Electronic Supplementary Information for Dalton Transactions

Regioselective functionalization of iminophosphoranes through Pd-mediated C-H bond activation: C-C and C-X bond formation.

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Electronic Supplementary Information

[(*p*-tol)$_3$P=N-1-C$_{10}$H$_7$] (2)

To a solution of 1-naphthylazide (0.501 g, 2.96 mmol) in dry CH_2Cl_2 (20 mL), a solution of P(*p*-tol)$_3$ (0.901 g, 2.96 mmol) in CH_2Cl_2 (25 mL) was added dropwise. The mixture was stirred at room temperature until N_2 evolution ceased (about 2 h), then the solvent was evaporated to a small volume (≈ 1-2 mL). By addition of Et_2O (15 mL) and subsequent stirring, **2** was obtained as a pale pink solid, which was filtered, washed with additional Et_2O (10 mL) and vacuum dried. Obtained: 0.75 g (57% yield). Anal. Calc. for [$C_{31}H_{28}NP$] (445.6): C, 83.57; H, 6.33; N, 3.14. Found: C, 83.02; H, 6.15; N, 3.03. IR: 1346 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 445 (75 %) $[M]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = 4.00. ^1H NMR ($CDCl_3$): δ = 2.42 (s, 9H, Me), 6.48 (d, 1H, H_2, $C_{10}H_7$, $^3J_{HH}$ = 7.4), 7.04 (t, 1H, H_3, $C_{10}H_7$, $^3J_{HH}$ = 7.6), 7.16 (d, 1H, H_4, $C_{10}H_7$, $^3J_{HH}$ = 8.0), 7.28 (m, 6H, H_m, P(*p*-tol)$_3$), 7.41-7.49 (m, 2H, H_6 + H_7, $C_{10}H_7$), 7.73-7.79 (m, 7H, H_5, $C_{10}H_7$ + H_o, P(*p*-tol)$_3$), 8.95 (dd, 1H, H_8, $C_{10}H_7$, $^3J_{HH}$ = 8.5, $^4J_{HH}$ = 1.4).

[PhMe$_2$P=N-C$_{10}$H$_7$-1] (3)

Compound **3** was obtained following a synthetic method similar to that described for **2**. 1-naphthylazide (1.370 g, 8.10 mmol) in dry CH_2Cl_2 (30 mL) reacted with a solution of $PPhMe_2$ (1.19 mL, 8.10 mmol) in CH_2Cl_2 (30 mL) to give **3** as a red solid. Obtained: 1.63 g (72% yield). Anal. Calc. for [$C_{18}H_{18}NP$] (279.3): C, 77.40; H, 6.50; N, 5.01. Found: C, 77.20; H, 6.31; N, 4.93. IR: 1337 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 279 (70 %) $[M]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = 7.65. ^1H NMR ($CDCl_3$): δ = 1.83 (d, 6H, PMe_2, $^2J_{HP}$ = 12.7), 6.31 (d, 1H, H_2, $C_{10}H_7$, $^3J_{HH}$ = 7.2), 7.02 (t, 1H, H_3, $C_{10}H_7$, $^3J_{HH}$ = 8.0), 7.09 (d, 1H, H_4, $C_{10}H_7$, $^3J_{HH}$ = 8.0), 7.32 (m, 2H, H_6 + H_7, $C_{10}H_7$,), 7.35-7.45 (m, 3H, H_m + H_p, PPh), 7.63 (dd, 1H, H_5, $C_{10}H_7$, $^3J_{HH}$ = 6.0, $^4J_{HH}$ = 3.2), 7.69 (m, 2H, H_o, PPh), 8.60 (dd, 1H, H_8, $C_{10}H_7$, $^3J_{HH}$ = 6.3, $^4J_{HH}$ = 3.3). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 15.82 (d, Me, PMe_2, $^1J_{PC}$ = 71.7), 113.61 (d, C_2, $C_{10}H_7$, $^3J_{PC}$ = 13.2), 116.71 (s, C_4, $C_{10}H_7$), 123.90 (s, $C_{10}H_7$), 125.12 (s, C_8, $C_{10}H_7$), 125.61 (s, $C_{10}H_7$), 126.25 (s, C_3, $C_{10}H_7$), 127.44 (s, C_5, $C_{10}H_7$), 128.98 (d, C_m, PPh, $^3J_{PC}$ = 11.3), 130.41 (d, C_o, PPh, $^2J_{PC}$ = 9.4), 131.64 (d, C_p, PPh, $^4J_{PC}$ = 2.8), 131.69 (d, C_{8a}, $C_{10}H_7$, $^3J_{PC}$ = 22.1), 132.91 (d, C_i, PPh, $^1J_{PC}$ = 87.3), 135.10 (d, C_{4a}, $C_{10}H_7$, $^4J_{PC}$ = 2.3), 148.78 (d, C_1, $C_{10}H_7$, $^2J_{PC}$ = 2.3).

[MePh$_2$P=N-C$_{10}$H$_7$-1] (4)

Compound **4** was obtained following a synthetic method similar to that described for **2**. 1-naphthylazide (0.560 g, 3.31 mmol) in dry CH_2Cl_2 (20 mL) reacted with a solution of PPh_2Me (0.63

mL, 3.31 mmol) in CH_2Cl_2 (20 mL) to give **4** as a pink solid. Obtained: 0.803 g (71% yield). Anal. Calc. for [$C_{23}H_{20}NP$] (341.4): C, 80.92; H, 5.90; N, 4.10. Found: C, 80.25; H, 5.50; N, 3.98. IR: 1340 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 341 (90 %) $[M]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = 4.40. ^1H NMR ($CDCl_3$): δ = 2.08 (d, 3H, PMe, $^2J_{HP}$ = 12.6), 6.26 (d, 1H, H_2, $C_{10}H_7$, $^3J_{HH}$ = 7.7), 6.96 (t, 1H, H_3, $C_{10}H_7$, $^3J_{HH}$ = 7.7), 7.07 (d, 1H, H_4, $C_{10}H_7$, $^3J_{HH}$ = 8.0), 7.30-7.44 (m, 8H, H_6 + H_7, $C_{10}H_7$, + H_m+H_p, PPh_2), 7.63 (dd, 1H, H_5, $C_{10}H_7$, $^3J_{HH}$ = 7.0, $^4J_{HH}$ = 2.0), 7.76 (m, 4H, H_o, PPh_2), 8.75 (dd, 1H, H_8, $C_{10}H_7$, $^3J_{HH}$= 7.4, $^4J_{HH}$= 2.1). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 14.15 (d, Me, PMe, $^1J_{PC}$ = 67.4), 113.86 (d, C_2, $C_{10}H_7$, $^3J_{PC}$ = 12.6), 116.73 (s, $C_{10}H_7$), 123.91 (s, $C_{10}H_7$), 125.40 (s, $C_{10}H_7$), 125.65 (s, $C_{10}H_7$), 126.39 (s, $C_{10}H_7$), 127.53 (s, $C_{10}H_7$), 128.91 (d, C_m, PPh, $^3J_{PC}$ = 11.8), 131.36 (d, C_o, PPh, $^2J_{PC}$ = 9.5), 131.73 (d, C_p, PPh, $^4J_{PC}$ = 2.7), 132.13 (d, C_8, $C_{10}H_7$, $^3J_{PC}$ = 22.1), 132.28 (d, C_i, PPh, $^1J_{PC}$ = 98.7), 135.18 (d, C_4, $C_{10}H_7$, $^4J_{PC}$ = 2.2), 148.57 (d, C_1, $C_{10}H_7$, $^2J_{PC}$ = 2.1).

[Pd(acac-O-O')(C_6H_4-(PPh_2=N-$C_{10}H_7$-1)-2)-κ-C,N] (8)

A suspension of **5** (0.415 g, 0.38 mmol) in CH_2Cl_2 (20 mL) was treated with Tl(acac) (0.231 g, 0.76 mmol). The color of the mixture changes clearly, and a grey suspension was obtained in few minutes. After 1 h stirring at 25 ºC it was filtered through a celite pad, and the resulting solution was evaporated to dryness. The residue was treated with cold Et_2O (15 mL) and stirred vigorously, giving **8** as an orange solid. Obtained: 0.205 g (44% yield). Anal. Calc. for [$C_{33}H_{28}NO_2PPd$] (607.97): C, 65.19; H, 4.64; N, 2.30. Found: C, 64.90; H, 4.38; N, 1.99. IR: 1586 (ν_{CO}, acac), 1513 (ν_{CO}, acac), 1281 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 507 (85 %) $[M\text{-acac}]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = 47.80. ^1H NMR ($CDCl_3$): δ = 0.93 (s, 3H, Me, acac), 1.92 (s, 3H, Me, acac), 4.98 (s, 1H, CH, acac), 6.88 (ddd, 1H, $H_{2'}$, $C_{10}H_7$, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.4, $^4J_{HP}$ = 9.2), 6.97-7.02 (m, 2H, $H_{3'}$, $C_{10}H_7$ + H_3, C_6H_4), 7.07 (d, 1H, $H_{4'}$, $C_{10}H_7$, $^3J_{HH}$ = 7.3), 7.15 (m, 2H, H_m, PPh), 7.21-7.26 (m, 3H, $H_{6'}$ + $H_{7'}$, $C_{10}H_7$ + H_p, PPh), 7.30 (td, 1H, H_4, C_6H_4, $^3J_{HH}$ = 7.4, $^4J_{HH}$ = 1.1), 7.37 (d, 1H, H_6, C_6H_4, $^3J_{HH}$ = 7.5), 7.43-7.50 (m, 4H, H_o+ H_m, PPh), 7.53-7.59 (m, 2H, H_5, C_6H_4 + H_p, PPh), 7.72 (d, $H_{5'}$, $C_{10}H_7$, $^3J_{HH}$ = 7.9), 8.05 (m, 2H, H_o, PPh), 9.10 (dd, 1H, $H_{8'}$, $C_{10}H_7$, $^3J_{HH}$ = 6.6, $^5J_{HP}$ = 3.0). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 26.75, 27.38 (2s, 2Me, acac), 99.86 (s, CH, acac), 122.71 (d, $C_{4'}$, $C_{10}H_7$, $^3J_{PC}$ = 7.1), 123.49 (d, C_6, C_6H_4, $^3J_{PC}$ = 2.4), 124.08 (s, $C_{10}H_7$), 124.35 (d, C_3, C_6H_4, $^2J_{PC}$ = 14.4), 125.06 (d, $C_{3'}$, $C_{10}H_7$, $^4J_{PC}$ = 2.3), 125.16 (s, $C_{10}H_7$), 125.51 (s, $C_{8'}$, $C_{10}H_7$), 126.30 (C_i, PPh, $^1J_{PC}$ = 86.3), 127.14 (s, C_5, C_6H_4), 128.07 (d, $C_{2'}$, $C_{10}H_7$, $^3J_{PC}$ = 20.3), 128.52 (d, C_m, PPh, $^3J_{PC}$ = 11.6), 128.98 (d, C_m, PPh, $^3J_{PC}$ = 11.7), 130.06 (d, C_p, PPh, $^4J_{PC}$ = 3.8), 131.59 (C_i, PPh, $^1J_{PC}$ = 84.2), 132.41 (s, $C_{5'}$, $C_{10}H_7$), 132.50 (d, C_4, C_6H_4, $^3J_{PC}$ = 11.9), 132.65 (d, C_p, PPh, $^4J_{PC}$ = 2.7), 133.09 (d, d, C_o, PPh, $^2J_{PC}$ = 9.7), 133.26 (d, C_o, PPh, $^2J_{PC}$ = 10.0), 134.38 ($C_{4a'}$ + $C_{8a'}$, $C_{10}H_7$), 139.86 (d, C_2, C_6H_4,

$^{1}J_{PC}$ = 140.7), 143.22 (d, $C_{1'}$, $C_{10}H_7$, $^{2}J_{PC}$ = 3.9), 152.96 (d, C_1, C_6H_4, $^{2}J_{PC}$ = 21.2), 185.05, 188.05 (2s, 2CO, acac).

