2)
C(40)-Fe(1)-C(36)-C(37)	-92.5(3)
C(41)-Fe(1)-C(36)-C(37)	-137.2(2)
C(44)-Fe(1)-C(36)-C(37)	-53.2(4)
C(34)-Fe(1)-C(36)-C(37)	82.2(3)
C(42)-Fe(1)-C(36)-C(37)	-176.8(2)
C(35)-Fe(1)-C(36)-C(37)	119.9(4)
C(43)-Fe(1)-C(36)-C(37)	123(3)
C(35)-C(36)-C(37)-C(38)	0.2(5)
Fe(1)-C(36)-C(37)-C(38)	-59.0(3)
C(35)-C(36)-C(37)-Fe(1)	59.2(3)
C(40)-Fe(1)-C(37)-C(38)	-135.9(3)
C(41)-Fe(1)-C(37)-C(38)	-174.1(3)
C(44)-Fe(1)-C(37)-C(38)	-91.6(3)
C(34)-Fe(1)-C(37)-C(38)	38.5(2)
C(42)-Fe(1)-C(37)-C(38)	169(4)
C(36)-Fe(1)-C(37)-C(38)	119.4(4)

C(35)-Fe(1)-C(37)-C(38)	82.4(3)
C(43)-Fe(1)-C(37)-C(38)	-55.8(4)
C(38)-Fe(1)-C(37)-C(36)	-119.4(4)
C(40)-Fe(1)-C(37)-C(36)	104.7(3)
C(41)-Fe(1)-C(37)-C(36)	66.5(3)
C(44)-Fe(1)-C(37)-C(36)	148.9(2)
C(34)-Fe(1)-C(37)-C(36)	-80.9(3)
C(42)-Fe(1)-C(37)-C(36)	50(4)
C(35)-Fe(1)-C(37)-C(36)	-37.0(2)
C(43)-Fe(1)-C(37)-C(36)	-175.2(3)
C(36)-C(37)-C(38)-C(34)	-0.4(5)
Fe(1)-C(37)-C(38)-C(34)	-60.1(3)
C(36)-C(37)-C(38)-Fe(1)	59.8(3)
C(35)-C(34)-C(38)-C(37)	0.4(4)
C(33)-C(34)-C(38)-C(37)	177.6(3)
Fe(1)-C(34)-C(38)-C(37)	60.4(3)
C(35)-C(34)-C(38)-Fe(1)	-60.0(3)
C(33)-C(34)-C(38)-Fe(1)	117.2(4)
C(40)-Fe(1)-C(38)-C(37)	66.1(4)
C(41)-Fe(1)-C(38)-C(37)	57(2)
C(44)-Fe(1)-C(38)-C(37)	103.8(3)
C(34)-Fe(1)-C(38)-C(37)	-118.4(4)
C(42)-Fe(1)-C(38)-C(37)	-179.1(3)
C(36)-Fe(1)-C(38)-C(37)	-37.4(3)
C(35)-Fe(1)-C(38)-C(37)	-80.7(3)
C(43)-Fe(1)-C(38)-C(37)	146.4(3)
C(40)-Fe(1)-C(38)-C(34)	-175.5(2)
C(41)-Fe(1)-C(38)-C(34)	175(2)
C(44)-Fe(1)-C(38)-C(34)	-137.9(2)
C(37)-Fe(1)-C(38)-C(34)	118.4(4)
C(42)-Fe(1)-C(38)-C(34)	-60.8(4)
C(36)-Fe(1)-C(38)-C(34)	80.9(3)
C(35)-Fe(1)-C(38)-C(34)	37.7(2)
C(43)-Fe(1)-C(38)-C(34)	-95.2(3)
O(3)-C(39)-C(40)-C(41)	170.5(4)
O(4)-C(39)-C(40)-C(41)	-10.0(5)
O(3)-C(39)-C(40)-C(44)	-5.8(6)
O(4)-C(39)-C(40)-C(44)	173.7(3)
O(3)-C(39)-C(40)-Fe(1)	81.4(5)
O(4)-C(39)-C(40)-Fe(1)	-99.1(4)
C(38)-Fe(1)-C(40)-C(41)	-178.8(3)
C(44)-Fe(1)-C(40)-C(41)	119.2(3)
C(34)-Fe(1)-C(40)-C(41)	148.1(16)
C(37)-Fe(1)-C(40)-C(41)	-139.5(3)

C(42)-Fe(1)-C(40)-C(41)	38.0(2)
C(36)-Fe(1)-C(40)-C(41)	-95.9(3)
C(35)-Fe(1)-C(40)-C(41)	-59.6(4)
C(43)-Fe(1)-C(40)-C(41)	81.8(3)
C(38)-Fe(1)-C(40)-C(44)	62.0(3)
C(41)-Fe(1)-C(40)-C(44)	-119.2(3)
C(34)-Fe(1)-C(40)-C(44)	28.9(17)
C(37)-Fe(1)-C(40)-C(44)	101.3(3)
C(42)-Fe(1)-C(40)-C(44)	-81.1(3)
C(36)-Fe(1)-C(40)-C(44)	144.9(3)
C(35)-Fe(1)-C(40)-C(44)	-178.8(3)
C(43)-Fe(1)-C(40)-C(44)	-37.4(2)
C(38)-Fe(1)-C(40)-C(39)	-56.6(4)
C(41)-Fe(1)-C(40)-C(39)	122.2(5)
C(44)-Fe(1)-C(40)-C(39)	-118.6(4)
C(34)-Fe(1)-C(40)-C(39)	-89.7(17)
C(37)-Fe(1)-C(40)-C(39)	-17.3(4)
C(42)-Fe(1)-C(40)-C(39)	160.2(4)
C(36)-Fe(1)-C(40)-C(39)	26.2(4)
C(35)-Fe(1)-C(40)-C(39)	62.6(5)
C(43)-Fe(1)-C(40)-C(39)	-156.0(4)
C(44)-C(40)-C(41)-C(42)	-1.0(4)
C(39)-C(40)-C(41)-C(42)	-177.8(4)
Fe(1)-C(40)-C(41)-C(42)	-60.3(3)
C(44)-C(40)-C(41)-Fe(1)	59.3(3)
C(39)-C(40)-C(41)-Fe(1)	-117.5(4)
C(38)-Fe(1)-C(41)-C(40)	10(2)
C(44)-Fe(1)-C(41)-C(40)	-38.0(2)
C(34)-Fe(1)-C(41)-C(40)	-175.1(3)
C(37)-Fe(1)-C(41)-C(40)	62.7(4)
C(42)-Fe(1)-C(41)-C(40)	-118.6(4)
C(36)-Fe(1)-C(41)-C(40)	102.5(3)
C(35)-Fe(1)-C(41)-C(40)	146.3(2)
C(43)-Fe(1)-C(41)-C(40)	-81.3(3)
C(38)-Fe(1)-C(41)-C(42)	129(2)
C(40)-Fe(1)-C(41)-C(42)	118.6(4)
C(44)-Fe(1)-C(41)-C(42)	80.6(3)
C(34)-Fe(1)-C(41)-C(42)	-56.6(4)
C(37)-Fe(1)-C(41)-C(42)	-178.8(3)
C(36)-Fe(1)-C(41)-C(42)	-138.9(3)
C(35)-Fe(1)-C(41)-C(42)	-95.1(3)
C(43)-Fe(1)-C(41)-C(42)	37.3(2)
C(40)-C(41)-C(42)-C(43)	0.6(5)
Fe(1)-C(41)-C(42)-C(43)	-59.2(3)

C(40)-C(41)-C(42)-Fe(1)	59.7(3)
C(38)-Fe(1)-C(42)-C(41)	-173.9(3)
C(40)-Fe(1)-C(42)-C(41)	-38.2(2)
C(44)-Fe(1)-C(42)-C(41)	-82.7(3)
C(34)-Fe(1)-C(42)-C(41)	147.4(2)
C(37)-Fe(1)-C(42)-C(41)	18(4)
C(36)-Fe(1)-C(42)-C(41)	65.0(3)
C(35)-Fe(1)-C(42)-C(41)	103.3(3)
C(43)-Fe(1)-C(42)-C(41)	-119.8(4)
C(38)-Fe(1)-C(42)-C(43)	-54.0(4)
C(40)-Fe(1)-C(42)-C(43)	81.6(3)
C(41)-Fe(1)-C(42)-C(43)	119.8(4)
C(44)-Fe(1)-C(42)-C(43)	37.1(2)
C(34)-Fe(1)-C(42)-C(43)	-92.8(3)
C(37)-Fe(1)-C(42)-C(43)	137(4)
C(36)-Fe(1)-C(42)-C(43)	-175.2(3)
C(35)-Fe(1)-C(42)-C(43)	-136.9(2)
C(41)-C(42)-C(43)-C(44)	0.1(5)
Fe(1)-C(42)-C(43)-C(44)	-58.3(3)
C(41)-C(42)-C(43)-Fe(1)	58.4(3)
C(38)-Fe(1)-C(43)-C(44)	-92.5(3)
C(40)-Fe(1)-C(43)-C(44)	38.2(2)
C(41)-Fe(1)-C(43)-C(44)	82.3(3)
C(34)-Fe(1)-C(43)-C(44)	-136.5(2)
C(37)-Fe(1)-C(43)-C(44)	-57.2(4)
C(42)-Fe(1)-C(43)-C(44)	119.8(3)
C(36)-Fe(1)-C(43)-C(44)	-176(3)
C(35)-Fe(1)-C(43)-C(44)	-173.5(3)
C(38)-Fe(1)-C(43)-C(42)	147.8(2)
C(40)-Fe(1)-C(43)-C(42)	-81.5(2)
C(41)-Fe(1)-C(43)-C(42)	-37.4(2)
C(44)-Fe(1)-C(43)-C(42)	-119.8(3)
C(34)-Fe(1)-C(43)-C(42)	103.7(2)
C(37)-Fe(1)-C(43)-C(42)	-176.9(3)
C(36)-Fe(1)-C(43)-C(42)	64(3)
C(35)-Fe(1)-C(43)-C(42)	66.7(3)
C(42)-C(43)-C(44)-C(40)	-0.7(4)
Fe(1)-C(43)-C(44)-C(40)	-59.4(3)
C(42)-C(43)-C(44)-Fe(1)	58.6(3)
C(41)-C(40)-C(44)-C(43)	1.1(4)
C(39)-C(40)-C(44)-C(43)	178.0(3)
Fe(1)-C(40)-C(44)-C(43)	60.4(3)
C(41)-C(40)-C(44)-Fe(1)	-59.3(3)
C(39)-C(40)-C(44)-Fe(1)	117.6(4)

C(38)-Fe(1)-C(44)-C(43)	102.5(3)
C(40)-Fe(1)-C(44)-C(43)	-119.1(3)
C(41)-Fe(1)-C(44)-C(43)	-81.3(3)
C(34)-Fe(1)-C(44)-C(43)	64.6(3)
C(37)-Fe(1)-C(44)-C(43)	145.5(2)
C(42)-Fe(1)-C(44)-C(43)	-37.4(2)
C(36)-Fe(1)-C(44)-C(43)	179.6(3)
C(35)-Fe(1)-C(44)-C(43)	54(2)
C(38)-Fe(1)-C(44)-C(40)	-138.5(2)
C(41)-Fe(1)-C(44)-C(40)	37.7(2)
C(34)-Fe(1)-C(44)-C(40)	-176.3(2)
C(37)-Fe(1)-C(44)-C(40)	-95.4(3)
C(42)-Fe(1)-C(44)-C(40)	81.6(2)
C(36)-Fe(1)-C(44)-C(40)	-61.3(4)
C(35)-Fe(1)-C(44)-C(40)	172.6(18)
C(43)-Fe(1)-C(44)-C(40)	119.1(3)

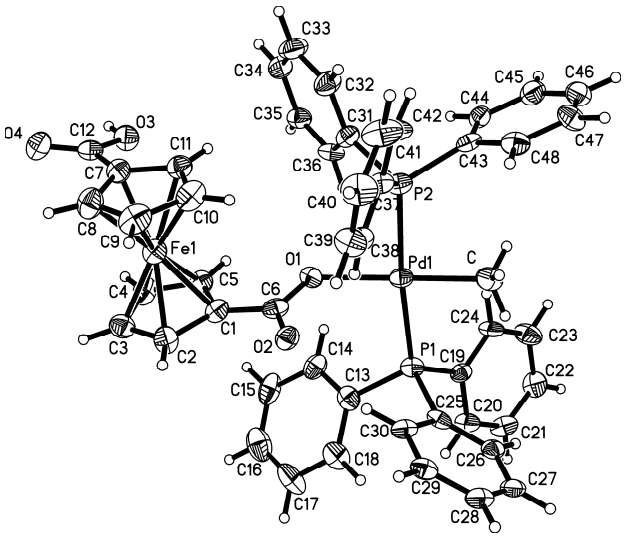
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **6c** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(1)#1	0.84	1.73	2.529(4)	159.2

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,-z+1

The X-ray structure of compound 6d



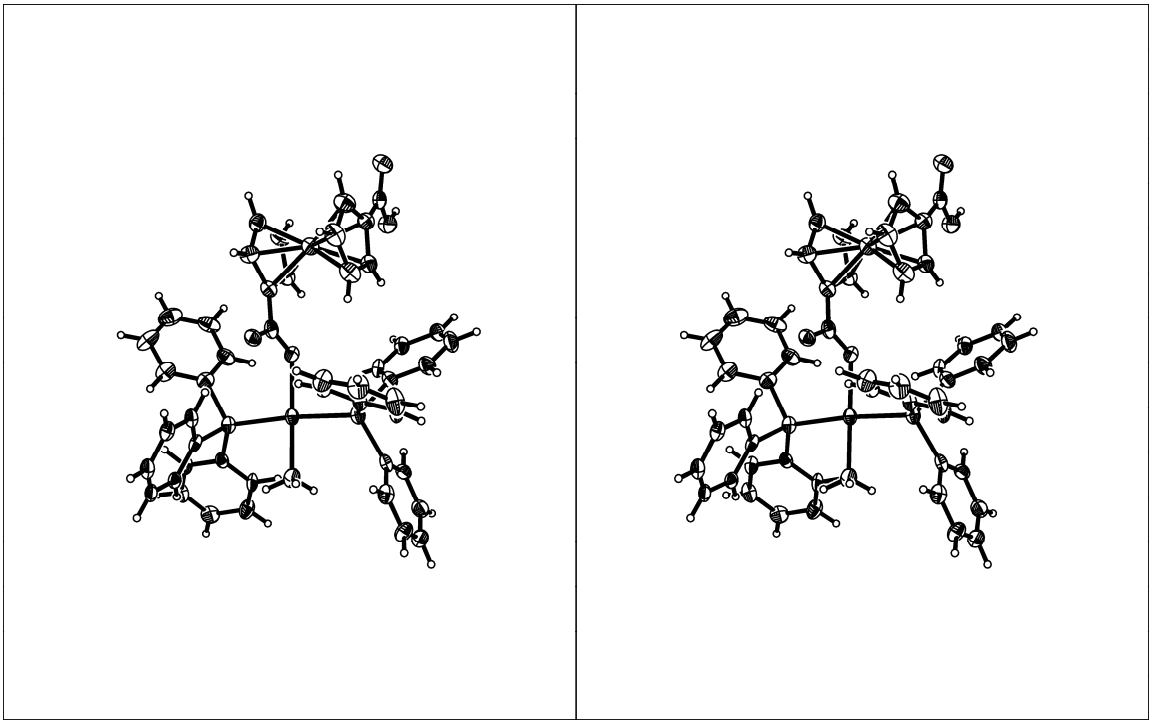


Table 1. Crystal data and structure refinement for **6d**.

Identification code	sa1599-b
Empirical formula	C50 H44 Cl2 Fe O4 P2 Pd
Formula weight	1003.94
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 17.696(3) A alpha = 90 deg.
	b = 13.606(3) A beta = 98.300(4) deg.
	c = 18.782(4) A gamma = 90 deg.
Volume	4474.8(16) A^3
Z, Calculated density	4, 1.490 Mg/m^3
Absorption coefficient	0.962 mm^-1
F(000)	2048
Crystal size	0.24 x 0.12 x 0.12 mm
Theta range for data collection	1.16 to 25.36 deg.
Limiting indices	-21<=h<=14, -16<=k<=16, -21<=l<=22
Reflections collected / unique	23010 / 8138 [R(int) = 0.0882]
Completeness to theta = 25.36	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8933 and 0.8020
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8138 / 0 / 543
Goodness-of-fit on F^2	1.297
Final R indices [I>2sigma(I)]	R1 = 0.1347, wR2 = 0.1872
R indices (all data)	R1 = 0.1629, wR2 = 0.1985
Largest diff. peak and hole	0.639 and -0.625 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6d**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	2015(1)	9778(1)	7783(1)	41(1)
Fe(1)	5127(1)	9916(1)	7296(1)	51(1)
Cl(1)	2069(2)	6553(3)	7790(3)	111(2)
Cl(2)	1193(4)	4796(5)	7627(4)	208(4)
P(1)	1340(2)	9712(2)	6637(1)	43(1)
P(2)	2587(2)	9883(2)	8982(2)	45(1)
O(1)	3082(4)	9578(5)	7417(3)	46(2)
O(2)	3161(4)	11120(5)	7028(4)	49(2)
O(3)	6065(4)	7741(5)	8075(5)	61(2)
O(4)	7096(5)	8599(6)	7880(5)	69(2)
C(1)	4061(6)	9931(7)	6751(6)	45(3)
C(2)	4545(6)	10514(8)	6383(6)	58(3)
C(3)	5131(7)	9912(8)	6204(6)	57(3)
C(4)	5024(6)	8958(8)	6444(6)	58(3)
C(5)	4364(6)	8968(8)	6776(5)	49(3)
C(6)	3393(6)	10253(8)	7091(5)	47(3)
C(7)	5972(6)	9454(8)	8068(6)	51(3)
C(8)	6136(7)	10414(8)	7831(7)	69(4)
C(9)	5532(8)	11035(9)	7963(7)	68(4)
C(10)	4996(7)	10465(9)	8278(7)	69(4)
C(11)	5259(6)	9502(8)	8342(6)	54(3)
C(12)	6435(7)	8573(9)	7999(6)	54(3)
C(13)	1903(6)	9480(8)	5912(6)	50(3)
C(14)	2430(6)	8742(8)	5971(6)	55(3)
C(15)	2854(7)	8549(9)	5421(8)	68(4)
C(16)	2703(9)	9067(11)	4784(8)	84(5)
C(17)	2161(9)	9780(10)	4692(7)	82(4)
C(18)	1769(7)	9989(8)	5258(6)	63(3)
C(19)	563(6)	8821(7)	6455(5)	41(2)
C(20)	145(6)	8732(8)	5765(6)	51(3)
C(21)	-463(7)	8115(7)	5642(6)	54(3)
C(22)	-682(7)	7569(8)	6179(7)	60(3)
C(23)	-247(7)	7592(8)	6863(6)	63(3)
C(24)	364(6)	8219(8)	6984(5)	50(3)
C(25)	879(6)	10896(7)	6439(5)	40(2)
C(26)	89(6)	11046(8)	6286(5)	44(3)
C(27)	-198(7)	11977(8)	6186(5)	49(3)

C(28)	283(7)	12775(8)	6235(5)	52(3)
C(29)	1056(7)	12656(7)	6373(5)	48(3)
C(30)	1362(6)	11720(7)	6476(5)	47(3)
C(31)	3389(6)	9045(8)	9193(6)	50(3)
C(32)	3930(7)	9127(9)	9808(6)	61(3)
C(33)	4491(7)	8430(10)	9969(6)	71(4)
C(34)	4519(7)	7626(9)	9525(6)	60(3)
C(35)	3995(6)	7534(8)	8915(6)	51(3)
C(36)	3444(6)	8247(7)	8748(5)	49(3)
C(37)	2921(6)	11130(7)	9236(5)	42(3)
C(38)	2916(6)	11814(7)	8688(6)	47(3)
C(39)	3106(7)	12768(8)	8877(7)	60(3)
C(40)	3303(7)	13063(8)	9569(7)	67(4)
C(41)	3286(8)	12397(8)	10110(7)	75(4)
C(42)	3089(7)	11436(8)	9964(6)	67(4)
C(43)	1970(6)	9544(7)	9644(5)	42(2)
C(44)	1871(6)	8560(8)	9792(6)	47(3)
C(45)	1338(7)	8257(9)	10215(6)	60(3)
C(46)	890(7)	8945(9)	10490(6)	63(3)
C(47)	977(7)	9911(9)	10362(6)	59(3)
C(48)	1510(6)	10208(8)	9930(5)	53(3)
C(49)	1708(9)	5533(13)	7292(9)	122(6)
C	990(6)	9996(8)	8135(6)	60(3)

Table 3. Bond lengths [A] and angles [deg] for **6d**.

Pd(1)-C	2.040(10)
Pd(1)-O(1)	2.120(7)
Pd(1)-P(1)	2.308(3)
Pd(1)-P(2)	2.336(3)
Fe(1)-C(1)	2.012(10)
Fe(1)-C(5)	2.014(10)
Fe(1)-C(11)	2.024(11)
Fe(1)-C(7)	2.027(11)
Fe(1)-C(10)	2.034(13)
Fe(1)-C(8)	2.035(12)
Fe(1)-C(9)	2.035(11)
Fe(1)-C(2)	2.038(12)
Fe(1)-C(4)	2.051(11)
Fe(1)-C(3)	2.052(11)
Cl(1)-C(49)	1.744(14)
Cl(2)-C(49)	1.550(16)
P(1)-C(25)	1.821(10)
P(1)-C(19)	1.827(10)
P(1)-C(13)	1.827(11)
P(2)-C(31)	1.820(11)
P(2)-C(43)	1.828(11)
P(2)-C(37)	1.837(10)
O(1)-C(6)	1.271(12)
O(2)-C(6)	1.249(11)
O(3)-C(12)	1.326(13)
O(3)-H(3)	0.8400
O(4)-C(12)	1.222(13)
C(1)-C(5)	1.414(13)
C(1)-C(2)	1.418(13)
C(1)-C(6)	1.487(14)
C(2)-C(3)	1.400(14)
C(2)-H(2)	0.9500
C(3)-C(4)	1.396(14)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.400(14)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(7)-C(8)	1.423(15)
C(7)-C(11)	1.431(14)
C(7)-C(12)	1.468(15)
C(8)-C(9)	1.413(16)
C(8)-H(8)	0.9500

C(9)-C(10)	1.418(16)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(14)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(13)-C(14)	1.364(14)
C(13)-C(18)	1.400(15)
C(14)-C(15)	1.386(15)
C(14)-H(14)	0.9500
C(15)-C(16)	1.382(18)
C(15)-H(15)	0.9500
C(16)-C(17)	1.358(18)
C(16)-H(16)	0.9500
C(17)-C(18)	1.380(15)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.373(13)
C(19)-C(20)	1.402(13)
C(20)-C(21)	1.358(14)
C(20)-H(20)	0.9500
C(21)-C(22)	1.353(14)
C(21)-H(21)	0.9500
C(22)-C(23)	1.399(15)
C(22)-H(22)	0.9500
C(23)-C(24)	1.370(14)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.401(13)
C(25)-C(30)	1.404(13)
C(26)-C(27)	1.368(13)
C(26)-H(26)	0.9500
C(27)-C(28)	1.373(14)
C(27)-H(27)	0.9500
C(28)-C(29)	1.365(14)
C(28)-H(28)	0.9500
C(29)-C(30)	1.387(13)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(36)	1.382(14)
C(31)-C(32)	1.393(14)
C(32)-C(33)	1.375(15)
C(32)-H(32)	0.9500
C(33)-C(34)	1.381(15)
C(33)-H(33)	0.9500

C(34)-C(35)	1.372(14)
C(34)-H(34)	0.9500
C(35)-C(36)	1.380(14)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.387(13)
C(37)-C(42)	1.418(14)
C(38)-C(39)	1.376(13)
C(38)-H(38)	0.9500
C(39)-C(40)	1.356(15)
C(39)-H(39)	0.9500
C(40)-C(41)	1.365(16)
C(40)-H(40)	0.9500
C(41)-C(42)	1.372(14)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
C(43)-C(48)	1.377(13)
C(43)-C(44)	1.383(13)
C(44)-C(45)	1.381(14)
C(44)-H(44)	0.9500
C(45)-C(46)	1.376(15)
C(45)-H(45)	0.9500
C(46)-C(47)	1.349(15)
C(46)-H(46)	0.9500
C(47)-C(48)	1.389(14)
C(47)-H(47)	0.9500
C(48)-H(48)	0.9500
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C-HA	0.9800
C-HC	0.9800
C-HB	0.9800

C-Pd(1)-O(1)	179.0(4)
C-Pd(1)-P(1)	86.8(3)
O(1)-Pd(1)-P(1)	93.27(19)
C-Pd(1)-P(2)	87.8(3)
O(1)-Pd(1)-P(2)	92.2(2)
P(1)-Pd(1)-P(2)	174.51(11)
C(1)-Fe(1)-C(5)	41.1(4)
C(1)-Fe(1)-C(11)	117.7(4)
C(5)-Fe(1)-C(11)	105.5(4)
C(1)-Fe(1)-C(7)	155.2(4)
C(5)-Fe(1)-C(7)	121.4(4)

C(11)-Fe(1)-C(7)	41.4(4)
C(1)-Fe(1)-C(10)	103.7(5)
C(5)-Fe(1)-C(10)	121.2(5)
C(11)-Fe(1)-C(10)	40.0(4)
C(7)-Fe(1)-C(10)	68.5(5)
C(1)-Fe(1)-C(8)	160.0(4)
C(5)-Fe(1)-C(8)	158.6(5)
C(11)-Fe(1)-C(8)	69.1(5)
C(7)-Fe(1)-C(8)	41.0(4)
C(10)-Fe(1)-C(8)	68.7(5)
C(1)-Fe(1)-C(9)	121.8(5)
C(5)-Fe(1)-C(9)	158.3(5)
C(11)-Fe(1)-C(9)	68.3(5)
C(7)-Fe(1)-C(9)	68.5(5)
C(10)-Fe(1)-C(9)	40.8(5)
C(8)-Fe(1)-C(9)	40.6(4)
C(1)-Fe(1)-C(2)	41.0(4)
C(5)-Fe(1)-C(2)	68.0(4)
C(11)-Fe(1)-C(2)	154.3(5)
C(7)-Fe(1)-C(2)	163.1(4)
C(10)-Fe(1)-C(2)	120.4(5)
C(8)-Fe(1)-C(2)	125.7(5)
C(9)-Fe(1)-C(2)	108.1(5)
C(1)-Fe(1)-C(4)	68.8(4)
C(5)-Fe(1)-C(4)	40.3(4)
C(11)-Fe(1)-C(4)	124.4(5)
C(7)-Fe(1)-C(4)	109.5(5)
C(10)-Fe(1)-C(4)	158.7(5)
C(8)-Fe(1)-C(4)	124.7(5)
C(9)-Fe(1)-C(4)	159.9(5)
C(2)-Fe(1)-C(4)	67.7(4)
C(1)-Fe(1)-C(3)	68.3(4)
C(5)-Fe(1)-C(3)	67.2(4)
C(11)-Fe(1)-C(3)	162.3(4)
C(7)-Fe(1)-C(3)	127.3(5)
C(10)-Fe(1)-C(3)	157.6(5)
C(8)-Fe(1)-C(3)	111.4(5)
C(9)-Fe(1)-C(3)	124.5(5)
C(2)-Fe(1)-C(3)	40.0(4)
C(4)-Fe(1)-C(3)	39.8(4)
C(25)-P(1)-C(19)	104.2(5)
C(25)-P(1)-C(13)	106.1(5)
C(19)-P(1)-C(13)	102.9(5)
C(25)-P(1)-Pd(1)	108.2(3)

C(19)-P(1)-Pd(1)	118.3(3)
C(13)-P(1)-Pd(1)	116.0(4)
C(31)-P(2)-C(43)	102.5(5)
C(31)-P(2)-C(37)	108.1(5)
C(43)-P(2)-C(37)	104.9(5)
C(31)-P(2)-Pd(1)	112.8(4)
C(43)-P(2)-Pd(1)	115.0(3)
C(37)-P(2)-Pd(1)	112.7(3)
C(6)-O(1)-Pd(1)	122.1(6)
C(12)-O(3)-H(3)	109.5
C(5)-C(1)-C(2)	106.3(9)
C(5)-C(1)-C(6)	125.5(10)
C(2)-C(1)-C(6)	128.1(9)
C(5)-C(1)-Fe(1)	69.5(6)
C(2)-C(1)-Fe(1)	70.5(6)
C(6)-C(1)-Fe(1)	122.0(7)
C(3)-C(2)-C(1)	108.1(9)
C(3)-C(2)-Fe(1)	70.6(7)
C(1)-C(2)-Fe(1)	68.5(6)
C(3)-C(2)-H(2)	126.0
C(1)-C(2)-H(2)	126.0
Fe(1)-C(2)-H(2)	126.5
C(4)-C(3)-C(2)	109.0(10)
C(4)-C(3)-Fe(1)	70.1(6)
C(2)-C(3)-Fe(1)	69.4(7)
C(4)-C(3)-H(3A)	125.5
C(2)-C(3)-H(3A)	125.5
Fe(1)-C(3)-H(3A)	126.6
C(3)-C(4)-C(5)	107.2(10)
C(3)-C(4)-Fe(1)	70.2(6)
C(5)-C(4)-Fe(1)	68.4(6)
C(3)-C(4)-H(4)	126.4
C(5)-C(4)-H(4)	126.4
Fe(1)-C(4)-H(4)	126.6
C(4)-C(5)-C(1)	109.3(10)
C(4)-C(5)-Fe(1)	71.3(6)
C(1)-C(5)-Fe(1)	69.4(6)
C(4)-C(5)-H(5)	125.3
C(1)-C(5)-H(5)	125.3
Fe(1)-C(5)-H(5)	125.6
O(2)-C(6)-O(1)	124.6(10)
O(2)-C(6)-C(1)	120.6(10)
O(1)-C(6)-C(1)	114.8(9)
C(8)-C(7)-C(11)	107.5(10)

C(8)-C(7)-C(12)	125.4(11)
C(11)-C(7)-C(12)	127.0(10)
C(8)-C(7)-Fe(1)	69.8(7)
C(11)-C(7)-Fe(1)	69.2(6)
C(12)-C(7)-Fe(1)	123.6(8)
C(9)-C(8)-C(7)	107.5(11)
C(9)-C(8)-Fe(1)	69.7(7)
C(7)-C(8)-Fe(1)	69.2(7)
C(9)-C(8)-H(8)	126.3
C(7)-C(8)-H(8)	126.3
Fe(1)-C(8)-H(8)	126.4
C(8)-C(9)-C(10)	108.3(11)
C(8)-C(9)-Fe(1)	69.7(7)
C(10)-C(9)-Fe(1)	69.6(7)
C(8)-C(9)-H(9)	125.8
C(10)-C(9)-H(9)	125.8
Fe(1)-C(9)-H(9)	126.5
C(11)-C(10)-C(9)	108.4(11)
C(11)-C(10)-Fe(1)	69.6(7)
C(9)-C(10)-Fe(1)	69.6(7)
C(11)-C(10)-H(10)	125.8
C(9)-C(10)-H(10)	125.8
Fe(1)-C(10)-H(10)	126.6
C(10)-C(11)-C(7)	108.3(11)
C(10)-C(11)-Fe(1)	70.4(7)
C(7)-C(11)-Fe(1)	69.4(6)
C(10)-C(11)-H(11)	125.8
C(7)-C(11)-H(11)	125.8
Fe(1)-C(11)-H(11)	125.9
O(4)-C(12)-O(3)	123.0(11)
O(4)-C(12)-C(7)	123.6(11)
O(3)-C(12)-C(7)	113.4(10)
C(14)-C(13)-C(18)	117.6(11)
C(14)-C(13)-P(1)	120.4(9)
C(18)-C(13)-P(1)	121.7(9)
C(13)-C(14)-C(15)	121.0(12)
C(13)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	119.5(13)
C(16)-C(15)-H(15)	120.3
C(14)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	121.2(13)
C(17)-C(16)-H(16)	119.4
C(15)-C(16)-H(16)	119.4

C(16)-C(17)-C(18)	118.3(14)
C(16)-C(17)-H(17)	120.8
C(18)-C(17)-H(17)	120.8
C(17)-C(18)-C(13)	122.1(12)
C(17)-C(18)-H(18)	118.9
C(13)-C(18)-H(18)	118.9
C(24)-C(19)-C(20)	117.4(10)
C(24)-C(19)-P(1)	121.7(8)
C(20)-C(19)-P(1)	120.9(8)
C(21)-C(20)-C(19)	120.7(10)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(22)-C(21)-C(20)	121.1(11)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(21)-C(22)-C(23)	119.6(11)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(24)-C(23)-C(22)	118.8(11)
C(24)-C(23)-H(23)	120.6
C(22)-C(23)-H(23)	120.6
C(23)-C(24)-C(19)	122.1(10)
C(23)-C(24)-H(24)	119.0
C(19)-C(24)-H(24)	119.0
C(26)-C(25)-C(30)	118.4(9)
C(26)-C(25)-P(1)	125.1(8)
C(30)-C(25)-P(1)	116.4(8)
C(27)-C(26)-C(25)	120.1(10)
C(27)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(26)-C(27)-C(28)	120.6(11)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(29)-C(28)-C(27)	120.8(10)
C(29)-C(28)-H(28)	119.6
C(27)-C(28)-H(28)	119.6
C(28)-C(29)-C(30)	119.7(11)
C(28)-C(29)-H(29)	120.1
C(30)-C(29)-H(29)	120.1
C(29)-C(30)-C(25)	120.2(10)
C(29)-C(30)-H(30)	119.9
C(25)-C(30)-H(30)	119.9
C(36)-C(31)-C(32)	117.7(10)
C(36)-C(31)-P(2)	118.7(9)

C(32)-C(31)-P(2)	123.4(9)
C(33)-C(32)-C(31)	121.0(11)
C(33)-C(32)-H(32)	119.5
C(31)-C(32)-H(32)	119.5
C(32)-C(33)-C(34)	120.0(12)
C(32)-C(33)-H(33)	120.0
C(34)-C(33)-H(33)	120.0
C(35)-C(34)-C(33)	119.9(11)
C(35)-C(34)-H(34)	120.1
C(33)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	119.7(11)
C(34)-C(35)-H(35)	120.1
C(36)-C(35)-H(35)	120.1
C(35)-C(36)-C(31)	121.6(10)
C(35)-C(36)-H(36)	119.2
C(31)-C(36)-H(36)	119.2
C(38)-C(37)-C(42)	119.8(10)
C(38)-C(37)-P(2)	117.3(8)
C(42)-C(37)-P(2)	122.4(8)
C(39)-C(38)-C(37)	117.8(10)
C(39)-C(38)-H(38)	121.1
C(37)-C(38)-H(38)	121.1
C(40)-C(39)-C(38)	123.1(11)
C(40)-C(39)-H(39)	118.5
C(38)-C(39)-H(39)	118.5
C(39)-C(40)-C(41)	119.2(11)
C(39)-C(40)-H(40)	120.4
C(41)-C(40)-H(40)	120.4
C(40)-C(41)-C(42)	121.1(12)
C(40)-C(41)-H(41)	119.5
C(42)-C(41)-H(41)	119.5
C(41)-C(42)-C(37)	119.0(11)
C(41)-C(42)-H(42)	120.5
C(37)-C(42)-H(42)	120.5
C(48)-C(43)-C(44)	117.2(10)
C(48)-C(43)-P(2)	123.0(8)
C(44)-C(43)-P(2)	119.1(8)
C(45)-C(44)-C(43)	121.4(10)
C(45)-C(44)-H(44)	119.3
C(43)-C(44)-H(44)	119.3
C(46)-C(45)-C(44)	119.5(11)
C(46)-C(45)-H(45)	120.3
C(44)-C(45)-H(45)	120.3
C(47)-C(46)-C(45)	120.6(11)

