Supporting Information

for

New Seven Membered Palladacycles:

C-Br Bond Activation of 2-Br-Pyridine Derivative by Pd(II)

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General information

All reactions involving sensitive compounds were carried out under an atmosphere of purified dinitrogen using standard Schlenk techniques. The palladacycles **I**[1] and 6-bromo-2-pyridinecarboxaldehyde[2] were prepared according to literature procedures, all other reagents were used as received from commercial sources. ^{1}H, ^{13}C-{^{1}H} and 2D Nuclear Magnetic Resonance (NMR) spectra were recorded on a Varian (300 MHz) spectrometer. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. ^{1}H NMR coupling constants (J) are reported in Hertz (Hz) and multiplicities are indicated as follows: s (singlet), d (doublet), t (triplet), m (multiplet).

Synthesis of 2-(6-bromopyridin-2-yl)-1-phenyl-1H-benzoimidazole (1)

N-phenyl-1,2-phenylenediamine (990 mg, 5.376 mmol), 6-bromo-2-pyridinecarboxaldehyde (1g, 5.376 mmol) and 50 mL of EtOH were placed in a 100 mL round bottom flask containing a magnetic stirring bar. The mixture was stirred for 24 h at room temperature. $NiCl_2(H_2O)_6$ was added and the mixture was stirred for 72 h. The solvent was removed under reduced pressure and the residue was extracted with a mixture of dichloromethane and water. The organic phase was dried with Na_2SO_4 and the solvent removed giving compound **1** as a brown solid. Yield: (755 mg, 40.10%). When the compound was prepared using the procedure reported by Hayashi et al[3] the yield of compound **I** was 60.00 %. Anal. Calcd. for $C_{18}H_{12}BrN_3$ (350.21 g mol^{-1}): C, 61.73; H, 3.45; N, 12.00. Found: C, 61.17; H, 3.52; N, 12.09.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.0-7.6 (m, 10H), 7.85 (d, $^{3}J_{HH}$= 7.6 Hz, 1H), 8.15 (d, $^{3}J_{HH}$= 7.6 Hz, 1H).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$): δ 111.3, 120.3, 123.2, 123.6, 124.6, 127.7, 128.4, 128.6, 129.4, 137.5, 138.0, 138.9, 140.8, 142.4, 148.7, 149.8,

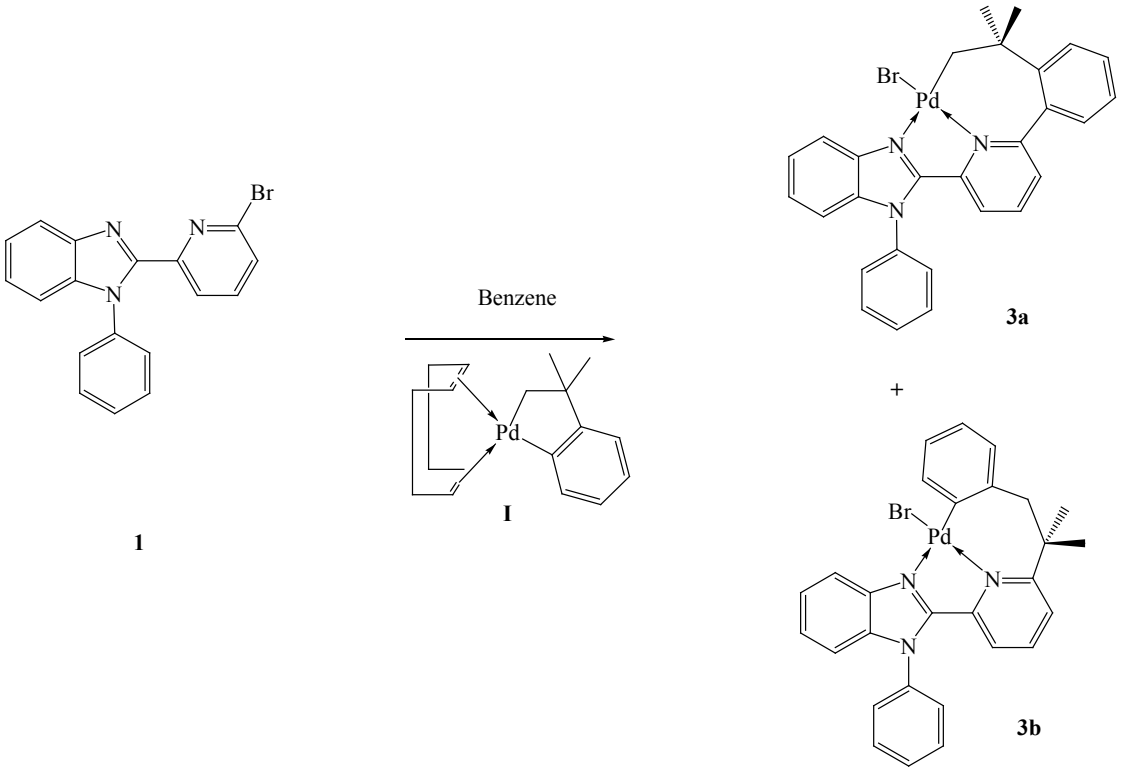
Synthesis of the complex 2.