[Pd(acac-O,O')(C_6H_3(P(*p*-tol)$_2$=N$C_{10}H_7$-1)-2-Me-5)-κ-C,N] (9)

Complex **9** was obtained following a synthetic method similar to that described for **8**. **6** (0.122 g, 0.10 mmol) reacted with Tlacac (0.063 g, 0.21 mmol) in dry CH_2Cl_2 (15 mL) to give **9** as a yellow solid. Obtained: 0.06 g (46% yield). Anal. Calc. for [$C_{36}H_{34}NO_2PPd$] (650.05): C, 66.51; H, 5.27; N, 2.15. Found: C, 66.04; H, 5.03; N, 2.01. IR: 1581 (ν_{CO}, acac), 1522 (ν_{CO}, acac), 1286 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 550 (35%) [M-acac]$^{+}$. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$): δ = 47.21. ^{1}H NMR ($CDCl_3$): δ = 0.99 (s, 3H, Me, acac), 1.99 (s, 3H, Me, acac), 2.22 (s, 3H, Me, P(*p*-tol)), 2.37 (s, 3H, Me, P(*p*-tol)), 2.44 (s, 3H, Me, C_6H_3-*Me*), 5.04 (s, 1H, CH, acac), 6.83-6.90 (m, 2H, *C_6H_3*-Me), 7.06 (t, 1H, $H_{3'}$, $C_{10}H_7$, $^{3}J_{HH}$ = 7.8), 7.13 (d, 1H, $C_{10}H_7$, $^{3}J_{HH}$ = 7.4), 7.29-7.35 (m, 6H, 2H, $C_{10}H_7$ + H_m, P(*p*-tol)$_2$), 7.41-7.46 (m, 3H, 1H, $C_{10}H_7$ + H_o, P(*p*-tol)), 7.59 (s, 1H, H_6, *C_6H_3*-Me), 7.65 (dd, 1H, $H_{5'}$, $C_{10}H_7$, $^{3}J_{HH}$ = 6.8, $^{4}J_{HH}$ = 2.5), 7.98 (m, 2H, H_o, P(*p*-tol)), 9.27 (dd, 1H, $H_{8'}$, $C_{10}H_7$, $^{3}J_{HH}$ = 7.0, $^{4}J_{HH}$ = 2.4). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$): δ = 21.51, 21.67, 22.12 (3Me, P(*p*-tol)$_2$ + C_6H_3-*Me*), 26.68, 27.41 (2s, 2Me, acac), 99.70 (s, CH, acac), 122.39 (d, $C_{2'}$, $C_{10}H_7$, $^{3}J_{PC}$ = 7.2), 123.12 (d, $C_{10}H_7$, J_{PC} = 2.3), 123.91, 125.01, 125.05 (s, $C_{10}H_7$), 125.43 (d, C_4, *C_6H_3*-Me, $^{3}J_{PC}$ = 14.7), 125.66 (s, $C_{10}H_7$), 127.83 (d, C_3, *C_6H_3*-Me, $^{2}J_{PC}$ = 22.3), 128.14 (s, $C_{4a'}$, $C_{10}H_7$), 129.21 (d, C_m, P(*p*-tol), $^{3}J_{PC}$ = 12.0), 129.61 (d, C_m, P(*p*-tol), $^{3}J_{PC}$ = 12.1), 132.69 (d, C_6, *C_6H_3*-Me, $^{3}J_{PC}$ = 15.2), 133.12 (d, C_o, P(*p*-tol), $^{2}J_{PC}$ = 10.2), 133.27 (d, C_o, P(*p*-tol), $^{2}J_{PC}$ = 10.5), 134.37 (s, $C_{8a'}$, $C_{10}H_7$), 136.74 (d, C_2, *C_6H_3*-Me, $^{1}J_{PC}$ = 143.2), 140.15 (d, C_5, *C_6H_3*-Me, $^{4}J_{PC}$ = 3.2), 142.86 (d, C_p, P(*p*-tol), $^{4}J_{PC}$ = 2.9), 143.17 (d, C_p, P(*p*-tol), $^{4}J_{PC}$ = 2.8), 143.72 (d, $C_{1'}$, $C_{10}H_7$, $^{2}J_{PC}$ = 3.8), 151.97 (d, C_1, *C_6H_3*-Me, $^{2}J_{PC}$ = 21.4), 185.03, 187.97 (s, CO, acac). Peaks due to C_i [P(*p*-tol)$_2$] and to one C atom of the $C_{10}H_7$ rings were not observed.

[Pd(acac-O,O')($C_{10}H_6$-(N=PPhMe$_2$)-8)-κ-C,N] (10)

Complex **10** was obtained following a synthetic method similar to that described for **8**. **7** (0.317 g, 0.38 mmol) reacted with Tlacac (0.229 g, 0.75 mmol) in dry CH_2Cl_2 (15 mL) to give **10** as a yellow solid. Obtained: 0.173 g (47% yield). Anal. Calc. for [$C_{23}H_{24}NO_2PPd$] (483.84): C, 57.09; H, 5.00; N, 2.89. Found: C, 56.52; H, 4.73; N, 2.56. IR: 1583 (ν_{CO}, acac), 1520 (ν_{CO}, acac), 1279 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 483 (50 %) [M-H]$^{+}$. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$): δ = 33.49. ^{1}H NMR ($CDCl_3$): δ = 1.74 (s, 3H, Me, acac), 1.99 (s, 3H, Me, acac), 2.20 (d, 6H, Me, PMe_2, $^{2}J_{HP}$ = 12.8), 5.21 (s, 1H, CH, acac), 5.98 (d, 1H, H_7, $C_{10}H_6$, $^{3}J_{HH}$ = 7.4), 6.87 (t, 1H, H_6, $C_{10}H_6$, $^{3}J_{HH}$ = 7.6), 6.97 (d, 1H, H_5, $C_{10}H_6$, $^{3}J_{HH}$ = 7.0), 7.17 (t,

1H, H_3, $C_{10}H_6$, $^3J_{HH}$ = 7.2), 7.25 (dd, 1H, H_4, $C_{10}H_6$, $^3J_{HH}$ = 7.1, $^4J_{HH}$ = 0.9), 7.29 (d, 1H, H_2, $C_{10}H_6$, $^3J_{HH}$ = 8.0), 7.45 (m, 2H, H_m, PPh), 7.53 (m, 1H, H_p, PPh), 7.76 (m, 2H, H_o, PPh). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 15.32 (d, Me, $PPhMe_2$, $^1J_{PC}$ = 70.2), 27.93, 27.97 (2s, 2Me, acac), 99.51 (s, CH, acac), 110.69 (d, C_7, $C_{10}H_6$, $^3J_{PC}$ = 8.2), 118.34 (s, C_5, $C_{10}H_6$), 122.31 (s, C_2, $C_{10}H_6$), 124.76, 124.86, 124.97 (s, C_3 + C_4 + C_6, $C_{10}H_6$), 129.34 (d, C_m, PPh, $^3J_{PC}$ = 12.0), 130.36 (d, C_i, PPh, $^1J_{PC}$ = 89.8), 130.46 (d, C_o, PPh, $^2J_{PC}$ = 10.0), 132.62 (d, C_p, PPh, $^4J_{PC}$ = 2.9), 133.92 (d, C_{4a}, $C_{10}H_6$, $^4J_{PC}$ = 2.3), 142.59 (d, C_{8a}, $C_{10}H_6$, $^3J_{PC}$ = 15.7), 145.07 (s, C_1, $C_{10}H_6$), 153.48 (d, C_8, $C_{10}H_6$, $^2J_{PC}$ = 3.1), 186.97, 186.55 (2s, 2CO, acac).

[Pd(acac-O,O')($C_{10}H_6$-(N=PPh_2Me)-8)-κ-C,N] (12exo)

Complex **12exo** was obtained following a synthetic method similar to that described for **8**. Therefore, **11exo** (0.093 g, 0.10 mmol) reacted with Tl(acac) (0.058 g, 0.20 mmol) in dry CH_2Cl_2 (15 mL) to give **12exo** as a yellow solid. Obtained: 0.092 g (84% yield). Anal. Calc. for [$C_{28}H_{26}NO_2PPd$] (545.91): C, 61.60; H, 4.80; N, 2.57. Found: C, 61.93; H, 4.91; N, 2.65. IR: 1585 (ν_{CO}, acac), 1512 (ν_{CO}, acac), 1262 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 544 (35 %) $[M-H]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = 30.25. ^1H NMR ($CDCl_3$): δ = 1.49 (s, 3H, Me, acac), 2.03 (s, 3H, Me, acac), 2.60 (d, 3H, Me, PMe, $^2J_{HP}$ = 13.5), 5.17 (s, 1H, CH, acac), 5.75 (d, 1H, H_7, $C_{10}H_6$, $^3J_{HH}$ = 7.5), 6.69 (t, 1H, H_6, $C_{10}H_6$, $^3J_{HH}$ = 7.8), 6.98 (d, 1H, H_5, $C_{10}H_6$, $^3J_{HH}$ = 7.9), 7.21 (t, 1H, H_3, $C_{10}H_6$, $^3J_{HH}$ = 7.2), 7.34-7.36 (m, 2H, 1H, H_4+ H_2, $C_{10}H_6$), 7.51 (m, 4H, H_m, PPh_2), 7.61 (m, 2H, H_p, PPh_2), 7.80 (m, 4H, H_o, PPh_2).

NMR monitoring of the conversion of 13exo into 13endo

A solution of **13exo** (0.030 g, 0.03 mmol) was dissolved in 0.6 mL of toluene-d_8. Only one peak at about 35 ppm is observed, due to **13exo**. This solution was heated at 80 ºC. The progress of the reaction was followed by the decrease of the peak at 35 ppm and the appearance of a broad signal at about 48-49 ppm, due to **13endo**.

[$Ph_2PCH_2P(Ph_2)$=N-$C_{10}H_7$-1] (14)

Compound **14** was prepared following the same synthetic method as that reported for **2-4**. Therefore, 1-naphthylazide (0.345 g, 2.04 mmol) reacted with $Ph_2PCH_2PPh_2$ (0.784 g, 2.04 mmol) in dry CH_2Cl_2 (20 mL) to give **14** as a red solid. Obtained: 0.743 g (70.0% yield). Anal. Calc. for [$C_{35}H_{29}NP_2$] (525.57): C, 79.99; H, 5.56; N, 2.67. Found: C, 79.30; H, 5.10; N, 2.23. IR: 1349 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 526 (65 %) $[M]^+$. $^{31}P\{^1H\}$ NMR ($CDCl_3$): δ = -26.76 (d, $^2J_{PP}$ = 49.5, PPh_2), 6.1 (d, $^2J_{PP}$ = 49.5, $NPPh_2$). ^1H NMR ($CDCl_3$): δ = 3.25 (d, 2H, CH_2, $^2J_{HP}$ = 12.2), 6.14 (d, 1H, H_2, $C_{10}H_7$, $^3J_{HH}$ = 7.6), 6.84 (t, 1H, H_3, $C_{10}H_7$, $^3J_{HH}$ = 7.6), 7.01 (d, 1H, H_4, $C_{10}H_7$, $^3J_{HH}$ = 8.1), 7.03-7.10 (m, 6H, H_m + H_p, N=PPh_2), 7.19-7.35 (m, 10H, H_6 + H_7, $C_{10}H_7$, H_o, N=PPh_2 + H_m, PPh_2),

7.41 (m, 2H, H_p, PPh_2), 7.58 (d, 1H, H_5, $C_{10}H_7$, $^3J_{HH}$ = 7.9), 7.77 (m, 4H, H_o, PPh_2), 8.51 (d, 1H, H_8, $C_{10}H_7$, $^3J_{HH}$ = 8.5). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = 29.34 (dd, CH_2, $^1J_{PC}$ = 33.6, $^1J_{PC}$ = 71.1), 113.92 (d, C_2, $C_{10}H_7$, $^3J_{PC}$ = 12.4), 116.56 (s, C_4, $C_{10}H_7$), 123.59 (s, C_6, $C_{10}H_7$), 125.39 (s, C_8, $C_{10}H_7$), 125.75 (s, C_7, $C_{10}H_7$), 126.09 (s, C_3, $C_{10}H_7$), 127.19 (s, C_5, $C_{10}H_7$), 128.68-128.90 (solapados C_m, PPh_2 + C_m, PPh_2 + C_p, PPh_2), 131.27 (d, C_i, PPh_2, $^1J_{PC}$ = 102.6), 131.70 (d, C_p, PPh_2, $^4J_{PC}$ = 2.6), 132.05 (d, C_o, PPh_2, $^2J_{PC}$ = 9.2), 132.77 (d, C_o, PPh_2, $^2J_{PC}$ = 20.6), 144.99 (d, C_1, $C_{10}H_7$, $^2J_{PC}$ = 3.0). Peaks due to C_{4a} and C_{8a} ($C_{10}H_7$) or to C_i (PPh_2) were not observed.