C(47)-C(46)-H(46)	119.7
C(45)-C(46)-H(46)	119.7
C(46)-C(47)-C(48)	119.5(11)
C(46)-C(47)-H(47)	120.2
C(48)-C(47)-H(47)	120.2
C(43)-C(48)-C(47)	121.7(10)
C(43)-C(48)-H(48)	119.1
C(47)-C(48)-H(48)	119.1
Cl(2)-C(49)-Cl(1)	119.2(10)
Cl(2)-C(49)-H(49A)	107.5
Cl(1)-C(49)-H(49A)	107.5
Cl(2)-C(49)-H(49B)	107.5
Cl(1)-C(49)-H(49B)	107.5
H(49A)-C(49)-H(49B)	107.0
Pd(1)-C-HA	109.5
Pd(1)-C-HC	109.5
HA-C-HC	109.5
Pd(1)-C-HB	109.5
HA-C-HB	109.5
HC-C-HB	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **6d**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	48(1)	36(1)	37(1)	0(1)	-2(1)	-2(1)
Fe(1)	51(1)	41(1)	59(1)	-3(1)	5(1)	-3(1)
Cl(1)	85(3)	106(3)	142(4)	-36(3)	18(3)	-11(3)
Cl(2)	183(6)	209(6)	266(8)	-161(6)	152(6)	-111(5)
P(1)	51(2)	38(1)	39(2)	-1(1)	1(1)	0(1)
P(2)	54(2)	35(1)	43(2)	0(1)	-3(1)	1(1)
O(1)	51(5)	48(4)	40(4)	4(3)	8(4)	-1(4)
O(2)	46(5)	44(4)	57(5)	1(4)	6(4)	8(4)
O(3)	64(6)	44(4)	76(6)	9(4)	13(5)	4(4)
O(4)	53(5)	65(5)	85(7)	1(5)	3(5)	-1(5)
C(1)	44(6)	33(5)	56(7)	-3(5)	-2(5)	-3(5)
C(2)	61(8)	43(6)	73(9)	1(6)	21(7)	4(6)
C(3)	66(8)	51(7)	55(7)	6(6)	10(6)	4(6)
C(4)	52(8)	55(7)	69(8)	-20(6)	15(6)	15(6)
C(5)	50(7)	50(6)	45(6)	-8(5)	3(5)	-9(6)
C(6)	55(7)	46(6)	37(6)	-5(5)	-6(5)	5(6)
C(7)	51(7)	51(7)	48(7)	-9(5)	1(6)	-12(6)
C(8)	59(8)	57(8)	91(10)	-5(7)	7(7)	-10(7)
C(9)	78(10)	47(7)	73(9)	-26(6)	-10(7)	-9(7)
C(10)	66(9)	56(8)	84(10)	-14(7)	1(7)	5(7)
C(11)	55(7)	52(7)	52(7)	1(5)	1(6)	-2(6)
C(12)	59(8)	66(8)	35(6)	0(6)	-1(6)	-1(7)
C(13)	53(7)	44(6)	54(7)	-4(5)	9(6)	-15(6)
C(14)	46(7)	54(7)	63(8)	-13(6)	-2(6)	0(6)
C(15)	47(8)	68(8)	88(10)	-36(8)	10(7)	4(7)
C(16)	90(12)	90(11)	80(11)	-29(9)	37(9)	-23(9)
C(17)	116(12)	70(9)	73(9)	2(8)	53(9)	-9(9)
C(18)	86(10)	42(7)	67(8)	-4(6)	26(7)	0(6)
C(19)	43(6)	45(6)	33(6)	-7(5)	-1(5)	10(5)
C(20)	63(8)	49(6)	37(6)	5(5)	-3(6)	-5(6)
C(21)	64(8)	34(6)	57(7)	-4(5)	-16(6)	-3(6)
C(22)	55(8)	48(7)	75(9)	-1(6)	3(7)	-23(6)
C(23)	82(9)	65(8)	39(7)	-3(6)	0(6)	-23(7)
C(24)	63(8)	55(7)	27(6)	8(5)	-7(5)	-5(6)
C(25)	61(7)	36(5)	24(5)	0(4)	7(5)	-11(5)
C(26)	46(7)	57(7)	28(5)	1(5)	-2(5)	-5(6)
C(27)	60(7)	53(7)	33(6)	12(5)	5(5)	15(6)
C(28)	69(8)	46(6)	38(6)	4(5)	2(6)	13(6)

C(29)	67(8)	38(6)	39(6)	4(5)	8(6)	1(6)
C(30)	58(7)	44(6)	38(6)	6(5)	-2(5)	9(6)
C(31)	41(7)	53(7)	52(7)	2(6)	-3(5)	0(6)
C(32)	56(8)	68(8)	55(8)	-13(6)	-2(6)	17(7)
C(33)	65(9)	95(10)	46(7)	-3(7)	-12(6)	14(8)
C(34)	54(8)	63(8)	61(8)	16(7)	5(7)	12(6)
C(35)	58(8)	45(6)	46(7)	4(5)	0(6)	-8(6)
C(36)	66(8)	47(6)	30(6)	7(5)	-2(5)	1(6)
C(37)	49(7)	38(6)	38(6)	2(5)	-1(5)	3(5)
C(38)	50(7)	40(6)	49(7)	-2(5)	5(5)	7(5)
C(39)	81(9)	37(6)	62(8)	0(6)	10(7)	-6(6)
C(40)	91(10)	33(6)	74(9)	-11(6)	-1(8)	-13(6)
C(41)	100(11)	46(7)	69(9)	-9(7)	-25(8)	-12(7)
C(42)	98(10)	55(7)	42(7)	0(6)	-15(7)	0(7)
C(43)	42(6)	40(6)	39(6)	-1(5)	-12(5)	6(5)
C(44)	38(6)	52(7)	51(7)	1(5)	1(5)	1(5)
C(45)	52(8)	60(8)	67(8)	11(6)	1(7)	1(6)
C(46)	61(8)	79(9)	49(7)	8(7)	8(6)	-7(7)
C(47)	82(9)	58(7)	42(6)	-11(6)	19(6)	0(7)
C(48)	65(8)	46(6)	44(6)	-8(5)	-4(6)	-10(6)
C(49)	95(12)	163(17)	101(13)	-47(12)	-9(10)	-57(12)
C	71(8)	60(7)	49(7)	5(6)	9(6)	4(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6d**.

	x	y	z	U(eq)
H(3)	6361	7263	8049	92
H(2)	4482	11194	6277	70
H(3A)	5536	10119	5958	69
H(4)	5339	8406	6392	70
H(5)	4154	8415	6986	58
H(8)	6572	10602	7623	83
H(9)	5491	11718	7859	82
H(10)	4536	10701	8422	83
H(11)	5008	8968	8534	64
H(14)	2509	8354	6396	66
H(15)	3245	8066	5482	81
H(16)	2983	8920	4402	101
H(17)	2054	10127	4250	99
H(18)	1395	10495	5203	76
H(20)	288	9107	5380	61
H(21)	-739	8065	5171	65
H(22)	-1128	7174	6092	72
H(23)	-374	7180	7237	75
H(24)	659	8237	7449	60
H(26)	-248	10499	6252	53
H(27)	-734	12073	6081	58
H(28)	74	13417	6171	62
H(29)	1383	13212	6399	57
H(30)	1900	11635	6572	57
H(32)	3910	9673	10120	73
H(33)	4860	8502	10387	85
H(34)	4900	7137	9642	71
H(35)	4011	6981	8609	61
H(36)	3093	8189	8317	58
H(38)	2786	11629	8198	56
H(39)	3100	13244	8506	72
H(40)	3451	13724	9676	81
H(41)	3412	12603	10596	90
H(42)	3065	10981	10344	81
H(44)	2176	8083	9598	57
H(45)	1282	7579	10315	73
H(46)	516	8738	10774	76
H(47)	676	10385	10565	71
H(48)	1558	10888	9830	63

H(49A)	1415	5778	6838	146
H(49B)	2149	5161	7161	146
HA	581	9999	7722	90
HC	997	10628	8386	90
HB	899	9466	8465	90

Table 6. Torsion angles [deg] for **6d**.

C-Pd(1)-P(1)-C(25)	62.5(5)
O(1)-Pd(1)-P(1)-C(25)	-116.5(4)
P(2)-Pd(1)-P(1)-C(25)	57.5(11)
C-Pd(1)-P(1)-C(19)	-55.6(5)
O(1)-Pd(1)-P(1)-C(19)	125.4(4)
P(2)-Pd(1)-P(1)-C(19)	-60.5(11)
C-Pd(1)-P(1)-C(13)	-178.5(5)
O(1)-Pd(1)-P(1)-C(13)	2.5(4)
P(2)-Pd(1)-P(1)-C(13)	176.5(10)
C-Pd(1)-P(2)-C(31)	143.2(5)
O(1)-Pd(1)-P(2)-C(31)	-37.8(4)
P(1)-Pd(1)-P(2)-C(31)	148.2(10)
C-Pd(1)-P(2)-C(43)	26.1(5)
O(1)-Pd(1)-P(2)-C(43)	-154.9(4)
P(1)-Pd(1)-P(2)-C(43)	31.1(12)
C-Pd(1)-P(2)-C(37)	-94.0(5)
O(1)-Pd(1)-P(2)-C(37)	85.0(4)
P(1)-Pd(1)-P(2)-C(37)	-89.1(11)
C-Pd(1)-O(1)-C(6)	-19(21)
P(1)-Pd(1)-O(1)-C(6)	72.8(7)
P(2)-Pd(1)-O(1)-C(6)	-106.6(7)
C(11)-Fe(1)-C(1)-C(5)	-81.9(7)
C(7)-Fe(1)-C(1)-C(5)	-54.0(12)
C(10)-Fe(1)-C(1)-C(5)	-122.2(7)
C(8)-Fe(1)-C(1)-C(5)	173.0(13)
C(9)-Fe(1)-C(1)-C(5)	-162.2(7)
C(2)-Fe(1)-C(1)-C(5)	116.8(9)
C(4)-Fe(1)-C(1)-C(5)	36.9(6)
C(3)-Fe(1)-C(1)-C(5)	79.8(7)
C(5)-Fe(1)-C(1)-C(2)	-116.8(9)
C(11)-Fe(1)-C(1)-C(2)	161.3(6)
C(7)-Fe(1)-C(1)-C(2)	-170.8(9)
C(10)-Fe(1)-C(1)-C(2)	121.0(7)
C(8)-Fe(1)-C(1)-C(2)	56.2(16)
C(9)-Fe(1)-C(1)-C(2)	81.0(8)
C(4)-Fe(1)-C(1)-C(2)	-79.9(7)
C(3)-Fe(1)-C(1)-C(2)	-37.0(6)
C(5)-Fe(1)-C(1)-C(6)	119.8(11)
C(11)-Fe(1)-C(1)-C(6)	38.0(10)
C(7)-Fe(1)-C(1)-C(6)	65.8(13)
C(10)-Fe(1)-C(1)-C(6)	-2.4(9)
C(8)-Fe(1)-C(1)-C(6)	-67.2(17)

C(9)-Fe(1)-C(1)-C(6)	-42.4(10)
C(2)-Fe(1)-C(1)-C(6)	-123.4(11)
C(4)-Fe(1)-C(1)-C(6)	156.7(10)
C(3)-Fe(1)-C(1)-C(6)	-160.4(9)
C(5)-C(1)-C(2)-C(3)	-0.9(12)
C(6)-C(1)-C(2)-C(3)	175.6(10)
Fe(1)-C(1)-C(2)-C(3)	59.7(8)
C(5)-C(1)-C(2)-Fe(1)	-60.6(7)
C(6)-C(1)-C(2)-Fe(1)	115.9(11)
C(1)-Fe(1)-C(2)-C(3)	-119.5(9)
C(5)-Fe(1)-C(2)-C(3)	-80.2(7)
C(11)-Fe(1)-C(2)-C(3)	-160.3(9)
C(7)-Fe(1)-C(2)-C(3)	47.2(17)
C(10)-Fe(1)-C(2)-C(3)	165.4(7)
C(8)-Fe(1)-C(2)-C(3)	81.0(8)
C(9)-Fe(1)-C(2)-C(3)	122.5(7)
C(4)-Fe(1)-C(2)-C(3)	-36.6(7)
C(5)-Fe(1)-C(2)-C(1)	39.3(6)
C(11)-Fe(1)-C(2)-C(1)	-40.8(13)
C(7)-Fe(1)-C(2)-C(1)	166.7(13)
C(10)-Fe(1)-C(2)-C(1)	-75.0(7)
C(8)-Fe(1)-C(2)-C(1)	-159.5(6)
C(9)-Fe(1)-C(2)-C(1)	-118.0(7)
C(4)-Fe(1)-C(2)-C(1)	82.9(6)
C(3)-Fe(1)-C(2)-C(1)	119.5(9)
C(1)-C(2)-C(3)-C(4)	0.6(13)
Fe(1)-C(2)-C(3)-C(4)	59.0(8)
C(1)-C(2)-C(3)-Fe(1)	-58.4(8)
C(1)-Fe(1)-C(3)-C(4)	-82.5(7)
C(5)-Fe(1)-C(3)-C(4)	-37.9(7)
C(11)-Fe(1)-C(3)-C(4)	30.8(18)
C(7)-Fe(1)-C(3)-C(4)	75.1(8)
C(10)-Fe(1)-C(3)-C(4)	-155.1(12)
C(8)-Fe(1)-C(3)-C(4)	119.0(7)
C(9)-Fe(1)-C(3)-C(4)	163.0(7)
C(2)-Fe(1)-C(3)-C(4)	-120.4(10)
C(1)-Fe(1)-C(3)-C(2)	37.9(6)
C(5)-Fe(1)-C(3)-C(2)	82.5(7)
C(11)-Fe(1)-C(3)-C(2)	151.3(14)
C(7)-Fe(1)-C(3)-C(2)	-164.5(6)
C(10)-Fe(1)-C(3)-C(2)	-34.7(16)
C(8)-Fe(1)-C(3)-C(2)	-120.5(7)
C(9)-Fe(1)-C(3)-C(2)	-76.5(8)
C(4)-Fe(1)-C(3)-C(2)	120.4(10)

C(2)-C(3)-C(4)-C(5)	0.0(14)
Fe(1)-C(3)-C(4)-C(5)	58.6(8)
C(2)-C(3)-C(4)-Fe(1)	-58.6(8)
C(1)-Fe(1)-C(4)-C(3)	81.1(7)
C(5)-Fe(1)-C(4)-C(3)	118.7(10)
C(11)-Fe(1)-C(4)-C(3)	-169.1(7)
C(7)-Fe(1)-C(4)-C(3)	-125.3(7)
C(10)-Fe(1)-C(4)-C(3)	153.9(12)
C(8)-Fe(1)-C(4)-C(3)	-82.1(9)
C(9)-Fe(1)-C(4)-C(3)	-44.6(17)
C(2)-Fe(1)-C(4)-C(3)	36.8(7)
C(1)-Fe(1)-C(4)-C(5)	-37.6(6)
C(11)-Fe(1)-C(4)-C(5)	72.1(8)
C(7)-Fe(1)-C(4)-C(5)	115.9(7)
C(10)-Fe(1)-C(4)-C(5)	35.1(16)
C(8)-Fe(1)-C(4)-C(5)	159.2(7)
C(9)-Fe(1)-C(4)-C(5)	-163.4(13)
C(2)-Fe(1)-C(4)-C(5)	-81.9(7)
C(3)-Fe(1)-C(4)-C(5)	-118.7(10)
C(3)-C(4)-C(5)-C(1)	-0.6(13)
Fe(1)-C(4)-C(5)-C(1)	59.1(7)
C(3)-C(4)-C(5)-Fe(1)	-59.7(8)
C(2)-C(1)-C(5)-C(4)	0.9(12)
C(6)-C(1)-C(5)-C(4)	-175.7(10)
Fe(1)-C(1)-C(5)-C(4)	-60.3(8)
C(2)-C(1)-C(5)-Fe(1)	61.2(7)
C(6)-C(1)-C(5)-Fe(1)	-115.4(10)
C(1)-Fe(1)-C(5)-C(4)	120.1(10)
C(11)-Fe(1)-C(5)-C(4)	-125.4(7)
C(7)-Fe(1)-C(5)-C(4)	-83.4(8)
C(10)-Fe(1)-C(5)-C(4)	-165.9(7)
C(8)-Fe(1)-C(5)-C(4)	-53.3(16)
C(9)-Fe(1)-C(5)-C(4)	164.6(12)
C(2)-Fe(1)-C(5)-C(4)	80.9(7)
C(3)-Fe(1)-C(5)-C(4)	37.5(7)
C(11)-Fe(1)-C(5)-C(1)	114.5(7)
C(7)-Fe(1)-C(5)-C(1)	156.5(6)
C(10)-Fe(1)-C(5)-C(1)	74.1(8)
C(8)-Fe(1)-C(5)-C(1)	-173.4(12)
C(9)-Fe(1)-C(5)-C(1)	44.5(16)
C(2)-Fe(1)-C(5)-C(1)	-39.2(6)
C(4)-Fe(1)-C(5)-C(1)	-120.1(10)
C(3)-Fe(1)-C(5)-C(1)	-82.6(7)
Pd(1)-O(1)-C(6)-O(2)	9.0(14)

Pd(1)-O(1)-C(6)-C(1)	-168.9(6)
C(5)-C(1)-C(6)-O(2)	-178.9(10)
C(2)-C(1)-C(6)-O(2)	5.2(17)
Fe(1)-C(1)-C(6)-O(2)	94.6(11)
C(5)-C(1)-C(6)-O(1)	-0.9(15)
C(2)-C(1)-C(6)-O(1)	-176.8(10)
Fe(1)-C(1)-C(6)-O(1)	-87.4(10)
C(1)-Fe(1)-C(7)-C(8)	-157.6(10)
C(5)-Fe(1)-C(7)-C(8)	163.8(7)
C(11)-Fe(1)-C(7)-C(8)	-118.9(10)
C(10)-Fe(1)-C(7)-C(8)	-81.8(8)
C(9)-Fe(1)-C(7)-C(8)	-37.8(7)
C(2)-Fe(1)-C(7)-C(8)	43.5(17)
C(4)-Fe(1)-C(7)-C(8)	120.9(7)
C(3)-Fe(1)-C(7)-C(8)	79.9(8)
C(1)-Fe(1)-C(7)-C(11)	-38.7(13)
C(5)-Fe(1)-C(7)-C(11)	-77.3(7)
C(10)-Fe(1)-C(7)-C(11)	37.1(6)
C(8)-Fe(1)-C(7)-C(11)	118.9(10)
C(9)-Fe(1)-C(7)-C(11)	81.1(7)
C(2)-Fe(1)-C(7)-C(11)	162.4(13)
C(4)-Fe(1)-C(7)-C(11)	-120.3(7)
C(3)-Fe(1)-C(7)-C(11)	-161.3(6)
C(1)-Fe(1)-C(7)-C(12)	82.7(14)
C(5)-Fe(1)-C(7)-C(12)	44.1(11)
C(11)-Fe(1)-C(7)-C(12)	121.4(12)
C(10)-Fe(1)-C(7)-C(12)	158.4(11)
C(8)-Fe(1)-C(7)-C(12)	-119.8(13)
C(9)-Fe(1)-C(7)-C(12)	-157.6(11)
C(2)-Fe(1)-C(7)-C(12)	-76.3(18)
C(4)-Fe(1)-C(7)-C(12)	1.1(11)
C(3)-Fe(1)-C(7)-C(12)	-39.9(12)
C(11)-C(7)-C(8)-C(9)	0.3(13)
C(12)-C(7)-C(8)-C(9)	177.0(10)
Fe(1)-C(7)-C(8)-C(9)	59.4(8)
C(11)-C(7)-C(8)-Fe(1)	-59.1(8)
C(12)-C(7)-C(8)-Fe(1)	117.5(11)
C(1)-Fe(1)-C(8)-C(9)	33.2(18)
C(5)-Fe(1)-C(8)-C(9)	-159.6(12)
C(11)-Fe(1)-C(8)-C(9)	-80.6(8)
C(7)-Fe(1)-C(8)-C(9)	-118.9(11)
C(10)-Fe(1)-C(8)-C(9)	-37.5(7)
C(2)-Fe(1)-C(8)-C(9)	75.4(9)
C(4)-Fe(1)-C(8)-C(9)	161.3(8)

C(3)-Fe(1)-C(8)-C(9)	118.4(8)
C(1)-Fe(1)-C(8)-C(7)	152.1(12)
C(5)-Fe(1)-C(8)-C(7)	-40.7(16)
C(11)-Fe(1)-C(8)-C(7)	38.3(7)
C(10)-Fe(1)-C(8)-C(7)	81.3(7)
C(9)-Fe(1)-C(8)-C(7)	118.9(11)
C(2)-Fe(1)-C(8)-C(7)	-165.8(6)
C(4)-Fe(1)-C(8)-C(7)	-79.8(8)
C(3)-Fe(1)-C(8)-C(7)	-122.7(7)
C(7)-C(8)-C(9)-C(10)	-0.1(14)
Fe(1)-C(8)-C(9)-C(10)	59.0(9)
C(7)-C(8)-C(9)-Fe(1)	-59.1(8)
C(1)-Fe(1)-C(9)-C(8)	-167.3(7)
C(5)-Fe(1)-C(9)-C(8)	159.9(12)
C(11)-Fe(1)-C(9)-C(8)	82.8(8)
C(7)-Fe(1)-C(9)-C(8)	38.1(7)
C(10)-Fe(1)-C(9)-C(8)	119.7(11)
C(2)-Fe(1)-C(9)-C(8)	-124.3(8)
C(4)-Fe(1)-C(9)-C(8)	-50.1(18)
C(3)-Fe(1)-C(9)-C(8)	-83.2(9)
C(1)-Fe(1)-C(9)-C(10)	73.0(9)
C(5)-Fe(1)-C(9)-C(10)	40.2(17)
C(11)-Fe(1)-C(9)-C(10)	-36.9(7)
C(7)-Fe(1)-C(9)-C(10)	-81.6(8)
C(8)-Fe(1)-C(9)-C(10)	-119.7(11)
C(2)-Fe(1)-C(9)-C(10)	116.0(7)
C(4)-Fe(1)-C(9)-C(10)	-169.9(13)
C(3)-Fe(1)-C(9)-C(10)	157.1(7)
C(8)-C(9)-C(10)-C(11)	-0.1(14)
Fe(1)-C(9)-C(10)-C(11)	58.9(9)
C(8)-C(9)-C(10)-Fe(1)	-59.1(9)
C(1)-Fe(1)-C(10)-C(11)	117.0(7)
C(5)-Fe(1)-C(10)-C(11)	76.4(8)
C(7)-Fe(1)-C(10)-C(11)	-38.3(7)
C(8)-Fe(1)-C(10)-C(11)	-82.5(8)
C(9)-Fe(1)-C(10)-C(11)	-119.8(11)
C(2)-Fe(1)-C(10)-C(11)	157.7(7)
C(4)-Fe(1)-C(10)-C(11)	50.6(16)
C(3)-Fe(1)-C(10)-C(11)	-177.2(11)
C(1)-Fe(1)-C(10)-C(9)	-123.2(7)
C(5)-Fe(1)-C(10)-C(9)	-163.8(7)
C(11)-Fe(1)-C(10)-C(9)	119.8(11)
C(7)-Fe(1)-C(10)-C(9)	81.6(8)
C(8)-Fe(1)-C(10)-C(9)	37.4(7)

C(2)-Fe(1)-C(10)-C(9)	-82.5(8)
C(4)-Fe(1)-C(10)-C(9)	170.4(12)
C(3)-Fe(1)-C(10)-C(9)	-57.3(16)
C(9)-C(10)-C(11)-C(7)	0.3(14)
Fe(1)-C(10)-C(11)-C(7)	59.3(8)
C(9)-C(10)-C(11)-Fe(1)	-59.0(9)
C(8)-C(7)-C(11)-C(10)	-0.4(13)
C(12)-C(7)-C(11)-C(10)	-177.0(11)
Fe(1)-C(7)-C(11)-C(10)	-59.9(8)
C(8)-C(7)-C(11)-Fe(1)	59.5(8)
C(12)-C(7)-C(11)-Fe(1)	-117.1(11)
C(1)-Fe(1)-C(11)-C(10)	-77.9(8)
C(5)-Fe(1)-C(11)-C(10)	-120.4(8)
C(7)-Fe(1)-C(11)-C(10)	119.3(10)
C(8)-Fe(1)-C(11)-C(10)	81.4(8)
C(9)-Fe(1)-C(11)-C(10)	37.6(7)
C(2)-Fe(1)-C(11)-C(10)	-49.0(13)
C(4)-Fe(1)-C(11)-C(10)	-160.1(7)
C(3)-Fe(1)-C(11)-C(10)	176.5(14)
C(1)-Fe(1)-C(11)-C(7)	162.7(6)
C(5)-Fe(1)-C(11)-C(7)	120.2(6)
C(10)-Fe(1)-C(11)-C(7)	-119.3(10)
C(8)-Fe(1)-C(11)-C(7)	-38.0(6)
C(9)-Fe(1)-C(11)-C(7)	-81.7(7)
C(2)-Fe(1)-C(11)-C(7)	-168.3(9)
C(4)-Fe(1)-C(11)-C(7)	80.6(8)
C(3)-Fe(1)-C(11)-C(7)	57.2(17)
C(8)-C(7)-C(12)-O(4)	17.1(18)
C(11)-C(7)-C(12)-O(4)	-166.9(11)
Fe(1)-C(7)-C(12)-O(4)	105.0(12)
C(8)-C(7)-C(12)-O(3)	-162.5(11)
C(11)-C(7)-C(12)-O(3)	13.5(16)
Fe(1)-C(7)-C(12)-O(3)	-74.6(12)
C(25)-P(1)-C(13)-C(14)	167.5(9)
C(19)-P(1)-C(13)-C(14)	-83.3(9)
Pd(1)-P(1)-C(13)-C(14)	47.4(10)
C(25)-P(1)-C(13)-C(18)	-17.9(10)
C(19)-P(1)-C(13)-C(18)	91.3(10)
Pd(1)-P(1)-C(13)-C(18)	-138.0(8)
C(18)-C(13)-C(14)-C(15)	4.3(16)
P(1)-C(13)-C(14)-C(15)	179.1(9)
C(13)-C(14)-C(15)-C(16)	-4.6(18)
C(14)-C(15)-C(16)-C(17)	2(2)
C(15)-C(16)-C(17)-C(18)	1(2)

C(16)-C(17)-C(18)-C(13)	-1(2)
C(14)-C(13)-C(18)-C(17)	-1.5(18)
P(1)-C(13)-C(18)-C(17)	-176.2(10)
C(25)-P(1)-C(19)-C(24)	-118.5(9)
C(13)-P(1)-C(19)-C(24)	131.0(9)
Pd(1)-P(1)-C(19)-C(24)	1.7(10)
C(25)-P(1)-C(19)-C(20)	61.3(9)
C(13)-P(1)-C(19)-C(20)	-49.3(9)
Pd(1)-P(1)-C(19)-C(20)	-178.5(7)
C(24)-C(19)-C(20)-C(21)	4.0(15)
P(1)-C(19)-C(20)-C(21)	-175.8(8)
C(19)-C(20)-C(21)-C(22)	0.0(17)
C(20)-C(21)-C(22)-C(23)	-4.2(18)
C(21)-C(22)-C(23)-C(24)	4.3(18)
C(22)-C(23)-C(24)-C(19)	-0.2(18)
C(20)-C(19)-C(24)-C(23)	-3.8(16)
P(1)-C(19)-C(24)-C(23)	176.0(9)
C(19)-P(1)-C(25)-C(26)	8.1(9)
C(13)-P(1)-C(25)-C(26)	116.3(9)
Pd(1)-P(1)-C(25)-C(26)	-118.6(8)
C(19)-P(1)-C(25)-C(30)	-174.9(7)
C(13)-P(1)-C(25)-C(30)	-66.6(8)
Pd(1)-P(1)-C(25)-C(30)	58.4(8)
C(30)-C(25)-C(26)-C(27)	-0.8(14)
P(1)-C(25)-C(26)-C(27)	176.2(7)
C(25)-C(26)-C(27)-C(28)	-0.2(15)
C(26)-C(27)-C(28)-C(29)	1.0(15)
C(27)-C(28)-C(29)-C(30)	-0.9(16)
C(28)-C(29)-C(30)-C(25)	-0.1(15)
C(26)-C(25)-C(30)-C(29)	0.9(14)
P(1)-C(25)-C(30)-C(29)	-176.3(7)
C(43)-P(2)-C(31)-C(36)	104.2(9)
C(37)-P(2)-C(31)-C(36)	-145.3(8)
Pd(1)-P(2)-C(31)-C(36)	-20.0(10)
C(43)-P(2)-C(31)-C(32)	-71.6(11)
C(37)-P(2)-C(31)-C(32)	38.9(11)
Pd(1)-P(2)-C(31)-C(32)	164.2(9)
C(36)-C(31)-C(32)-C(33)	-0.9(18)
P(2)-C(31)-C(32)-C(33)	175.0(9)
C(31)-C(32)-C(33)-C(34)	-1.0(19)
C(32)-C(33)-C(34)-C(35)	1.3(19)
C(33)-C(34)-C(35)-C(36)	0.1(17)
C(34)-C(35)-C(36)-C(31)	-2.1(16)
C(32)-C(31)-C(36)-C(35)	2.4(16)

P(2)-C(31)-C(36)-C(35)	-173.7(8)
C(31)-P(2)-C(37)-C(38)	115.3(9)
C(43)-P(2)-C(37)-C(38)	-135.9(8)
Pd(1)-P(2)-C(37)-C(38)	-10.1(9)
C(31)-P(2)-C(37)-C(42)	-72.5(10)
C(43)-P(2)-C(37)-C(42)	36.4(11)
Pd(1)-P(2)-C(37)-C(42)	162.1(9)
C(42)-C(37)-C(38)-C(39)	2.4(16)
P(2)-C(37)-C(38)-C(39)	174.9(8)
C(37)-C(38)-C(39)-C(40)	0.7(18)
C(38)-C(39)-C(40)-C(41)	-3(2)
C(39)-C(40)-C(41)-C(42)	1(2)
C(40)-C(41)-C(42)-C(37)	2(2)
C(38)-C(37)-C(42)-C(41)	-3.6(18)
P(2)-C(37)-C(42)-C(41)	-175.6(10)
C(31)-P(2)-C(43)-C(48)	148.1(9)
C(37)-P(2)-C(43)-C(48)	35.2(10)
Pd(1)-P(2)-C(43)-C(48)	-89.1(9)
C(31)-P(2)-C(43)-C(44)	-41.6(9)
C(37)-P(2)-C(43)-C(44)	-154.4(8)
Pd(1)-P(2)-C(43)-C(44)	81.2(8)
C(48)-C(43)-C(44)-C(45)	-0.7(15)
P(2)-C(43)-C(44)-C(45)	-171.6(9)
C(43)-C(44)-C(45)-C(46)	0.7(17)
C(44)-C(45)-C(46)-C(47)	-1.3(18)
C(45)-C(46)-C(47)-C(48)	1.8(18)
C(44)-C(43)-C(48)-C(47)	1.3(15)
P(2)-C(43)-C(48)-C(47)	171.8(8)
C(46)-C(47)-C(48)-C(43)	-1.9(17)

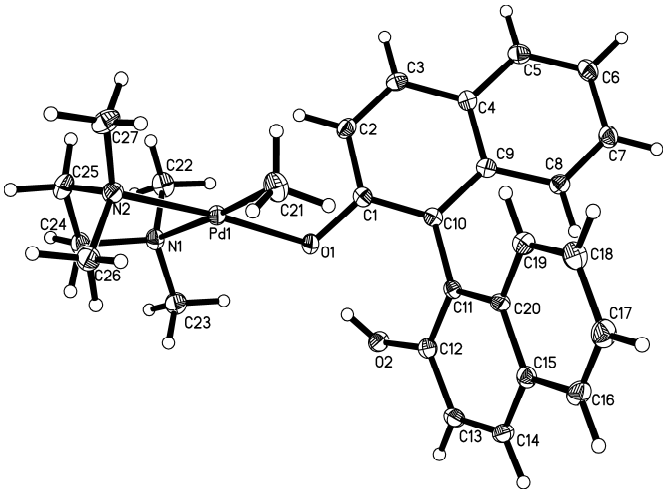
Symmetry transformations used to generate equivalent atoms:

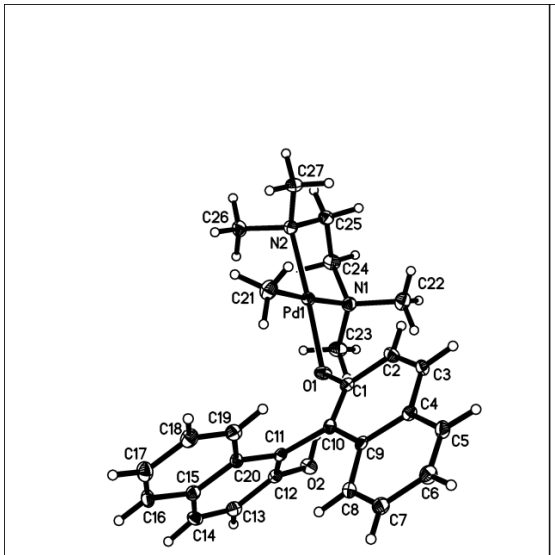
Table 7. Hydrogen bonds for **6d** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(2)#1	0.84	1.79	2.617(10)	169.8

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+3/2

The X-ray structure of compound 7a





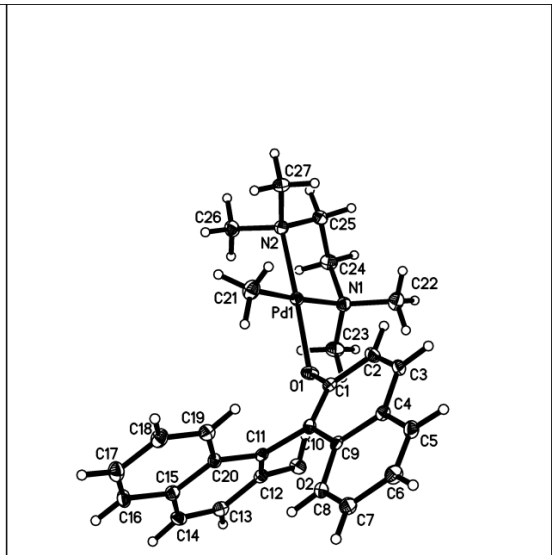


Table 1. Crystal data and structure refinement for **7a**.

Identification code	a
Empirical formula	C28 H34 C12 N2 O2 Pd
Formula weight	607.87
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 10.754(2) A alpha = 66.21(3) deg.
	b = 11.776(2) A beta = 77.67(3) deg.
	c = 12.101(2) A gamma = 89.24(3) deg.
Volume	1365.4(5) A^3
Z, Calculated density	2, 1.479 Mg/m^3
Absorption coefficient	0.903 mm^-1
F(000)	624
Crystal size	0.42 x 0.22 x 0.12 mm
Theta range for data collection	1.94 to 27.49 deg.
Limiting indices	-13<=h<=13, -15<=k<=15, -15<=l<=15
Reflections collected / unique	17486 / 11389 [R(int) = 0.0356]
Completeness to theta = 27.49	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.6389
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11389 / 3 / 641
Goodness-of-fit on F^2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.0855
R indices (all data)	R1 = 0.0391, wR2 = 0.0867
Absolute structure parameter	-0.030(19)
Largest diff. peak and hole	1.024 and -0.408 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	6763(1)	9764(1)	8056(1)	22(1)
Pd(2)	2361(1)	9849(1)	5510(1)	22(1)
Cl(1)	9617(2)	9992(2)	-8(1)	61(1)
Cl(2)	11984(2)	9582(2)	845(1)	63(1)
Cl(3)	6145(2)	9813(2)	3080(2)	68(1)
Cl(4)	8849(1)	9763(1)	3079(1)	49(1)
O(1)	7365(3)	8287(2)	7647(2)	27(1)
O(2)	7464(3)	7219(3)	6135(3)	28(1)
O(3)	2771(3)	11357(2)	5849(2)	26(1)
O(4)	2193(3)	12362(3)	7385(3)	29(1)
N(1)	8045(3)	11139(3)	6386(3)	26(1)
N(2)	6105(3)	11317(3)	8339(3)	26(1)
N(3)	1849(3)	8263(3)	5313(3)	24(1)
N(4)	2936(3)	8537(3)	7167(3)	25(1)
C(1)	7846(3)	7344(3)	8469(3)	22(1)
C(2)	8740(4)	7614(4)	9055(4)	27(1)
C(3)	9328(4)	6694(4)	9830(4)	25(1)
C(4)	9068(3)	5439(4)	10053(3)	23(1)
C(5)	9678(4)	4474(4)	10829(4)	29(1)
C(6)	9382(4)	3252(4)	11097(4)	31(1)
C(7)	8499(4)	2950(4)	10541(4)	29(1)
C(8)	7902(4)	3859(4)	9768(4)	25(1)
C(9)	8128(3)	5141(4)	9509(3)	21(1)
C(10)	7486(3)	6108(3)	8739(3)	20(1)
C(11)	6461(4)	5801(4)	8222(4)	20(1)
C(12)	6553(4)	6296(4)	6950(3)	23(1)
C(13)	5694(4)	5860(4)	6432(4)	26(1)
C(14)	4699(4)	5019(4)	7173(4)	27(1)
C(15)	4464(4)	4600(4)	8477(4)	25(1)
C(16)	3357(4)	3802(4)	9271(4)	31(1)
C(17)	3127(4)	3419(4)	10532(4)	34(1)
C(18)	4002(4)	3805(4)	11051(4)	31(1)
C(19)	5062(4)	4573(4)	10320(4)	28(1)
C(20)	5346(4)	4989(3)	9004(4)	21(1)
C(21)	5581(4)	8552(4)	9635(4)	37(1)
C(22)	9359(4)	11129(4)	6557(4)	36(1)
C(23)	8040(5)	10917(4)	5271(4)	35(1)

C(24)	7522(4)	12349(4)	6250(4)	31(1)
C(25)	7082(4)	12368(4)	7513(4)	31(1)
C(26)	4861(4)	11570(4)	7970(4)	33(1)
C(27)	5919(4)	11219(4)	9624(4)	35(1)
C(28)	3634(4)	12274(4)	5021(3)	24(1)
C(29)	4786(4)	11986(4)	4388(4)	29(1)
C(30)	5730(4)	12882(4)	3616(4)	30(1)
C(31)	5606(3)	14131(4)	3456(3)	22(1)
C(32)	6608(4)	15074(4)	2698(4)	31(1)
C(33)	6482(4)	16282(4)	2508(4)	34(1)
C(34)	5356(4)	16602(4)	3113(4)	33(1)
C(35)	4376(4)	15721(4)	3869(3)	24(1)
C(36)	4455(3)	14454(3)	4043(3)	19(1)
C(37)	3431(3)	13508(3)	4799(3)	20(1)
C(38)	2168(4)	13849(3)	5334(3)	19(1)
C(39)	1645(4)	13306(3)	6605(4)	22(1)
C(40)	534(4)	13713(4)	7131(4)	29(1)
C(41)	−127(4)	14585(4)	6405(4)	28(1)
C(42)	285(4)	15085(4)	5091(4)	25(1)
C(43)	−427(4)	15934(4)	4319(4)	33(1)
C(44)	−7(5)	16430(4)	3054(4)	36(1)
C(45)	1132(4)	16066(4)	2523(4)	33(1)
C(46)	1827(4)	15240(4)	3229(4)	26(1)
C(47)	1442(4)	14715(3)	4555(3)	22(1)
C(48)	1876(4)	11017(4)	3937(4)	34(1)
C(49)	2215(4)	8318(4)	4037(4)	34(1)
C(50)	437(4)	7992(4)	5762(4)	32(1)
C(51)	2501(4)	7242(4)	6110(4)	28(1)
C(52)	2410(4)	7295(4)	7359(4)	28(1)
C(53)	4348(4)	8595(4)	6927(4)	35(1)
C(54)	2442(4)	8772(4)	8278(4)	34(1)
C(55)	10953(5)	10673(5)	196(5)	45(1)
C(56)	7468(5)	8927(5)	3215(5)	48(1)

Table 3. Bond lengths [A] and angles [deg] for **7a**.