1 equivalent of **1** (175 mg, 0.5 mmol) was added to a **II** (198 mg, 0.5 mmol) dissolved in CH_2Cl_2 , and the resultant solution was stirred for 30 min at room temperature. After removal of the solvent under reduced pressure complex **1** was obtained as yellow solid. Yield: (0.243 g, 95.00 %). Anal. Calcd. for $C_{28}H_{24}BrN_3Pd$ (588.83 g mol^{-1}): C, 57.11; H, 7.14; N, 12.00. Found: C, 57.23; H, 7.09; N, 12.42.

Selected data for 2: ^{1}H NMR (300 MHz, C_6D_6): δ 1.12 (s, 6H), 1.39 (s, 2H), 6.61-7.23 (m, 14H), 8.07 (d, $^{2}J_{HH}$= 7.5 Hz, 1H), 8.35 (d, $^{2}J_{HH}$= 7.5 Hz, 1H).

C^{13}-{^{1}H} NMR (75 MHz, C_6D_6): δ 29.1, 37.4, 39.1, 111.3, 120.8, 122.9, 123.4, 124.41, 125.6, 126.1, 126.5, 127.6, 128.4, 129.1, 138.7, 149.3.

Synthesis of complexes 3a and 3b.



20 mL of benzene were added to a mixture of palladacycle **I** (540 mg, 1.55 mmol) and **1** (545 mg, 1.55) and the mixture was stirred for 24 h at 35 °C, the formation of a precipitate was observed. After filtration, the precipitate was washed with ethyl ether twice and dried under reduced pressure. Compounds **3a** and **3b** were obtained as a yellow powder. Yield: (512 mg, 56 %). m.p.= 180 °C (decomposition). Anal. Calcd. for $C_{28}H_{24}BrN_3Pd$ (588.83 g mol^{-1}): C, 57.11; H, 7.14; N, 12.00. Found: C, 56.78; H, 7.22; N, 12.38.

Selected data for 3a: ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.90 (s, 3H, CH_3), 1.50 (s, 3H, CH_3), 2.46 (d, $^2J_{HH}$ = 9.9 Hz, 1H), 2.71 (d, $^2J_{HH}$ = 9.6 Hz, 1H), 6.90-7.10 (m, 3H), 7.20-7.80 (m, 13H), 8.70 (d, $^3J_{HH}$= 6.20 Hz, 1H).

C^{13}-{^{1}H} NMR (75 MHz, $CDCl_3$): δ 28.6 (CH_3), 31.2 (CH_3), 36.9 (CH_2), 38.9 ($\underline{C}(CH_2)$), 111.2, 121.1, 122.3, 125.1, 126.2, 127.3, 129.4, 130.2, 131.3, 133.2, 136.3, 137.1, 138.2, 141.2, 148.7, 148.5, 169.0.