[Pd(Cl)($C_{10}H_6$-(N=$PPh_2CH_2PPh_2$)-8)-κ-C,N,P] (15)

To a solution of **14** (0.180 g, 0.34 mmol) in dry toluene (20 mL), $Pd(OAc)_2$ (0.077 g, 0.34 mmol) was added, and the resulting solution was refluxed for 2h. After the reaction time, the cool solution was filtered to discard any remaining solid, and the resulting clear orange solution was evaporated to dryness. The orange residue was dissolved in MeOH (20 mL) and treated with anhydrous LiCl (0.058 g, 1.37 mmol), resulting in the formation of a yellow precipitate of **15**. This solid was filtered, washed with MeOH (5 mL) and Et_2O (10 mL) and recrystallized from $CHCl_3$ / Et_2O to give yellow crystals of **15**. Obtained: 0.095 g (42% yield). Anal. Calc. for [$C_{35}H_{28}ClNP_2Pd$] (666.42): C, 63.08; H, 4.23; N, 2.10. Found: C, 62.59; H, 4.09; N, 2.33. IR: 1293 ($\nu_{P=N}$) cm^{-1}. MS (FAB +): 666 (30 %) $[M]^+$. $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ = -3.34 (d, $^2J_{PP}$ = 35.6, PPh_2), 36.57 (d, $^2J_{PP}$ = 35.6, $NPPh_2$). ^1H NMR (CD_2Cl_2): δ = 3.57 (dd, 2H, CH_2, $^2J_{PH}$ = 6.8, $^2J_{HP}$ = 8.8), 5.85 (d, 1H, H_7, $C_{10}H_6$, $^3J_{HH}$ = 7.5), 6.67 (t, 1H, H_6, $C_{10}H_6$, $^3J_{HH}$ = 7.7), 7.01 (d, 1H, H_5, $C_{10}H_6$, $^3J_{HH}$ = 7.9), 7.19-7.30 (m, 7H, 1H, $C_{10}H_6$ + H_m + H_p, PPh_2), 7.34-7.40 (m, 5H, 1 H, $C_{10}H_6$ + H_m, PPh_2), 7.51 (m, 2H, H_p, PPh_2), 7.65 (m, 4H, H_o, PPh_2), 7.72-7.82 (m, 5H, 1H, $C_{10}H_6$ + H_o, PPh_2). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ = 39.29 (dd, CH_2, $^1J_{PC}$ = 6.0, $^1J_{PC}$ = 60.5), 112.93 (d, C_7, $C_{10}H_6$, $^3J_{PC}$ = 8.5), 120.89 (s, C_5, $C_{10}H_6$), 124.50 (s, $C_{10}H_6$), 125.08 (d, C_i, PPh_2, $^1J_{PC}$ = 90.1), 125.26 (s, $C_{10}H_6$), 126.68 (s, C_6, $C_{10}H_6$), 127.58 (d, C_i, PPh_2, $^1J_{PC}$ = 88.9), 130.61 (d, C_m, PPh_2, $^3J_{PC}$ = 11.9), 131.48 (d, C_m, PPh_2, $^3J_{PC}$ = 12.0), 132.68 (d, C_p, PPh_2, $^4J_{PC}$ = 2.8), 132.79 (s, $C_{10}H_6$), 135.74 (d, C_p, PPh_2, $^4J_{PC}$ = 2.7), 134.21 (d, C_o, PPh_2, $^2J_{PC}$ = 10.8), 135.19 (d, C_o, PPh_2, $^2J_{PC}$ = 10.5), 140.53 (s, C_1, $C_{10}H_6$), 145.38 (d, C_8, $C_{10}H_6$, $^2J_{PC}$ = 2.9).

Table S1. Crystal data and structure refinement for **13exo·2OEt$_2$**.

Empirical formula	C58 H64 N2 O6 P2 Pd2	
Formula weight	1159.85	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.3627(3) Å	α= 110.605(2)°.
	b = 19.7929(3) Å	β= 100.030(2)°.
	c = 20.9124(4) Å	γ = 96.153(2)°.
Volume	5387.30(17) Å^3	
Z	4	
Density (calculated)	1.430 Mg/m^3	
Absorption coefficient	0.778 mm^{-1}	
F(000)	2384	
Crystal size	0.42 x 0.37 x 0.19 mm^3	
Theta range for data collection	2.64 to 25.00°.	
Index ranges	-17<=h<=17, -23<=k<=20, -24<=l<=24	
Reflections collected	83766	
Independent reflections	18641 [R(int) = 0.0243]	
Completeness to theta = 25.00°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.863 and 0.778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18641 / 0 / 1276	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0299, wR2 = 0.0718	
R indices (all data)	R1 = 0.0438, wR2 = 0.0754	
Largest diff. peak and hole	0.463 and -0.591 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13exo·2OEt$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2941(1)	1524(1)	2919(1)	23(1)
Pd(2)	4446(1)	937(1)	2040(1)	18(1)
Pd(3)	1766(1)	3303(1)	6995(1)	21(1)
Pd(4)	505(1)	4094(1)	7992(1)	18(1)
P(1)	3467(1)	653(1)	4013(1)	19(1)
P(2)	2852(1)	-477(1)	810(1)	17(1)
P(3)	1340(1)	4181(1)	5897(1)	25(1)
P(4)	2245(1)	5456(1)	9144(1)	18(1)
N(1)	2709(2)	813(1)	3436(1)	21(1)
N(2)	3859(1)	-148(1)	1395(1)	19(1)
N(3)	2067(2)	3974(1)	6453(1)	25(1)
N(4)	1214(2)	5167(1)	8583(1)	20(1)
O(1)	3624(1)	1545(1)	1541(1)	25(1)
O(2)	2960(2)	2217(1)	2385(1)	34(1)
O(3)	5202(1)	1962(1)	2674(1)	29(1)
O(4)	4337(2)	2167(1)	3499(1)	32(1)
O(5)	1675(1)	2640(1)	7547(1)	27(1)
O(6)	1312(1)	3473(1)	8475(1)	26(1)
O(7)	280(1)	2773(1)	6496(1)	30(1)
O(8)	-377(1)	3104(1)	7435(1)	26(1)
C(101)	1571(2)	1150(2)	2497(1)	28(1)
C(102)	1004(2)	1351(2)	2021(2)	40(1)
C(103)	23(2)	1051(2)	1781(2)	56(1)
C(104)	-408(2)	556(2)	2011(2)	52(1)
C(105)	142(2)	341(2)	2507(2)	35(1)
C(106)	-245(2)	-151(2)	2789(2)	38(1)
C(107)	333(2)	-315(2)	3278(2)	32(1)
C(108)	1326(2)	-19(2)	3515(1)	26(1)
C(109)	1733(2)	459(2)	3254(1)	22(1)
C(110)	1141(2)	643(2)	2746(1)	26(1)
C(111)	3219(2)	1004(2)	4875(1)	21(1)
C(112)	3791(2)	928(2)	5451(1)	26(1)
C(113)	3621(2)	1245(2)	6113(1)	32(1)
C(114)	2891(2)	1646(2)	6212(1)	34(1)
C(115)	2332(2)	1733(2)	5649(2)	34(1)
C(116)	2492(2)	1413(2)	4980(1)	27(1)
C(117)	3520(2)	-313(2)	3745(1)	23(1)
C(118)	3653(2)	-655(2)	3070(2)	32(1)
C(119)	3770(2)	-1379(2)	2830(2)	39(1)
C(120)	3773(2)	-1764(2)	3262(2)	38(1)
C(121)	3642(2)	-1437(2)	3934(2)	33(1)
C(122)	3506(2)	-719(2)	4173(1)	26(1)
C(123)	4665(2)	1072(2)	4099(1)	27(1)
C(124)	5005(2)	2344(2)	3247(1)	27(1)
C(125)	5646(3)	3076(2)	3657(2)	47(1)
C(201)	5434(2)	475(2)	2405(1)	21(1)
C(202)	6264(2)	820(2)	2910(1)	28(1)
C(203)	6952(2)	416(2)	3081(2)	34(1)
C(204)	6810(2)	-329(2)	2751(2)	33(1)
C(205)	5971(2)	-719(2)	2220(1)	25(1)
C(206)	5782(2)	-1487(2)	1847(2)	31(1)
C(207)	4972(2)	-1809(2)	1330(2)	28(1)
C(208)	4300(2)	-1398(2)	1148(1)	24(1)

C(209)	4450(2)	-646(2)	1508(1)	19(1)
C(210)	5293(2)	-300(2)	2052(1)	20(1)
C(211)	3034(2)	-856(1)	-69(1)	19(1)
C(212)	3954(2)	-743(2)	-182(1)	24(1)
C(213)	4093(2)	-977(2)	-859(2)	30(1)
C(214)	3326(2)	-1326(2)	-1426(1)	30(1)
C(215)	2411(2)	-1439(2)	-1322(1)	32(1)
C(216)	2260(2)	-1199(2)	-647(1)	26(1)
C(217)	2099(2)	-1162(1)	971(1)	18(1)
C(218)	1814(2)	-928(2)	1603(1)	28(1)
C(219)	1232(2)	-1412(2)	1769(2)	35(1)
C(220)	926(2)	-2130(2)	1312(2)	33(1)
C(221)	1199(2)	-2369(2)	677(2)	29(1)
C(222)	1788(2)	-1888(2)	508(1)	22(1)
C(223)	2160(2)	215(2)	822(1)	25(1)
C(224)	3246(2)	2077(2)	1821(1)	23(1)
C(225)	3107(2)	2613(2)	1465(2)	40(1)
C(301)	3154(2)	3592(2)	7386(1)	22(1)
C(302)	3694(2)	3357(2)	7848(1)	28(1)
C(303)	4695(2)	3607(2)	8076(2)	35(1)
C(304)	5158(2)	4086(2)	7847(2)	34(1)
C(305)	4638(2)	4332(2)	7365(1)	27(1)
C(306)	5065(2)	4807(2)	7085(2)	35(1)
C(307)	4517(2)	4992(2)	6597(2)	36(1)
C(308)	3519(2)	4735(2)	6362(2)	32(1)
C(309)	3066(2)	4282(2)	6631(1)	24(1)
C(310)	3628(2)	4076(2)	7135(1)	22(1)
C(311)	1526(2)	3804(2)	5019(1)	28(1)
C(312)	2191(2)	3342(2)	4882(2)	39(1)
C(313)	2324(3)	3030(2)	4207(2)	54(1)
C(314)	1797(3)	3171(2)	3670(2)	54(1)
C(315)	1120(3)	3619(2)	3793(2)	46(1)
C(316)	980(2)	3936(2)	4465(2)	35(1)
C(317)	1436(2)	5164(2)	6177(1)	28(1)
C(318)	1643(2)	5569(2)	5775(2)	32(1)
C(319)	1731(2)	6322(2)	6053(2)	43(1)
C(320)	1635(3)	6678(2)	6729(2)	50(1)
C(321)	1428(3)	6286(2)	7130(2)	50(1)
C(322)	1331(2)	5529(2)	6855(2)	38(1)
C(323)	124(2)	3837(2)	5844(2)	35(1)
C(324)	1536(2)	2871(2)	8165(1)	23(1)
C(325)	1674(2)	2364(2)	8554(2)	35(1)
C(401)	-449(2)	4599(2)	7652(1)	20(1)
C(402)	-1314(2)	4290(2)	7183(1)	27(1)
C(403)	-1952(2)	4731(2)	7026(2)	33(1)
C(404)	-1737(2)	5478(2)	7333(1)	30(1)
C(405)	-854(2)	5833(2)	7829(1)	24(1)
C(406)	-591(2)	6600(2)	8183(1)	29(1)
C(407)	250(2)	6889(2)	8675(1)	27(1)
C(408)	877(2)	6443(2)	8838(1)	24(1)
C(409)	662(2)	5693(2)	8491(1)	19(1)
C(410)	-223(2)	5378(2)	7982(1)	19(1)
C(411)	3021(2)	6115(2)	8965(1)	20(1)
C(412)	3279(2)	5865(2)	8321(2)	33(1)
C(413)	3856(2)	6334(2)	8137(2)	42(1)
C(414)	4194(2)	7050(2)	8583(2)	40(1)
C(415)	3953(2)	7306(2)	9230(2)	32(1)
C(416)	3368(2)	6843(2)	9419(1)	25(1)
C(417)	2108(2)	5840(1)	10035(1)	19(1)