Pd(1)-C(21)	2.028(4)
Pd(1)-O(1)	2.054(3)
Pd(1)-N(2)	2.081(3)
Pd(1)-N(1)	2.200(3)
Pd(2)-C(48)	2.020(4)
Pd(2)-O(3)	2.050(3)
Pd(2)-N(3)	2.071(3)
Pd(2)-N(4)	2.190(3)
Cl(1)-C(55)	1.764(6)
Cl(2)-C(55)	1.736(6)
Cl(3)-C(56)	1.750(6)
Cl(4)-C(56)	1.734(5)
O(1)-C(1)	1.343(4)
O(2)-C(12)	1.365(5)
O(2)-H(2)	0.8399
O(3)-C(28)	1.337(5)
O(4)-C(39)	1.359(5)
O(4)-H(4)	0.8401
N(1)-C(22)	1.471(5)
N(1)-C(23)	1.475(5)
N(1)-C(24)	1.484(5)
N(2)-C(27)	1.480(5)
N(2)-C(26)	1.489(5)
N(2)-C(25)	1.491(5)
N(3)-C(51)	1.483(5)
N(3)-C(49)	1.484(5)
N(3)-C(50)	1.491(5)
N(4)-C(54)	1.470(5)
N(4)-C(53)	1.481(5)
N(4)-C(52)	1.484(5)
C(1)-C(10)	1.397(5)
C(1)-C(2)	1.418(5)
C(2)-C(3)	1.367(6)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.411(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.410(5)
C(4)-C(9)	1.434(5)
C(5)-C(6)	1.367(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.399(6)
C(6)-H(6)	0.9500

C(7)-C(8)	1.366(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.425(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.428(5)
C(10)-C(11)	1.492(5)
C(11)-C(12)	1.389(5)
C(11)-C(20)	1.436(5)
C(12)-C(13)	1.425(5)
C(13)-C(14)	1.353(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.415(6)
C(14)-H(14)	0.9500
C(15)-C(20)	1.422(5)
C(15)-C(16)	1.427(5)
C(16)-C(17)	1.371(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.408(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.362(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.427(5)
C(19)-H(19)	0.9500
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22C)	0.9800
C(22)-H(22B)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(23)-H(23A)	0.9800
C(24)-C(25)	1.509(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25B)	0.9900
C(25)-H(25A)	0.9900
C(26)-H(26A)	0.9800
C(26)-H(26C)	0.9800
C(26)-H(26B)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27C)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(37)	1.390(5)

C(28)-C(29)	1.424(5)
C(29)-C(30)	1.358(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.413(6)
C(30)-H(30)	0.9500
C(31)-C(36)	1.417(5)
C(31)-C(32)	1.422(5)
C(32)-C(33)	1.357(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.405(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.370(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.425(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.439(5)
C(37)-C(38)	1.498(5)
C(38)-C(39)	1.392(5)
C(38)-C(47)	1.435(5)
C(39)-C(40)	1.403(5)
C(40)-C(41)	1.360(6)
C(40)-H(40)	0.9500
C(41)-C(42)	1.422(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.411(6)
C(42)-C(47)	1.424(5)
C(43)-C(44)	1.371(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.403(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.348(6)
C(45)-H(45)	0.9500
C(46)-C(47)	1.432(5)
C(46)-H(46)	0.9500
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(48)-H(48A)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49C)	0.9800
C(49)-H(49B)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(50)-H(50A)	0.9800
C(51)-C(52)	1.521(6)

C(51)-H(51B)	0.9900
C(51)-H(51A)	0.9900
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(53)-H(53A)	0.9800
C(54)-H(54A)	0.9800
C(54)-H(54C)	0.9800
C(54)-H(54B)	0.9800
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-H(56B)	0.9900
C(56)-H(56A)	0.9900

C(21)-Pd(1)-O(1)	88.99(15)
C(21)-Pd(1)-N(2)	93.30(16)
O(1)-Pd(1)-N(2)	175.43(12)
C(21)-Pd(1)-N(1)	177.30(16)
O(1)-Pd(1)-N(1)	93.46(12)
N(2)-Pd(1)-N(1)	84.33(13)
C(48)-Pd(2)-O(3)	89.07(15)
C(48)-Pd(2)-N(3)	93.73(16)
O(3)-Pd(2)-N(3)	175.30(12)
C(48)-Pd(2)-N(4)	177.32(16)
O(3)-Pd(2)-N(4)	92.80(12)
N(3)-Pd(2)-N(4)	84.52(12)
C(1)-O(1)-Pd(1)	119.5(2)
C(12)-O(2)-H(2)	109.4
C(28)-O(3)-Pd(2)	120.6(2)
C(39)-O(4)-H(4)	109.5
C(22)-N(1)-C(23)	109.2(3)
C(22)-N(1)-C(24)	110.8(3)
C(23)-N(1)-C(24)	109.8(3)
C(22)-N(1)-Pd(1)	110.6(3)
C(23)-N(1)-Pd(1)	112.2(3)
C(24)-N(1)-Pd(1)	104.3(2)
C(27)-N(2)-C(26)	107.9(3)
C(27)-N(2)-C(25)	108.4(3)
C(26)-N(2)-C(25)	110.2(3)
C(27)-N(2)-Pd(1)	115.8(3)
C(26)-N(2)-Pd(1)	108.5(2)
C(25)-N(2)-Pd(1)	106.0(2)
C(51)-N(3)-C(49)	107.8(3)

C(51)-N(3)-C(50)	109.9(3)
C(49)-N(3)-C(50)	108.5(3)
C(51)-N(3)-Pd(2)	106.3(2)
C(49)-N(3)-Pd(2)	115.8(3)
C(50)-N(3)-Pd(2)	108.4(2)
C(54)-N(4)-C(53)	108.8(3)
C(54)-N(4)-C(52)	109.8(3)
C(53)-N(4)-C(52)	110.5(3)
C(54)-N(4)-Pd(2)	113.6(3)
C(53)-N(4)-Pd(2)	109.3(3)
C(52)-N(4)-Pd(2)	104.9(2)
O(1)-C(1)-C(10)	120.8(3)
O(1)-C(1)-C(2)	119.3(3)
C(10)-C(1)-C(2)	120.0(3)
C(3)-C(2)-C(1)	121.6(4)
C(3)-C(2)-H(2A)	119.2
C(1)-C(2)-H(2A)	119.2
C(2)-C(3)-C(4)	120.3(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	121.5(4)
C(5)-C(4)-C(9)	119.5(3)
C(3)-C(4)-C(9)	119.0(3)
C(6)-C(5)-C(4)	121.6(4)
C(6)-C(5)-H(5)	119.2
C(4)-C(5)-H(5)	119.2
C(5)-C(6)-C(7)	119.5(4)
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
C(8)-C(7)-C(6)	120.6(4)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	122.1(4)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(8)-C(9)-C(10)	123.3(3)
C(8)-C(9)-C(4)	116.6(3)
C(10)-C(9)-C(4)	120.1(3)
C(1)-C(10)-C(9)	118.8(3)
C(1)-C(10)-C(11)	120.7(3)
C(9)-C(10)-C(11)	120.4(3)
C(12)-C(11)-C(20)	117.2(3)
C(12)-C(11)-C(10)	120.8(3)
C(20)-C(11)-C(10)	122.0(3)

O(2)-C(12)-C(11)	122.1(3)
O(2)-C(12)-C(13)	116.6(3)
C(11)-C(12)-C(13)	121.3(4)
C(14)-C(13)-C(12)	120.7(4)
C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
C(13)-C(14)-C(15)	120.3(4)
C(13)-C(14)-H(14)	119.8
C(15)-C(14)-H(14)	119.8
C(14)-C(15)-C(20)	119.2(4)
C(14)-C(15)-C(16)	121.3(4)
C(20)-C(15)-C(16)	119.5(4)
C(17)-C(16)-C(15)	120.8(4)
C(17)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6
C(16)-C(17)-C(18)	119.6(4)
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-H(17)	120.2
C(19)-C(18)-C(17)	121.1(4)
C(19)-C(18)-H(18)	119.5
C(17)-C(18)-H(18)	119.5
C(18)-C(19)-C(20)	121.3(4)
C(18)-C(19)-H(19)	119.3
C(20)-C(19)-H(19)	119.3
C(15)-C(20)-C(19)	117.7(4)
C(15)-C(20)-C(11)	120.4(3)
C(19)-C(20)-C(11)	121.9(3)
Pd(1)-C(21)-H(21A)	109.5
Pd(1)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Pd(1)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-H(22A)	109.5
N(1)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
N(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
H(22C)-C(22)-H(22B)	109.5
N(1)-C(23)-H(23B)	109.5
N(1)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(1)-C(23)-H(23A)	109.5
H(23B)-C(23)-H(23A)	109.5

H(23C)-C(23)-H(23A)	109.5
N(1)-C(24)-C(25)	109.5(3)
N(1)-C(24)-H(24A)	109.8
C(25)-C(24)-H(24A)	109.8
N(1)-C(24)-H(24B)	109.8
C(25)-C(24)-H(24B)	109.8
H(24A)-C(24)-H(24B)	108.2
N(2)-C(25)-C(24)	111.0(3)
N(2)-C(25)-H(25B)	109.4
C(24)-C(25)-H(25B)	109.4
N(2)-C(25)-H(25A)	109.4
C(24)-C(25)-H(25A)	109.4
H(25B)-C(25)-H(25A)	108.0
N(2)-C(26)-H(26A)	109.5
N(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
N(2)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
H(26C)-C(26)-H(26B)	109.5
N(2)-C(27)-H(27A)	109.5
N(2)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
N(2)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
H(27C)-C(27)-H(27B)	109.5
O(3)-C(28)-C(37)	120.4(3)
O(3)-C(28)-C(29)	119.9(3)
C(37)-C(28)-C(29)	119.7(3)
C(30)-C(29)-C(28)	121.7(4)
C(30)-C(29)-H(29)	119.1
C(28)-C(29)-H(29)	119.1
C(29)-C(30)-C(31)	120.1(4)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(30)-C(31)-C(36)	119.4(3)
C(30)-C(31)-C(32)	121.0(4)
C(36)-C(31)-C(32)	119.5(4)
C(33)-C(32)-C(31)	121.5(4)
C(33)-C(32)-H(32)	119.3
C(31)-C(32)-H(32)	119.3
C(32)-C(33)-C(34)	119.2(4)
C(32)-C(33)-H(33)	120.4
C(34)-C(33)-H(33)	120.4
C(35)-C(34)-C(33)	121.3(4)

C(35)-C(34)-H(34)	119.4
C(33)-C(34)-H(34)	119.4
C(34)-C(35)-C(36)	120.8(4)
C(34)-C(35)-H(35)	119.6
C(36)-C(35)-H(35)	119.6
C(31)-C(36)-C(35)	117.6(3)
C(31)-C(36)-C(37)	119.9(3)
C(35)-C(36)-C(37)	122.5(3)
C(28)-C(37)-C(36)	118.8(3)
C(28)-C(37)-C(38)	120.7(3)
C(36)-C(37)-C(38)	120.5(3)
C(39)-C(38)-C(47)	117.8(3)
C(39)-C(38)-C(37)	120.9(3)
C(47)-C(38)-C(37)	121.3(3)
O(4)-C(39)-C(38)	121.3(3)
O(4)-C(39)-C(40)	117.4(3)
C(38)-C(39)-C(40)	121.3(4)
C(41)-C(40)-C(39)	121.0(4)
C(41)-C(40)-H(40)	119.5
C(39)-C(40)-H(40)	119.5
C(40)-C(41)-C(42)	120.3(4)
C(40)-C(41)-H(41)	119.8
C(42)-C(41)-H(41)	119.8
C(43)-C(42)-C(41)	121.3(4)
C(43)-C(42)-C(47)	119.9(4)
C(41)-C(42)-C(47)	118.8(4)
C(44)-C(43)-C(42)	120.8(4)
C(44)-C(43)-H(43)	119.6
C(42)-C(43)-H(43)	119.6
C(43)-C(44)-C(45)	119.4(4)
C(43)-C(44)-H(44)	120.3
C(45)-C(44)-H(44)	120.3
C(46)-C(45)-C(44)	121.5(4)
C(46)-C(45)-H(45)	119.3
C(44)-C(45)-H(45)	119.3
C(45)-C(46)-C(47)	121.2(4)
C(45)-C(46)-H(46)	119.4
C(47)-C(46)-H(46)	119.4
C(42)-C(47)-C(46)	117.2(4)
C(42)-C(47)-C(38)	120.2(3)
C(46)-C(47)-C(38)	122.7(3)
Pd(2)-C(48)-H(48B)	109.5
Pd(2)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5

Pd(2)-C(48)-H(48A)	109.5
H(48B)-C(48)-H(48A)	109.5
H(48C)-C(48)-H(48A)	109.5
N(3)-C(49)-H(49A)	109.5
N(3)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
N(3)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
H(49C)-C(49)-H(49B)	109.5
N(3)-C(50)-H(50B)	109.5
N(3)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
N(3)-C(50)-H(50A)	109.5
H(50B)-C(50)-H(50A)	109.5
H(50C)-C(50)-H(50A)	109.5
N(3)-C(51)-C(52)	111.1(3)
N(3)-C(51)-H(51B)	109.4
C(52)-C(51)-H(51B)	109.4
N(3)-C(51)-H(51A)	109.4
C(52)-C(51)-H(51A)	109.4
H(51B)-C(51)-H(51A)	108.0
N(4)-C(52)-C(51)	109.6(3)
N(4)-C(52)-H(52A)	109.8
C(51)-C(52)-H(52A)	109.8
N(4)-C(52)-H(52B)	109.8
C(51)-C(52)-H(52B)	109.8
H(52A)-C(52)-H(52B)	108.2
N(4)-C(53)-H(53B)	109.5
N(4)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
N(4)-C(53)-H(53A)	109.5
H(53B)-C(53)-H(53A)	109.5
H(53C)-C(53)-H(53A)	109.5
N(4)-C(54)-H(54A)	109.5
N(4)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
N(4)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
H(54C)-C(54)-H(54B)	109.5
Cl(2)-C(55)-Cl(1)	112.5(3)
Cl(2)-C(55)-H(55A)	109.1
Cl(1)-C(55)-H(55A)	109.1
Cl(2)-C(55)-H(55B)	109.1
Cl(1)-C(55)-H(55B)	109.1

H(55A)-C(55)-H(55B)	107.8
Cl(4)-C(56)-Cl(3)	113.2(3)
Cl(4)-C(56)-H(56B)	108.9
Cl(3)-C(56)-H(56B)	108.9
Cl(4)-C(56)-H(56A)	108.9
Cl(3)-C(56)-H(56A)	108.9
H(56B)-C(56)-H(56A)	107.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **7a**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	22(1)	20(1)	25(1)	-9(1)	-7(1)	2(1)
Pd(2)	22(1)	19(1)	24(1)	-9(1)	-5(1)	3(1)
Cl(1)	71(1)	75(1)	51(1)	-40(1)	-15(1)	2(1)
Cl(2)	74(1)	73(1)	36(1)	-17(1)	-12(1)	18(1)
Cl(3)	54(1)	68(1)	97(1)	-50(1)	-18(1)	16(1)
Cl(4)	54(1)	59(1)	35(1)	-19(1)	-8(1)	-5(1)
O(1)	37(2)	19(1)	26(1)	-10(1)	-10(1)	5(1)
O(2)	32(2)	28(2)	23(1)	-9(1)	-3(1)	-4(1)
O(3)	30(2)	19(1)	29(1)	-12(1)	1(1)	-1(1)
O(4)	33(2)	28(2)	23(1)	-10(1)	-3(1)	7(1)
N(1)	26(2)	23(2)	30(2)	-11(1)	-6(1)	4(1)
N(2)	24(2)	27(2)	30(2)	-14(1)	-9(1)	5(1)
N(3)	25(2)	25(2)	26(2)	-13(1)	-7(1)	4(1)
N(4)	27(2)	23(2)	28(2)	-11(1)	-9(1)	1(1)
C(1)	21(2)	23(2)	21(2)	-10(2)	-3(1)	5(2)
C(2)	28(2)	24(2)	30(2)	-12(2)	-6(2)	-3(2)
C(3)	21(2)	31(2)	28(2)	-15(2)	-9(2)	1(2)
C(4)	20(2)	23(2)	23(2)	-9(2)	-2(1)	2(2)
C(5)	23(2)	34(2)	31(2)	-14(2)	-10(2)	5(2)
C(6)	32(2)	27(2)	33(2)	-9(2)	-14(2)	9(2)
C(7)	29(2)	23(2)	34(2)	-10(2)	-10(2)	6(2)
C(8)	21(2)	27(2)	29(2)	-13(2)	-7(2)	4(2)
C(9)	15(2)	26(2)	21(2)	-11(2)	-2(1)	5(1)
C(10)	17(2)	22(2)	18(2)	-6(2)	-2(1)	0(1)
C(11)	18(2)	19(2)	25(2)	-10(2)	-8(2)	8(2)
C(12)	22(2)	23(2)	25(2)	-11(2)	-4(2)	5(2)
C(13)	30(2)	27(2)	23(2)	-11(2)	-10(2)	8(2)
C(14)	30(2)	27(2)	34(2)	-18(2)	-16(2)	7(2)
C(15)	23(2)	22(2)	29(2)	-10(2)	-7(2)	5(2)
C(16)	20(2)	31(2)	46(2)	-17(2)	-11(2)	1(2)
C(17)	27(2)	31(2)	37(2)	-9(2)	-4(2)	-4(2)
C(18)	28(2)	31(2)	27(2)	-8(2)	2(2)	1(2)
C(19)	27(2)	28(2)	28(2)	-12(2)	-6(2)	2(2)
C(20)	19(2)	22(2)	24(2)	-9(2)	-9(1)	4(1)
C(21)	32(2)	32(2)	37(2)	-8(2)	-2(2)	2(2)
C(22)	29(2)	33(2)	39(2)	-11(2)	-4(2)	3(2)
C(23)	46(3)	32(2)	30(2)	-14(2)	-11(2)	5(2)
C(24)	38(2)	21(2)	30(2)	-7(2)	-7(2)	1(2)

C(25)	29(2)	26(2)	41(2)	-18(2)	-4(2)	-1(2)
C(26)	28(2)	32(2)	47(3)	-19(2)	-16(2)	8(2)
C(27)	35(2)	45(3)	35(2)	-28(2)	-4(2)	3(2)
C(28)	26(2)	23(2)	23(2)	-11(2)	-8(2)	2(2)
C(29)	31(2)	25(2)	29(2)	-9(2)	-7(2)	9(2)
C(30)	24(2)	40(2)	28(2)	-18(2)	-2(2)	6(2)
C(31)	21(2)	29(2)	18(2)	-10(2)	-6(1)	4(2)
C(32)	23(2)	41(2)	28(2)	-15(2)	1(2)	0(2)
C(33)	28(2)	40(3)	27(2)	-9(2)	0(2)	-11(2)
C(34)	38(2)	29(2)	29(2)	-8(2)	-9(2)	-4(2)
C(35)	21(2)	27(2)	23(2)	-10(2)	-4(2)	-1(2)
C(36)	20(2)	24(2)	16(2)	-9(2)	-6(1)	0(2)
C(37)	21(2)	23(2)	18(2)	-9(2)	-5(1)	3(2)
C(38)	20(2)	17(2)	21(2)	-9(2)	-4(2)	2(2)
C(39)	24(2)	21(2)	27(2)	-14(2)	-8(2)	1(2)
C(40)	28(2)	30(2)	27(2)	-13(2)	1(2)	-5(2)
C(41)	17(2)	26(2)	42(2)	-19(2)	1(2)	1(2)
C(42)	23(2)	20(2)	36(2)	-14(2)	-8(2)	2(2)
C(43)	24(2)	33(2)	48(3)	-23(2)	-12(2)	10(2)
C(44)	43(3)	34(2)	38(2)	-17(2)	-24(2)	15(2)
C(45)	37(2)	36(2)	28(2)	-11(2)	-16(2)	5(2)
C(46)	28(2)	27(2)	26(2)	-14(2)	-11(2)	6(2)
C(47)	23(2)	22(2)	27(2)	-14(2)	-7(2)	2(2)
C(48)	38(2)	29(2)	29(2)	-4(2)	-12(2)	5(2)
C(49)	37(2)	38(2)	31(2)	-19(2)	-6(2)	6(2)
C(50)	22(2)	34(2)	41(2)	-17(2)	-7(2)	2(2)
C(51)	32(2)	21(2)	33(2)	-13(2)	-9(2)	8(2)
C(52)	35(2)	18(2)	29(2)	-9(2)	-9(2)	6(2)
C(53)	27(2)	40(2)	42(2)	-18(2)	-16(2)	10(2)
C(54)	38(2)	35(2)	29(2)	-15(2)	-7(2)	-2(2)
C(55)	59(3)	35(3)	39(3)	-16(2)	-4(2)	-2(3)
C(56)	56(3)	34(3)	48(3)	-14(2)	-10(3)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7a**.

	x	y	z	U(eq)
H(2)	7529	7755	6417	34
H(4)	2474	11888	7041	34
H(2A)	8936	8455	8906	32
H(3)	9913	6899	10221	30
H(5)	10311	4678	11175	34
H(6)	9773	2614	11657	37
H(7)	8313	2103	10703	34
H(8)	7318	3631	9390	30
H(13)	5822	6162	5557	31
H(14)	4155	4709	6816	33
H(16)	2773	3532	8921	38
H(17)	2381	2897	11052	41
H(18)	3849	3524	11927	38
H(19)	5625	4838	10693	33
H(21A)	5552	7727	9620	55
H(21B)	4722	8842	9695	55
H(21C)	5900	8501	10353	55
H(22A)	9690	10327	6636	53
H(22C)	9365	11252	7310	53
H(22B)	9900	11801	5839	53
H(23B)	8321	10089	5393	53
H(23C)	8621	11549	4551	53
H(23A)	7174	10966	5128	53
H(24A)	6795	12466	5842	37
H(24B)	8188	13038	5724	37
H(25B)	7823	12306	7893	38
H(25A)	6714	13167	7422	38
H(26A)	4947	11591	7139	50
H(26C)	4609	12374	7964	50
H(26B)	4208	10910	8563	50
H(27A)	5274	10535	10179	53
H(27C)	5633	12001	9655	53
H(27B)	6728	11056	9888	53
H(29)	4897	11146	4510	35
H(30)	6475	12669	3182	36
H(32)	7383	14852	2318	37
H(33)	7147	16905	1971	41
H(34)	5274	17444	2996	40
H(35)	3633	15959	4282	29

H(40)	238	13374	8007	35
H(41)	-868	14862	6778	33
H(43)	-1208	16165	4680	39
H(44)	-482	17015	2541	43
H(45)	1420	16409	1646	39
H(46)	2586	15002	2840	31
H(48B)	2545	11080	3219	51
H(48C)	1783	11842	3945	51
H(48A)	1066	10694	3883	51
H(49A)	1922	7532	4041	51
H(49C)	3146	8453	3745	51
H(49B)	1820	9006	3484	51
H(50B)	14	8657	5215	47
H(50C)	181	7945	6608	47
H(50A)	190	7195	5759	47
H(51B)	3411	7308	5688	33
H(51A)	2105	6430	6240	33
H(52A)	1506	7146	7821	33
H(52B)	2896	6639	7856	33
H(53B)	4609	7985	7655	52
H(53C)	4682	9432	6762	52
H(53A)	4687	8407	6207	52
H(54A)	1510	8773	8424	50
H(54C)	2810	9582	8156	50
H(54B)	2675	8116	8997	50
H(55A)	11423	11298	-618	54
H(55B)	10656	11110	740	54
H(56B)	7276	8205	4030	57
H(56A)	7618	8602	2564	57

Table 6. Torsion angles [deg] for **7a**.

C(21)-Pd(1)-O(1)-C(1)	-56.0(3)
N(2)-Pd(1)-O(1)-C(1)	-176.2(15)
N(1)-Pd(1)-O(1)-C(1)	122.9(3)
C(48)-Pd(2)-O(3)-C(28)	-57.6(3)
N(3)-Pd(2)-O(3)-C(28)	175.7(15)
N(4)-Pd(2)-O(3)-C(28)	120.5(3)
C(21)-Pd(1)-N(1)-C(22)	77(4)
O(1)-Pd(1)-N(1)-C(22)	-77.7(3)
N(2)-Pd(1)-N(1)-C(22)	106.3(3)
C(21)-Pd(1)-N(1)-C(23)	-160(3)
O(1)-Pd(1)-N(1)-C(23)	44.4(3)
N(2)-Pd(1)-N(1)-C(23)	-131.6(3)
C(21)-Pd(1)-N(1)-C(24)	-42(4)
O(1)-Pd(1)-N(1)-C(24)	163.2(3)
N(2)-Pd(1)-N(1)-C(24)	-12.8(3)
C(21)-Pd(1)-N(2)-C(27)	42.8(3)
O(1)-Pd(1)-N(2)-C(27)	162.8(15)
N(1)-Pd(1)-N(2)-C(27)	-135.9(3)
C(21)-Pd(1)-N(2)-C(26)	-78.7(3)
O(1)-Pd(1)-N(2)-C(26)	41.3(17)
N(1)-Pd(1)-N(2)-C(26)	102.6(3)
C(21)-Pd(1)-N(2)-C(25)	163.0(3)
O(1)-Pd(1)-N(2)-C(25)	-77.0(16)
N(1)-Pd(1)-N(2)-C(25)	-15.7(3)
C(48)-Pd(2)-N(3)-C(51)	161.1(3)
O(3)-Pd(2)-N(3)-C(51)	-72.4(16)
N(4)-Pd(2)-N(3)-C(51)	-16.9(2)
C(48)-Pd(2)-N(3)-C(49)	41.4(3)
O(3)-Pd(2)-N(3)-C(49)	167.9(15)
N(4)-Pd(2)-N(3)-C(49)	-136.6(3)
C(48)-Pd(2)-N(3)-C(50)	-80.8(3)
O(3)-Pd(2)-N(3)-C(50)	45.8(17)
N(4)-Pd(2)-N(3)-C(50)	101.3(3)
C(48)-Pd(2)-N(4)-C(54)	180(100)
O(3)-Pd(2)-N(4)-C(54)	45.1(3)
N(3)-Pd(2)-N(4)-C(54)	-131.0(3)
C(48)-Pd(2)-N(4)-C(53)	58(3)
O(3)-Pd(2)-N(4)-C(53)	-76.5(3)
N(3)-Pd(2)-N(4)-C(53)	107.4(3)
C(48)-Pd(2)-N(4)-C(52)	-61(3)
O(3)-Pd(2)-N(4)-C(52)	165.0(2)
N(3)-Pd(2)-N(4)-C(52)	-11.1(2)

Pd(1)-O(1)-C(1)-C(10)	135.9(3)
Pd(1)-O(1)-C(1)-C(2)	-44.8(4)
O(1)-C(1)-C(2)-C(3)	-175.2(3)
C(10)-C(1)-C(2)-C(3)	4.0(6)
C(1)-C(2)-C(3)-C(4)	1.0(6)
C(2)-C(3)-C(4)-C(5)	178.8(4)
C(2)-C(3)-C(4)-C(9)	-3.4(5)
C(3)-C(4)-C(5)-C(6)	176.6(4)
C(9)-C(4)-C(5)-C(6)	-1.2(6)
C(4)-C(5)-C(6)-C(7)	3.3(6)
C(5)-C(6)-C(7)-C(8)	-2.2(6)
C(6)-C(7)-C(8)-C(9)	-1.1(6)
C(7)-C(8)-C(9)-C(10)	-177.8(4)
C(7)-C(8)-C(9)-C(4)	3.1(5)
C(5)-C(4)-C(9)-C(8)	-2.0(5)
C(3)-C(4)-C(9)-C(8)	-179.8(3)
C(5)-C(4)-C(9)-C(10)	178.9(3)
C(3)-C(4)-C(9)-C(10)	1.0(5)
O(1)-C(1)-C(10)-C(9)	172.9(3)
C(2)-C(1)-C(10)-C(9)	-6.3(5)
O(1)-C(1)-C(10)-C(11)	-6.3(5)
C(2)-C(1)-C(10)-C(11)	174.4(3)
C(8)-C(9)-C(10)-C(1)	-175.3(3)
C(4)-C(9)-C(10)-C(1)	3.8(5)
C(8)-C(9)-C(10)-C(11)	4.0(5)
C(4)-C(9)-C(10)-C(11)	-176.9(3)
C(1)-C(10)-C(11)-C(12)	56.6(5)
C(9)-C(10)-C(11)-C(12)	-122.6(4)
C(1)-C(10)-C(11)-C(20)	-123.4(4)
C(9)-C(10)-C(11)-C(20)	57.3(5)
C(20)-C(11)-C(12)-O(2)	169.9(3)
C(10)-C(11)-C(12)-O(2)	-10.2(6)
C(20)-C(11)-C(12)-C(13)	-10.2(6)
C(10)-C(11)-C(12)-C(13)	169.7(3)
O(2)-C(12)-C(13)-C(14)	-174.7(4)
C(11)-C(12)-C(13)-C(14)	5.4(6)
C(12)-C(13)-C(14)-C(15)	2.7(6)
C(13)-C(14)-C(15)-C(20)	-5.3(6)
C(13)-C(14)-C(15)-C(16)	174.3(4)
C(14)-C(15)-C(16)-C(17)	-178.8(4)
C(20)-C(15)-C(16)-C(17)	0.8(6)
C(15)-C(16)-C(17)-C(18)	-0.8(7)
C(16)-C(17)-C(18)-C(19)	1.3(7)
C(17)-C(18)-C(19)-C(20)	-1.7(6)

C(14)-C(15)-C(20)-C(19)	178.5(4)
C(16)-C(15)-C(20)-C(19)	-1.1(5)
C(14)-C(15)-C(20)-C(11)	0.1(5)
C(16)-C(15)-C(20)-C(11)	-179.5(4)
C(18)-C(19)-C(20)-C(15)	1.6(6)
C(18)-C(19)-C(20)-C(11)	179.9(4)
C(12)-C(11)-C(20)-C(15)	7.5(5)
C(10)-C(11)-C(20)-C(15)	-172.5(3)
C(12)-C(11)-C(20)-C(19)	-170.8(3)
C(10)-C(11)-C(20)-C(19)	9.2(6)
C(22)-N(1)-C(24)-C(25)	-79.8(4)
C(23)-N(1)-C(24)-C(25)	159.5(4)
Pd(1)-N(1)-C(24)-C(25)	39.1(4)
C(27)-N(2)-C(25)-C(24)	167.9(4)
C(26)-N(2)-C(25)-C(24)	-74.2(4)
Pd(1)-N(2)-C(25)-C(24)	42.9(4)
N(1)-C(24)-C(25)-N(2)	-57.7(5)
Pd(2)-O(3)-C(28)-C(37)	141.1(3)
Pd(2)-O(3)-C(28)-C(29)	-40.7(5)
O(3)-C(28)-C(29)-C(30)	-174.7(4)
C(37)-C(28)-C(29)-C(30)	3.5(6)
C(28)-C(29)-C(30)-C(31)	2.3(6)
C(29)-C(30)-C(31)-C(36)	-4.1(6)
C(29)-C(30)-C(31)-C(32)	176.9(4)
C(30)-C(31)-C(32)-C(33)	177.9(4)
C(36)-C(31)-C(32)-C(33)	-1.0(6)
C(31)-C(32)-C(33)-C(34)	2.7(7)
C(32)-C(33)-C(34)-C(35)	-1.4(7)
C(33)-C(34)-C(35)-C(36)	-1.4(6)
C(30)-C(31)-C(36)-C(35)	179.3(3)
C(32)-C(31)-C(36)-C(35)	-1.8(5)
C(30)-C(31)-C(36)-C(37)	0.3(5)
C(32)-C(31)-C(36)-C(37)	179.2(3)
C(34)-C(35)-C(36)-C(31)	3.0(5)
C(34)-C(35)-C(36)-C(37)	-178.1(4)
O(3)-C(28)-C(37)-C(36)	171.0(3)
C(29)-C(28)-C(37)-C(36)	-7.2(5)
O(3)-C(28)-C(37)-C(38)	-9.0(5)
C(29)-C(28)-C(37)-C(38)	172.7(3)
C(31)-C(36)-C(37)-C(28)	5.4(5)
C(35)-C(36)-C(37)-C(28)	-173.6(3)
C(31)-C(36)-C(37)-C(38)	-174.6(3)
C(35)-C(36)-C(37)-C(38)	6.5(5)
C(28)-C(37)-C(38)-C(39)	55.7(5)

C(36)-C(37)-C(38)-C(39)	-124.3(4)
C(28)-C(37)-C(38)-C(47)	-122.4(4)
C(36)-C(37)-C(38)-C(47)	57.6(5)
C(47)-C(38)-C(39)-O(4)	171.4(3)
C(37)-C(38)-C(39)-O(4)	-6.8(6)
C(47)-C(38)-C(39)-C(40)	-8.7(6)
C(37)-C(38)-C(39)-C(40)	173.1(3)
O(4)-C(39)-C(40)-C(41)	-174.8(3)
C(38)-C(39)-C(40)-C(41)	5.2(6)
C(39)-C(40)-C(41)-C(42)	1.3(6)
C(40)-C(41)-C(42)-C(43)	176.2(4)
C(40)-C(41)-C(42)-C(47)	-3.9(6)
C(41)-C(42)-C(43)-C(44)	178.6(4)
C(47)-C(42)-C(43)-C(44)	-1.3(6)
C(42)-C(43)-C(44)-C(45)	1.4(7)
C(43)-C(44)-C(45)-C(46)	-0.2(7)
C(44)-C(45)-C(46)-C(47)	-1.0(6)
C(43)-C(42)-C(47)-C(46)	0.1(5)
C(41)-C(42)-C(47)-C(46)	-179.8(4)
C(43)-C(42)-C(47)-C(38)	-179.8(3)
C(41)-C(42)-C(47)-C(38)	0.3(5)
C(45)-C(46)-C(47)-C(42)	1.1(6)
C(45)-C(46)-C(47)-C(38)	-179.0(4)
C(39)-C(38)-C(47)-C(42)	5.9(5)
C(37)-C(38)-C(47)-C(42)	-175.9(3)
C(39)-C(38)-C(47)-C(46)	-174.0(4)
C(37)-C(38)-C(47)-C(46)	4.2(6)
C(49)-N(3)-C(51)-C(52)	167.9(3)
C(50)-N(3)-C(51)-C(52)	-74.1(4)
Pd(2)-N(3)-C(51)-C(52)	43.1(4)
C(54)-N(4)-C(52)-C(51)	159.2(3)
C(53)-N(4)-C(52)-C(51)	-80.9(4)
Pd(2)-N(4)-C(52)-C(51)	36.8(4)
N(3)-C(51)-C(52)-N(4)	-55.9(5)

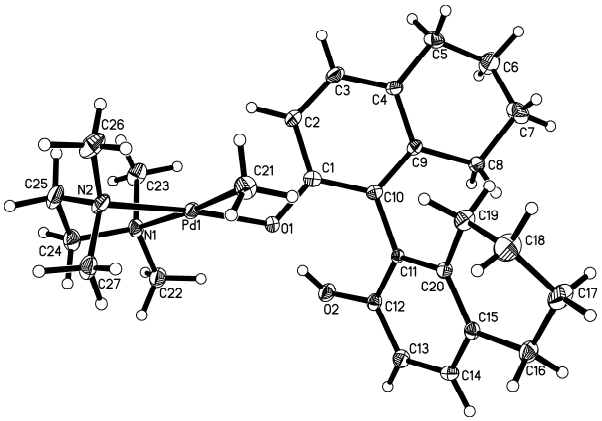
Symmetry transformations used to generate equivalent atoms:

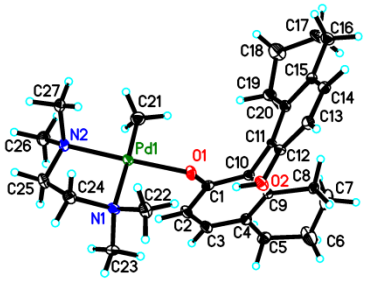
Table 7. Hydrogen bonds for **7a** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)	0.84	1.81	2.591(4)	153.9
O(4)-H(4)...O(3)	0.84	1.76	2.551(4)	155.8

Symmetry transformations used to generate equivalent atoms:

The X-ray structure of compound 7b





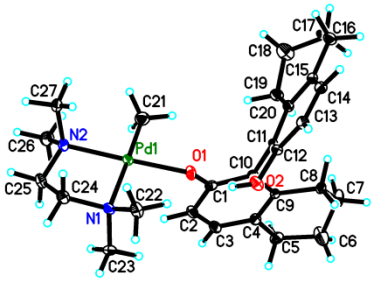


Table 1. Crystal data and structure refinement for **7b**.