C(418)	1199(2)	5701(2)	10161(1)	24(1)
C(419)	1072(2)	5938(2)	10842(2)	30(1)
C(420)	1838(2)	6316(2)	11399(1)	30(1)
C(421)	2743(2)	6455(2)	11283(1)	29(1)
C(422)	2885(2)	6209(2)	10606(1)	25(1)
C(423)	2886(2)	4732(2)	9105(1)	28(1)
C(424)	-334(2)	2682(2)	6828(1)	25(1)
C(425)	-1113(2)	2012(2)	6488(2)	39(1)
O(9)	3881(2)	7320(1)	4737(1)	35(1)
C(501)	2876(2)	7115(2)	4630(2)	42(1)
C(502)	4296(2)	6800(2)	4260(2)	47(1)
C(503)	5346(2)	7063(2)	4421(2)	56(1)
C(504)	2518(2)	7708(2)	5156(2)	50(1)
O(10)	2857(2)	3811(1)	10261(1)	42(1)
C(505)	3846(2)	4053(2)	10528(2)	55(1)
C(506)	2274(3)	4150(2)	10702(2)	49(1)
C(507)	1256(2)	3858(2)	10354(2)	57(1)
C(508)	4369(3)	3673(3)	10004(2)	75(1)
O(11)	9163(2)	1225(1)	4338(1)	51(1)
C(509)	9918(3)	1669(2)	4239(2)	58(1)
C(510)	9486(3)	844(2)	4758(2)	57(1)
C(511)	8682(3)	341(2)	4755(2)	61(1)
C(512)	9483(4)	1974(3)	3725(3)	112(2)
O(12)	1978(2)	1109(2)	-254(1)	50(1)
C(513)	1083(3)	1217(3)	-427(2)	77(2)
C(514)	2654(3)	1132(3)	-612(2)	88(2)
C(515)	3565(3)	1020(3)	-376(2)	74(1)
C(516)	444(3)	1175(3)	-7(2)	89(2)

Table S3. Bond lengths [Å] and angles [°] for **13exo·2OEt$_2$**.

Pd(1)-C(101)	1.954(3)
Pd(1)-O(2)	2.0524(19)
Pd(1)-N(1)	2.086(2)
Pd(1)-O(4)	2.153(2)
Pd(1)-Pd(2)	3.1346(3)
Pd(2)-C(201)	1.956(3)
Pd(2)-O(3)	2.0466(18)
Pd(2)-N(2)	2.079(2)
Pd(2)-O(1)	2.1658(18)
Pd(3)-C(301)	1.955(3)
Pd(3)-O(5)	2.0379(19)
Pd(3)-N(3)	2.083(2)
Pd(3)-O(7)	2.1728(19)
Pd(3)-Pd(4)	3.1155(3)
Pd(4)-C(401)	1.960(3)
Pd(4)-O(8)	2.0360(18)
Pd(4)-N(4)	2.081(2)
Pd(4)-O(6)	2.1536(19)
P(1)-N(1)	1.621(2)
P(1)-C(123)	1.777(3)
P(1)-C(111)	1.805(3)
P(1)-C(117)	1.808(3)
P(2)-N(2)	1.622(2)
P(2)-C(223)	1.772(3)
P(2)-C(211)	1.801(3)
P(2)-C(217)	1.805(3)
P(3)-N(3)	1.617(2)
P(3)-C(323)	1.776(3)
P(3)-C(311)	1.803(3)
P(3)-C(317)	1.805(3)
P(4)-N(4)	1.624(2)
P(4)-C(423)	1.770(3)
P(4)-C(417)	1.803(3)
P(4)-C(411)	1.805(3)
N(1)-C(109)	1.419(3)
N(2)-C(209)	1.421(3)
N(3)-C(309)	1.426(3)
N(4)-C(409)	1.419(3)
O(1)-C(224)	1.242(3)
O(2)-C(224)	1.265(3)
O(3)-C(124)	1.270(3)
O(4)-C(124)	1.247(3)
O(5)-C(324)	1.270(3)
O(6)-C(324)	1.247(3)
O(7)-C(424)	1.250(3)
O(8)-C(424)	1.267(3)
C(101)-C(102)	1.372(4)
C(101)-C(110)	1.417(4)
C(102)-C(103)	1.397(5)
C(102)-H(10A)	0.9300
C(103)-C(104)	1.370(5)
C(103)-H(10B)	0.9300
C(104)-C(105)	1.408(4)
C(104)-H(10C)	0.9300
C(105)-C(106)	1.416(5)
C(105)-C(110)	1.421(4)
C(106)-C(107)	1.356(4)

C(106)-H(10D)	0.9300
C(107)-C(108)	1.411(4)
C(107)-H(10E)	0.9300
C(108)-C(109)	1.376(4)
C(108)-H(10F)	0.9300
C(109)-C(110)	1.418(4)
C(111)-C(116)	1.390(4)
C(111)-C(112)	1.398(4)
C(112)-C(113)	1.382(4)
C(112)-H(11A)	0.9300
C(113)-C(114)	1.381(4)
C(113)-H(11B)	0.9300
C(114)-C(115)	1.379(4)
C(114)-H(11C)	0.9300
C(115)-C(116)	1.390(4)
C(115)-H(11D)	0.9300
C(116)-H(11E)	0.9300
C(117)-C(118)	1.392(4)
C(117)-C(122)	1.397(4)
C(118)-C(119)	1.381(4)
C(118)-H(11F)	0.9300
C(119)-C(120)	1.372(4)
C(119)-H(11G)	0.9300
C(120)-C(121)	1.381(4)
C(120)-H(12A)	0.9300
C(121)-C(122)	1.379(4)
C(121)-H(12B)	0.9300
C(122)-H(12C)	0.9300
C(123)-H(12D)	0.9600
C(123)-H(12E)	0.9600
C(123)-H(12F)	0.9600
C(124)-C(125)	1.499(4)
C(125)-H(12G)	0.9600
C(125)-H(12H)	0.9600
C(125)-H(12I)	0.9600
C(201)-C(202)	1.372(4)
C(201)-C(210)	1.422(4)
C(202)-C(203)	1.411(4)
C(202)-H(20A)	0.9300
C(203)-C(204)	1.365(4)
C(203)-H(20B)	0.9300
C(204)-C(205)	1.418(4)
C(204)-H(20C)	0.9300
C(205)-C(206)	1.413(4)
C(205)-C(210)	1.420(4)
C(206)-C(207)	1.360(4)
C(206)-H(20D)	0.9300
C(207)-C(208)	1.413(4)
C(207)-H(20E)	0.9300
C(208)-C(209)	1.384(4)
C(208)-H(20F)	0.9300
C(209)-C(210)	1.422(3)
C(211)-C(212)	1.390(4)
C(211)-C(216)	1.397(4)
C(212)-C(213)	1.385(4)
C(212)-H(21A)	0.9300
C(213)-C(214)	1.379(4)
C(213)-H(21B)	0.9300
C(214)-C(215)	1.377(4)

C(214)-H(21C)	0.9300
C(215)-C(216)	1.386(4)
C(215)-H(21D)	0.9300
C(216)-H(21E)	0.9300
C(217)-C(218)	1.387(4)
C(217)-C(222)	1.391(4)
C(218)-C(219)	1.378(4)
C(218)-H(21F)	0.9300
C(219)-C(220)	1.374(4)
C(219)-H(21G)	0.9300
C(220)-C(221)	1.386(4)
C(220)-H(22A)	0.9300
C(221)-C(222)	1.384(4)
C(221)-H(22B)	0.9300
C(222)-H(22C)	0.9300
C(223)-H(22D)	0.9600
C(223)-H(22E)	0.9600
C(223)-H(22F)	0.9600
C(224)-C(225)	1.506(4)
C(225)-H(22G)	0.9600
C(225)-H(22H)	0.9600
C(225)-H(22I)	0.9600
C(301)-C(302)	1.371(4)
C(301)-C(310)	1.413(4)
C(302)-C(303)	1.409(4)
C(302)-H(30A)	0.9300
C(303)-C(304)	1.366(4)
C(303)-H(30B)	0.9300
C(304)-C(305)	1.405(4)
C(304)-H(30C)	0.9300
C(305)-C(306)	1.411(4)
C(305)-C(310)	1.421(4)
C(306)-C(307)	1.358(4)
C(306)-H(30D)	0.9300
C(307)-C(308)	1.406(4)
C(307)-H(30E)	0.9300
C(308)-C(309)	1.379(4)
C(308)-H(30F)	0.9300
C(309)-C(310)	1.418(4)
C(311)-C(312)	1.389(4)
C(311)-C(316)	1.401(4)
C(312)-C(313)	1.383(4)
C(312)-H(31A)	0.9300
C(313)-C(314)	1.374(5)
C(313)-H(31B)	0.9300
C(314)-C(315)	1.381(5)
C(314)-H(31C)	0.9300
C(315)-C(316)	1.385(4)
C(315)-H(31D)	0.9300
C(316)-H(31E)	0.9300
C(317)-C(322)	1.390(4)
C(317)-C(318)	1.397(4)
C(318)-C(319)	1.378(5)
C(318)-H(31F)	0.9300
C(319)-C(320)	1.380(5)
C(319)-H(31G)	0.9300
C(320)-C(321)	1.375(5)
C(320)-H(32A)	0.9300
C(321)-C(322)	1.383(5)

C(321)-H(32B)	0.9300
C(322)-H(32C)	0.9300
C(323)-H(32D)	0.9600
C(323)-H(32E)	0.9600
C(323)-H(32F)	0.9600
C(324)-C(325)	1.506(4)
C(325)-H(32G)	0.9600
C(325)-H(32H)	0.9600
C(325)-H(32I)	0.9600
C(401)-C(402)	1.368(4)
C(401)-C(410)	1.422(4)
C(402)-C(403)	1.405(4)
C(402)-H(40A)	0.9300
C(403)-C(404)	1.364(4)
C(403)-H(40B)	0.9300
C(404)-C(405)	1.420(4)
C(404)-H(40C)	0.9300
C(405)-C(406)	1.408(4)
C(405)-C(410)	1.418(4)
C(406)-C(407)	1.360(4)
C(406)-H(40D)	0.9300
C(407)-C(408)	1.408(4)
C(407)-H(40E)	0.9300
C(408)-C(409)	1.376(4)
C(408)-H(40F)	0.9300
C(409)-C(410)	1.426(3)
C(411)-C(412)	1.393(4)
C(411)-C(416)	1.394(4)
C(412)-C(413)	1.376(4)
C(412)-H(41A)	0.9300
C(413)-C(414)	1.370(5)
C(413)-H(41B)	0.9300
C(414)-C(415)	1.388(4)
C(414)-H(41C)	0.9300
C(415)-C(416)	1.381(4)
C(415)-H(41D)	0.9300
C(416)-H(41E)	0.9300
C(417)-C(418)	1.395(4)
C(417)-C(422)	1.397(4)
C(418)-C(419)	1.385(4)
C(418)-H(41F)	0.9300
C(419)-C(420)	1.375(4)
C(419)-H(41G)	0.9300
C(420)-C(421)	1.380(4)
C(420)-H(42A)	0.9300
C(421)-C(422)	1.387(4)
C(421)-H(42B)	0.9300
C(422)-H(42C)	0.9300
C(423)-H(42D)	0.9600
C(423)-H(42E)	0.9600
C(423)-H(42F)	0.9600
C(424)-C(425)	1.502(4)
C(425)-H(42G)	0.9600
C(425)-H(42H)	0.9600
C(425)-H(42I)	0.9600
O(9)-C(501)	1.414(4)
O(9)-C(502)	1.424(4)
C(501)-C(504)	1.507(5)
C(501)-H(50A)	0.9700

C(501)-H(50B)	0.9700
C(502)-C(503)	1.481(5)
C(502)-H(50C)	0.9700
C(502)-H(50D)	0.9700
C(503)-H(50E)	0.9600
C(503)-H(50F)	0.9600
C(503)-H(50G)	0.9600
C(504)-H(50H)	0.9600
C(504)-H(50I)	0.9600
C(504)-H(50J)	0.9600
O(10)-C(505)	1.396(4)
O(10)-C(506)	1.399(4)
C(505)-C(508)	1.469(5)
C(505)-H(50K)	0.9700
C(505)-H(50L)	0.9700
C(506)-C(507)	1.468(5)
C(506)-H(50M)	0.9700
C(506)-H(50N)	0.9700
C(507)-H(50O)	0.9600
C(507)-H(50P)	0.9600
C(507)-H(50Q)	0.9600
C(508)-H(50R)	0.9600
C(508)-H(50S)	0.9600
C(508)-H(50T)	0.9600
O(11)-C(510)	1.400(4)
O(11)-C(509)	1.411(4)
C(509)-C(512)	1.488(6)
C(509)-H(50U)	0.9700
C(509)-H(50V)	0.9700
C(510)-C(511)	1.439(5)
C(510)-H(51A)	0.9700
C(510)-H(51B)	0.9700
C(511)-H(51C)	0.9600
C(511)-H(51D)	0.9600
C(511)-H(51E)	0.9600
C(512)-H(51F)	0.9600
C(512)-H(51G)	0.9600
C(512)-H(51H)	0.9600
O(12)-C(514)	1.331(4)
O(12)-C(513)	1.335(4)
C(513)-C(516)	1.392(5)
C(513)-H(51I)	0.9700
C(513)-H(51J)	0.9700
C(514)-C(515)	1.386(5)
C(514)-H(51K)	0.9700
C(514)-H(51L)	0.9700
C(515)-H(51M)	0.9600
C(515)-H(51N)	0.9600
C(515)-H(51O)	0.9600
C(516)-H(51P)	0.9600
C(516)-H(51Q)	0.9600
C(516)-H(51R)	0.9600

C(101)-Pd(1)-O(2)	90.48(11)
C(101)-Pd(1)-N(1)	81.81(10)
O(2)-Pd(1)-N(1)	171.80(8)
C(101)-Pd(1)-O(4)	166.81(10)
O(2)-Pd(1)-O(4)	84.19(8)
N(1)-Pd(1)-O(4)	102.74(8)

C(101)-Pd(1)-Pd(2)	119.09(8)
O(2)-Pd(1)-Pd(2)	80.44(5)
N(1)-Pd(1)-Pd(2)	105.73(6)
O(4)-Pd(1)-Pd(2)	71.97(5)
C(201)-Pd(2)-O(3)	91.40(10)
C(201)-Pd(2)-N(2)	81.91(10)
O(3)-Pd(2)-N(2)	172.22(8)
C(201)-Pd(2)-O(1)	166.38(9)
O(3)-Pd(2)-O(1)	82.91(7)
N(2)-Pd(2)-O(1)	102.75(8)
C(201)-Pd(2)-Pd(1)	119.32(7)
O(3)-Pd(2)-Pd(1)	80.32(5)
N(2)-Pd(2)-Pd(1)	106.39(6)
O(1)-Pd(2)-Pd(1)	72.03(5)
C(301)-Pd(3)-O(5)	90.22(10)
C(301)-Pd(3)-N(3)	82.11(10)
O(5)-Pd(3)-N(3)	171.87(8)
C(301)-Pd(3)-O(7)	169.17(10)
O(5)-Pd(3)-O(7)	83.71(8)
N(3)-Pd(3)-O(7)	103.42(8)
C(301)-Pd(3)-Pd(4)	114.96(7)
O(5)-Pd(3)-Pd(4)	80.04(5)
N(3)-Pd(3)-Pd(4)	105.61(6)
O(7)-Pd(3)-Pd(4)	72.88(5)
C(401)-Pd(4)-O(8)	90.87(10)
C(401)-Pd(4)-N(4)	81.95(10)
O(8)-Pd(4)-N(4)	171.24(8)
C(401)-Pd(4)-O(6)	167.32(9)
O(8)-Pd(4)-O(6)	83.63(7)
N(4)-Pd(4)-O(6)	102.38(8)
C(401)-Pd(4)-Pd(3)	118.55(7)
O(8)-Pd(4)-Pd(3)	79.13(5)
N(4)-Pd(4)-Pd(3)	108.69(6)
O(6)-Pd(4)-Pd(3)	71.69(5)
N(1)-P(1)-C(123)	111.61(12)
N(1)-P(1)-C(111)	112.36(12)
C(123)-P(1)-C(111)	106.47(13)
N(1)-P(1)-C(117)	111.60(12)
C(123)-P(1)-C(117)	103.70(13)
C(111)-P(1)-C(117)	110.64(13)
N(2)-P(2)-C(223)	111.41(12)
N(2)-P(2)-C(211)	112.33(11)
C(223)-P(2)-C(211)	105.99(12)
N(2)-P(2)-C(217)	111.95(11)
C(223)-P(2)-C(217)	105.34(13)
C(211)-P(2)-C(217)	109.43(12)
N(3)-P(3)-C(323)	111.16(13)
N(3)-P(3)-C(311)	112.94(13)
C(323)-P(3)-C(311)	106.28(14)
N(3)-P(3)-C(317)	110.68(13)
C(323)-P(3)-C(317)	105.53(14)
C(311)-P(3)-C(317)	109.90(14)
N(4)-P(4)-C(423)	111.62(12)
N(4)-P(4)-C(417)	111.84(11)
C(423)-P(4)-C(417)	105.76(13)
N(4)-P(4)-C(411)	111.78(12)
C(423)-P(4)-C(411)	105.38(13)
C(417)-P(4)-C(411)	110.10(12)
C(109)-N(1)-P(1)	118.79(18)

C(109)-N(1)-Pd(1)	112.30(16)
P(1)-N(1)-Pd(1)	128.86(12)
C(209)-N(2)-P(2)	118.45(17)
C(209)-N(2)-Pd(2)	112.55(15)
P(2)-N(2)-Pd(2)	129.00(12)
C(309)-N(3)-P(3)	119.03(18)
C(309)-N(3)-Pd(3)	111.74(17)
P(3)-N(3)-Pd(3)	129.23(13)
C(409)-N(4)-P(4)	118.55(17)
C(409)-N(4)-Pd(4)	112.47(16)
P(4)-N(4)-Pd(4)	128.87(13)
C(224)-O(1)-Pd(2)	128.13(17)
C(224)-O(2)-Pd(1)	123.58(18)
C(124)-O(3)-Pd(2)	123.09(18)
C(124)-O(4)-Pd(1)	126.38(18)
C(324)-O(5)-Pd(3)	122.19(18)
C(324)-O(6)-Pd(4)	126.39(17)
C(424)-O(7)-Pd(3)	123.39(17)
C(424)-O(8)-Pd(4)	124.28(17)
C(102)-C(101)-C(110)	118.8(3)
C(102)-C(101)-Pd(1)	126.8(2)
C(110)-C(101)-Pd(1)	114.4(2)
C(101)-C(102)-C(103)	120.2(3)
C(101)-C(102)-H(10A)	119.9
C(103)-C(102)-H(10A)	119.9
C(104)-C(103)-C(102)	122.1(3)
C(104)-C(103)-H(10B)	118.9
C(102)-C(103)-H(10B)	118.9
C(103)-C(104)-C(105)	119.8(3)
C(103)-C(104)-H(10C)	120.1
C(105)-C(104)-H(10C)	120.1
C(104)-C(105)-C(106)	123.8(3)
C(104)-C(105)-C(110)	118.0(3)
C(106)-C(105)-C(110)	118.2(3)
C(107)-C(106)-C(105)	119.8(3)
C(107)-C(106)-H(10D)	120.1
C(105)-C(106)-H(10D)	120.1
C(106)-C(107)-C(108)	122.2(3)
C(106)-C(107)-H(10E)	118.9
C(108)-C(107)-H(10E)	118.9
C(109)-C(108)-C(107)	120.0(3)
C(109)-C(108)-H(10F)	120.0
C(107)-C(108)-H(10F)	120.0
C(108)-C(109)-C(110)	118.8(2)
C(108)-C(109)-N(1)	127.6(2)
C(110)-C(109)-N(1)	113.6(2)
C(101)-C(110)-C(109)	117.9(3)
C(101)-C(110)-C(105)	121.2(3)
C(109)-C(110)-C(105)	120.9(3)
C(116)-C(111)-C(112)	119.2(2)
C(116)-C(111)-P(1)	118.9(2)
C(112)-C(111)-P(1)	121.7(2)
C(113)-C(112)-C(111)	120.2(3)
C(113)-C(112)-H(11A)	119.9
C(111)-C(112)-H(11A)	119.9
C(114)-C(113)-C(112)	120.2(3)
C(114)-C(113)-H(11B)	119.9
C(112)-C(113)-H(11B)	119.9
C(115)-C(114)-C(113)	120.0(3)