Identification code	a
Empirical formula	C28 H42 C12 N2 O2 Pd
Formula weight	615.94
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 10.839(2) A alpha = 62.30(3) deg.
	b = 12.056(2) A beta = 78.85(3) deg.
	c = 12.660(3) A gamma = 89.82(3) deg.
Volume	1430.1(5) A^3
Z, Calculated density	2, 1.430 Mg/m^3
Absorption coefficient	0.863 mm^-1
F(000)	640
Crystal size	0.28 x 0.13 x 0.05 mm
Theta range for data collection	1.92 to 27.45 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -16<=l<=16
Reflections collected / unique	18592 / 11701 [R(int) = 0.0723]
Completeness to theta = 27.45	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.5278
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11701 / 3 / 643
Goodness-of-fit on F^2	1.435
Final R indices [I>2sigma(I)]	R1 = 0.0847, wR2 = 0.2123
R indices (all data)	R1 = 0.0861, wR2 = 0.2143
Absolute structure parameter	0.01(4)
Largest diff. peak and hole	7.143 and -1.254 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	5935(1)	7344(1)	7024(1)	20(1)
Pd(2)	1451(1)	7230(1)	4760(1)	21(1)
Cl(1)	1391(4)	7249(3)	9921(3)	67(1)
Cl(2)	-1026(4)	7292(4)	9207(3)	69(1)
Cl(3)	5443(4)	7273(5)	2353(6)	93(2)
Cl(4)	8152(3)	7248(3)	2197(2)	49(1)
O(1)	6387(6)	5797(5)	6814(5)	26(1)
O(2)	6657(6)	4804(6)	5344(5)	30(1)
O(3)	1827(6)	8765(5)	4957(5)	28(1)
O(4)	1410(6)	9722(6)	6445(5)	29(1)
N(1)	7251(6)	8643(6)	5324(6)	24(1)
N(2)	5417(6)	8986(7)	7100(7)	27(1)
N(3)	2032(6)	5949(6)	6462(6)	22(1)
N(4)	962(6)	5591(6)	4719(6)	26(1)
C(1)	6875(7)	4863(7)	7665(6)	22(1)
C(2)	7736(8)	5115(8)	8250(7)	27(2)
C(3)	8327(8)	4139(8)	9015(8)	29(2)
C(4)	8148(7)	2918(7)	9219(7)	23(1)
C(5)	8879(8)	1926(8)	10026(8)	30(2)
C(6)	8859(12)	735(10)	9899(14)	63(4)
C(7)	7662(12)	340(10)	9758(11)	50(3)
C(8)	7172(7)	1341(7)	8731(7)	23(1)
C(9)	7292(7)	2644(7)	8648(7)	19(1)
C(10)	6616(7)	3614(7)	7904(6)	19(1)
C(11)	5608(6)	3301(6)	7399(7)	16(1)
C(12)	5733(7)	3850(7)	6127(7)	21(1)
C(13)	4922(8)	3424(7)	5633(7)	26(2)
C(14)	3929(8)	2535(8)	6398(7)	24(2)
C(15)	3680(7)	2079(7)	7666(7)	21(1)
C(16)	2508(8)	1167(8)	8457(8)	30(2)
C(17)	2456(11)	566(11)	9776(9)	46(3)
C(18)	2894(11)	1487(11)	10166(9)	49(3)
C(19)	4222(8)	2082(8)	9522(7)	29(2)
C(20)	4523(7)	2477(7)	8162(7)	21(1)
C(21)	4777(9)	6189(9)	8642(8)	36(2)
C(22)	7221(9)	8379(8)	4311(8)	33(2)
C(23)	8536(7)	8576(9)	5559(9)	35(2)

C(24)	6826(8)	9914(8)	5055(8)	32(2)
C(25)	6420(9)	9984(9)	6233(10)	37(2)
C(26)	5277(10)	8906(10)	8340(10)	41(2)
C(27)	4194(8)	9262(8)	6722(10)	36(2)
C(28)	2700(7)	9700(7)	4108(6)	22(1)
C(29)	3800(8)	9466(8)	3501(7)	27(2)
C(30)	4747(8)	10450(8)	2725(8)	29(2)
C(31)	4630(7)	11659(8)	2579(7)	26(2)
C(32)	5709(8)	12685(9)	1747(8)	33(2)
C(33)	5658(9)	13864(10)	1873(10)	41(2)
C(34)	4324(10)	14209(10)	1981(9)	43(2)
C(35)	3414(8)	13224(7)	3065(7)	26(2)
C(36)	3519(7)	11916(7)	3151(6)	21(1)
C(37)	2521(7)	10945(7)	3870(7)	21(1)
C(38)	1279(7)	11257(7)	4393(6)	17(1)
C(39)	851(7)	10690(7)	5666(6)	20(1)
C(40)	−215(8)	11079(8)	6178(7)	27(2)
C(41)	−856(8)	12014(8)	5413(8)	26(2)
C(42)	−511(7)	12490(7)	4140(7)	22(2)
C(43)	−1309(8)	13449(8)	3374(8)	28(2)
C(44)	−1055(9)	13696(10)	2056(8)	38(2)
C(45)	342(10)	13785(9)	1553(9)	41(2)
C(46)	884(7)	12555(7)	2267(7)	25(2)
C(47)	544(7)	12110(7)	3641(6)	20(1)
C(48)	976(8)	8357(8)	3145(7)	32(2)
C(49)	3423(9)	6037(10)	6221(11)	42(2)
C(50)	1544(10)	6208(8)	7473(8)	37(2)
C(51)	1504(9)	4700(8)	6753(9)	35(2)
C(52)	1621(9)	4596(8)	5576(10)	36(2)
C(53)	1351(9)	5618(10)	3513(9)	38(2)
C(54)	−427(7)	5291(8)	5129(9)	30(2)
C(55)	208(11)	8194(10)	9264(10)	45(3)
C(56)	6752(12)	6437(11)	2412(11)	49(3)

Table 3. Bond lengths [A] and angles [deg] for **7b**.

Pd(1)-C(21)	2.018(9)
Pd(1)-O(1)	2.048(5)
Pd(1)-N(2)	2.096(7)
Pd(1)-N(1)	2.194(7)
Pd(2)-C(48)	2.027(8)
Pd(2)-O(3)	2.032(6)
Pd(2)-N(4)	2.074(7)
Pd(2)-N(3)	2.202(6)
Cl(1)-C(55)	1.776(11)
Cl(2)-C(55)	1.760(13)
Cl(3)-C(56)	1.731(14)
Cl(4)-C(56)	1.714(12)
O(1)-C(1)	1.341(9)
O(2)-C(12)	1.368(9)
O(2)-H(2)	0.8400
O(3)-C(28)	1.345(9)
O(4)-C(39)	1.364(9)
O(4)-H(4)	0.8400
N(1)-C(22)	1.464(11)
N(1)-C(23)	1.474(10)
N(1)-C(24)	1.499(10)
N(2)-C(25)	1.468(12)
N(2)-C(27)	1.480(10)
N(2)-C(26)	1.506(11)
N(3)-C(50)	1.458(11)
N(3)-C(51)	1.462(10)
N(3)-C(49)	1.473(11)
N(4)-C(54)	1.481(10)
N(4)-C(53)	1.487(11)
N(4)-C(52)	1.487(11)
C(1)-C(10)	1.409(11)
C(1)-C(2)	1.411(10)
C(2)-C(3)	1.382(11)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.379(11)
C(3)-H(3)	0.9500
C(4)-C(9)	1.406(9)
C(4)-C(5)	1.508(10)
C(5)-C(6)	1.517(14)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.454(15)

C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.495(11)
C(7)-H(7B)	0.9900
C(7)-H(7A)	0.9900
C(8)-C(9)	1.529(10)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.425(9)
C(10)-C(11)	1.496(9)
C(11)-C(12)	1.406(10)
C(11)-C(20)	1.407(10)
C(12)-C(13)	1.393(10)
C(13)-C(14)	1.373(11)
C(13)-H(13)	0.9500
C(14)-C(15)	1.402(11)
C(14)-H(14)	0.9500
C(15)-C(20)	1.402(10)
C(15)-C(16)	1.523(11)
C(16)-C(17)	1.468(13)
C(16)-H(16B)	0.9900
C(16)-H(16A)	0.9900
C(17)-C(18)	1.519(15)
C(17)-H(17B)	0.9900
C(17)-H(17A)	0.9900
C(18)-C(19)	1.504(13)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.523(10)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22C)	0.9800
C(22)-H(22B)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23C)	0.9800
C(23)-H(23B)	0.9800
C(24)-C(25)	1.512(13)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-H(25B)	0.9900

C(25)-H(25A)	0.9900
C(26)-H(26A)	0.9800
C(26)-H(26C)	0.9800
C(26)-H(26B)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27C)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(29)	1.391(11)
C(28)-C(37)	1.408(11)
C(29)-C(30)	1.401(12)
C(29)-H(29)	0.9500
C(30)-C(31)	1.391(12)
C(30)-H(30)	0.9500
C(31)-C(36)	1.392(11)
C(31)-C(32)	1.526(11)
C(32)-C(33)	1.501(13)
C(32)-H(32B)	0.9900
C(32)-H(32A)	0.9900
C(33)-C(34)	1.502(15)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.495(12)
C(34)-H(34B)	0.9900
C(34)-H(34A)	0.9900
C(35)-C(36)	1.535(10)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(37)	1.416(10)
C(37)-C(38)	1.507(10)
C(38)-C(39)	1.404(9)
C(38)-C(47)	1.407(10)
C(39)-C(40)	1.402(11)
C(40)-C(41)	1.389(12)
C(40)-H(40)	0.9500
C(41)-C(42)	1.406(12)
C(41)-H(41)	0.9500
C(42)-C(47)	1.379(11)
C(42)-C(43)	1.516(10)
C(43)-C(44)	1.520(12)
C(43)-H(43B)	0.9900
C(43)-H(43A)	0.9900
C(44)-C(45)	1.508(14)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900

C(45)-C(46)	1.522(12)
C(45)-H(45B)	0.9900
C(45)-H(45A)	0.9900
C(46)-C(47)	1.528(10)
C(46)-H(46B)	0.9900
C(46)-H(46A)	0.9900
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(48)-H(48A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(49)-H(49A)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50C)	0.9800
C(50)-H(50B)	0.9800
C(51)-C(52)	1.534(13)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-H(52B)	0.9900
C(52)-H(52A)	0.9900
C(53)-H(53A)	0.9800
C(53)-H(53C)	0.9800
C(53)-H(53B)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(54)-H(54A)	0.9800
C(55)-H(55B)	0.9900
C(55)-H(55A)	0.9900
C(56)-H(56B)	0.9900
C(56)-H(56A)	0.9900

C(21)-Pd(1)-O(1)	88.7(3)
C(21)-Pd(1)-N(2)	93.8(3)
O(1)-Pd(1)-N(2)	175.1(2)
C(21)-Pd(1)-N(1)	176.5(3)
O(1)-Pd(1)-N(1)	93.3(2)
N(2)-Pd(1)-N(1)	84.4(3)
C(48)-Pd(2)-O(3)	89.9(3)
C(48)-Pd(2)-N(4)	93.4(3)
O(3)-Pd(2)-N(4)	174.7(3)
C(48)-Pd(2)-N(3)	176.7(3)
O(3)-Pd(2)-N(3)	92.4(2)
N(4)-Pd(2)-N(3)	84.5(2)
C(1)-O(1)-Pd(1)	119.4(5)

C(12)-O(2)-H(2)	109.5
C(28)-O(3)-Pd(2)	120.3(5)
C(39)-O(4)-H(4)	109.5
C(22)-N(1)-C(23)	110.1(7)
C(22)-N(1)-C(24)	110.9(6)
C(23)-N(1)-C(24)	110.0(7)
C(22)-N(1)-Pd(1)	113.1(5)
C(23)-N(1)-Pd(1)	108.5(5)
C(24)-N(1)-Pd(1)	104.1(5)
C(25)-N(2)-C(27)	110.9(7)
C(25)-N(2)-C(26)	108.9(7)
C(27)-N(2)-C(26)	108.5(7)
C(25)-N(2)-Pd(1)	106.1(5)
C(27)-N(2)-Pd(1)	107.9(5)
C(26)-N(2)-Pd(1)	114.6(6)
C(50)-N(3)-C(51)	109.6(7)
C(50)-N(3)-C(49)	109.9(7)
C(51)-N(3)-C(49)	110.9(7)
C(50)-N(3)-Pd(2)	113.5(5)
C(51)-N(3)-Pd(2)	104.3(5)
C(49)-N(3)-Pd(2)	108.6(6)
C(54)-N(4)-C(53)	108.3(6)
C(54)-N(4)-C(52)	111.0(7)
C(53)-N(4)-C(52)	107.1(7)
C(54)-N(4)-Pd(2)	108.7(5)
C(53)-N(4)-Pd(2)	115.7(6)
C(52)-N(4)-Pd(2)	105.9(5)
O(1)-C(1)-C(10)	119.5(6)
O(1)-C(1)-C(2)	121.3(7)
C(10)-C(1)-C(2)	119.0(7)
C(3)-C(2)-C(1)	119.2(7)
C(3)-C(2)-H(2A)	120.4
C(1)-C(2)-H(2A)	120.4
C(4)-C(3)-C(2)	123.4(7)
C(4)-C(3)-H(3)	118.3
C(2)-C(3)-H(3)	118.3
C(3)-C(4)-C(9)	118.4(7)
C(3)-C(4)-C(5)	119.6(7)
C(9)-C(4)-C(5)	122.1(7)
C(4)-C(5)-C(6)	113.4(7)
C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5A)	108.9
C(4)-C(5)-H(5B)	108.9
C(6)-C(5)-H(5B)	108.9

H(5A)-C(5)-H(5B)	107.7
C(7)-C(6)-C(5)	115.3(9)
C(7)-C(6)-H(6A)	108.5
C(5)-C(6)-H(6A)	108.4
C(7)-C(6)-H(6B)	108.4
C(5)-C(6)-H(6B)	108.4
H(6A)-C(6)-H(6B)	107.5
C(6)-C(7)-C(8)	113.7(9)
C(6)-C(7)-H(7B)	108.8
C(8)-C(7)-H(7B)	108.8
C(6)-C(7)-H(7A)	108.8
C(8)-C(7)-H(7A)	108.8
H(7B)-C(7)-H(7A)	107.7
C(7)-C(8)-C(9)	114.1(7)
C(7)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8B)	108.7
C(9)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(4)-C(9)-C(10)	119.8(7)
C(4)-C(9)-C(8)	120.1(6)
C(10)-C(9)-C(8)	119.9(6)
C(1)-C(10)-C(9)	120.0(6)
C(1)-C(10)-C(11)	120.0(6)
C(9)-C(10)-C(11)	120.0(6)
C(12)-C(11)-C(20)	118.5(6)
C(12)-C(11)-C(10)	119.6(6)
C(20)-C(11)-C(10)	121.9(6)
O(2)-C(12)-C(13)	118.4(7)
O(2)-C(12)-C(11)	121.1(7)
C(13)-C(12)-C(11)	120.5(7)
C(14)-C(13)-C(12)	119.5(7)
C(14)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	121.5(7)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(14)-C(15)-C(20)	118.7(7)
C(14)-C(15)-C(16)	119.0(7)
C(20)-C(15)-C(16)	122.3(7)
C(17)-C(16)-C(15)	114.6(7)
C(17)-C(16)-H(16B)	108.6
C(15)-C(16)-H(16B)	108.6
C(17)-C(16)-H(16A)	108.6

C(15)-C(16)-H(16A)	108.6
H(16B)-C(16)-H(16A)	107.6
C(16)-C(17)-C(18)	112.0(9)
C(16)-C(17)-H(17B)	109.2
C(18)-C(17)-H(17B)	109.2
C(16)-C(17)-H(17A)	109.2
C(18)-C(17)-H(17A)	109.2
H(17B)-C(17)-H(17A)	107.9
C(19)-C(18)-C(17)	112.9(9)
C(19)-C(18)-H(18A)	109.0
C(17)-C(18)-H(18A)	109.0
C(19)-C(18)-H(18B)	109.0
C(17)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
C(18)-C(19)-C(20)	114.0(7)
C(18)-C(19)-H(19A)	108.7
C(20)-C(19)-H(19A)	108.7
C(18)-C(19)-H(19B)	108.7
C(20)-C(19)-H(19B)	108.7
H(19A)-C(19)-H(19B)	107.6
C(15)-C(20)-C(11)	120.3(7)
C(15)-C(20)-C(19)	119.8(7)
C(11)-C(20)-C(19)	119.7(6)
Pd(1)-C(21)-H(21A)	109.5
Pd(1)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
Pd(1)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(1)-C(22)-H(22A)	109.5
N(1)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
N(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
H(22C)-C(22)-H(22B)	109.5
N(1)-C(23)-H(23A)	109.5
N(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
N(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
H(23C)-C(23)-H(23B)	109.5
N(1)-C(24)-C(25)	109.7(7)
N(1)-C(24)-H(24A)	109.7
C(25)-C(24)-H(24A)	109.7

N(1)-C(24)-H(24B)	109.7
C(25)-C(24)-H(24B)	109.7
H(24A)-C(24)-H(24B)	108.2
N(2)-C(25)-C(24)	111.6(7)
N(2)-C(25)-H(25B)	109.3
C(24)-C(25)-H(25B)	109.3
N(2)-C(25)-H(25A)	109.3
C(24)-C(25)-H(25A)	109.3
H(25B)-C(25)-H(25A)	108.0
N(2)-C(26)-H(26A)	109.5
N(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
N(2)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
H(26C)-C(26)-H(26B)	109.5
N(2)-C(27)-H(27A)	109.5
N(2)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
N(2)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
H(27C)-C(27)-H(27B)	109.5
O(3)-C(28)-C(29)	121.9(7)
O(3)-C(28)-C(37)	118.8(7)
C(29)-C(28)-C(37)	119.2(7)
C(28)-C(29)-C(30)	120.0(7)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	121.0(7)
C(31)-C(30)-H(30)	119.5
C(29)-C(30)-H(30)	119.5
C(30)-C(31)-C(36)	119.5(7)
C(30)-C(31)-C(32)	118.7(7)
C(36)-C(31)-C(32)	121.8(8)
C(33)-C(32)-C(31)	115.2(7)
C(33)-C(32)-H(32B)	108.5
C(31)-C(32)-H(32B)	108.5
C(33)-C(32)-H(32A)	108.5
C(31)-C(32)-H(32A)	108.5
H(32B)-C(32)-H(32A)	107.5
C(32)-C(33)-C(34)	109.7(8)
C(32)-C(33)-H(33A)	109.7
C(34)-C(33)-H(33A)	109.7
C(32)-C(33)-H(33B)	109.7
C(34)-C(33)-H(33B)	109.7

H(33A)-C(33)-H(33B)	108.2
C(35)-C(34)-C(33)	113.7(9)
C(35)-C(34)-H(34B)	108.8
C(33)-C(34)-H(34B)	108.8
C(35)-C(34)-H(34A)	108.8
C(33)-C(34)-H(34A)	108.8
H(34B)-C(34)-H(34A)	107.7
C(34)-C(35)-C(36)	112.0(8)
C(34)-C(35)-H(35A)	109.2
C(36)-C(35)-H(35A)	109.2
C(34)-C(35)-H(35B)	109.2
C(36)-C(35)-H(35B)	109.2
H(35A)-C(35)-H(35B)	107.9
C(31)-C(36)-C(37)	119.7(7)
C(31)-C(36)-C(35)	119.9(7)
C(37)-C(36)-C(35)	120.3(7)
C(28)-C(37)-C(36)	120.0(7)
C(28)-C(37)-C(38)	120.6(6)
C(36)-C(37)-C(38)	119.4(6)
C(39)-C(38)-C(47)	119.0(7)
C(39)-C(38)-C(37)	119.1(6)
C(47)-C(38)-C(37)	121.9(6)
O(4)-C(39)-C(40)	117.6(6)
O(4)-C(39)-C(38)	122.1(7)
C(40)-C(39)-C(38)	120.2(7)
C(41)-C(40)-C(39)	119.4(7)
C(41)-C(40)-H(40)	120.3
C(39)-C(40)-H(40)	120.3
C(40)-C(41)-C(42)	120.6(8)
C(40)-C(41)-H(41)	119.7
C(42)-C(41)-H(41)	119.7
C(47)-C(42)-C(41)	119.5(7)
C(47)-C(42)-C(43)	123.1(7)
C(41)-C(42)-C(43)	117.3(7)
C(42)-C(43)-C(44)	113.5(7)
C(42)-C(43)-H(43B)	108.9
C(44)-C(43)-H(43B)	108.9
C(42)-C(43)-H(43A)	108.9
C(44)-C(43)-H(43A)	108.9
H(43B)-C(43)-H(43A)	107.7
C(45)-C(44)-C(43)	111.0(7)
C(45)-C(44)-H(44A)	109.4
C(43)-C(44)-H(44A)	109.4
C(45)-C(44)-H(44B)	109.4

C(43)-C(44)-H(44B)	109.4
H(44A)-C(44)-H(44B)	108.0
C(44)-C(45)-C(46)	111.1(8)
C(44)-C(45)-H(45B)	109.4
C(46)-C(45)-H(45B)	109.4
C(44)-C(45)-H(45A)	109.4
C(46)-C(45)-H(45A)	109.4
H(45B)-C(45)-H(45A)	108.0
C(45)-C(46)-C(47)	111.7(7)
C(45)-C(46)-H(46B)	109.3
C(47)-C(46)-H(46B)	109.3
C(45)-C(46)-H(46A)	109.3
C(47)-C(46)-H(46A)	109.3
H(46B)-C(46)-H(46A)	107.9
C(42)-C(47)-C(38)	120.7(7)
C(42)-C(47)-C(46)	120.2(7)
C(38)-C(47)-C(46)	119.0(7)
Pd(2)-C(48)-H(48B)	109.5
Pd(2)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
Pd(2)-C(48)-H(48A)	109.5
H(48B)-C(48)-H(48A)	109.5
H(48C)-C(48)-H(48A)	109.5
N(3)-C(49)-H(49B)	109.5
N(3)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
N(3)-C(49)-H(49A)	109.5
H(49B)-C(49)-H(49A)	109.5
H(49C)-C(49)-H(49A)	109.5
N(3)-C(50)-H(50A)	109.5
N(3)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
N(3)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
H(50C)-C(50)-H(50B)	109.5
N(3)-C(51)-C(52)	109.8(7)
N(3)-C(51)-H(51A)	109.7
C(52)-C(51)-H(51A)	109.7
N(3)-C(51)-H(51B)	109.7
C(52)-C(51)-H(51B)	109.7
H(51A)-C(51)-H(51B)	108.2
N(4)-C(52)-C(51)	110.2(7)
N(4)-C(52)-H(52B)	109.6
C(51)-C(52)-H(52B)	109.6

N(4)-C(52)-H(52A)	109.6
C(51)-C(52)-H(52A)	109.6
H(52B)-C(52)-H(52A)	108.1
N(4)-C(53)-H(53A)	109.5
N(4)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
N(4)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
H(53C)-C(53)-H(53B)	109.5
N(4)-C(54)-H(54B)	109.5
N(4)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(4)-C(54)-H(54A)	109.5
H(54B)-C(54)-H(54A)	109.5
H(54C)-C(54)-H(54A)	109.5
Cl(2)-C(55)-Cl(1)	111.6(6)
Cl(2)-C(55)-H(55B)	109.3
Cl(1)-C(55)-H(55B)	109.3
Cl(2)-C(55)-H(55A)	109.3
Cl(1)-C(55)-H(55A)	109.3
H(55B)-C(55)-H(55A)	108.0
Cl(4)-C(56)-Cl(3)	115.0(7)
Cl(4)-C(56)-H(56B)	108.5
Cl(3)-C(56)-H(56B)	108.5
Cl(4)-C(56)-H(56A)	108.5
Cl(3)-C(56)-H(56A)	108.5
H(56B)-C(56)-H(56A)	107.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **7b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	20(1)	19(1)	24(1)	-11(1)	-5(1)	0(1)
Pd(2)	18(1)	20(1)	24(1)	-11(1)	-3(1)	2(1)
Cl(1)	77(2)	47(2)	62(2)	-15(1)	-13(2)	14(2)
Cl(2)	74(2)	82(2)	61(2)	-48(2)	-1(2)	-12(2)
Cl(3)	58(2)	102(3)	152(5)	-83(3)	-36(3)	22(2)
Cl(4)	56(2)	50(2)	34(1)	-17(1)	-5(1)	-7(1)
O(1)	33(3)	17(3)	30(3)	-11(2)	-17(2)	5(2)
O(2)	34(3)	28(3)	24(3)	-11(2)	-2(2)	-7(2)
O(3)	31(3)	20(3)	33(3)	-15(2)	0(2)	0(2)
O(4)	35(3)	29(3)	20(3)	-10(2)	-6(2)	12(3)
N(1)	20(3)	18(3)	28(3)	-7(2)	-4(3)	-2(2)
N(2)	25(3)	28(4)	39(4)	-25(3)	-9(3)	2(3)
N(3)	21(3)	21(3)	25(3)	-11(2)	-3(2)	1(2)
N(4)	22(3)	29(3)	33(3)	-19(3)	-8(3)	5(3)
C(1)	17(3)	27(4)	19(3)	-11(3)	-1(3)	2(3)
C(2)	28(4)	24(4)	31(4)	-14(3)	-11(3)	-1(3)
C(3)	25(4)	31(4)	36(4)	-19(3)	-12(3)	-1(3)
C(4)	24(3)	26(4)	23(3)	-14(3)	-9(3)	4(3)
C(5)	25(4)	36(4)	34(4)	-17(4)	-14(3)	12(3)
C(6)	62(8)	34(6)	106(11)	-28(6)	-63(8)	19(5)
C(7)	74(8)	34(5)	56(6)	-23(5)	-37(6)	33(5)
C(8)	23(3)	22(4)	28(4)	-14(3)	-9(3)	7(3)
C(9)	17(3)	21(3)	24(3)	-14(3)	-5(3)	2(3)
C(10)	17(3)	23(3)	19(3)	-11(3)	-3(3)	2(3)
C(11)	11(3)	14(3)	22(3)	-8(3)	-5(3)	2(2)
C(12)	17(3)	20(3)	24(3)	-10(3)	-2(3)	-1(3)
C(13)	29(4)	25(4)	22(3)	-11(3)	-3(3)	0(3)
C(14)	23(4)	28(4)	23(4)	-13(3)	-9(3)	5(3)
C(15)	20(3)	19(4)	24(4)	-10(3)	-4(3)	2(3)
C(16)	27(4)	29(4)	31(4)	-12(3)	-2(3)	-5(3)
C(17)	35(5)	59(7)	31(5)	-15(5)	8(4)	-27(5)
C(18)	55(6)	57(7)	31(5)	-21(5)	3(4)	-13(5)
C(19)	26(4)	34(4)	24(4)	-14(3)	1(3)	-4(3)
C(20)	22(3)	20(3)	21(3)	-10(3)	-4(3)	1(3)
C(21)	32(4)	35(5)	36(4)	-14(4)	-4(4)	2(4)
C(22)	43(5)	25(4)	31(4)	-12(3)	-6(4)	-3(3)
C(23)	16(4)	39(5)	55(5)	-29(4)	1(4)	-2(3)
C(24)	31(4)	23(4)	35(4)	-9(3)	-3(3)	-2(3)

C(25)	36(5)	27(4)	54(6)	−24(4)	−9(4)	−3(4)
C(26)	37(5)	52(6)	51(6)	−41(5)	−6(4)	2(4)
C(27)	28(4)	27(4)	60(6)	−26(4)	−12(4)	7(3)
C(28)	19(3)	27(4)	18(3)	−11(3)	−2(3)	−1(3)
C(29)	27(4)	25(4)	31(4)	−13(3)	−7(3)	5(3)
C(30)	23(4)	43(5)	31(4)	−27(4)	0(3)	8(3)
C(31)	17(3)	36(4)	27(4)	−18(3)	−1(3)	−3(3)
C(32)	17(3)	45(5)	41(5)	−28(4)	5(3)	−10(3)
C(33)	24(4)	44(6)	47(5)	−21(4)	7(4)	−12(4)
C(34)	42(6)	36(5)	37(5)	−8(4)	3(4)	−12(4)
C(35)	26(4)	17(3)	33(4)	−11(3)	−3(3)	−8(3)
C(36)	25(4)	20(3)	18(3)	−11(3)	−4(3)	−1(3)
C(37)	16(3)	20(3)	22(3)	−7(3)	−4(3)	0(3)
C(38)	14(3)	15(3)	18(3)	−6(3)	0(3)	0(3)
C(39)	21(3)	18(3)	16(3)	−5(3)	−1(3)	−2(3)
C(40)	25(4)	27(4)	28(4)	−14(3)	−2(3)	1(3)
C(41)	24(4)	29(4)	30(4)	−19(3)	−2(3)	3(3)
C(42)	20(4)	20(4)	29(4)	−13(3)	−8(3)	4(3)
C(43)	21(3)	29(4)	37(4)	−15(3)	−14(3)	9(3)
C(44)	30(4)	46(5)	25(4)	−7(4)	−7(4)	8(4)
C(45)	45(5)	39(5)	32(4)	−11(4)	−9(4)	7(4)
C(46)	21(3)	30(4)	20(3)	−9(3)	−5(3)	−3(3)
C(47)	22(3)	18(3)	20(3)	−9(3)	−3(3)	−5(3)
C(48)	25(4)	32(4)	26(4)	−3(3)	−5(3)	0(3)
C(49)	29(4)	43(5)	69(7)	−32(5)	−27(5)	8(4)
C(50)	53(6)	27(4)	29(4)	−12(3)	−8(4)	−2(4)
C(51)	41(5)	22(4)	44(5)	−14(4)	−19(4)	5(3)
C(52)	38(5)	23(4)	55(6)	−23(4)	−19(5)	10(4)
C(53)	32(5)	53(6)	49(5)	−41(5)	−7(4)	11(4)
C(54)	19(4)	31(4)	45(5)	−22(4)	−5(3)	−1(3)
C(55)	66(7)	27(5)	40(5)	−17(4)	−5(5)	16(5)
C(56)	59(7)	42(6)	44(6)	−18(5)	−11(5)	−10(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7b**.

	x	y	z	U(eq)
H(2)	6761	5275	5649	44
H(4)	1728	9306	6099	43
H(2A)	7907	5947	8120	32
H(3)	8885	4318	9422	34
H(5A)	8520	1706	10888	37
H(5B)	9767	2280	9823	37
H(6A)	9522	866	9182	75
H(6B)	9082	43	10631	75
H(7B)	7027	74	10528	60
H(7A)	7770	-400	9617	60
H(8A)	6270	1093	8831	27
H(8B)	7637	1394	7952	27
H(13)	5056	3746	4773	31
H(14)	3399	2221	6060	28
H(16B)	1751	1627	8292	37
H(16A)	2469	502	8211	37
H(17B)	2998	-137	9995	55
H(17A)	1578	210	10225	55
H(18A)	2315	2158	9996	59
H(18B)	2843	1040	11058	59
H(19A)	4818	1478	9916	34
H(19B)	4363	2832	9628	34
H(21A)	4719	5333	8742	54
H(21B)	3934	6486	8662	54
H(21C)	5115	6187	9307	54
H(22A)	7098	7466	4622	50
H(22C)	8022	8719	3708	50
H(22B)	6524	8773	3926	50
H(23A)	8783	7724	5792	53
H(23C)	8550	8777	6222	53
H(23B)	9129	9181	4817	53
H(24A)	6111	10062	4639	39
H(24B)	7527	10574	4504	39
H(25B)	7157	9905	6610	44
H(25A)	6113	10814	6051	44
H(26A)	4619	8232	8929	61
H(26C)	5041	9709	8297	61
H(26B)	6081	8726	8602	61
H(27A)	4221	9169	5990	53

H(27C)	4037	10127	6543	53
H(27B)	3513	8675	7384	53
H(29)	3908	8639	3613	33
H(30)	5482	10289	2291	35
H(32B)	6518	12336	1919	39
H(32A)	5708	12912	889	39
H(33A)	6213	14559	1149	49
H(33B)	5965	13728	2607	49
H(34B)	4310	15003	2033	52
H(34A)	4038	14365	1231	52
H(35A)	2543	13453	3009	32
H(35B)	3582	13197	3818	32
H(40)	−497	10707	7040	32
H(41)	−1532	12334	5753	32
H(43B)	−1144	14251	3384	34
H(43A)	−2213	13147	3752	34
H(44A)	−1497	13007	2012	45
H(44B)	−1392	14492	1552	45
H(45B)	784	14475	1598	49
H(45A)	486	13987	683	49
H(46B)	1815	12673	1987	30
H(46A)	554	11900	2101	30
H(48B)	1607	8357	2476	48
H(48C)	949	9216	3034	48
H(48A)	144	8042	3145	48
H(49B)	3694	5484	6976	64
H(49C)	3758	6908	5928	64
H(49A)	3741	5778	5599	64
H(50A)	680	5803	7865	55
H(50C)	1544	7119	7164	55
H(50B)	2082	5875	8072	55
H(51A)	604	4558	7173	42
H(51B)	1963	4048	7310	42
H(52B)	2525	4687	5183	43
H(52A)	1245	3756	5775	43
H(53A)	1176	4775	3610	57
H(53C)	2258	5887	3193	57
H(53B)	876	6211	2942	57
H(54B)	−840	5981	4575	45
H(54C)	−691	5185	5959	45
H(54A)	−668	4511	5125	45
H(55B)	−139	8614	9753	54
H(55A)	592	8856	8426	54
H(56B)	6605	5671	3217	59

H(56A)	6832	6160	1780	59

Table 6. Torsion angles [deg] for **7b**.

C(21)-Pd(1)-O(1)-C(1)	-57.7(6)
N(2)-Pd(1)-O(1)-C(1)	-179(3)
N(1)-Pd(1)-O(1)-C(1)	119.5(6)
C(48)-Pd(2)-O(3)-C(28)	-58.6(6)
N(4)-Pd(2)-O(3)-C(28)	173(3)
N(3)-Pd(2)-O(3)-C(28)	119.0(6)
C(21)-Pd(1)-N(1)-C(22)	168(5)
O(1)-Pd(1)-N(1)-C(22)	42.9(6)
N(2)-Pd(1)-N(1)-C(22)	-132.8(6)
C(21)-Pd(1)-N(1)-C(23)	45(6)
O(1)-Pd(1)-N(1)-C(23)	-79.7(5)
N(2)-Pd(1)-N(1)-C(23)	104.7(6)
C(21)-Pd(1)-N(1)-C(24)	-72(5)
O(1)-Pd(1)-N(1)-C(24)	163.3(5)
N(2)-Pd(1)-N(1)-C(24)	-12.4(5)
C(21)-Pd(1)-N(2)-C(25)	161.3(6)
O(1)-Pd(1)-N(2)-C(25)	-78(3)
N(1)-Pd(1)-N(2)-C(25)	-15.7(5)
C(21)-Pd(1)-N(2)-C(27)	-79.8(6)
O(1)-Pd(1)-N(2)-C(27)	41(3)
N(1)-Pd(1)-N(2)-C(27)	103.2(6)
C(21)-Pd(1)-N(2)-C(26)	41.1(6)
O(1)-Pd(1)-N(2)-C(26)	162(3)
N(1)-Pd(1)-N(2)-C(26)	-135.9(6)
C(48)-Pd(2)-N(3)-C(50)	178(5)
O(3)-Pd(2)-N(3)-C(50)	44.4(6)
N(4)-Pd(2)-N(3)-C(50)	-131.4(6)
C(48)-Pd(2)-N(3)-C(51)	-63(5)
O(3)-Pd(2)-N(3)-C(51)	163.5(5)
N(4)-Pd(2)-N(3)-C(51)	-12.2(5)
C(48)-Pd(2)-N(3)-C(49)	55(5)
O(3)-Pd(2)-N(3)-C(49)	-78.1(6)
N(4)-Pd(2)-N(3)-C(49)	106.2(6)
C(48)-Pd(2)-N(4)-C(54)	-80.1(6)
O(3)-Pd(2)-N(4)-C(54)	48(3)
N(3)-Pd(2)-N(4)-C(54)	102.4(5)
C(48)-Pd(2)-N(4)-C(53)	42.0(6)
O(3)-Pd(2)-N(4)-C(53)	170(3)
N(3)-Pd(2)-N(4)-C(53)	-135.5(6)
C(48)-Pd(2)-N(4)-C(52)	160.5(6)
O(3)-Pd(2)-N(4)-C(52)	-71(3)
N(3)-Pd(2)-N(4)-C(52)	-17.0(6)

Pd(1)-O(1)-C(1)-C(10)	148.2(6)
Pd(1)-O(1)-C(1)-C(2)	-37.6(9)
O(1)-C(1)-C(2)-C(3)	-172.5(8)
C(10)-C(1)-C(2)-C(3)	1.7(12)
C(1)-C(2)-C(3)-C(4)	1.8(13)
C(2)-C(3)-C(4)-C(9)	-2.0(13)
C(2)-C(3)-C(4)-C(5)	177.3(8)
C(3)-C(4)-C(5)-C(6)	-164.5(10)
C(9)-C(4)-C(5)-C(6)	14.7(13)
C(4)-C(5)-C(6)-C(7)	-38.7(15)
C(5)-C(6)-C(7)-C(8)	54.1(16)
C(6)-C(7)-C(8)-C(9)	-43.2(13)
C(3)-C(4)-C(9)-C(10)	-1.4(11)
C(5)-C(4)-C(9)-C(10)	179.4(7)
C(3)-C(4)-C(9)-C(8)	173.2(7)
C(5)-C(4)-C(9)-C(8)	-6.0(11)
C(7)-C(8)-C(9)-C(4)	19.6(11)
C(7)-C(8)-C(9)-C(10)	-165.8(8)
O(1)-C(1)-C(10)-C(9)	169.4(7)
C(2)-C(1)-C(10)-C(9)	-5.0(11)
O(1)-C(1)-C(10)-C(11)	-12.0(10)
C(2)-C(1)-C(10)-C(11)	173.6(7)
C(4)-C(9)-C(10)-C(1)	4.9(11)
C(8)-C(9)-C(10)-C(1)	-169.7(7)
C(4)-C(9)-C(10)-C(11)	-173.7(7)
C(8)-C(9)-C(10)-C(11)	11.7(10)
C(1)-C(10)-C(11)-C(12)	62.3(10)
C(9)-C(10)-C(11)-C(12)	-119.2(8)
C(1)-C(10)-C(11)-C(20)	-117.1(8)
C(9)-C(10)-C(11)-C(20)	61.4(10)
C(20)-C(11)-C(12)-O(2)	169.6(7)
C(10)-C(11)-C(12)-O(2)	-9.8(11)
C(20)-C(11)-C(12)-C(13)	-11.1(11)
C(10)-C(11)-C(12)-C(13)	169.5(7)
O(2)-C(12)-C(13)-C(14)	-175.1(7)
C(11)-C(12)-C(13)-C(14)	5.5(12)
C(12)-C(13)-C(14)-C(15)	2.6(12)
C(13)-C(14)-C(15)-C(20)	-4.8(12)
C(13)-C(14)-C(15)-C(16)	175.5(7)
C(14)-C(15)-C(16)-C(17)	169.1(9)
C(20)-C(15)-C(16)-C(17)	-10.6(13)
C(15)-C(16)-C(17)-C(18)	41.4(13)
C(16)-C(17)-C(18)-C(19)	-58.6(14)
C(17)-C(18)-C(19)-C(20)	42.4(12)

C(14)-C(15)-C(20)-C(11)	-1.1(11)
C(16)-C(15)-C(20)-C(11)	178.7(7)
C(14)-C(15)-C(20)-C(19)	175.1(7)
C(16)-C(15)-C(20)-C(19)	-5.1(11)
C(12)-C(11)-C(20)-C(15)	8.8(11)
C(10)-C(11)-C(20)-C(15)	-171.8(7)
C(12)-C(11)-C(20)-C(19)	-167.4(7)
C(10)-C(11)-C(20)-C(19)	12.0(11)
C(18)-C(19)-C(20)-C(15)	-11.2(11)
C(18)-C(19)-C(20)-C(11)	165.0(8)
C(22)-N(1)-C(24)-C(25)	160.0(7)
C(23)-N(1)-C(24)-C(25)	-78.0(9)
Pd(1)-N(1)-C(24)-C(25)	38.1(7)
C(27)-N(2)-C(25)-C(24)	-74.3(9)
C(26)-N(2)-C(25)-C(24)	166.4(8)
Pd(1)-N(2)-C(25)-C(24)	42.6(8)
N(1)-C(24)-C(25)-N(2)	-57.0(10)
Pd(2)-O(3)-C(28)-C(29)	-36.2(9)
Pd(2)-O(3)-C(28)-C(37)	146.8(5)
O(3)-C(28)-C(29)-C(30)	-172.9(7)
C(37)-C(28)-C(29)-C(30)	4.0(11)
C(28)-C(29)-C(30)-C(31)	2.3(12)
C(29)-C(30)-C(31)-C(36)	-4.2(12)
C(29)-C(30)-C(31)-C(32)	178.4(7)
C(30)-C(31)-C(32)-C(33)	-165.7(8)
C(36)-C(31)-C(32)-C(33)	16.9(11)
C(31)-C(32)-C(33)-C(34)	-41.9(11)
C(32)-C(33)-C(34)-C(35)	60.5(12)
C(33)-C(34)-C(35)-C(36)	-50.2(11)
C(30)-C(31)-C(36)-C(37)	-0.2(11)
C(32)-C(31)-C(36)-C(37)	177.1(7)
C(30)-C(31)-C(36)-C(35)	176.0(7)
C(32)-C(31)-C(36)-C(35)	-6.7(11)
C(34)-C(35)-C(36)-C(31)	22.7(10)
C(34)-C(35)-C(36)-C(37)	-161.2(7)
O(3)-C(28)-C(37)-C(36)	168.7(6)
C(29)-C(28)-C(37)-C(36)	-8.4(10)
O(3)-C(28)-C(37)-C(38)	-10.3(10)
C(29)-C(28)-C(37)-C(38)	172.6(7)
C(31)-C(36)-C(37)-C(28)	6.5(10)
C(35)-C(36)-C(37)-C(28)	-169.7(6)
C(31)-C(36)-C(37)-C(38)	-174.5(6)
C(35)-C(36)-C(37)-C(38)	9.3(10)
C(28)-C(37)-C(38)-C(39)	60.8(9)

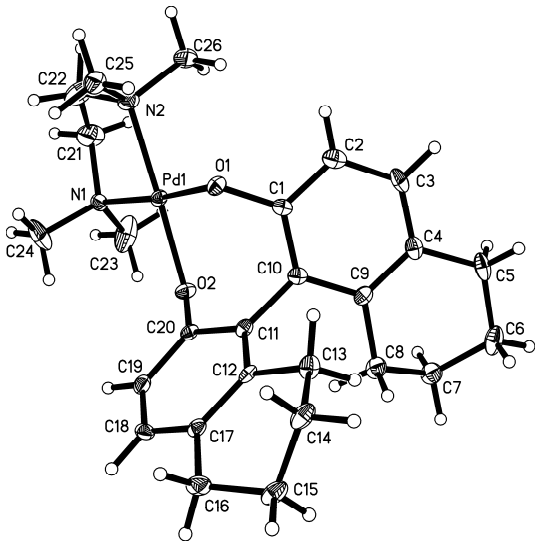
C(36)-C(37)-C(38)-C(39)	-118.2(8)
C(28)-C(37)-C(38)-C(47)	-120.0(8)
C(36)-C(37)-C(38)-C(47)	61.1(9)
C(47)-C(38)-C(39)-O(4)	170.1(7)
C(37)-C(38)-C(39)-O(4)	-10.6(11)
C(47)-C(38)-C(39)-C(40)	-7.3(11)
C(37)-C(38)-C(39)-C(40)	172.0(7)
O(4)-C(39)-C(40)-C(41)	-176.4(7)
C(38)-C(39)-C(40)-C(41)	1.1(11)
C(39)-C(40)-C(41)-C(42)	5.6(12)
C(40)-C(41)-C(42)-C(47)	-6.0(12)
C(40)-C(41)-C(42)-C(43)	176.2(7)
C(47)-C(42)-C(43)-C(44)	14.9(11)
C(41)-C(42)-C(43)-C(44)	-167.4(8)
C(42)-C(43)-C(44)-C(45)	-41.9(11)
C(43)-C(44)-C(45)-C(46)	61.8(11)
C(44)-C(45)-C(46)-C(47)	-51.9(10)
C(41)-C(42)-C(47)-C(38)	-0.3(11)
C(43)-C(42)-C(47)-C(38)	177.3(7)
C(41)-C(42)-C(47)-C(46)	176.2(7)
C(43)-C(42)-C(47)-C(46)	-6.2(11)
C(39)-C(38)-C(47)-C(42)	6.9(11)
C(37)-C(38)-C(47)-C(42)	-172.4(7)
C(39)-C(38)-C(47)-C(46)	-169.7(6)
C(37)-C(38)-C(47)-C(46)	11.1(10)
C(45)-C(46)-C(47)-C(42)	24.4(10)
C(45)-C(46)-C(47)-C(38)	-159.1(7)
C(50)-N(3)-C(51)-C(52)	160.4(7)
C(49)-N(3)-C(51)-C(52)	-78.1(9)
Pd(2)-N(3)-C(51)-C(52)	38.6(7)
C(54)-N(4)-C(52)-C(51)	-74.4(9)
C(53)-N(4)-C(52)-C(51)	167.6(7)
Pd(2)-N(4)-C(52)-C(51)	43.5(8)
N(3)-C(51)-C(52)-N(4)	-58.0(9)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **7b** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

The X-ray structure of compound 7c



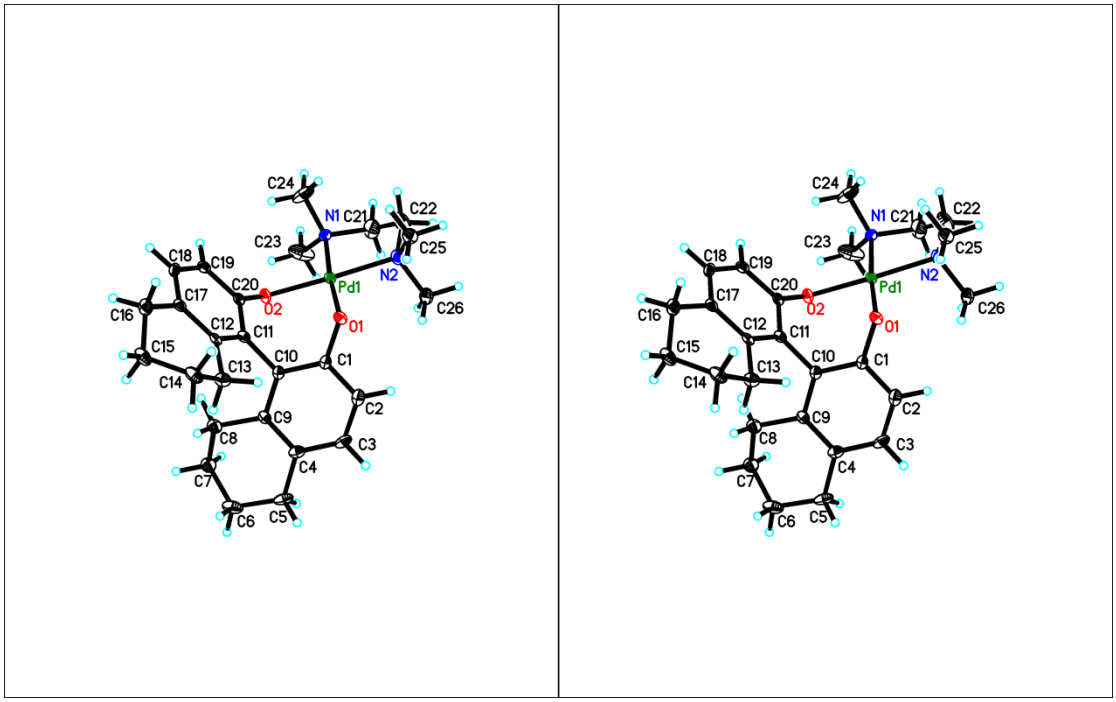


Table 1. Crystal data and structure refinement for **7c**.

Identification code	mx1321
Empirical formula	C27 H37 C13 N2 O2 Pd
Formula weight	634.34
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.8418(15) A alpha = 90 deg.
	b = 11.4447(18) A beta = 90 deg.
	c = 24.284(4) A gamma = 90 deg.
Volume	2735.2(7) A^3
Z, Calculated density	4, 1.540 Mg/m^3
Absorption coefficient	0.999 mm^-1
F(000)	1304
Crystal size	0.18 x 0.08 x 0.06 mm
Theta range for data collection	1.68 to 27.48 deg.
Limiting indices	-12<=h<=12, -14<=k<=14, -31<=l<=31
Reflections collected / unique	17508 / 6166 [R(int) = 0.0546]
Completeness to theta = 27.48	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9425 and 0.8406
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6166 / 0 / 320
Goodness-of-fit on F^2	1.138
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.0919
R indices (all data)	R1 = 0.0590, wR2 = 0.0951
Absolute structure parameter	0.00(4)
Largest diff. peak and hole	0.797 and -0.378 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7c**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd(1)	589(1)	6479(1)	9992(1)	20(1)
Cl(1)	1966(2)	1710(1)	10608(1)	45(1)
Cl(2)	4348(2)	3172(1)	10509(1)	52(1)
Cl(3)	3395(2)	2442(2)	11582(1)	58(1)
O(1)	1368(3)	7526(3)	9402(1)	24(1)
O(2)	382(3)	5063(3)	9507(1)	24(1)
N(1)	-118(4)	5513(4)	10654(2)	28(1)
N(2)	686(5)	7857(4)	10536(2)	29(1)
C(1)	649(5)	7508(4)	8924(2)	19(1)
C(2)	-116(5)	8492(5)	8778(2)	29(1)
C(3)	-916(5)	8454(5)	8308(2)	30(1)
C(4)	-1002(5)	7456(5)	7980(2)	26(1)
C(5)	-1961(5)	7435(5)	7493(2)	35(1)
C(6)	-1871(6)	6347(6)	7139(2)	41(1)
C(7)	-1660(5)	5263(5)	7489(2)	33(1)
C(8)	-315(5)	5368(5)	7791(2)	30(1)
C(9)	-207(4)	6494(4)	8119(2)	21(1)
C(10)	679(5)	6541(4)	8580(2)	21(1)
C(11)	1640(4)	5578(4)	8694(2)	19(1)
C(12)	2761(5)	5378(4)	8350(2)	19(1)
C(13)	3032(5)	6186(4)	7869(2)	27(1)
C(14)	4392(5)	5989(5)	7585(2)	31(1)
C(15)	4704(5)	4714(5)	7518(2)	33(1)
C(16)	4801(5)	4142(5)	8074(2)	31(1)
C(17)	3611(5)	4413(4)	8445(2)	22(1)
C(18)	3337(5)	3677(4)	8889(2)	25(1)
C(19)	2275(5)	3902(4)	9245(2)	25(1)
C(20)	1424(5)	4867(4)	9162(2)	19(1)
C(21)	-610(8)	6411(6)	11051(2)	54(2)
C(22)	285(7)	7377(6)	11091(3)	54(2)
C(23)	-1270(7)	4737(7)	10538(3)	61(2)
C(24)	978(7)	4794(6)	10863(3)	56(2)
C(25)	2067(5)	8342(5)	10583(2)	37(1)
C(26)	-268(6)	8767(5)	10362(2)	44(2)
C(27)	3586(6)	2045(5)	10886(2)	34(1)

Table 3. Bond lengths [A] and angles [deg] for **7c**.

Pd(1)-O(2)	2.013(3)
Pd(1)-O(1)	2.020(3)
Pd(1)-N(2)	2.060(4)
Pd(1)-N(1)	2.071(4)
Cl(1)-C(27)	1.774(6)
Cl(2)-C(27)	1.752(6)
Cl(3)-C(27)	1.759(6)
O(1)-C(1)	1.358(6)
O(2)-C(20)	1.343(5)
N(1)-C(24)	1.448(7)
N(1)-C(23)	1.467(8)
N(1)-C(21)	1.491(7)
N(2)-C(26)	1.465(7)
N(2)-C(25)	1.472(7)
N(2)-C(22)	1.507(7)
C(1)-C(10)	1.388(6)
C(1)-C(2)	1.400(7)
C(2)-C(3)	1.388(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.395(7)
C(3)-H(3)	0.9500
C(4)-C(9)	1.392(7)
C(4)-C(5)	1.513(7)
C(5)-C(6)	1.515(8)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.518(7)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.518(7)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.519(7)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.418(6)
C(10)-C(11)	1.479(6)
C(11)-C(12)	1.403(6)
C(11)-C(20)	1.414(6)
C(12)-C(17)	1.404(6)
C(12)-C(13)	1.514(6)
C(13)-C(14)	1.523(7)

C(13)-H(13B)	0.9900
C(13)-H(13A)	0.9900
C(14)-C(15)	1.500(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.504(7)
C(15)-H(15B)	0.9900
C(15)-H(15A)	0.9900
C(16)-C(17)	1.510(6)
C(16)-H(16B)	0.9900
C(16)-H(16A)	0.9900
C(17)-C(18)	1.393(7)
C(18)-C(19)	1.381(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.401(7)
C(19)-H(19)	0.9500
C(21)-C(22)	1.417(10)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(23)-H(23A)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24C)	0.9800
C(24)-H(24B)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(25)-H(25A)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26C)	0.9800
C(26)-H(26B)	0.9800
C(27)-H(27)	1.0000

O(2)-Pd(1)-O(1)	95.75(13)
O(2)-Pd(1)-N(2)	174.99(15)
O(1)-Pd(1)-N(2)	89.06(15)
O(2)-Pd(1)-N(1)	89.46(16)
O(1)-Pd(1)-N(1)	174.33(15)
N(2)-Pd(1)-N(1)	85.80(17)
C(1)-O(1)-Pd(1)	113.5(3)
C(20)-O(2)-Pd(1)	115.0(3)
C(24)-N(1)-C(23)	107.4(5)

C(24)-N(1)-C(21)	114.0(5)
C(23)-N(1)-C(21)	106.9(5)
C(24)-N(1)-Pd(1)	108.9(4)
C(23)-N(1)-Pd(1)	115.7(3)
C(21)-N(1)-Pd(1)	104.1(3)
C(26)-N(2)-C(25)	110.3(4)
C(26)-N(2)-C(22)	110.4(5)
C(25)-N(2)-C(22)	108.1(5)
C(26)-N(2)-Pd(1)	109.2(3)
C(25)-N(2)-Pd(1)	112.4(3)
C(22)-N(2)-Pd(1)	106.4(3)
O(1)-C(1)-C(10)	121.0(4)
O(1)-C(1)-C(2)	119.0(4)
C(10)-C(1)-C(2)	120.0(5)
C(3)-C(2)-C(1)	119.3(5)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	121.9(5)
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-H(3)	119.0
C(9)-C(4)-C(3)	118.4(4)
C(9)-C(4)-C(5)	121.9(5)
C(3)-C(4)-C(5)	119.8(5)
C(4)-C(5)-C(6)	114.8(4)
C(4)-C(5)-H(5A)	108.6
C(6)-C(5)-H(5A)	108.6
C(4)-C(5)-H(5B)	108.6
C(6)-C(5)-H(5B)	108.6
H(5A)-C(5)-H(5B)	107.5
C(5)-C(6)-C(7)	111.2(4)
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6B)	109.4
C(7)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(6)-C(7)-C(8)	109.0(4)
C(6)-C(7)-H(7A)	109.9
C(8)-C(7)-H(7A)	109.9
C(6)-C(7)-H(7B)	109.9
C(8)-C(7)-H(7B)	109.9
H(7A)-C(7)-H(7B)	108.3
C(7)-C(8)-C(9)	112.5(4)
C(7)-C(8)-H(8A)	109.1
C(9)-C(8)-H(8A)	109.1

C(7)-C(8)-H(8B)	109.1
C(9)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.8
C(4)-C(9)-C(10)	120.4(4)
C(4)-C(9)-C(8)	120.3(4)
C(10)-C(9)-C(8)	119.3(4)
C(1)-C(10)-C(9)	119.5(4)
C(1)-C(10)-C(11)	119.6(4)
C(9)-C(10)-C(11)	120.9(4)
C(12)-C(11)-C(20)	120.2(4)
C(12)-C(11)-C(10)	120.9(4)
C(20)-C(11)-C(10)	118.9(4)
C(11)-C(12)-C(17)	120.0(4)
C(11)-C(12)-C(13)	119.9(4)
C(17)-C(12)-C(13)	120.2(4)
C(12)-C(13)-C(14)	114.4(4)
C(12)-C(13)-H(13B)	108.7
C(14)-C(13)-H(13B)	108.7
C(12)-C(13)-H(13A)	108.7
C(14)-C(13)-H(13A)	108.7
H(13B)-C(13)-H(13A)	107.6
C(15)-C(14)-C(13)	111.9(4)
C(15)-C(14)-H(14A)	109.2
C(13)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14B)	109.2
C(13)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
C(14)-C(15)-C(16)	109.8(4)
C(14)-C(15)-H(15B)	109.7
C(16)-C(15)-H(15B)	109.7
C(14)-C(15)-H(15A)	109.7
C(16)-C(15)-H(15A)	109.7
H(15B)-C(15)-H(15A)	108.2
C(15)-C(16)-C(17)	113.4(4)
C(15)-C(16)-H(16B)	108.9
C(17)-C(16)-H(16B)	108.9
C(15)-C(16)-H(16A)	108.9
C(17)-C(16)-H(16A)	108.9
H(16B)-C(16)-H(16A)	107.7
C(18)-C(17)-C(12)	119.1(4)
C(18)-C(17)-C(16)	119.2(4)
C(12)-C(17)-C(16)	121.7(4)
C(19)-C(18)-C(17)	121.2(4)
C(19)-C(18)-H(18)	119.4

C(17)-C(18)-H(18)	119.4
C(18)-C(19)-C(20)	120.7(5)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
O(2)-C(20)-C(19)	119.9(4)
O(2)-C(20)-C(11)	121.4(4)
C(19)-C(20)-C(11)	118.6(4)
C(22)-C(21)-N(1)	112.3(5)
C(22)-C(21)-H(21A)	109.1
N(1)-C(21)-H(21A)	109.1
C(22)-C(21)-H(21B)	109.1
N(1)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.9
C(21)-C(22)-N(2)	112.7(5)
C(21)-C(22)-H(22A)	109.0
N(2)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22B)	109.0
N(2)-C(22)-H(22B)	109.0
H(22A)-C(22)-H(22B)	107.8
N(1)-C(23)-H(23B)	109.5
N(1)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(1)-C(23)-H(23A)	109.5
H(23B)-C(23)-H(23A)	109.5
H(23C)-C(23)-H(23A)	109.5
N(1)-C(24)-H(24A)	109.5
N(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
N(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24C)-C(24)-H(24B)	109.5
N(2)-C(25)-H(25B)	109.5
N(2)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(2)-C(25)-H(25A)	109.5
H(25B)-C(25)-H(25A)	109.5
H(25C)-C(25)-H(25A)	109.5
N(2)-C(26)-H(26A)	109.5
N(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
N(2)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
H(26C)-C(26)-H(26B)	109.5
Cl(2)-C(27)-Cl(3)	111.0(3)

Cl(2)-C(27)-Cl(1)	110.2(3)
Cl(3)-C(27)-Cl(1)	109.0(3)
Cl(2)-C(27)-H(27)	108.9
Cl(3)-C(27)-H(27)	108.9
Cl(1)-C(27)-H(27)	108.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **7c**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd(1)	21(1)	24(1)	15(1)	-2(1)	2(1)	2(1)
Cl(1)	38(1)	38(1)	59(1)	-6(1)	-5(1)	0(1)
Cl(2)	43(1)	46(1)	68(1)	13(1)	9(1)	-3(1)
Cl(3)	63(1)	69(1)	42(1)	-5(1)	-2(1)	6(1)
O(1)	26(2)	27(2)	18(2)	-1(2)	2(1)	-3(2)
O(2)	29(2)	22(2)	21(2)	-5(1)	6(1)	-2(2)
N(1)	40(2)	27(2)	16(2)	3(2)	3(2)	12(2)
N(2)	38(2)	29(2)	20(2)	-5(2)	5(2)	2(2)
C(1)	18(2)	17(2)	22(2)	2(2)	10(2)	-2(2)
C(2)	34(3)	23(2)	30(2)	0(2)	14(2)	-1(2)
C(3)	27(3)	30(3)	32(3)	16(2)	6(2)	7(2)
C(4)	21(2)	33(3)	26(2)	9(2)	3(2)	0(2)
C(5)	24(3)	45(3)	38(3)	17(3)	-7(2)	5(3)
C(6)	31(3)	64(4)	29(3)	6(3)	-10(2)	-4(3)
C(7)	25(3)	40(3)	34(3)	-4(2)	-3(2)	2(3)
C(8)	21(3)	38(3)	31(3)	-5(2)	-6(2)	0(2)
C(9)	20(2)	26(2)	18(2)	-1(2)	3(2)	-4(2)
C(10)	22(2)	20(2)	22(2)	0(2)	5(2)	-2(2)
C(11)	17(2)	24(2)	16(2)	-1(2)	2(2)	-3(2)
C(12)	22(2)	23(2)	12(2)	-4(2)	0(2)	-6(2)
C(13)	23(2)	36(3)	21(2)	6(2)	6(2)	-3(2)
C(14)	28(3)	46(3)	20(2)	-4(2)	4(2)	-11(3)
C(15)	22(3)	51(3)	24(2)	-11(2)	5(2)	-5(2)
C(16)	24(3)	36(3)	31(3)	-6(2)	7(2)	5(2)
C(17)	17(2)	28(3)	20(2)	-7(2)	-4(2)	-1(2)
C(18)	24(2)	18(2)	33(2)	-7(2)	-7(2)	3(2)
C(19)	32(3)	22(2)	20(2)	0(2)	-6(2)	-4(2)
C(20)	22(2)	21(2)	13(2)	-2(2)	5(2)	-3(2)
C(21)	88(5)	46(3)	28(3)	3(3)	23(3)	9(4)
C(22)	65(5)	68(5)	28(3)	-18(3)	15(3)	-2(4)
C(23)	55(4)	92(6)	35(3)	26(4)	-3(3)	-36(4)
C(24)	54(4)	52(4)	61(4)	32(4)	7(3)	22(4)
C(25)	36(3)	37(3)	38(3)	-6(3)	-8(2)	1(3)
C(26)	50(4)	44(4)	38(3)	-16(3)	-2(3)	22(3)
C(27)	32(3)	28(3)	41(3)	4(2)	-1(2)	10(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7c**.

	x	y	z	U(eq)
H(2)	-87	9177	8998	35
H(3)	-1419	9129	8206	36
H(5A)	-1772	8124	7259	42
H(5B)	-2903	7510	7631	42
H(6A)	-1106	6428	6877	50
H(6B)	-2718	6263	6923	50
H(7A)	-1654	4560	7252	39
H(7B)	-2412	5185	7757	39
H(8A)	436	5336	7521	36
H(8B)	-212	4696	8044	36
H(13B)	2994	7003	8001	32
H(13A)	2297	6084	7595	32
H(14A)	4377	6366	7218	38
H(14B)	5120	6361	7805	38
H(15B)	5574	4620	7318	39
H(15A)	3979	4335	7298	39
H(16B)	5647	4403	8256	37
H(16A)	4861	3285	8023	37
H(18)	3892	3010	8948	30
H(19)	2119	3397	9548	30
H(21A)	-1516	6690	10933	65
H(21B)	-711	6049	11419	65
H(22A)	1113	7134	11292	65
H(22B)	-159	8003	11307	65
H(23B)	-2054	5204	10422	91
H(23C)	-1502	4296	10870	91
H(23A)	-1022	4193	10243	91
H(24A)	1221	4204	10587	84
H(24C)	686	4406	11202	84
H(24B)	1770	5287	10940	84
H(25B)	2696	7725	10699	56
H(25C)	2071	8973	10856	56
H(25A)	2354	8650	10225	56
H(26A)	-13	9051	9996	66
H(26C)	-242	9415	10625	66
H(26B)	-1189	8442	10349	66
H(27)	4174	1334	10864	40

Table 6. Torsion angles [deg] for **7c**.

O(2)-Pd(1)-O(1)-C(1)	48.5(3)
N(2)-Pd(1)-O(1)-C(1)	-130.0(3)
N(1)-Pd(1)-O(1)-C(1)	-154.8(15)
O(1)-Pd(1)-O(2)-C(20)	41.4(3)
N(2)-Pd(1)-O(2)-C(20)	-155.2(18)
N(1)-Pd(1)-O(2)-C(20)	-136.3(3)
O(2)-Pd(1)-N(1)-C(24)	79.4(4)
O(1)-Pd(1)-N(1)-C(24)	-77.3(17)
N(2)-Pd(1)-N(1)-C(24)	-102.2(4)
O(2)-Pd(1)-N(1)-C(23)	-41.6(5)
O(1)-Pd(1)-N(1)-C(23)	161.6(14)
N(2)-Pd(1)-N(1)-C(23)	136.7(5)
O(2)-Pd(1)-N(1)-C(21)	-158.6(4)
O(1)-Pd(1)-N(1)-C(21)	44.7(17)
N(2)-Pd(1)-N(1)-C(21)	19.8(4)
O(2)-Pd(1)-N(2)-C(26)	-97.0(19)
O(1)-Pd(1)-N(2)-C(26)	66.4(4)
N(1)-Pd(1)-N(2)-C(26)	-115.9(4)
O(2)-Pd(1)-N(2)-C(25)	140.3(18)
O(1)-Pd(1)-N(2)-C(25)	-56.3(4)
N(1)-Pd(1)-N(2)-C(25)	121.3(4)
O(2)-Pd(1)-N(2)-C(22)	22(2)
O(1)-Pd(1)-N(2)-C(22)	-174.4(4)
N(1)-Pd(1)-N(2)-C(22)	3.2(4)
Pd(1)-O(1)-C(1)-C(10)	-72.1(5)
Pd(1)-O(1)-C(1)-C(2)	108.9(4)
O(1)-C(1)-C(2)-C(3)	-176.3(4)
C(10)-C(1)-C(2)-C(3)	4.7(7)
C(1)-C(2)-C(3)-C(4)	1.2(7)
C(2)-C(3)-C(4)-C(9)	-3.1(7)
C(2)-C(3)-C(4)-C(5)	175.9(5)
C(9)-C(4)-C(5)-C(6)	-6.3(7)
C(3)-C(4)-C(5)-C(6)	174.7(5)
C(4)-C(5)-C(6)-C(7)	38.6(6)
C(5)-C(6)-C(7)-C(8)	-62.6(6)
C(6)-C(7)-C(8)-C(9)	53.9(6)
C(3)-C(4)-C(9)-C(10)	-0.8(7)
C(5)-C(4)-C(9)-C(10)	-179.8(4)
C(3)-C(4)-C(9)-C(8)	177.1(4)
C(5)-C(4)-C(9)-C(8)	-1.9(7)
C(7)-C(8)-C(9)-C(4)	-22.5(6)
C(7)-C(8)-C(9)-C(10)	155.4(4)

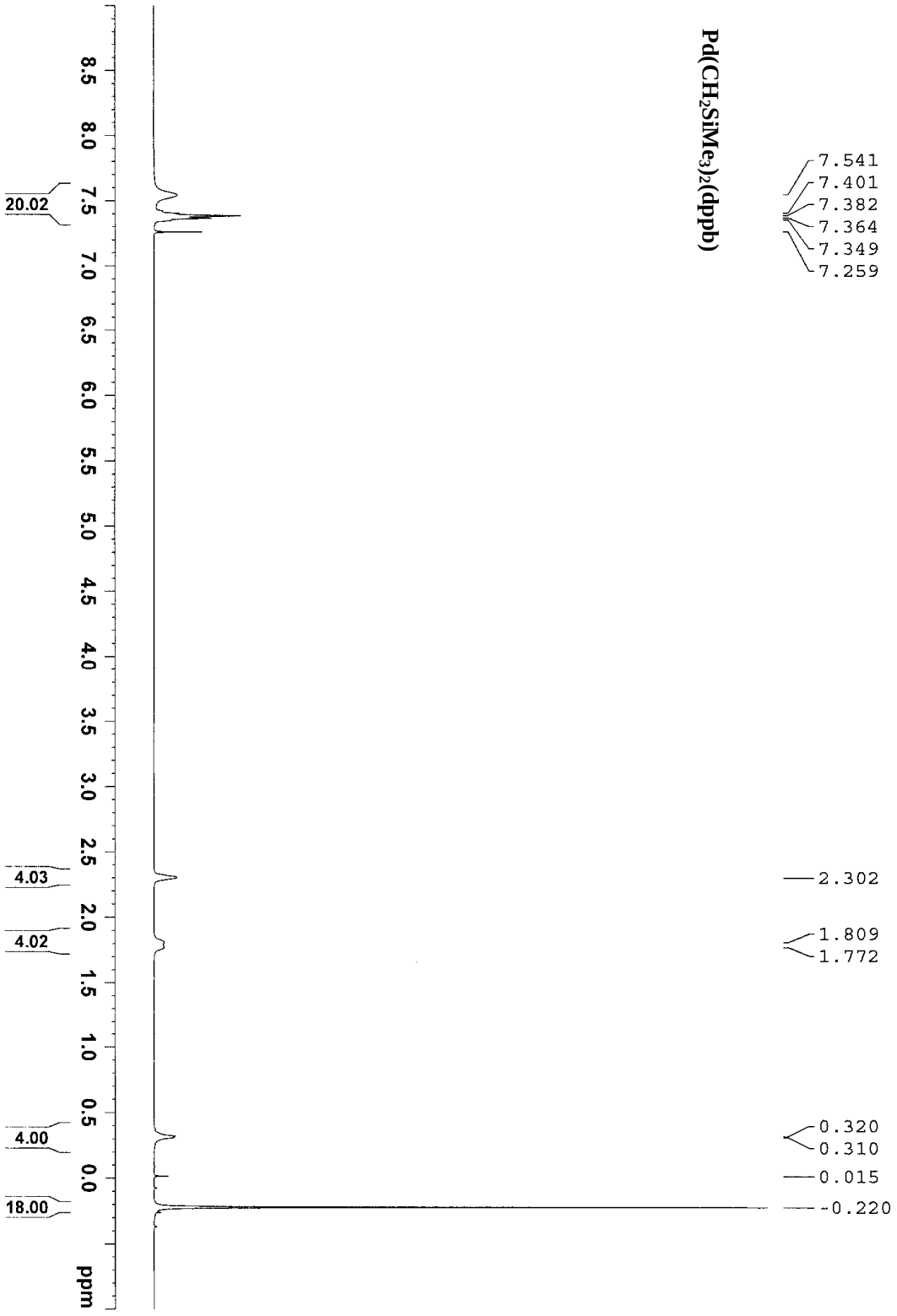
O(1)-C(1)-C(10)-C(9)	172.5(4)
C(2)-C(1)-C(10)-C(9)	-8.5(7)
O(1)-C(1)-C(10)-C(11)	-7.9(7)
C(2)-C(1)-C(10)-C(11)	171.1(4)
C(4)-C(9)-C(10)-C(1)	6.6(6)
C(8)-C(9)-C(10)-C(1)	-171.3(4)
C(4)-C(9)-C(10)-C(11)	-173.0(4)
C(8)-C(9)-C(10)-C(11)	9.1(6)
C(1)-C(10)-C(11)-C(12)	-109.8(5)
C(9)-C(10)-C(11)-C(12)	69.7(6)
C(1)-C(10)-C(11)-C(20)	69.3(6)
C(9)-C(10)-C(11)-C(20)	-111.1(5)
C(20)-C(11)-C(12)-C(17)	5.1(7)
C(10)-C(11)-C(12)-C(17)	-175.8(4)
C(20)-C(11)-C(12)-C(13)	-176.5(4)
C(10)-C(11)-C(12)-C(13)	2.7(6)
C(11)-C(12)-C(13)-C(14)	170.8(4)
C(17)-C(12)-C(13)-C(14)	-10.7(6)
C(12)-C(13)-C(14)-C(15)	41.9(6)
C(13)-C(14)-C(15)-C(16)	-61.8(6)
C(14)-C(15)-C(16)-C(17)	49.7(6)
C(11)-C(12)-C(17)-C(18)	-1.2(7)
C(13)-C(12)-C(17)-C(18)	-179.6(4)
C(11)-C(12)-C(17)-C(16)	177.9(4)
C(13)-C(12)-C(17)-C(16)	-0.5(7)
C(15)-C(16)-C(17)-C(18)	159.7(4)
C(15)-C(16)-C(17)-C(12)	-19.4(7)
C(12)-C(17)-C(18)-C(19)	-2.0(7)
C(16)-C(17)-C(18)-C(19)	178.9(4)
C(17)-C(18)-C(19)-C(20)	1.2(7)
Pd(1)-O(2)-C(20)-C(19)	110.8(4)
Pd(1)-O(2)-C(20)-C(11)	-72.9(5)
C(18)-C(19)-C(20)-O(2)	179.0(4)
C(18)-C(19)-C(20)-C(11)	2.6(7)
C(12)-C(11)-C(20)-O(2)	177.9(4)
C(10)-C(11)-C(20)-O(2)	-1.2(7)
C(12)-C(11)-C(20)-C(19)	-5.7(7)
C(10)-C(11)-C(20)-C(19)	175.1(4)
C(24)-N(1)-C(21)-C(22)	76.4(7)
C(23)-N(1)-C(21)-C(22)	-165.0(6)
Pd(1)-N(1)-C(21)-C(22)	-42.2(6)
N(1)-C(21)-C(22)-N(2)	49.0(8)
C(26)-N(2)-C(22)-C(21)	90.1(7)
C(25)-N(2)-C(22)-C(21)	-149.2(6)