C(115)-C(114)-H(11C)	120.0
C(113)-C(114)-H(11C)	120.0
C(114)-C(115)-C(116)	120.3(3)
C(114)-C(115)-H(11D)	119.8
C(116)-C(115)-H(11D)	119.8
C(111)-C(116)-C(115)	120.0(3)
C(111)-C(116)-H(11E)	120.0
C(115)-C(116)-H(11E)	120.0
C(118)-C(117)-C(122)	118.6(3)
C(118)-C(117)-P(1)	115.8(2)
C(122)-C(117)-P(1)	125.4(2)
C(119)-C(118)-C(117)	120.6(3)
C(119)-C(118)-H(11F)	119.7
C(117)-C(118)-H(11F)	119.7
C(120)-C(119)-C(118)	120.0(3)
C(120)-C(119)-H(11G)	120.0
C(118)-C(119)-H(11G)	120.0
C(119)-C(120)-C(121)	120.4(3)
C(119)-C(120)-H(12A)	119.8
C(121)-C(120)-H(12A)	119.8
C(122)-C(121)-C(120)	120.0(3)
C(122)-C(121)-H(12B)	120.0
C(120)-C(121)-H(12B)	120.0
C(121)-C(122)-C(117)	120.4(3)
C(121)-C(122)-H(12C)	119.8
C(117)-C(122)-H(12C)	119.8
P(1)-C(123)-H(12D)	109.5
P(1)-C(123)-H(12E)	109.5
H(12D)-C(123)-H(12E)	109.5
P(1)-C(123)-H(12F)	109.5
H(12D)-C(123)-H(12F)	109.5
H(12E)-C(123)-H(12F)	109.5
O(4)-C(124)-O(3)	126.3(3)
O(4)-C(124)-C(125)	117.4(3)
O(3)-C(124)-C(125)	116.2(3)
C(124)-C(125)-H(12G)	109.5
C(124)-C(125)-H(12H)	109.5
H(12G)-C(125)-H(12H)	109.5
C(124)-C(125)-H(12I)	109.5
H(12G)-C(125)-H(12I)	109.5
H(12H)-C(125)-H(12I)	109.5
C(202)-C(201)-C(210)	118.2(3)
C(202)-C(201)-Pd(2)	127.2(2)
C(210)-C(201)-Pd(2)	114.44(18)
C(201)-C(202)-C(203)	120.9(3)
C(201)-C(202)-H(20A)	119.6
C(203)-C(202)-H(20A)	119.6
C(204)-C(203)-C(202)	121.0(3)
C(204)-C(203)-H(20B)	119.5
C(202)-C(203)-H(20B)	119.5
C(203)-C(204)-C(205)	120.9(3)
C(203)-C(204)-H(20C)	119.5
C(205)-C(204)-H(20C)	119.5
C(206)-C(205)-C(204)	124.1(3)
C(206)-C(205)-C(210)	118.8(2)
C(204)-C(205)-C(210)	117.1(3)
C(207)-C(206)-C(205)	119.9(3)
C(207)-C(206)-H(20D)	120.1
C(205)-C(206)-H(20D)	120.1

C(206)-C(207)-C(208)	122.0(3)
C(206)-C(207)-H(20E)	119.0
C(208)-C(207)-H(20E)	119.0
C(209)-C(208)-C(207)	120.0(2)
C(209)-C(208)-H(20F)	120.0
C(207)-C(208)-H(20F)	120.0
C(208)-C(209)-N(2)	127.7(2)
C(208)-C(209)-C(210)	118.7(2)
N(2)-C(209)-C(210)	113.6(2)
C(205)-C(210)-C(201)	121.9(2)
C(205)-C(210)-C(209)	120.7(2)
C(201)-C(210)-C(209)	117.4(2)
C(212)-C(211)-C(216)	119.0(2)
C(212)-C(211)-P(2)	119.35(19)
C(216)-C(211)-P(2)	121.4(2)
C(213)-C(212)-C(211)	120.0(3)
C(213)-C(212)-H(21A)	120.0
C(211)-C(212)-H(21A)	120.0
C(214)-C(213)-C(212)	120.5(3)
C(214)-C(213)-H(21B)	119.7
C(212)-C(213)-H(21B)	119.7
C(215)-C(214)-C(213)	120.0(3)
C(215)-C(214)-H(21C)	120.0
C(213)-C(214)-H(21C)	120.0
C(214)-C(215)-C(216)	120.0(3)
C(214)-C(215)-H(21D)	120.0
C(216)-C(215)-H(21D)	120.0
C(215)-C(216)-C(211)	120.4(3)
C(215)-C(216)-H(21E)	119.8
C(211)-C(216)-H(21E)	119.8
C(218)-C(217)-C(222)	119.2(2)
C(218)-C(217)-P(2)	116.2(2)
C(222)-C(217)-P(2)	124.6(2)
C(219)-C(218)-C(217)	120.2(3)
C(219)-C(218)-H(21F)	119.9
C(217)-C(218)-H(21F)	119.9
C(220)-C(219)-C(218)	120.6(3)
C(220)-C(219)-H(21G)	119.7
C(218)-C(219)-H(21G)	119.7
C(219)-C(220)-C(221)	119.8(3)
C(219)-C(220)-H(22A)	120.1
C(221)-C(220)-H(22A)	120.1
C(222)-C(221)-C(220)	120.0(3)
C(222)-C(221)-H(22B)	120.0
C(220)-C(221)-H(22B)	120.0
C(221)-C(222)-C(217)	120.1(2)
C(221)-C(222)-H(22C)	119.9
C(217)-C(222)-H(22C)	119.9
P(2)-C(223)-H(22D)	109.5
P(2)-C(223)-H(22E)	109.5
H(22D)-C(223)-H(22E)	109.5
P(2)-C(223)-H(22F)	109.5
H(22D)-C(223)-H(22F)	109.5
H(22E)-C(223)-H(22F)	109.5
O(1)-C(224)-O(2)	126.1(3)
O(1)-C(224)-C(225)	118.1(2)
O(2)-C(224)-C(225)	115.8(3)
C(224)-C(225)-H(22G)	109.5
C(224)-C(225)-H(22H)	109.5

H(22G)-C(225)-H(22H)	109.5
C(224)-C(225)-H(22I)	109.5
H(22G)-C(225)-H(22I)	109.5
H(22H)-C(225)-H(22I)	109.5
C(302)-C(301)-C(310)	118.5(3)
C(302)-C(301)-Pd(3)	127.0(2)
C(310)-C(301)-Pd(3)	114.48(19)
C(301)-C(302)-C(303)	120.5(3)
C(301)-C(302)-H(30A)	119.7
C(303)-C(302)-H(30A)	119.7
C(304)-C(303)-C(302)	121.5(3)
C(304)-C(303)-H(30B)	119.3
C(302)-C(303)-H(30B)	119.3
C(303)-C(304)-C(305)	120.1(3)
C(303)-C(304)-H(30C)	120.0
C(305)-C(304)-H(30C)	120.0
C(304)-C(305)-C(306)	123.6(3)
C(304)-C(305)-C(310)	118.1(3)
C(306)-C(305)-C(310)	118.2(3)
C(307)-C(306)-C(305)	120.0(3)
C(307)-C(306)-H(30D)	120.0
C(305)-C(306)-H(30D)	120.0
C(306)-C(307)-C(308)	122.1(3)
C(306)-C(307)-H(30E)	119.0
C(308)-C(307)-H(30E)	119.0
C(309)-C(308)-C(307)	120.1(3)
C(309)-C(308)-H(30F)	120.0
C(307)-C(308)-H(30F)	120.0
C(308)-C(309)-C(310)	118.6(3)
C(308)-C(309)-N(3)	127.3(3)
C(310)-C(309)-N(3)	114.0(2)
C(301)-C(310)-C(309)	117.6(2)
C(301)-C(310)-C(305)	121.3(3)
C(309)-C(310)-C(305)	121.0(3)
C(312)-C(311)-C(316)	119.4(3)
C(312)-C(311)-P(3)	119.1(2)
C(316)-C(311)-P(3)	121.4(2)
C(313)-C(312)-C(311)	120.0(3)
C(313)-C(312)-H(31A)	120.0
C(311)-C(312)-H(31A)	120.0
C(314)-C(313)-C(312)	120.3(3)
C(314)-C(313)-H(31B)	119.8
C(312)-C(313)-H(31B)	119.8
C(313)-C(314)-C(315)	120.6(3)
C(313)-C(314)-H(31C)	119.7
C(315)-C(314)-H(31C)	119.7
C(314)-C(315)-C(316)	119.8(3)
C(314)-C(315)-H(31D)	120.1
C(316)-C(315)-H(31D)	120.1
C(315)-C(316)-C(311)	120.0(3)
C(315)-C(316)-H(31E)	120.0
C(311)-C(316)-H(31E)	120.0
C(322)-C(317)-C(318)	119.2(3)
C(322)-C(317)-P(3)	116.0(2)
C(318)-C(317)-P(3)	124.7(2)
C(319)-C(318)-C(317)	119.7(3)
C(319)-C(318)-H(31F)	120.2
C(317)-C(318)-H(31F)	120.2
C(318)-C(319)-C(320)	120.4(3)

C(318)-C(319)-H(31G)	119.8
C(320)-C(319)-H(31G)	119.8
C(321)-C(320)-C(319)	120.5(3)
C(321)-C(320)-H(32A)	119.7
C(319)-C(320)-H(32A)	119.7
C(320)-C(321)-C(322)	119.5(3)
C(320)-C(321)-H(32B)	120.2
C(322)-C(321)-H(32B)	120.2
C(321)-C(322)-C(317)	120.6(3)
C(321)-C(322)-H(32C)	119.7
C(317)-C(322)-H(32C)	119.7
P(3)-C(323)-H(32D)	109.5
P(3)-C(323)-H(32E)	109.5
H(32D)-C(323)-H(32E)	109.5
P(3)-C(323)-H(32F)	109.5
H(32D)-C(323)-H(32F)	109.5
H(32E)-C(323)-H(32F)	109.5
O(6)-C(324)-O(5)	126.1(3)
O(6)-C(324)-C(325)	118.1(2)
O(5)-C(324)-C(325)	115.7(3)
C(324)-C(325)-H(32G)	109.5
C(324)-C(325)-H(32H)	109.5
H(32G)-C(325)-H(32H)	109.5
C(324)-C(325)-H(32I)	109.5
H(32G)-C(325)-H(32I)	109.5
H(32H)-C(325)-H(32I)	109.5
C(402)-C(401)-C(410)	117.9(3)
C(402)-C(401)-Pd(4)	127.6(2)
C(410)-C(401)-Pd(4)	114.28(18)
C(401)-C(402)-C(403)	120.8(3)
C(401)-C(402)-H(40A)	119.6
C(403)-C(402)-H(40A)	119.6
C(404)-C(403)-C(402)	121.8(3)
C(404)-C(403)-H(40B)	119.1
C(402)-C(403)-H(40B)	119.1
C(403)-C(404)-C(405)	120.2(3)
C(403)-C(404)-H(40C)	119.9
C(405)-C(404)-H(40C)	119.9
C(406)-C(405)-C(410)	119.2(2)
C(406)-C(405)-C(404)	123.7(3)
C(410)-C(405)-C(404)	117.1(3)
C(407)-C(406)-C(405)	119.6(3)
C(407)-C(406)-H(40D)	120.2
C(405)-C(406)-H(40D)	120.2
C(406)-C(407)-C(408)	121.8(3)
C(406)-C(407)-H(40E)	119.1
C(408)-C(407)-H(40E)	119.1
C(409)-C(408)-C(407)	120.5(2)
C(409)-C(408)-H(40F)	119.7
C(407)-C(408)-H(40F)	119.7
C(408)-C(409)-N(4)	127.8(2)
C(408)-C(409)-C(410)	118.5(2)
N(4)-C(409)-C(410)	113.7(2)
C(405)-C(410)-C(401)	122.2(2)
C(405)-C(410)-C(409)	120.4(2)
C(401)-C(410)-C(409)	117.5(2)
C(412)-C(411)-C(416)	118.7(3)
C(412)-C(411)-P(4)	116.4(2)
C(416)-C(411)-P(4)	124.9(2)