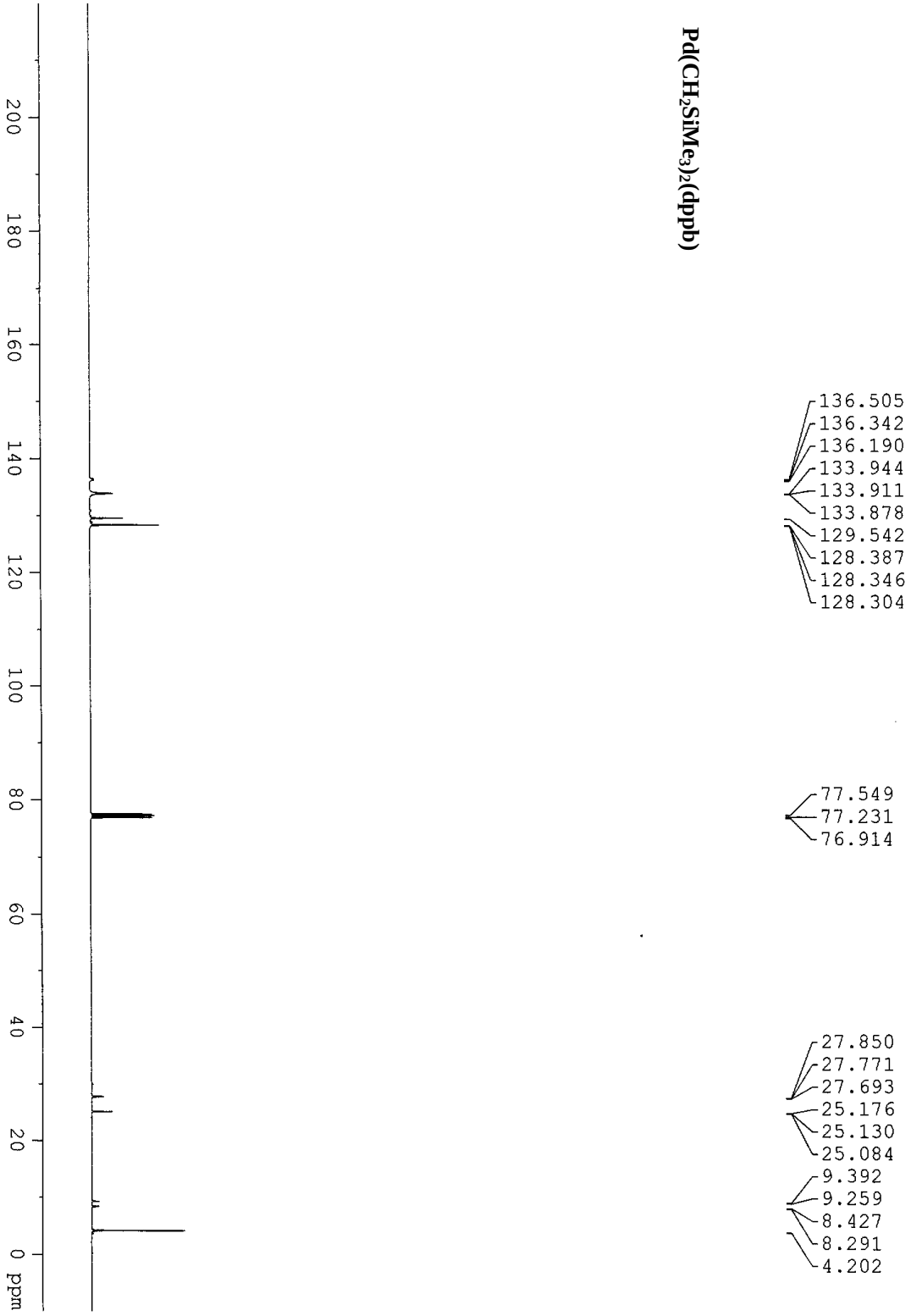
Pd(1)-N(2)-C(22)-C(21)	-28.3(7)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **7c** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

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133.911
133.878
129.542
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128.346
128.304
77.549
77.231
76.914
27.850
27.771
27.693
25.176
25.130
25.084
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8.291
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140
120
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60
40
20
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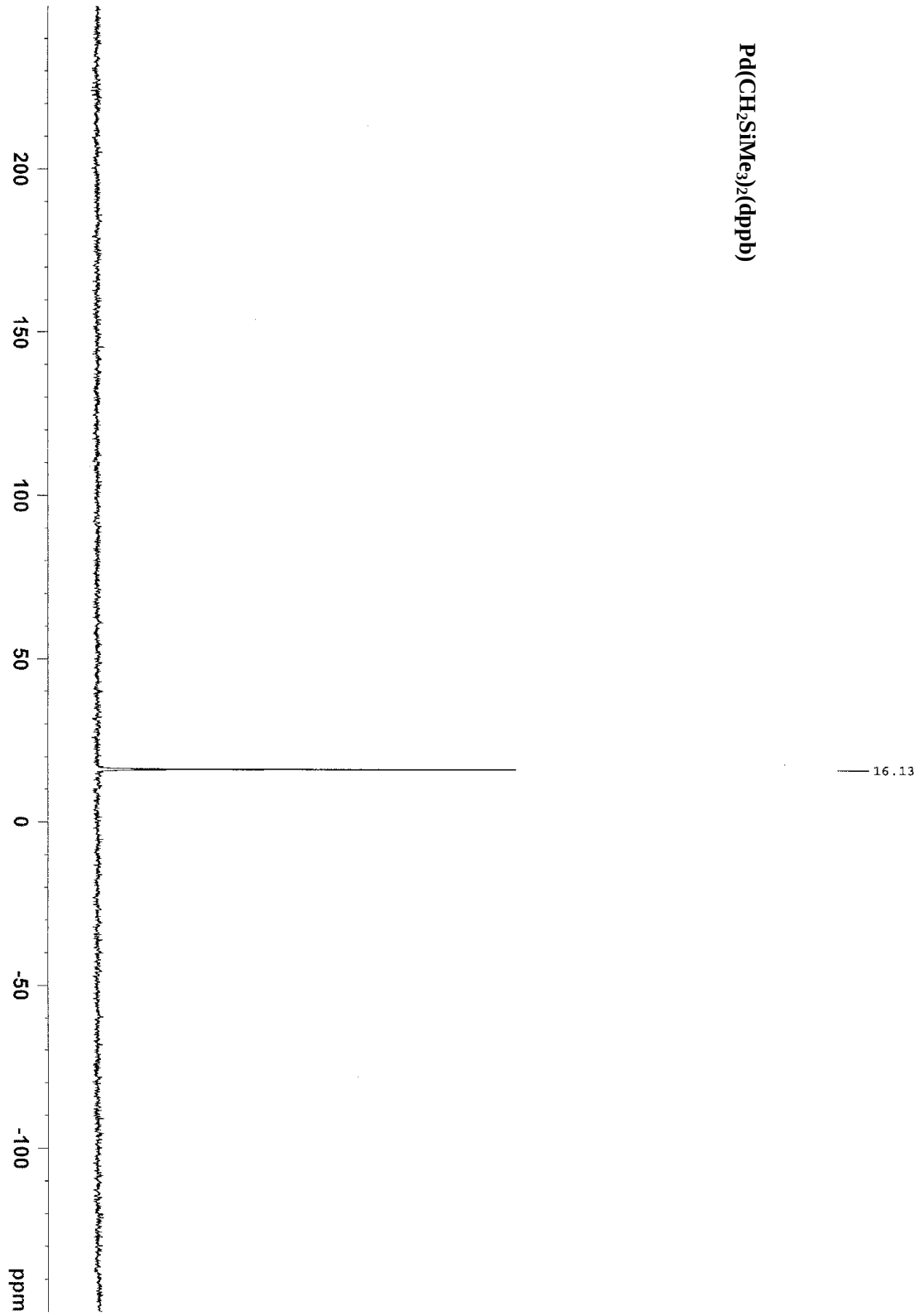

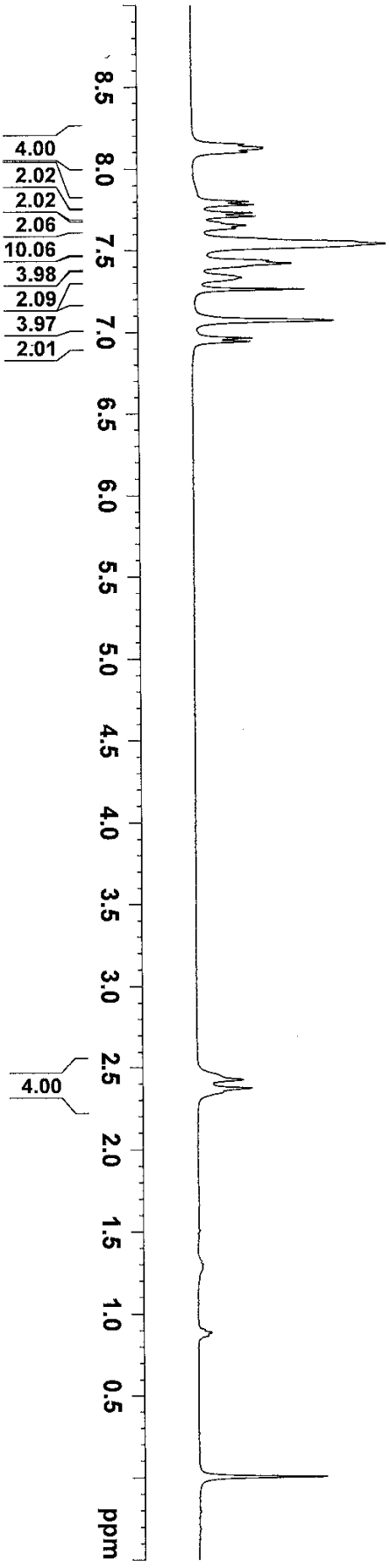

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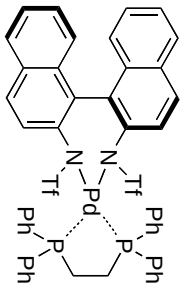

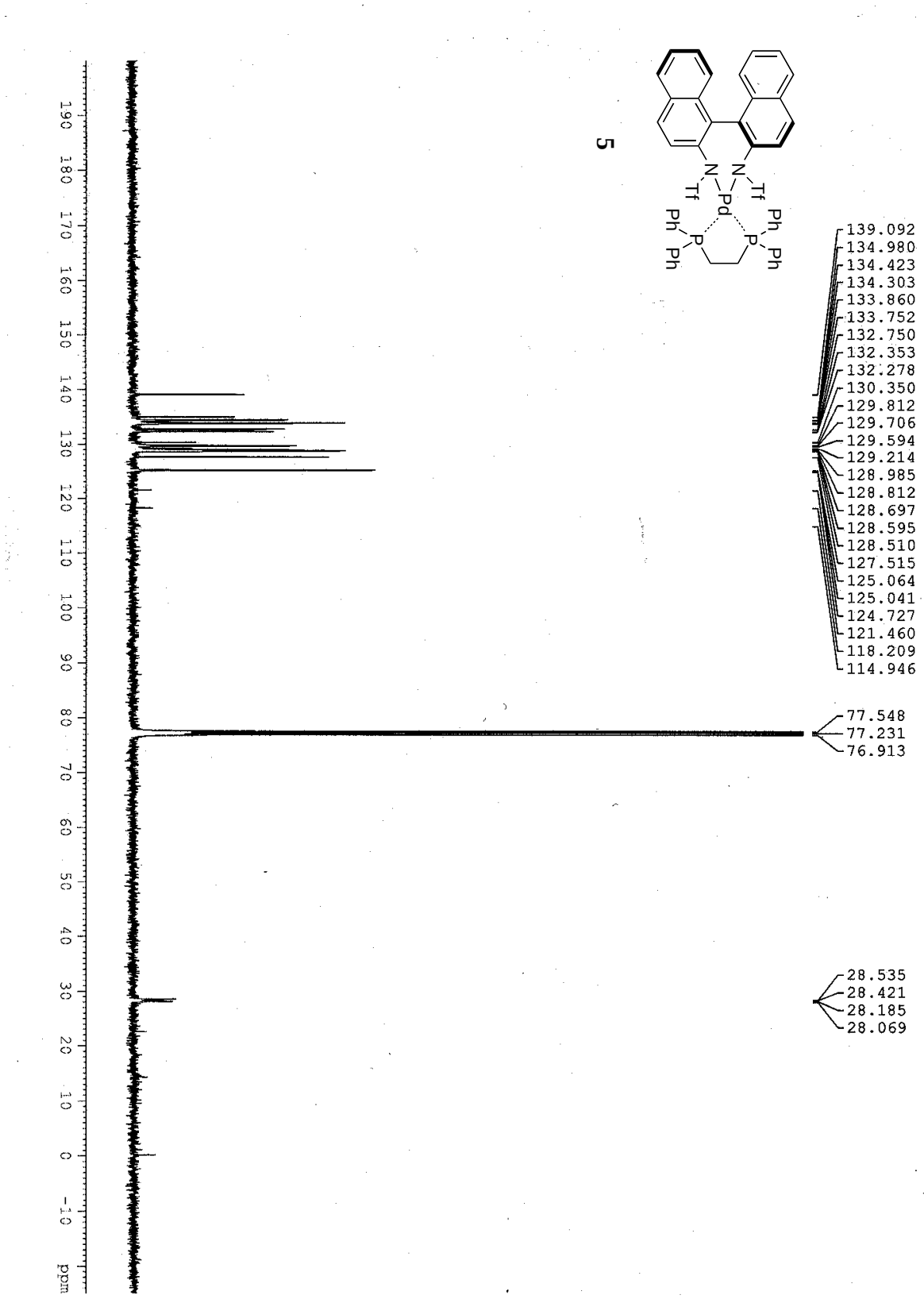
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Ph
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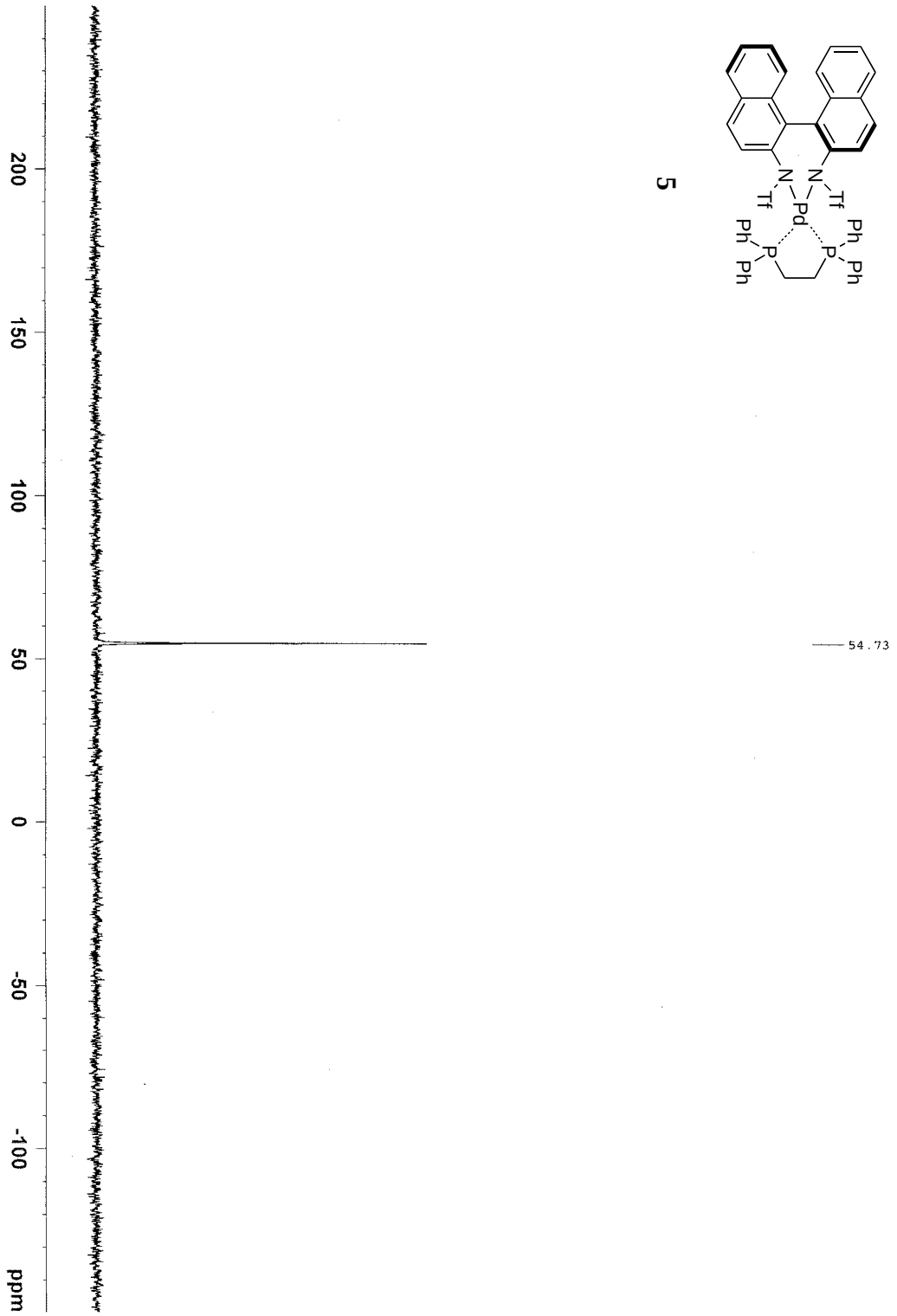

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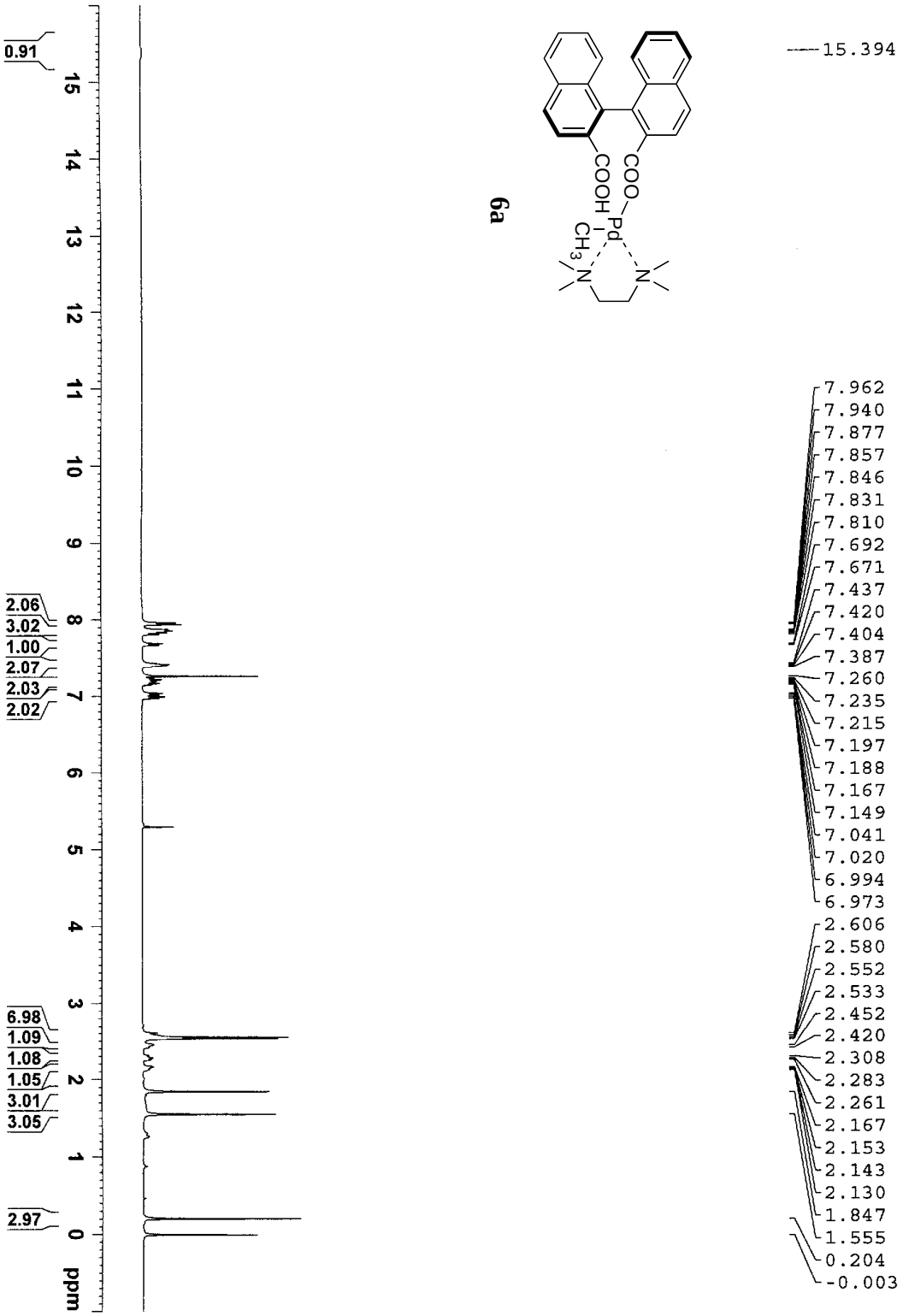
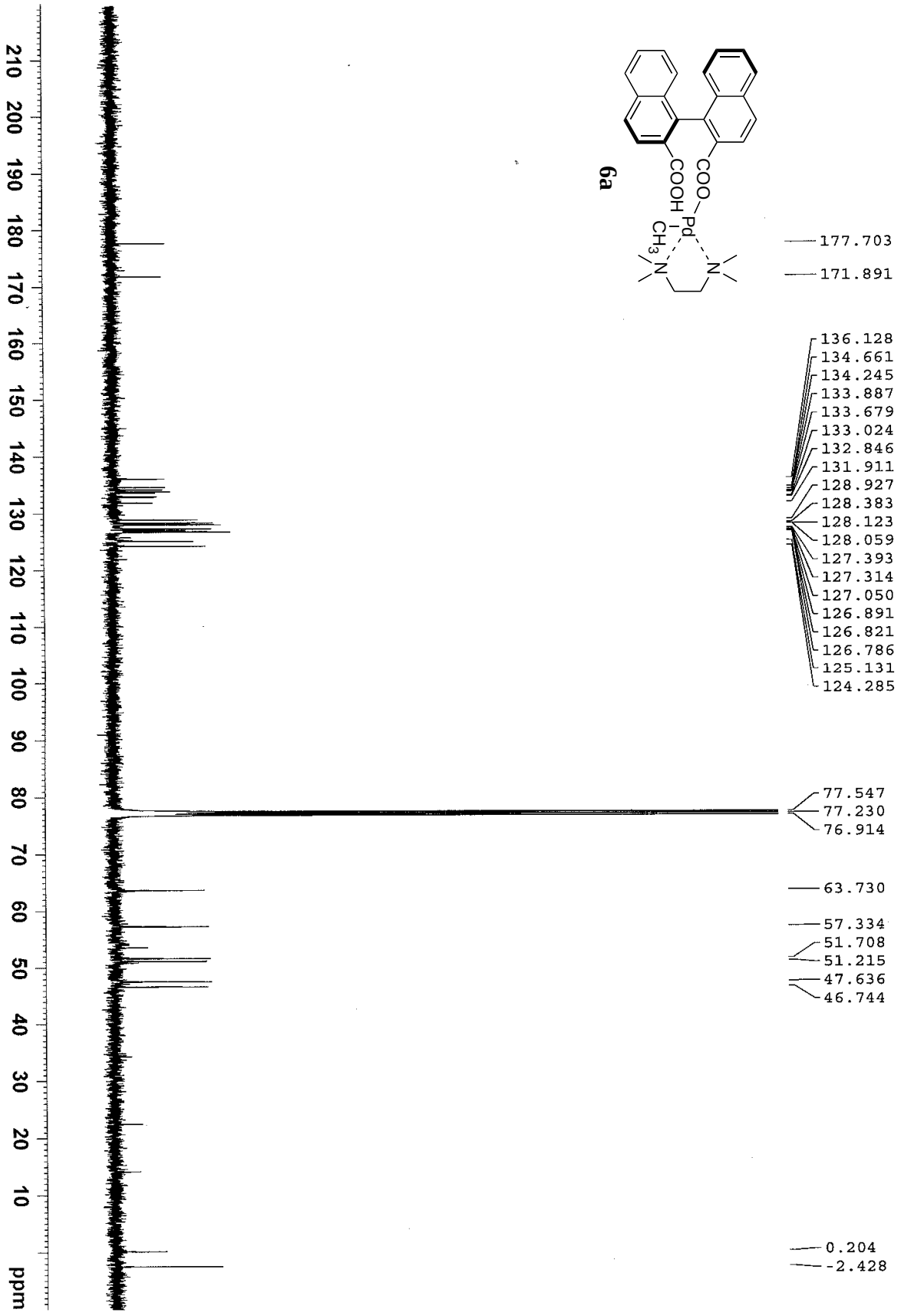
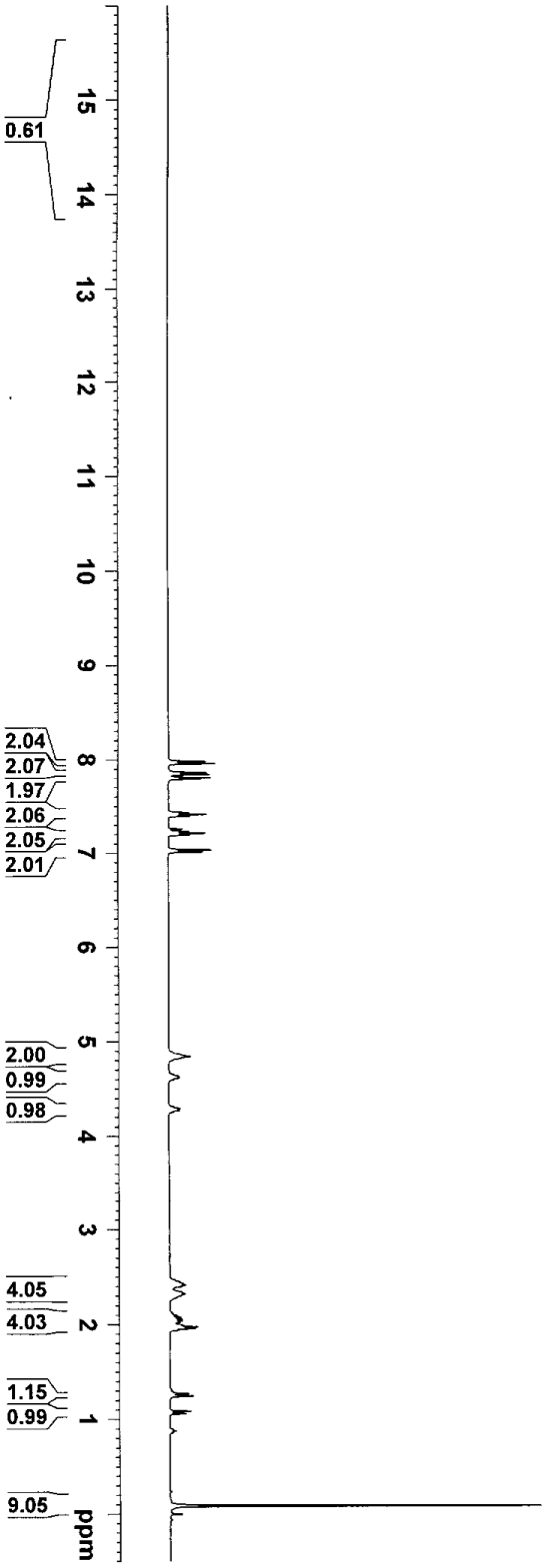
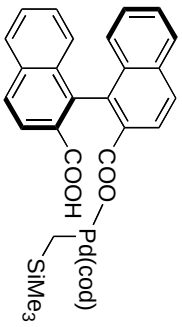
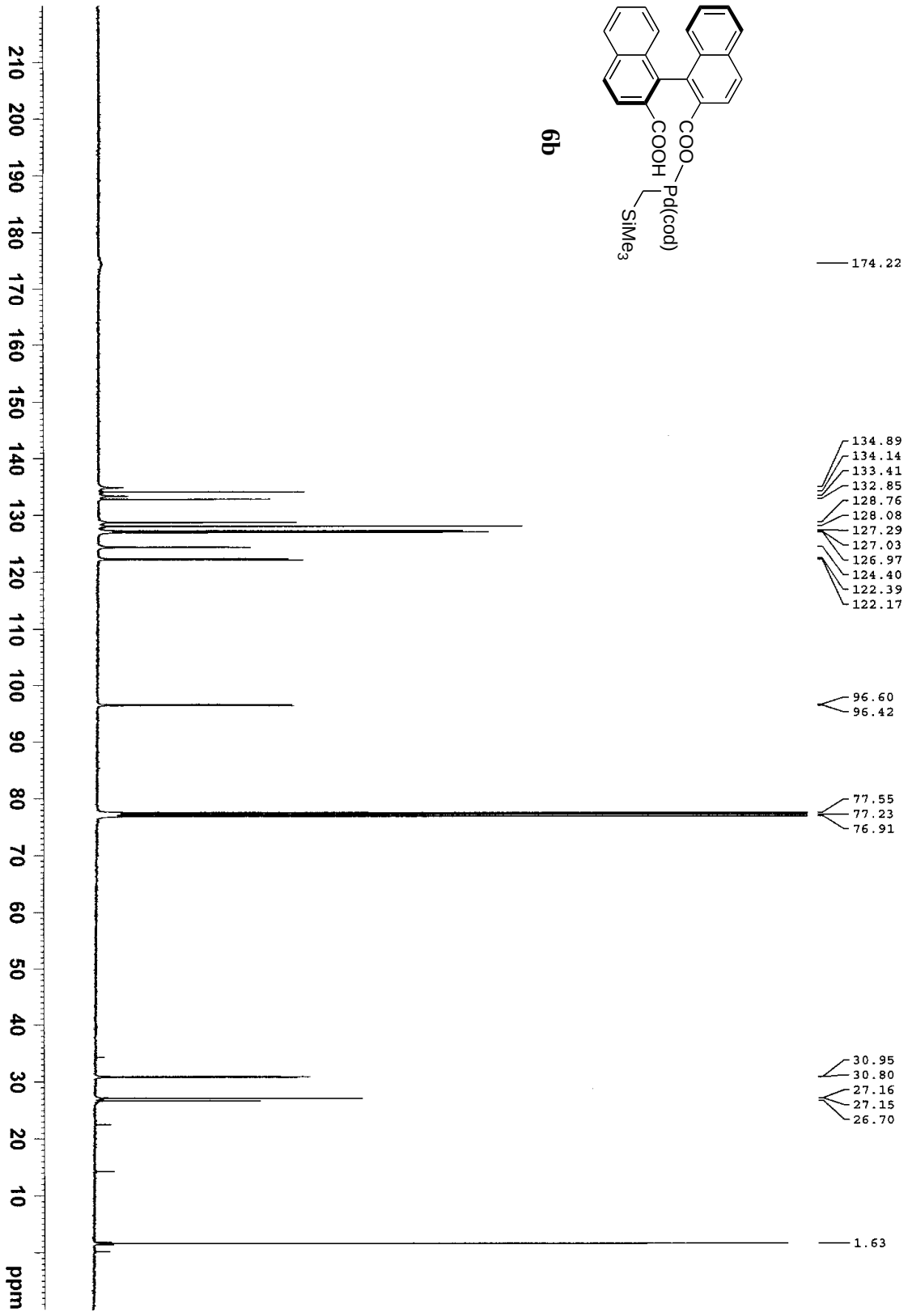

0.91
2.06
3.02
1.00
2.07
2.03
2.02
6.98
1.09
1.08
1.05
3.01
3.05
2.97
ppm
6a
COOH
COO
Pd
CH3
N
N
15.394
7.962
7.940
7.877
7.857
7.846
7.831
7.810
7.692
7.671
7.437
7.420
7.404
7.387
7.260
7.235
7.215
7.197
7.188
7.167
7.149
7.041
7.020
6.994
6.973
2.606
2.580
2.552
2.533
2.452
2.420
2.308
2.283
2.261
2.167
2.153
2.143
2.130
1.847
1.555
0.204
-0.003

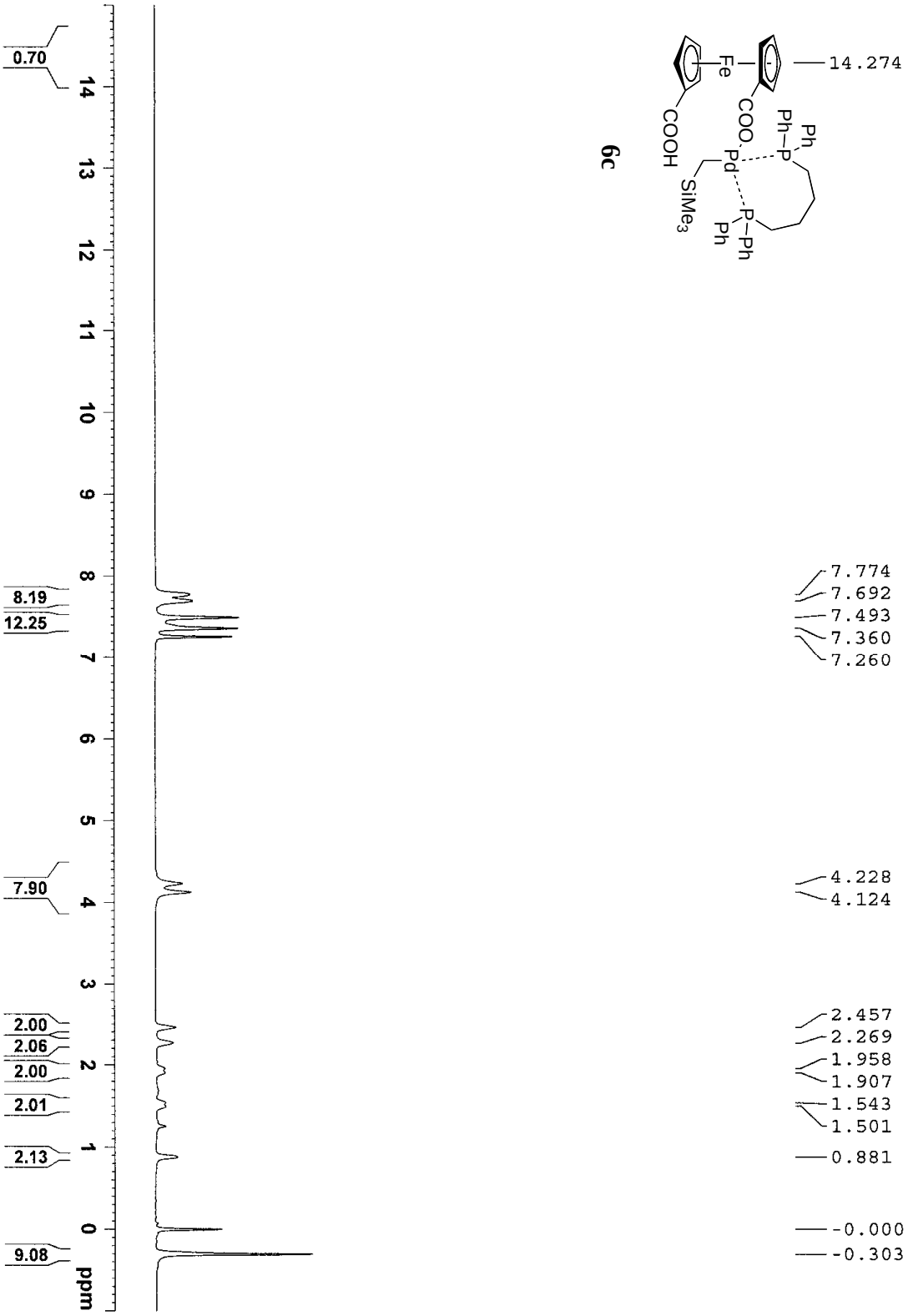


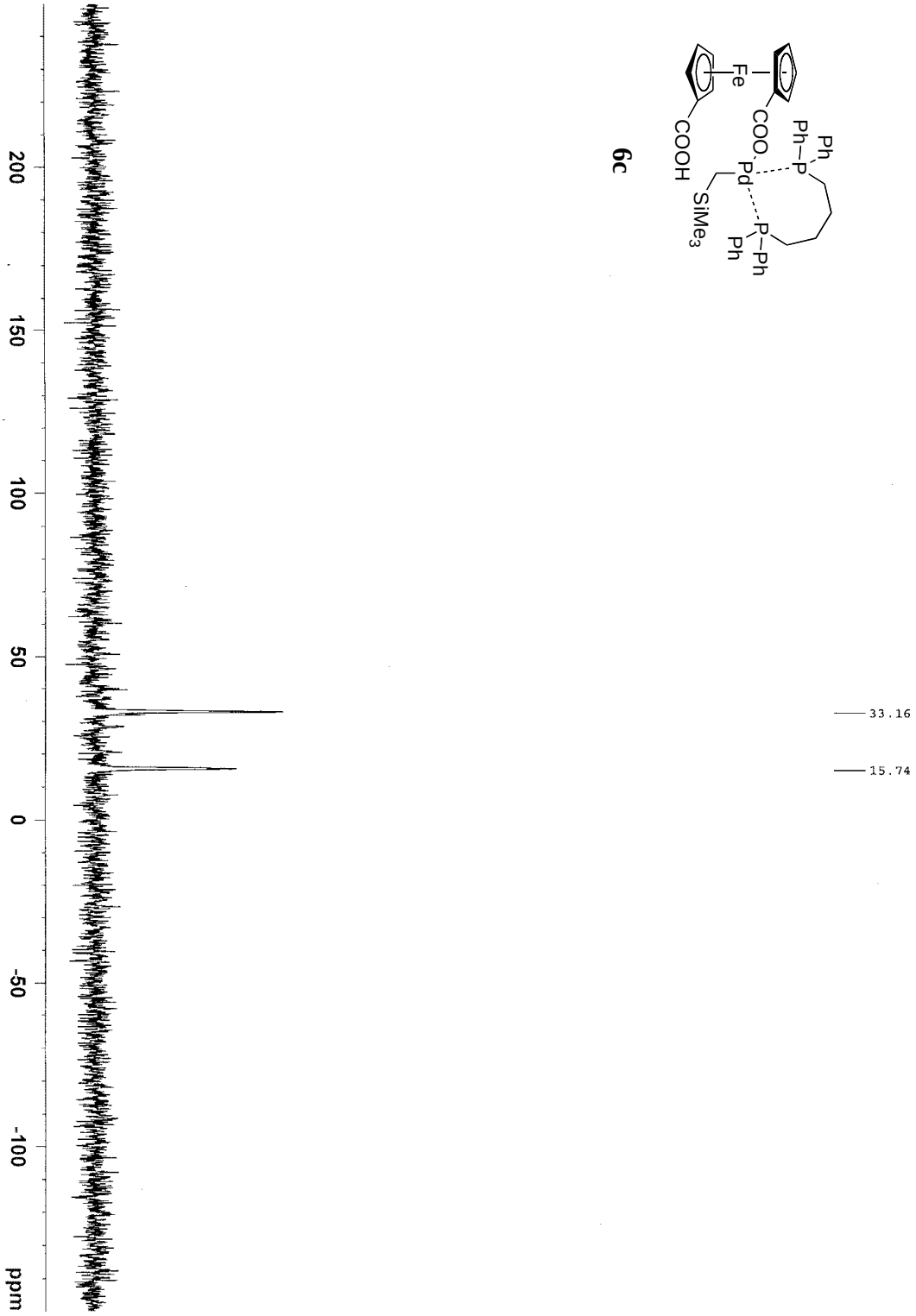

0.61
2.04
2.07
1.97
2.06
2.05
2.01
2.00
0.99
0.98
4.05
4.03
1.15
0.99
9.05
ppm

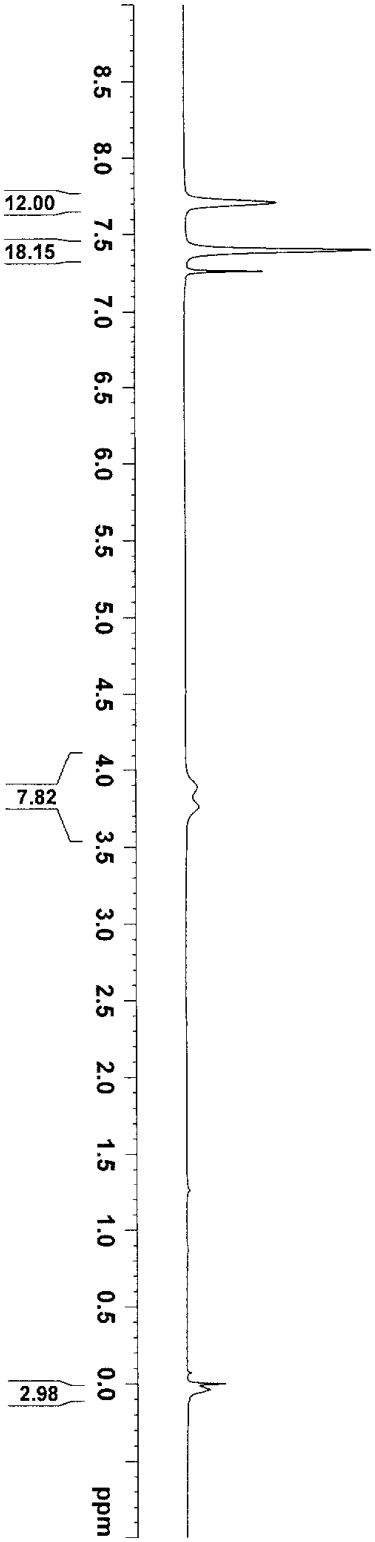

COO
COOH
Pd(cod)
SiMe3

6b

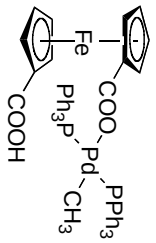

6b
COOH
COO
Pd(cod)
SiMe3
174.22
134.89
134.14
133.41
132.85
128.76
128.08
127.29
127.03
126.97
124.40
122.39
122.17
96.60
96.42
77.55
77.23
76.91
30.95
30.80
27.16
27.15
26.70
1.63
ppm


0.70
8.19
12.25
7.90
2.00
2.06
2.00
2.01
2.13
9.08
ppm
6c
Fe
COOH
COO
Pd
SiMe3
Ph
Ph–P
P–Ph
Ph
14.274
7.774
7.692
7.493
7.360
7.260
4.228
4.124
2.457
2.269
1.958
1.907
1.543
1.501
0.881
-0.000
-0.303


200
150
100
50
0
-50
-100
ppm
6c
Fe
COO
Pd
Ph
Ph–P
P–Ph
Ph
COOH
SiMe3
33.16
15.74



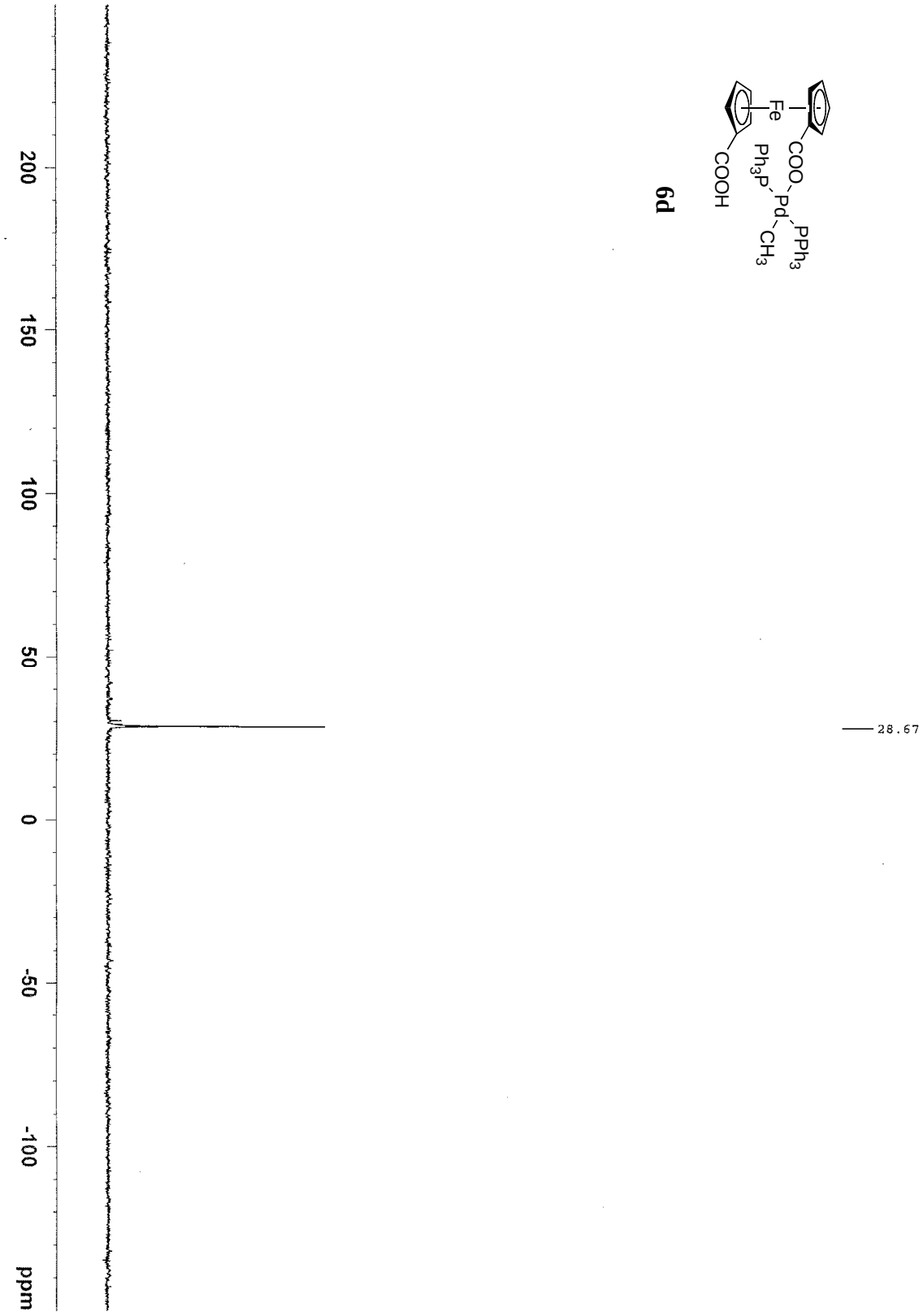
6d



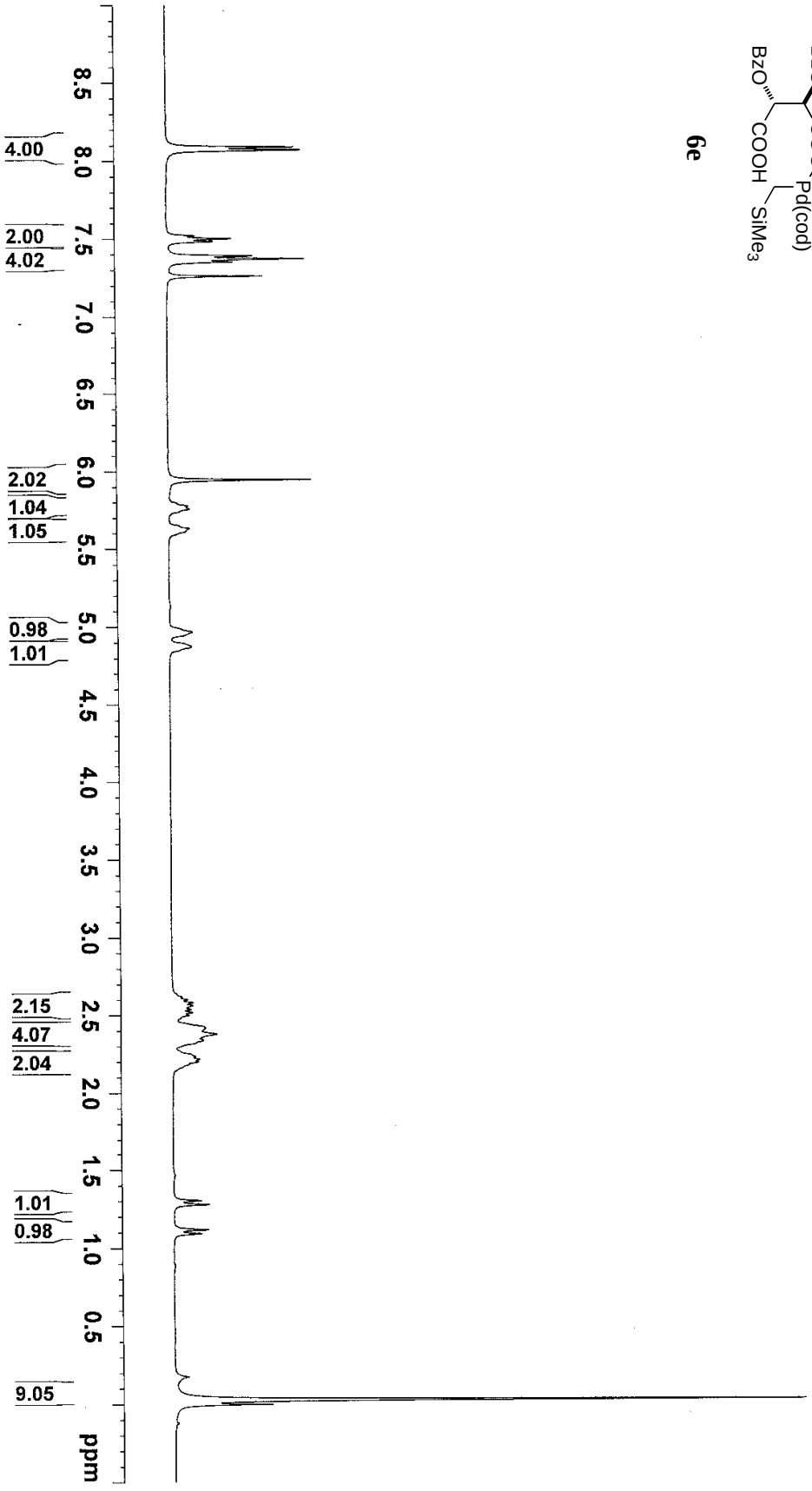
7.705
7.398
7.260

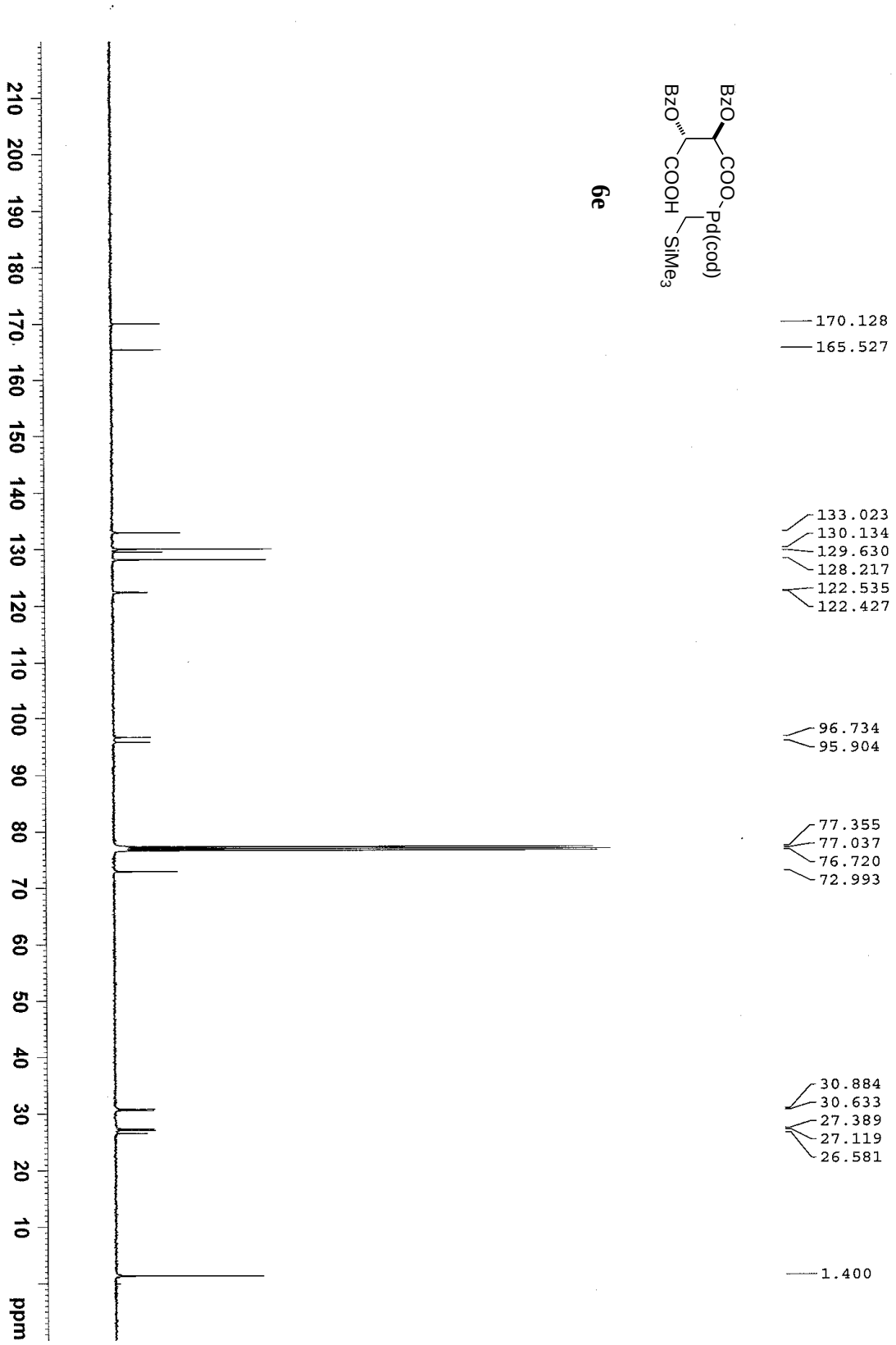
3.886
3.766

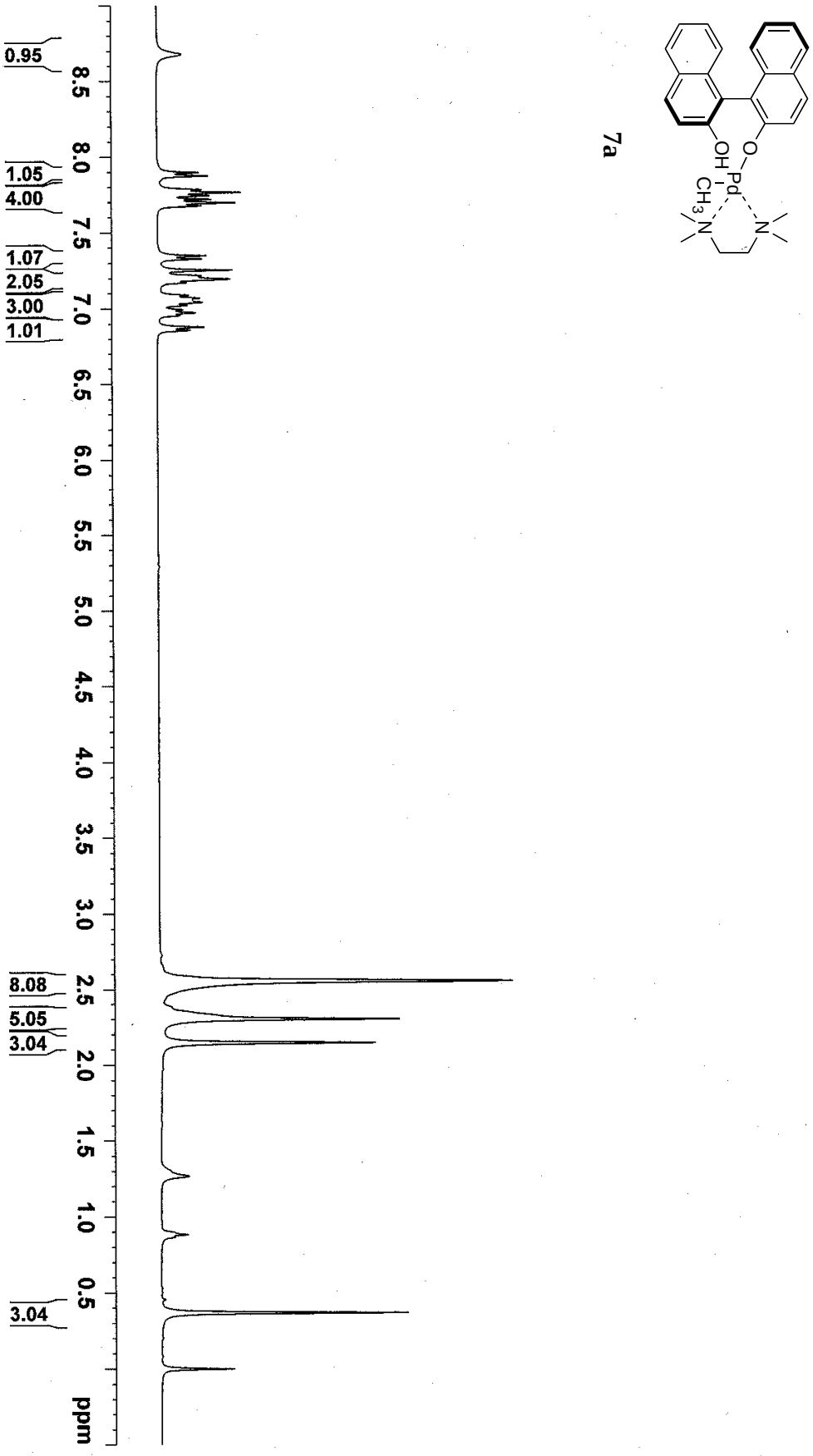
0.002
-0.037

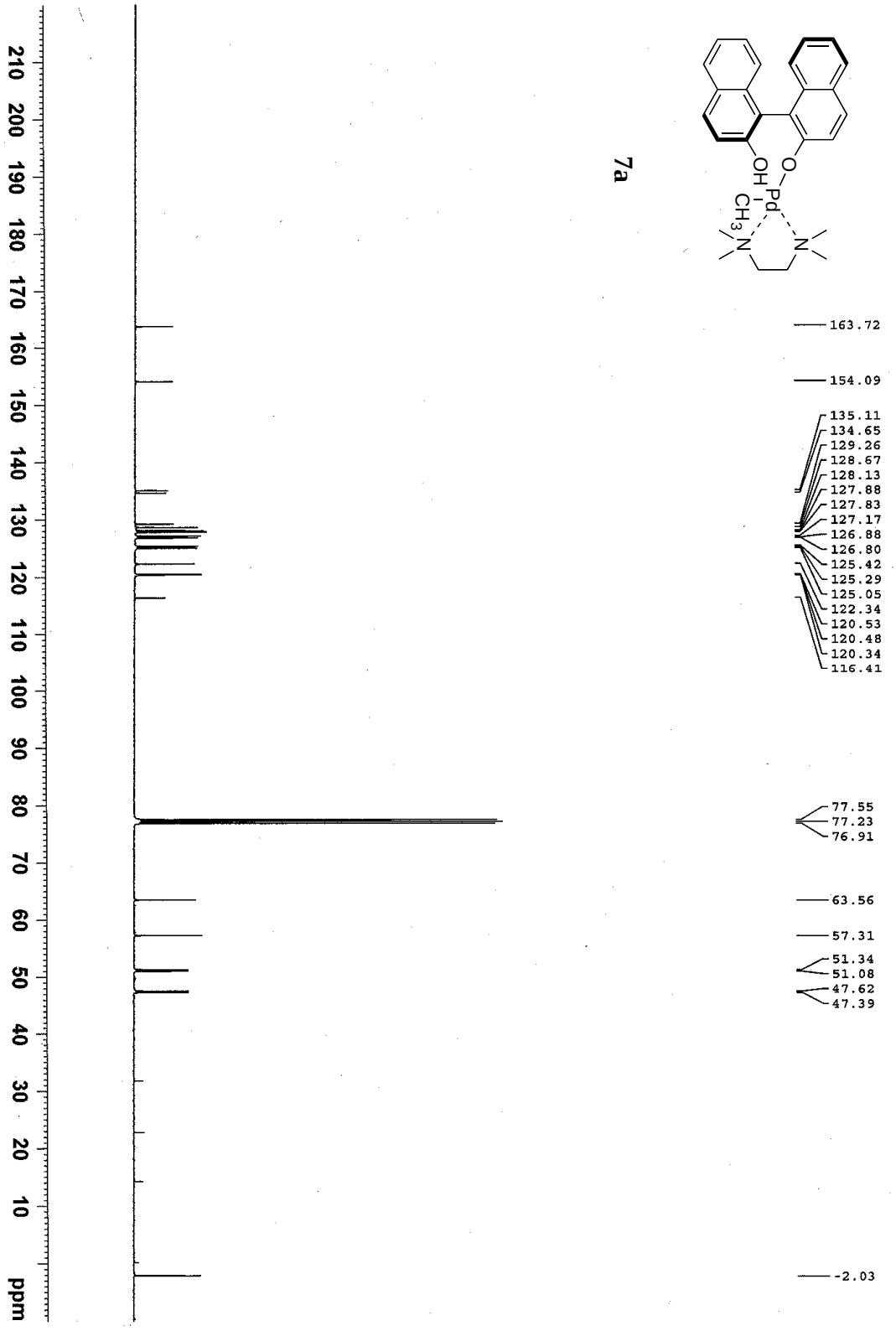


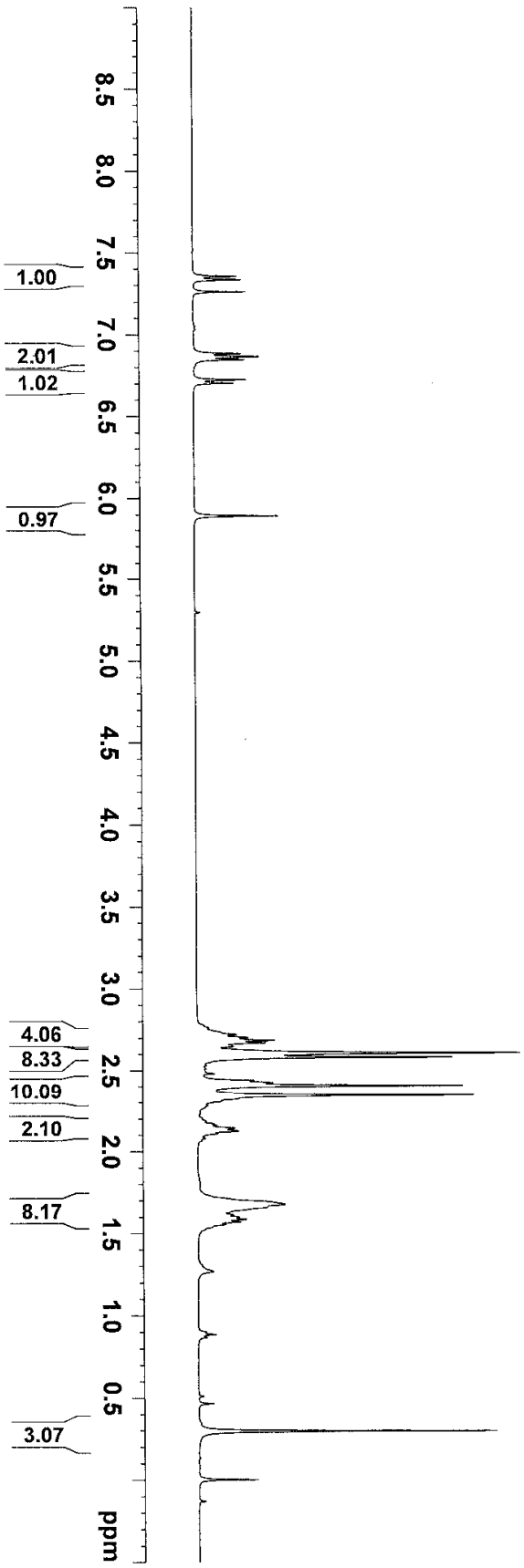
6d

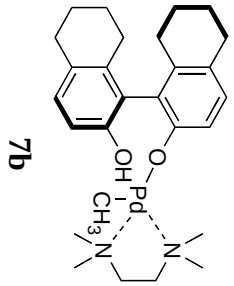



6e
BzO
COO
Pd(cod)
BzO
COOH
SiMe3
170.128
165.527
133.023
130.134
129.630
128.217
122.535
122.427
96.734
95.904
77.355
77.037
76.720
72.993
30.884
30.633
27.389
27.119
26.581
1.400
ppm