C(413)-C(412)-C(411)	120.2(3)
C(413)-C(412)-H(41A)	119.9
C(411)-C(412)-H(41A)	119.9
C(414)-C(413)-C(412)	121.0(3)
C(414)-C(413)-H(41B)	119.5
C(412)-C(413)-H(41B)	119.5
C(413)-C(414)-C(415)	119.6(3)
C(413)-C(414)-H(41C)	120.2
C(415)-C(414)-H(41C)	120.2
C(416)-C(415)-C(414)	120.0(3)
C(416)-C(415)-H(41D)	120.0
C(414)-C(415)-H(41D)	120.0
C(415)-C(416)-C(411)	120.5(3)
C(415)-C(416)-H(41E)	119.8
C(411)-C(416)-H(41E)	119.8
C(418)-C(417)-C(422)	118.9(2)
C(418)-C(417)-P(4)	118.06(19)
C(422)-C(417)-P(4)	122.8(2)
C(419)-C(418)-C(417)	120.2(3)
C(419)-C(418)-H(41F)	119.9
C(417)-C(418)-H(41F)	119.9
C(420)-C(419)-C(418)	120.5(3)
C(420)-C(419)-H(41G)	119.8
C(418)-C(419)-H(41G)	119.8
C(419)-C(420)-C(421)	120.0(3)
C(419)-C(420)-H(42A)	120.0
C(421)-C(420)-H(42A)	120.0
C(420)-C(421)-C(422)	120.2(3)
C(420)-C(421)-H(42B)	119.9
C(422)-C(421)-H(42B)	119.9
C(421)-C(422)-C(417)	120.2(3)
C(421)-C(422)-H(42C)	119.9
C(417)-C(422)-H(42C)	119.9
P(4)-C(423)-H(42D)	109.5
P(4)-C(423)-H(42E)	109.5
H(42D)-C(423)-H(42E)	109.5
P(4)-C(423)-H(42F)	109.5
H(42D)-C(423)-H(42F)	109.5
H(42E)-C(423)-H(42F)	109.5
O(7)-C(424)-O(8)	126.5(2)
O(7)-C(424)-C(425)	118.3(3)
O(8)-C(424)-C(425)	115.1(3)
C(424)-C(425)-H(42G)	109.5
C(424)-C(425)-H(42H)	109.5
H(42G)-C(425)-H(42H)	109.5
C(424)-C(425)-H(42I)	109.5
H(42G)-C(425)-H(42I)	109.5
H(42H)-C(425)-H(42I)	109.5
C(501)-O(9)-C(502)	113.5(2)
O(9)-C(501)-C(504)	108.7(3)
O(9)-C(501)-H(50A)	109.9
C(504)-C(501)-H(50A)	109.9
O(9)-C(501)-H(50B)	109.9
C(504)-C(501)-H(50B)	109.9
H(50A)-C(501)-H(50B)	108.3
O(9)-C(502)-C(503)	109.1(3)
O(9)-C(502)-H(50C)	109.9
C(503)-C(502)-H(50C)	109.9
O(9)-C(502)-H(50D)	109.9

C(503)-C(502)-H(50D)	109.9
H(50C)-C(502)-H(50D)	108.3
C(502)-C(503)-H(50E)	109.5
C(502)-C(503)-H(50F)	109.5
H(50E)-C(503)-H(50F)	109.5
C(502)-C(503)-H(50G)	109.5
H(50E)-C(503)-H(50G)	109.5
H(50F)-C(503)-H(50G)	109.5
C(501)-C(504)-H(50H)	109.5
C(501)-C(504)-H(50I)	109.5
H(50H)-C(504)-H(50I)	109.5
C(501)-C(504)-H(50J)	109.5
H(50H)-C(504)-H(50J)	109.5
H(50I)-C(504)-H(50J)	109.5
C(505)-O(10)-C(506)	115.7(3)
O(10)-C(505)-C(508)	110.0(3)
O(10)-C(505)-H(50K)	109.7
C(508)-C(505)-H(50K)	109.7
O(10)-C(505)-H(50L)	109.7
C(508)-C(505)-H(50L)	109.7
H(50K)-C(505)-H(50L)	108.2
O(10)-C(506)-C(507)	110.1(3)
O(10)-C(506)-H(50M)	109.6
C(507)-C(506)-H(50M)	109.6
O(10)-C(506)-H(50N)	109.6
C(507)-C(506)-H(50N)	109.6
H(50M)-C(506)-H(50N)	108.1
C(506)-C(507)-H(50O)	109.5
C(506)-C(507)-H(50P)	109.5
H(50O)-C(507)-H(50P)	109.5
C(506)-C(507)-H(50Q)	109.5
H(50O)-C(507)-H(50Q)	109.5
H(50P)-C(507)-H(50Q)	109.5
C(505)-C(508)-H(50R)	109.5
C(505)-C(508)-H(50S)	109.5
H(50R)-C(508)-H(50S)	109.5
C(505)-C(508)-H(50T)	109.5
H(50R)-C(508)-H(50T)	109.5
H(50S)-C(508)-H(50T)	109.5
C(510)-O(11)-C(509)	113.0(3)
O(11)-C(509)-C(512)	107.1(3)
O(11)-C(509)-H(50U)	110.3
C(512)-C(509)-H(50U)	110.3
O(11)-C(509)-H(50V)	110.3
C(512)-C(509)-H(50V)	110.3
H(50U)-C(509)-H(50V)	108.5
O(11)-C(510)-C(511)	108.8(3)
O(11)-C(510)-H(51A)	109.9
C(511)-C(510)-H(51A)	109.9
O(11)-C(510)-H(51B)	109.9
C(511)-C(510)-H(51B)	109.9
H(51A)-C(510)-H(51B)	108.3
C(510)-C(511)-H(51C)	109.5
C(510)-C(511)-H(51D)	109.5
H(51C)-C(511)-H(51D)	109.5
C(510)-C(511)-H(51E)	109.5
H(51C)-C(511)-H(51E)	109.5
H(51D)-C(511)-H(51E)	109.5
C(509)-C(512)-H(51F)	109.5

C(509)-C(512)-H(51G)	109.5
H(51F)-C(512)-H(51G)	109.5
C(509)-C(512)-H(51H)	109.5
H(51F)-C(512)-H(51H)	109.5
H(51G)-C(512)-H(51H)	109.5
C(514)-O(12)-C(513)	125.4(3)
O(12)-C(513)-C(516)	119.6(3)
O(12)-C(513)-H(51I)	107.4
C(516)-C(513)-H(51I)	107.4
O(12)-C(513)-H(51J)	107.4
C(516)-C(513)-H(51J)	107.4
H(51I)-C(513)-H(51J)	107.0
O(12)-C(514)-C(515)	120.3(3)
O(12)-C(514)-H(51K)	107.3
C(515)-C(514)-H(51K)	107.3
O(12)-C(514)-H(51L)	107.3
C(515)-C(514)-H(51L)	107.3
H(51K)-C(514)-H(51L)	106.9
C(514)-C(515)-H(51M)	109.5
C(514)-C(515)-H(51N)	109.5
H(51M)-C(515)-H(51N)	109.5
C(514)-C(515)-H(51O)	109.5
H(51M)-C(515)-H(51O)	109.5
H(51N)-C(515)-H(51O)	109.5
C(513)-C(516)-H(51P)	109.5
C(513)-C(516)-H(51Q)	109.5
H(51P)-C(516)-H(51Q)	109.5
C(513)-C(516)-H(51R)	109.5
H(51P)-C(516)-H(51R)	109.5
H(51Q)-C(516)-H(51R)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13exo·2OEt₂**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	30(1)	26(1)	18(1)	11(1)	11(1)	13(1)
Pd(2)	18(1)	19(1)	15(1)	5(1)	5(1)	3(1)
Pd(3)	25(1)	22(1)	17(1)	7(1)	8(1)	7(1)
Pd(4)	18(1)	17(1)	15(1)	3(1)	4(1)	2(1)
P(1)	20(1)	25(1)	15(1)	8(1)	5(1)	5(1)
P(2)	16(1)	18(1)	15(1)	5(1)	3(1)	4(1)
P(3)	26(1)	34(1)	19(1)	12(1)	9(1)	11(1)
P(4)	17(1)	18(1)	16(1)	3(1)	2(1)	4(1)
N(1)	22(1)	27(1)	16(1)	10(1)	6(1)	7(1)
N(2)	18(1)	19(1)	16(1)	4(1)	2(1)	4(1)
N(3)	26(1)	31(1)	22(1)	13(1)	10(1)	8(1)
N(4)	20(1)	18(1)	17(1)	2(1)	3(1)	5(1)
O(1)	31(1)	23(1)	24(1)	10(1)	8(1)	7(1)
O(2)	49(1)	33(1)	32(1)	19(1)	21(1)	22(1)
O(3)	28(1)	24(1)	30(1)	5(1)	7(1)	-2(1)
O(4)	43(1)	30(1)	23(1)	8(1)	10(1)	3(1)
O(5)	35(1)	23(1)	28(1)	10(1)	13(1)	8(1)
O(6)	30(1)	24(1)	23(1)	7(1)	5(1)	7(1)
O(7)	30(1)	31(1)	22(1)	6(1)	4(1)	1(1)
O(8)	25(1)	20(1)	27(1)	3(1)	6(1)	-2(1)
C(101)	31(2)	38(2)	22(1)	12(1)	16(1)	20(1)
C(102)	37(2)	64(2)	36(2)	31(2)	17(1)	30(2)
C(103)	36(2)	106(3)	47(2)	48(2)	11(2)	36(2)
C(104)	23(2)	95(3)	46(2)	37(2)	5(1)	18(2)
C(105)	25(2)	50(2)	31(2)	14(2)	8(1)	15(2)
C(106)	20(2)	51(2)	37(2)	11(2)	5(1)	4(2)
C(107)	29(2)	34(2)	34(2)	11(1)	14(1)	4(1)
C(108)	26(1)	29(2)	21(1)	8(1)	7(1)	6(1)
C(109)	24(1)	25(2)	16(1)	4(1)	9(1)	10(1)
C(110)	26(2)	39(2)	17(1)	8(1)	9(1)	16(1)
C(111)	23(1)	24(2)	15(1)	6(1)	7(1)	1(1)
C(112)	26(1)	29(2)	21(1)	7(1)	5(1)	4(1)
C(113)	39(2)	36(2)	16(1)	10(1)	1(1)	-2(2)
C(114)	46(2)	33(2)	17(1)	0(1)	11(1)	2(2)
C(115)	41(2)	32(2)	29(2)	6(1)	15(1)	12(2)
C(116)	34(2)	25(2)	20(1)	7(1)	6(1)	8(1)
C(117)	19(1)	29(2)	22(1)	9(1)	5(1)	6(1)
C(118)	42(2)	33(2)	28(2)	13(1)	16(1)	12(2)
C(119)	57(2)	35(2)	30(2)	10(2)	22(2)	17(2)
C(120)	43(2)	27(2)	45(2)	12(2)	14(2)	10(2)
C(121)	31(2)	34(2)	37(2)	20(2)	6(1)	3(1)
C(122)	26(1)	30(2)	23(1)	11(1)	6(1)	3(1)
C(123)	22(1)	35(2)	26(2)	14(1)	6(1)	3(1)
C(124)	34(2)	21(2)	22(2)	8(1)	-3(1)	3(1)
C(125)	56(2)	24(2)	45(2)	3(2)	-2(2)	-6(2)
C(201)	19(1)	30(2)	16(1)	11(1)	7(1)	3(1)
C(202)	25(1)	33(2)	21(1)	9(1)	2(1)	-1(1)
C(203)	21(2)	49(2)	28(2)	18(2)	-3(1)	1(1)
C(204)	20(1)	52(2)	37(2)	29(2)	4(1)	10(2)
C(205)	19(1)	36(2)	27(2)	18(1)	9(1)	8(1)
C(206)	28(2)	40(2)	38(2)	24(2)	14(1)	18(1)
C(207)	34(2)	23(2)	32(2)	12(1)	14(1)	13(1)
C(208)	22(1)	27(2)	22(1)	9(1)	5(1)	6(1)

C(209)	18(1)	24(2)	16(1)	9(1)	7(1)	7(1)
C(210)	18(1)	28(2)	18(1)	12(1)	8(1)	6(1)
C(211)	23(1)	17(2)	17(1)	8(1)	4(1)	4(1)
C(212)	24(1)	24(2)	23(1)	8(1)	6(1)	1(1)
C(213)	31(2)	34(2)	29(2)	13(1)	15(1)	0(1)
C(214)	43(2)	31(2)	20(1)	12(1)	13(1)	7(2)
C(215)	35(2)	37(2)	18(1)	7(1)	0(1)	6(1)
C(216)	24(1)	36(2)	19(1)	11(1)	4(1)	5(1)
C(217)	17(1)	20(2)	19(1)	8(1)	4(1)	5(1)
C(218)	33(2)	25(2)	23(1)	3(1)	10(1)	4(1)
C(219)	44(2)	36(2)	30(2)	9(2)	23(1)	7(2)
C(220)	31(2)	33(2)	44(2)	21(2)	20(1)	6(1)
C(221)	32(2)	19(2)	34(2)	6(1)	10(1)	1(1)
C(222)	26(1)	22(2)	20(1)	6(1)	9(1)	7(1)
C(223)	21(1)	26(2)	25(1)	9(1)	2(1)	8(1)
C(224)	21(1)	26(2)	25(2)	13(1)	6(1)	4(1)
C(225)	45(2)	46(2)	49(2)	34(2)	22(2)	23(2)
C(301)	26(1)	24(2)	18(1)	6(1)	10(1)	10(1)
C(302)	33(2)	29(2)	29(2)	14(1)	13(1)	13(1)
C(303)	31(2)	47(2)	31(2)	19(2)	5(1)	17(2)
C(304)	23(2)	43(2)	36(2)	15(2)	4(1)	9(1)
C(305)	27(2)	28(2)	27(2)	8(1)	10(1)	8(1)
C(306)	26(2)	40(2)	41(2)	15(2)	11(1)	5(1)
C(307)	35(2)	40(2)	46(2)	25(2)	20(1)	9(2)
C(308)	33(2)	44(2)	31(2)	23(2)	14(1)	15(2)
C(309)	27(2)	27(2)	19(1)	7(1)	10(1)	10(1)
C(310)	26(1)	22(2)	18(1)	6(1)	10(1)	8(1)
C(311)	35(2)	33(2)	21(1)	12(1)	11(1)	12(1)
C(312)	58(2)	44(2)	22(2)	15(1)	13(1)	26(2)
C(313)	75(3)	59(3)	34(2)	13(2)	23(2)	43(2)
C(314)	83(3)	63(3)	22(2)	13(2)	22(2)	37(2)
C(315)	59(2)	57(2)	22(2)	15(2)	5(2)	20(2)
C(316)	39(2)	46(2)	25(2)	15(1)	9(1)	17(2)
C(317)	25(1)	38(2)	26(2)	15(1)	11(1)	12(1)
C(318)	35(2)	40(2)	26(2)	15(1)	13(1)	13(2)
C(319)	45(2)	45(2)	46(2)	24(2)	13(2)	9(2)
C(320)	63(2)	35(2)	49(2)	10(2)	13(2)	12(2)
C(321)	74(3)	44(2)	35(2)	10(2)	22(2)	25(2)
C(322)	50(2)	42(2)	31(2)	16(2)	19(1)	18(2)
C(323)	27(2)	48(2)	33(2)	20(2)	6(1)	10(2)
C(324)	16(1)	25(2)	28(2)	12(1)	6(1)	2(1)
C(325)	39(2)	38(2)	41(2)	25(2)	18(1)	13(2)
C(401)	22(1)	25(2)	13(1)	6(1)	8(1)	5(1)
C(402)	24(1)	29(2)	21(1)	4(1)	2(1)	3(1)
C(403)	23(2)	43(2)	25(2)	10(1)	-3(1)	3(1)
C(404)	26(2)	35(2)	28(2)	12(1)	2(1)	10(1)
C(405)	22(1)	30(2)	22(1)	11(1)	8(1)	8(1)
C(406)	31(2)	29(2)	29(2)	12(1)	8(1)	13(1)
C(407)	31(2)	20(2)	28(2)	5(1)	8(1)	8(1)
C(408)	20(1)	21(2)	23(1)	2(1)	2(1)	3(1)
C(409)	19(1)	23(2)	16(1)	7(1)	7(1)	6(1)
C(410)	21(1)	23(2)	14(1)	6(1)	6(1)	5(1)
C(411)	17(1)	22(2)	20(1)	6(1)	4(1)	5(1)
C(412)	38(2)	31(2)	26(2)	5(1)	13(1)	5(2)
C(413)	52(2)	48(2)	36(2)	16(2)	30(2)	13(2)
C(414)	36(2)	42(2)	55(2)	27(2)	24(2)	8(2)
C(415)	31(2)	22(2)	42(2)	10(1)	12(1)	2(1)
C(416)	26(2)	24(2)	24(1)	7(1)	8(1)	7(1)
C(417)	21(1)	17(2)	18(1)	6(1)	4(1)	4(1)

C(418)	23(1)	21(2)	25(1)	6(1)	3(1)	0(1)
C(419)	30(2)	32(2)	34(2)	15(1)	14(1)	5(1)
C(420)	42(2)	33(2)	20(1)	11(1)	12(1)	11(2)
C(421)	31(2)	35(2)	18(1)	7(1)	0(1)	8(1)
C(422)	21(1)	30(2)	21(1)	8(1)	3(1)	6(1)
C(423)	24(1)	25(2)	27(2)	4(1)	1(1)	7(1)
C(424)	20(1)	21(2)	29(2)	9(1)	-1(1)	1(1)
C(425)	37(2)	25(2)	40(2)	3(1)	1(1)	-5(2)
O(9)	37(1)	32(1)	33(1)	8(1)	7(1)	7(1)
C(501)	38(2)	42(2)	39(2)	10(2)	4(1)	1(2)
C(502)	52(2)	33(2)	48(2)	3(2)	17(2)	11(2)
C(503)	44(2)	43(2)	69(3)	4(2)	22(2)	12(2)
C(504)	47(2)	56(2)	51(2)	23(2)	16(2)	10(2)
O(10)	31(1)	54(2)	41(1)	17(1)	9(1)	12(1)
C(505)	37(2)	75(3)	50(2)	24(2)	0(2)	11(2)
C(506)	54(2)	65(3)	39(2)	24(2)	19(2)	23(2)
C(507)	44(2)	82(3)	63(3)	39(2)	29(2)	23(2)
C(508)	39(2)	116(4)	93(3)	57(3)	24(2)	35(2)
O(11)	38(1)	53(2)	68(2)	28(1)	16(1)	12(1)
C(509)	43(2)	38(2)	95(3)	20(2)	31(2)	2(2)
C(510)	74(3)	73(3)	33(2)	19(2)	18(2)	45(2)
C(511)	75(3)	70(3)	38(2)	22(2)	10(2)	19(2)
C(512)	146(5)	87(4)	187(6)	98(4)	124(5)	72(4)
O(12)	28(1)	91(2)	49(1)	44(1)	14(1)	22(1)
C(513)	34(2)	158(5)	51(2)	53(3)	9(2)	28(3)
C(514)	42(2)	195(6)	46(2)	62(3)	18(2)	29(3)
C(515)	45(2)	137(4)	82(3)	75(3)	38(2)	42(3)
C(516)	40(2)	180(6)	83(3)	81(4)	26(2)	49(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **13exo·2OEt$_2$**.

	x	y	z	U(eq)
H(10A)	1272	1689	1857	47
H(10B)	-349	1192	1456	67
H(10C)	-1061	364	1839	62
H(10D)	-895	-360	2639	46
H(10E)	67	-633	3464	38
H(10F)	1704	-147	3848	31
H(11A)	4287	662	5388	31
H(11B)	4000	1190	6493	38
H(11C)	2777	1857	6658	41
H(11D)	1845	2007	5718	41
H(11E)	2113	1473	4602	32
H(11F)	3664	-393	2778	39
H(11G)	3847	-1605	2375	47
H(12A)	3864	-2249	3101	46
H(12B)	3645	-1700	4224	39
H(12C)	3404	-503	4622	31
H(12D)	4833	895	3652	40
H(12E)	5097	952	4431	40
H(12F)	4710	1595	4259	40
H(12G)	6231	3088	3494	71
H(12H)	5794	3152	4146	71
H(12I)	5325	3457	3594	71
H(20A)	6374	1327	3143	33
H(20B)	7510	661	3424	40
H(20C)	7270	-584	2875	40
H(20D)	6212	-1771	1956	37
H(20E)	4857	-2315	1089	33
H(20F)	3757	-1633	787	28
H(21A)	4476	-511	198	28
H(21B)	4709	-898	-933	36
H(21C)	3427	-1486	-1879	36
H(21D)	1894	-1677	-1704	38
H(21E)	1640	-1267	-578	31
H(21F)	2017	-444	1915	34
H(21G)	1045	-1251	2194	43
H(22A)	538	-2454	1429	39
H(22B)	986	-2853	364	35
H(22C)	1975	-2050	83	27
H(22D)	2054	445	1284	37
H(22E)	1553	-1	493	37
H(22F)	2499	576	695	37
H(22G)	2684	2364	1010	60
H(22H)	3717	2813	1416	60
H(22I)	2830	3003	1743	60
H(30A)	3396	3030	8011	34
H(30B)	5049	3443	8390	41
H(30C)	5819	4250	8011	41
H(30D)	5722	4992	7234	42
H(30E)	4811	5300	6412	44
H(30F)	3164	4870	6024	39
H(31A)	2547	3242	5244	46
H(31B)	2773	2724	4118	64

H(31C)	1896	2963	3219	65
H(31D)	759	3707	3425	55
H(31E)	524	4237	4550	42
H(31F)	1720	5332	5322	38
H(31G)	1857	6592	5783	51
H(32A)	1709	7187	6915	60
H(32B)	1355	6527	7583	60
H(32C)	1193	5263	7126	46
H(32D)	30	3313	5706	52
H(32E)	-291	3957	5503	52
H(32F)	-26	4054	6294	52
H(32G)	2017	2643	9030	52
H(32H)	2036	2006	8329	52
H(32I)	1058	2119	8551	52
H(40A)	-1483	3781	6965	32
H(40B)	-2535	4507	6704	39
H(40C)	-2172	5756	7218	36
H(40D)	-990	6906	8081	34
H(40E)	416	7396	8909	33
H(40F)	1441	6658	9184	28
H(41A)	3061	5379	8014	39
H(41B)	4019	6163	7704	51
H(41C)	4582	7362	8453	48
H(41D)	4186	7790	9537	39
H(41E)	3204	7017	9851	30
H(41F)	676	5450	9787	29
H(41G)	465	5841	10922	37
H(42A)	1746	6477	11854	36
H(42B)	3259	6714	11660	35
H(42C)	3500	6289	10531	30
H(42D)	2963	4495	8635	41
H(42E)	2535	4382	9238	41
H(42F)	3507	4926	9420	41
H(42G)	-1273	1888	5990	58
H(42H)	-1673	2111	6673	58
H(42I)	-892	1610	6585	58
H(50A)	2728	6653	4687	51
H(50B)	2562	7052	4157	51
H(50C)	4012	6740	3782	56
H(50D)	4169	6328	4301	56
H(50E)	5468	7500	4324	83
H(50F)	5639	6690	4136	83
H(50G)	5613	7169	4907	83
H(50H)	2820	7759	5622	75
H(50I)	1833	7578	5083	75
H(50J)	2672	8164	5099	75
H(50K)	4041	3957	10951	66
H(50L)	4001	4579	10648	66
H(50M)	2405	4676	10818	59
H(50N)	2418	4065	11135	59
H(50O)	1118	3936	9922	85
H(50P)	862	4105	10655	85
H(50Q)	1121	3342	10258	85
H(50R)	4226	3155	9894	112
H(50S)	5048	3848	10189	112
H(50T)	4175	3770	9586	112
H(50U)	10386	1379	4060	70
H(50V)	10239	2063	4680	70
H(51A)	9770	1187	5234	68

H(51B)	9973	576	4578	68
H(51C)	8230	612	4971	91
H(51D)	8904	49	5011	91
H(51E)	8376	27	4280	91
H(51F)	9061	1586	3328	167
H(51G)	9983	2196	3572	167
H(51H)	9124	2337	3943	167
H(51I)	795	861	-897	92
H(51J)	1127	1699	-453	92
H(51K)	2728	1608	-651	106
H(51L)	2405	768	-1084	106
H(51M)	3725	1212	127	110
H(51N)	4025	1267	-541	110
H(51O)	3578	504	-552	110
H(51P)	258	673	-65	133
H(51Q)	-117	1362	-142	133
H(51R)	748	1462	475	133