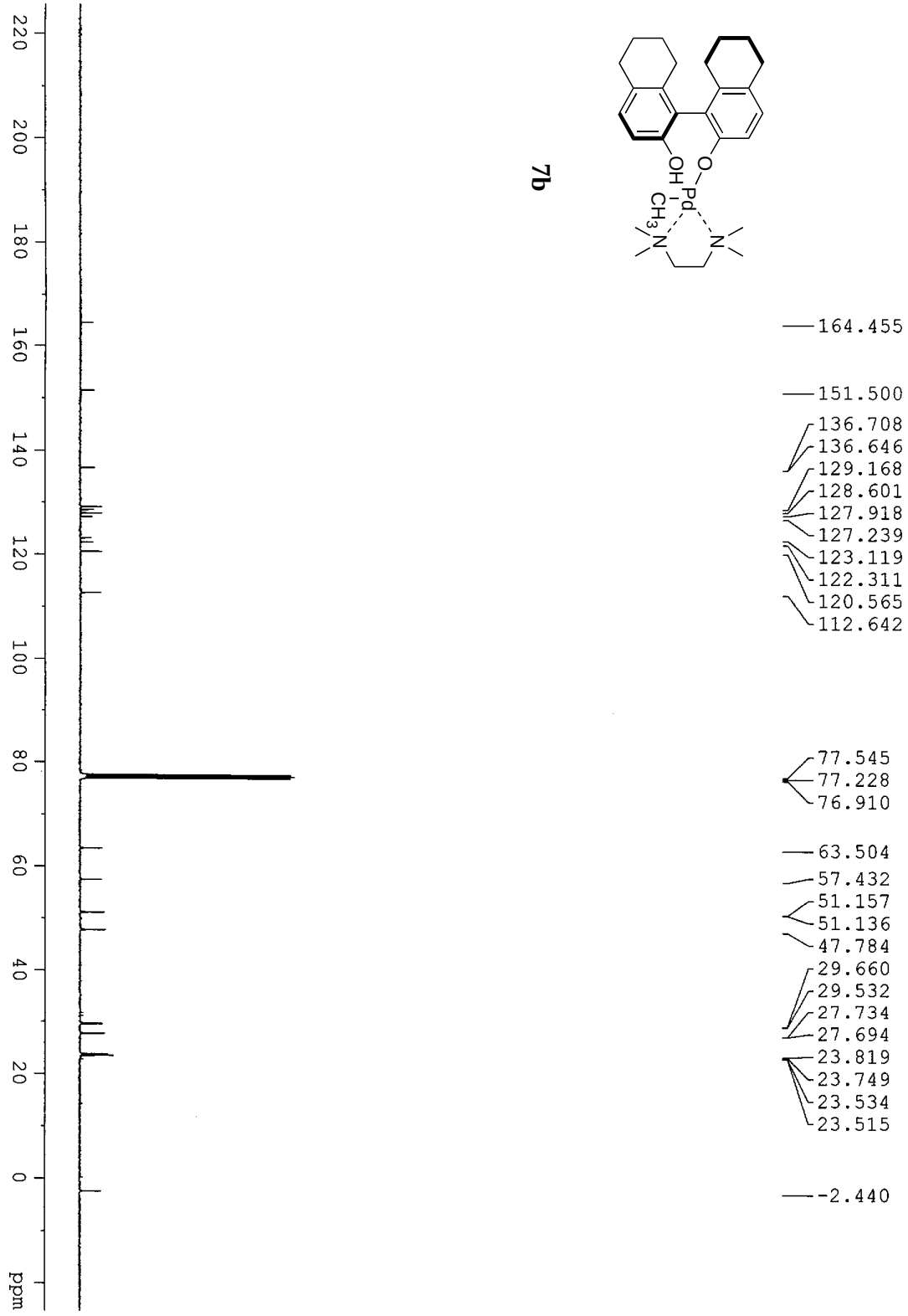


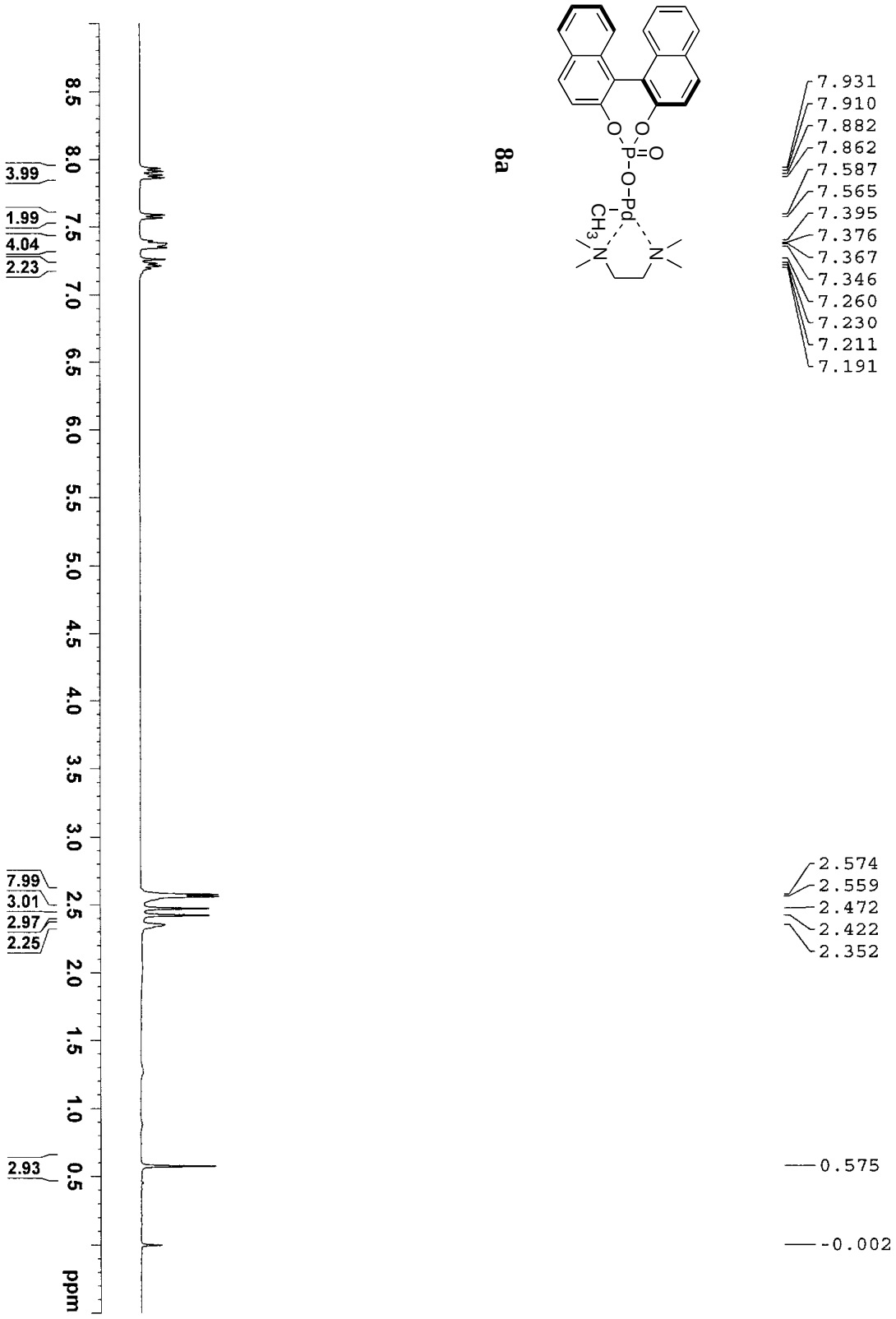


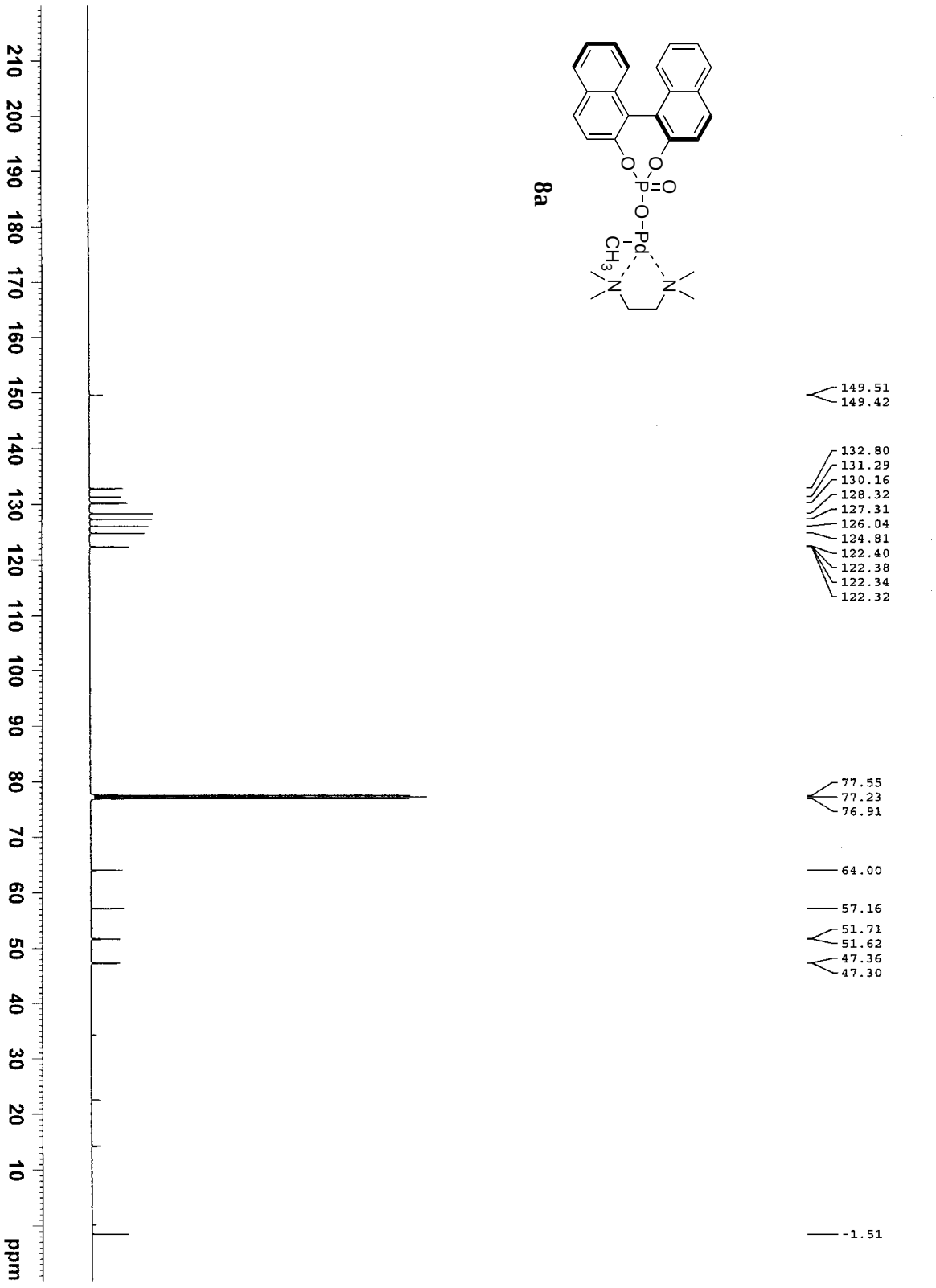


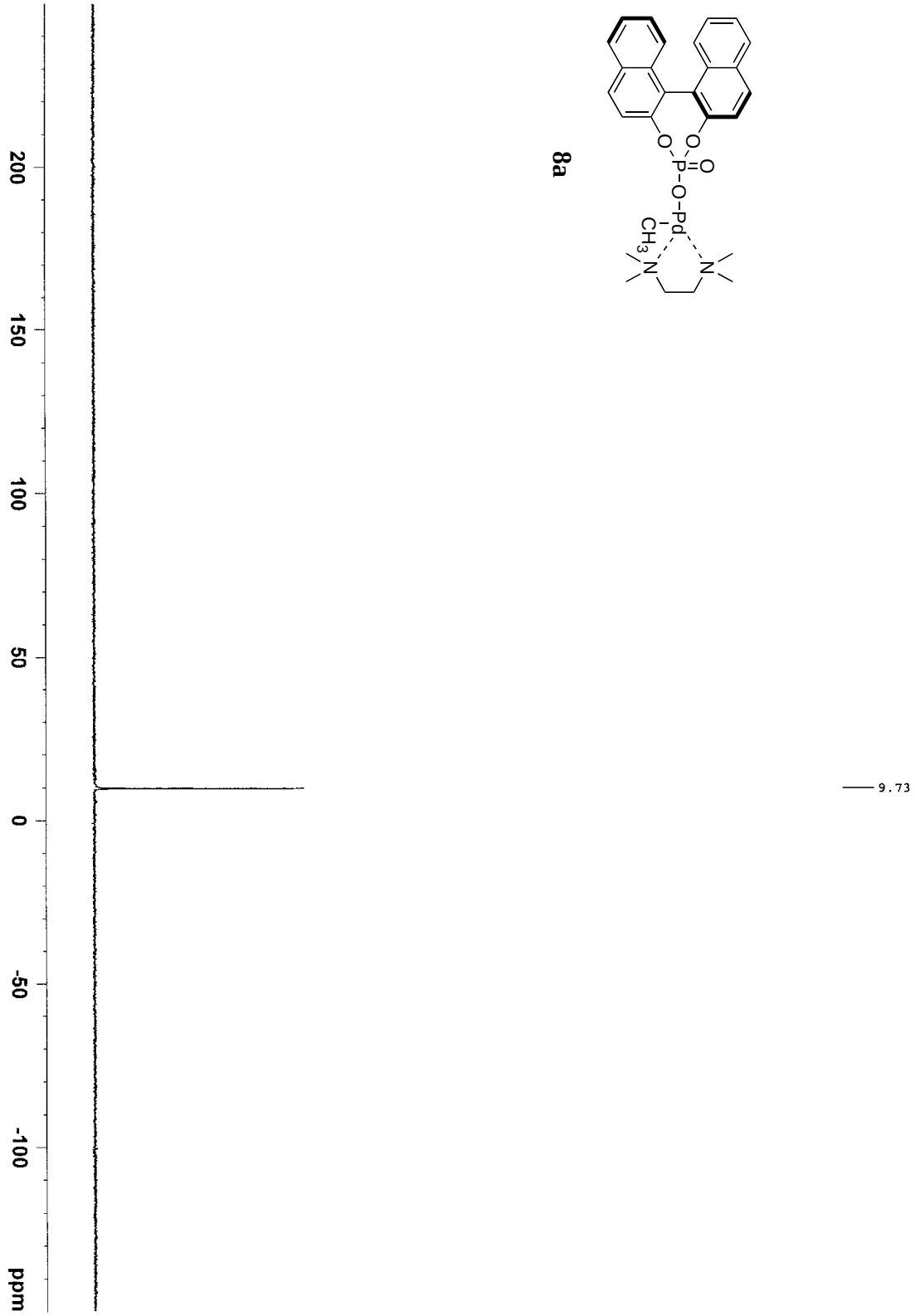


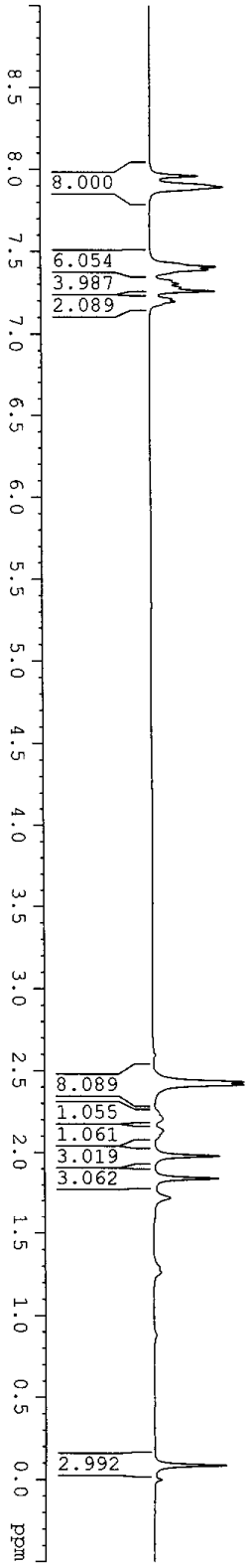
7b


7b
OH
O
Pd
I
CH3
N
N
164.455
151.500
136.708
136.646
129.168
128.601
127.918
127.239
123.119
122.311
120.565
112.642
77.545
77.228
76.910
63.504
57.432
51.157
51.136
47.784
29.660
29.532
27.734
27.694
23.819
23.749
23.534
23.515
-2.440
220
200
180
160
140
120
100
80
60
40
20
0
ppm

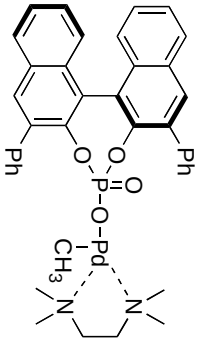





8a
9.73
200
150
100
50
0
-50
-100
ppm



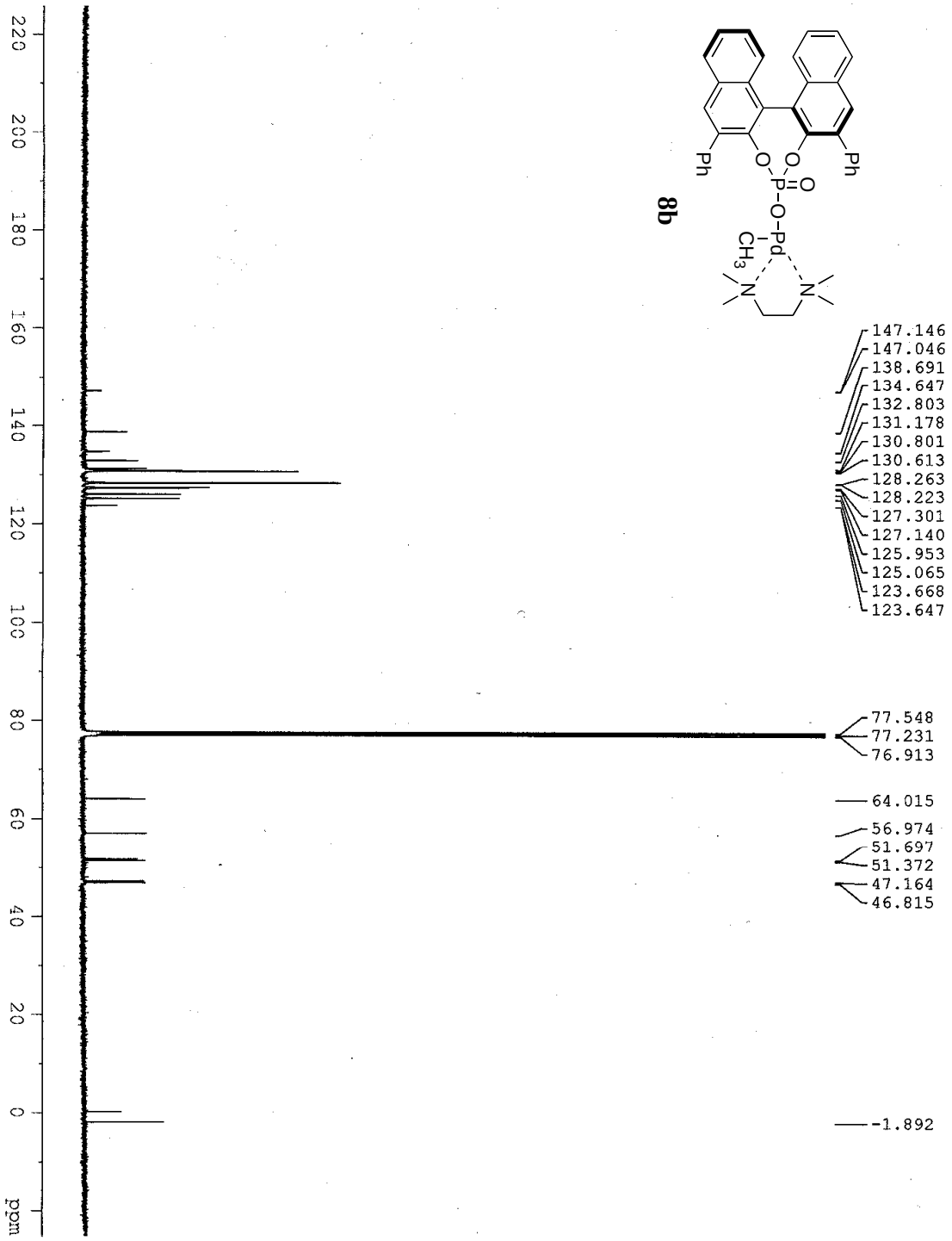
8b

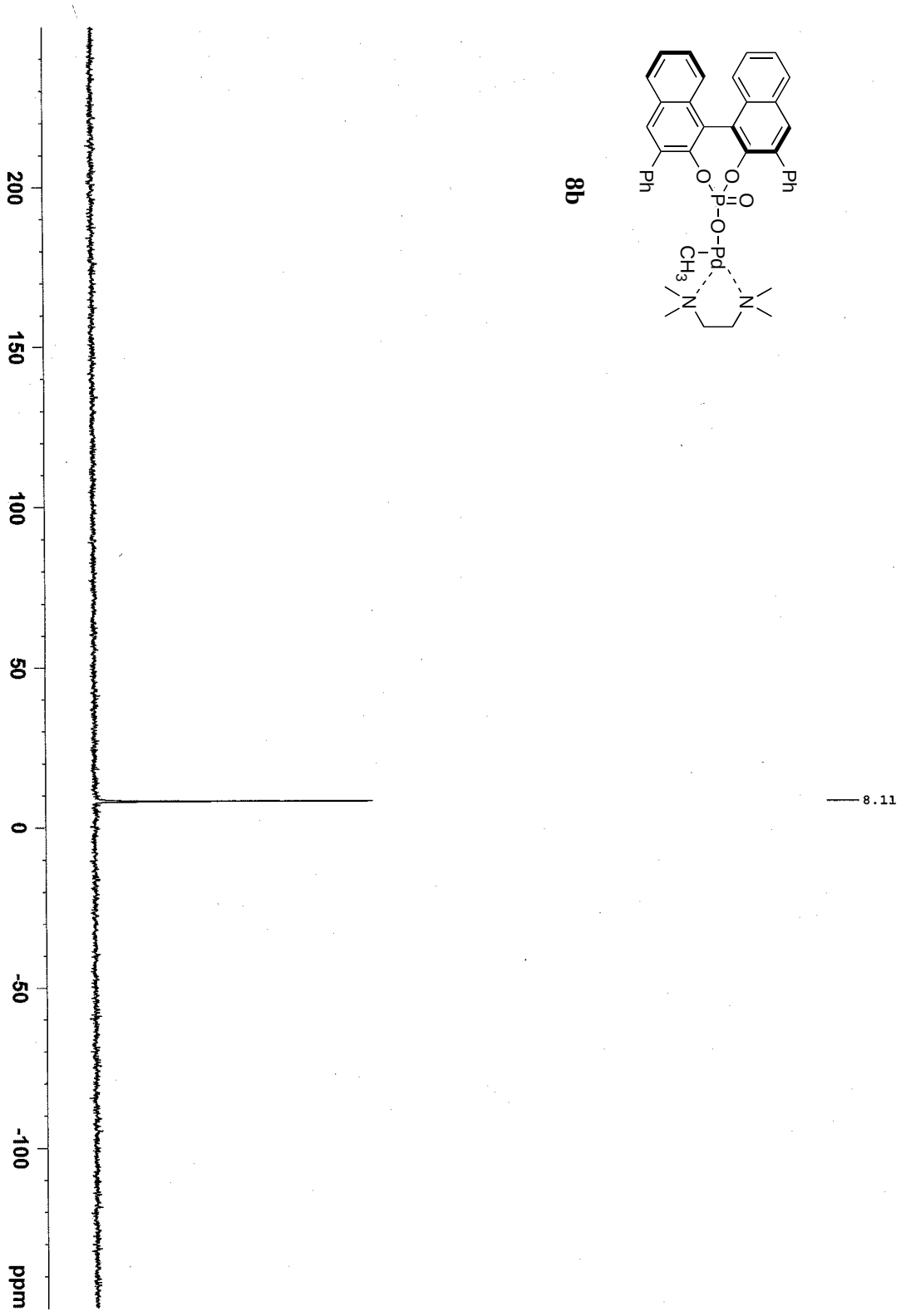


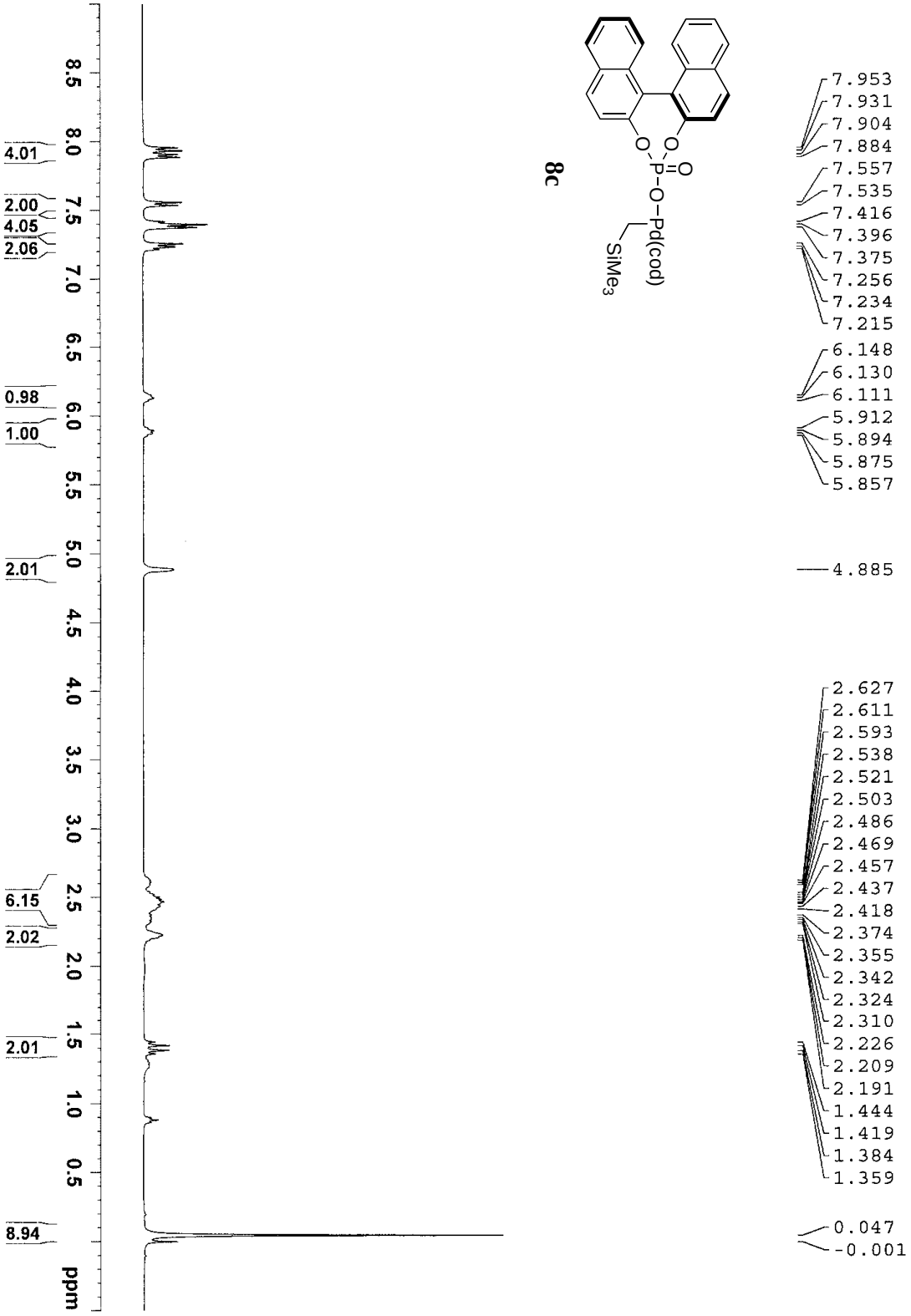
7.960
7.893
7.406
7.389
7.321
7.304
7.281
7.260
7.212
7.196

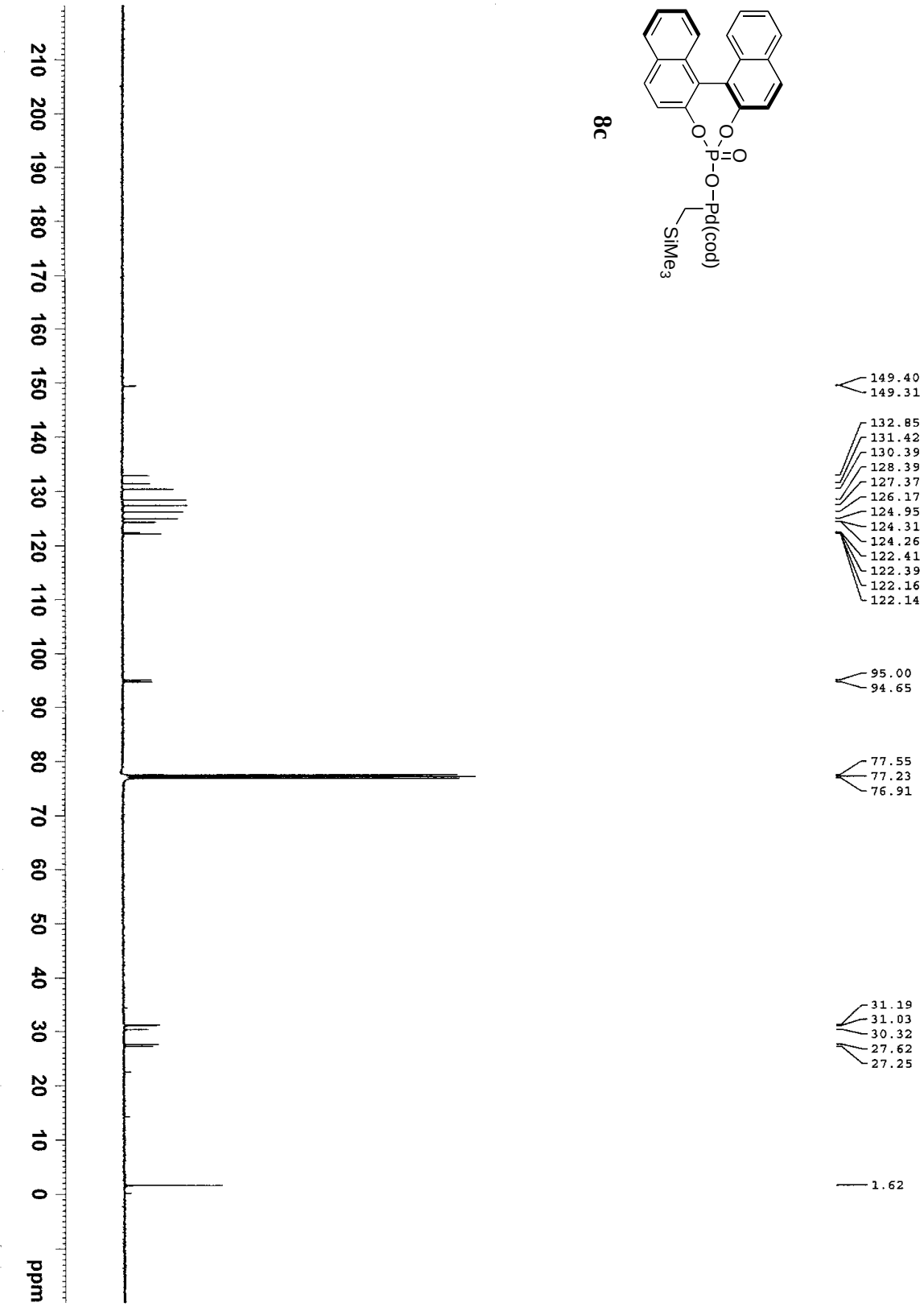
2.432
2.415
2.207
2.133
1.978
1.840

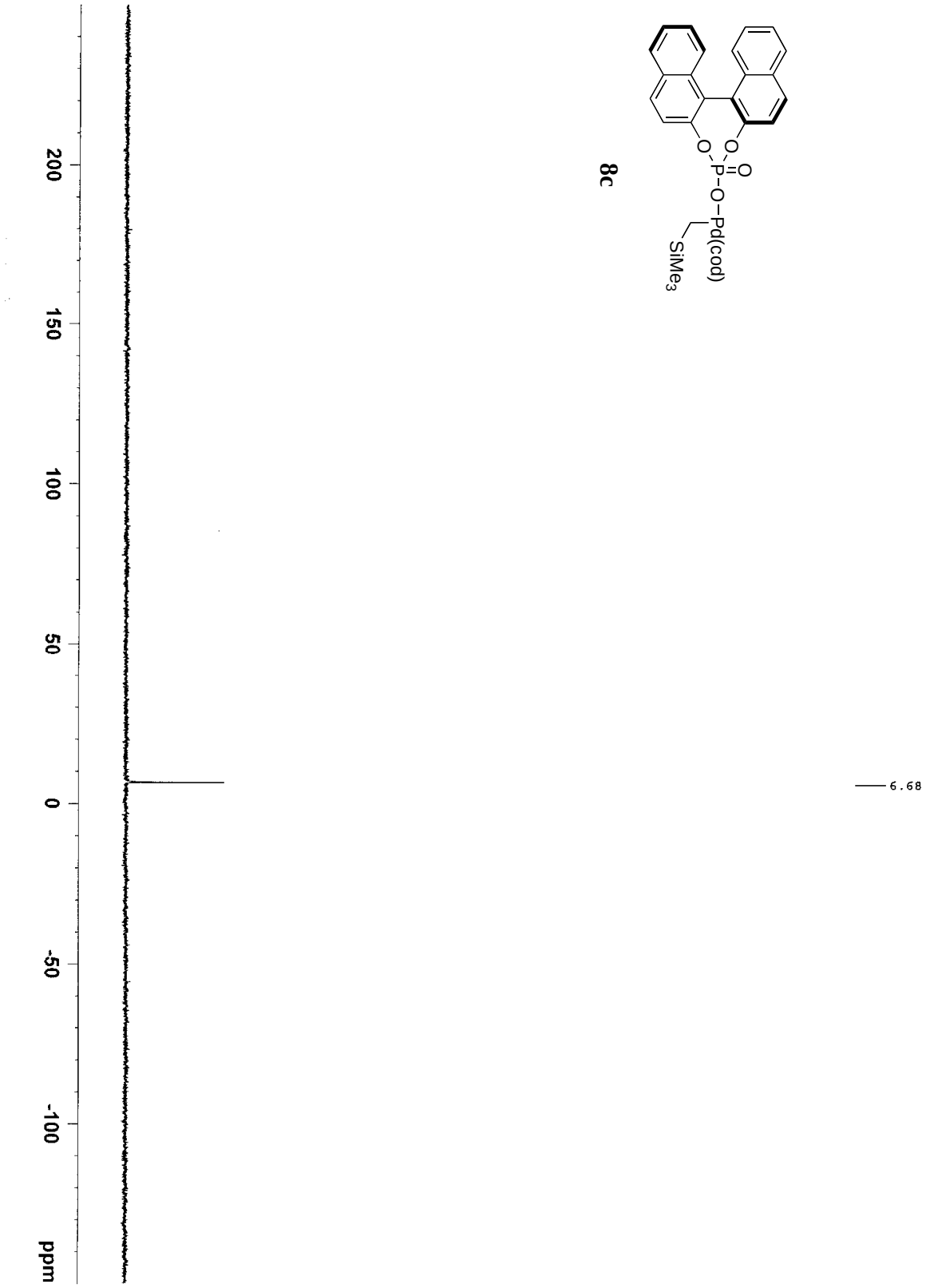
0.088
-0.000

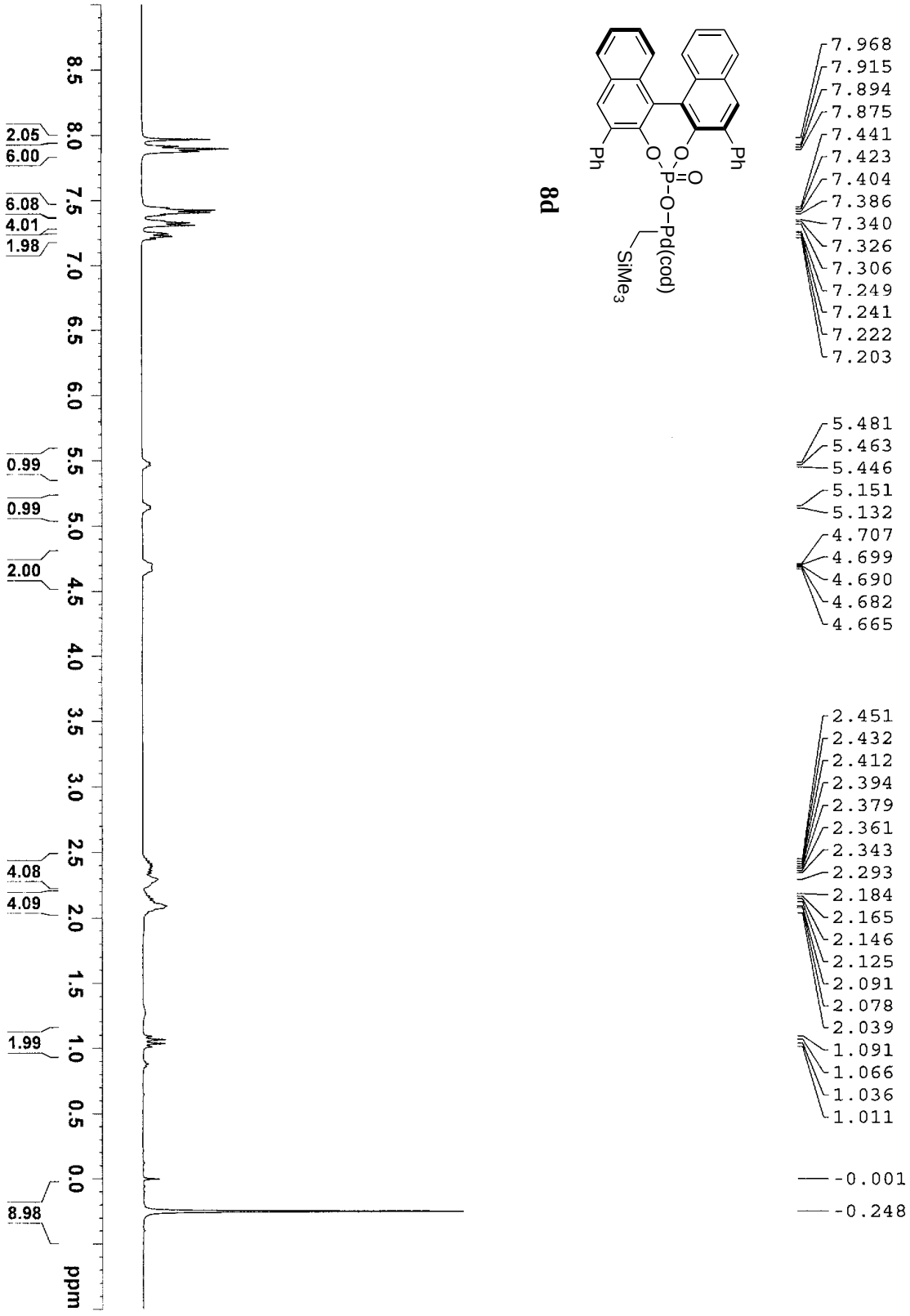


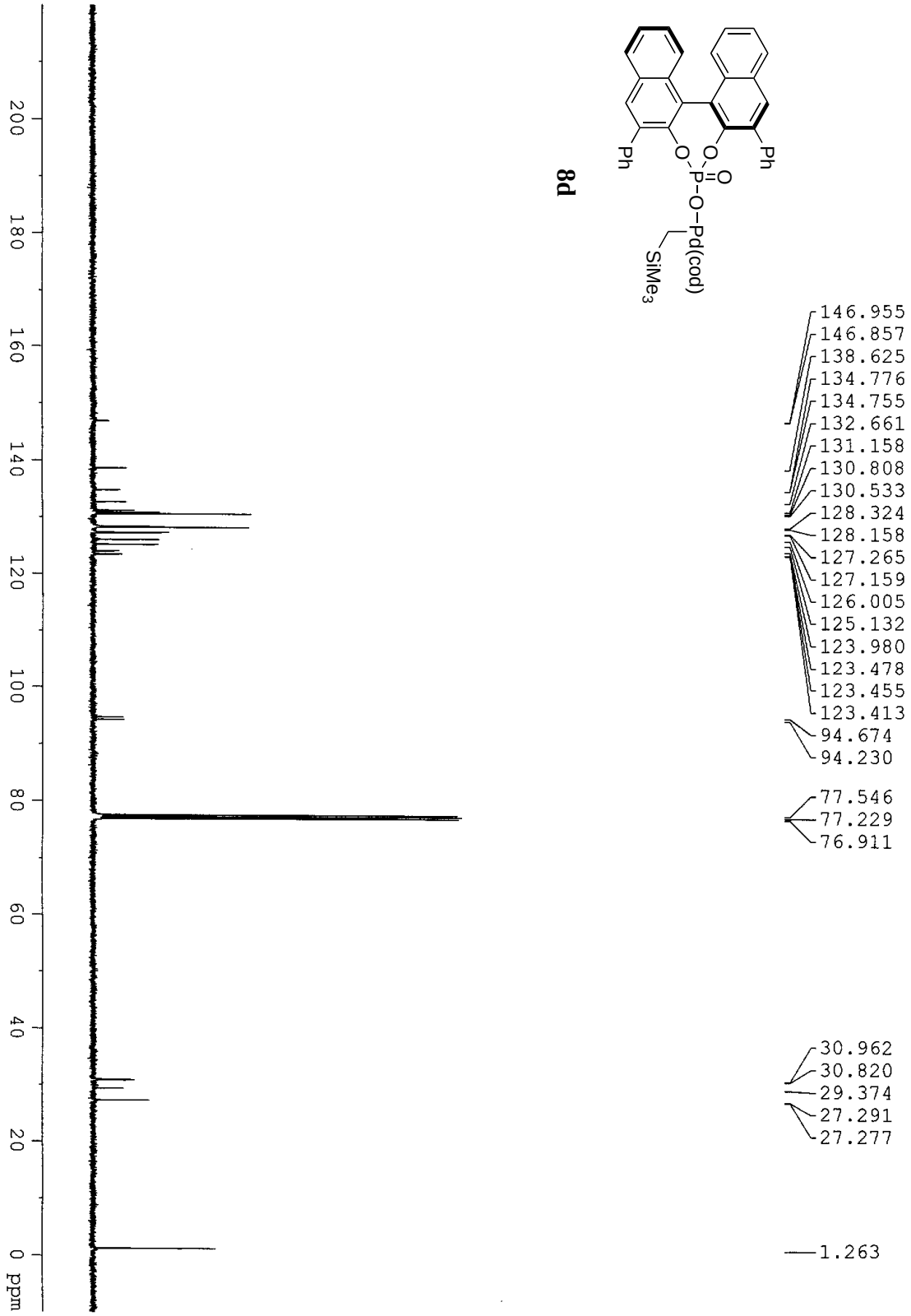



8c
SiMe3
Pd(cod)
7.953
7.931
7.904
7.884
7.557
7.535
7.416
7.396
7.375
7.256
7.234
7.215
6.148
6.130
6.111
5.912
5.894
5.875
5.857
4.885
2.627
2.611
2.593
2.538
2.521
2.503
2.486
2.469
2.457
2.437
2.418
2.374
2.355
2.342
2.324
2.310
2.226
2.209
2.191
1.444
1.419
1.384
1.359
0.047
-0.001
4.01
2.00
4.05
2.06
0.98
1.00
2.01
6.15
2.02
2.01
8.94
ppm


8c
O
O
P=O
O
Pd(cod)
SiMe3
149.40
149.31
132.85
131.42
130.39
128.39
127.37
126.17
124.95
124.31
124.26
122.41
122.39
122.16
122.14
95.00
94.65
77.55
77.23
76.91
31.19
31.03
30.32
27.62
27.25
1.62
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm






8d
Ph
Ph
O
O
O
P
O
Pd(cod)
SiMe3
146.955
146.857
138.625
134.776
134.755
132.661
131.158
130.808
130.533
128.324
128.158
127.265
127.159
126.005
125.132
123.980
123.478
123.455
123.413
94.674
94.230
77.546
77.229
76.911
30.962
30.820
29.374
27.291
27.277
1.263
200
180
160
140
120
100
80
60
40
20
0 ppm