Selected data for 3b: ^{1}H NMR (300 MHz, CD_2Cl_2): δ 0.93 (s, 3H), 1.47 (s, 3H), 2.34 (d, $^{2}J_{HH}$ = 9.9 Hz, 1H), 2.61 (d, $^{2}J_{HH}$ = 10.2 Hz, 1H), 6.9-7.1 (m, 3H), 7.2-7.8 (m, 13H), 8.50 (d, $^{3}J_{HH}$= 6.21 Hz, 1H).

C^{13}-{^{1}H} NMR (75 MHz, CD_2Cl_2): δ 28.6 (CH_3), 31.0 (CH_3), 39.0 (CH_2), 39.1 ($\underline{C}(CH_2)$), 111.1, 121.6, 122.3, 124.7, 124.9, 125.9, 126.1, 128.51, 128.7, 131.3, 133.2 137.0, 140.0, 148.4, 148.9, 169.1.

Computational Details.

We have performed all the calculations in Gaussian03 series of programs.[4] Geometry optimizations were done using the hybrid-GGA B3LYP density functional[5] in combination with several basis sets; namely LANL2DZdp[6] for Pd and Br atoms and 6-31G(d,p)[7] for C, N and H atoms. We report energies from single-point calculations employing augmented basis sets: LANL2TZ+f[6,8] for Pd, LANL08d[8] for Br and 6-311+G(2d,2p)[9] for C, N and H atoms. Therefore, in this work we refer to this mix of methodological basis set as *mix-basis* for simplicity. Moreover, the nature of stationary points located over the potential energy surface (PES) was confirmed by computing a frequency analysis; the number of negative eigenvalues of Hessian was rigorously one for transition state and zero for minima. We also checked that the transition state was connected to both minima by following the transition vector when integrating the intrinsic reaction coordinate (IRC calculation) in both directions.[10]

Reported values contain three different corrections to the energy: 1) zero-point energy and enthalpy corrections were added initially from thermochemistry in the output of frequency calculations; 2) solvent effects were taken into account by performing single-point calculations on the optimized geometries using the conductor-like polarizable continuum model (cPCM) method,[11] where a solvent cavity is formed as a surface of constant charge density of the solvated molecule with the UAHF radii (united atom topological model). The dielectric constant was set up to 4.9 (corresponding to chloroform); 3) lately, we have made use of Grimme's DFT-D method[12] to obtain long-range energy corrections (where parametrization for B3LYP uses a scaling factor (s^6) of 1.05 and we used a damping factor alpha of 20).

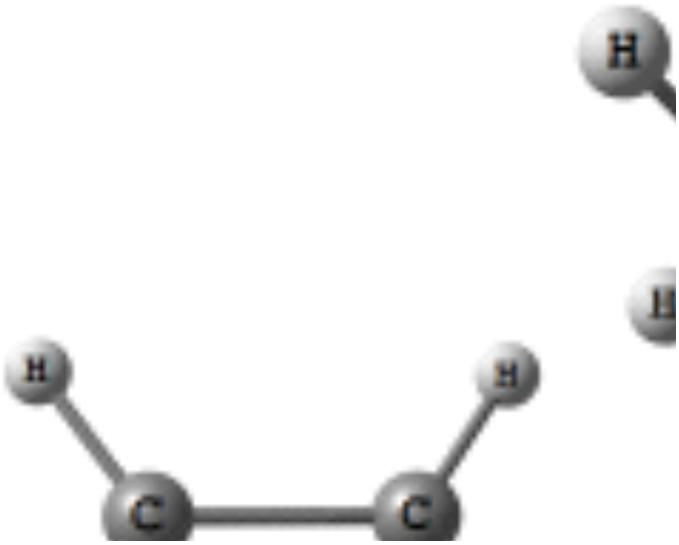


Figure S1. Optimized geometries of the initial part of the reaction mechanism calculated at B3LYP/*mix-basis* level. Bonding distances are given in angstroms.

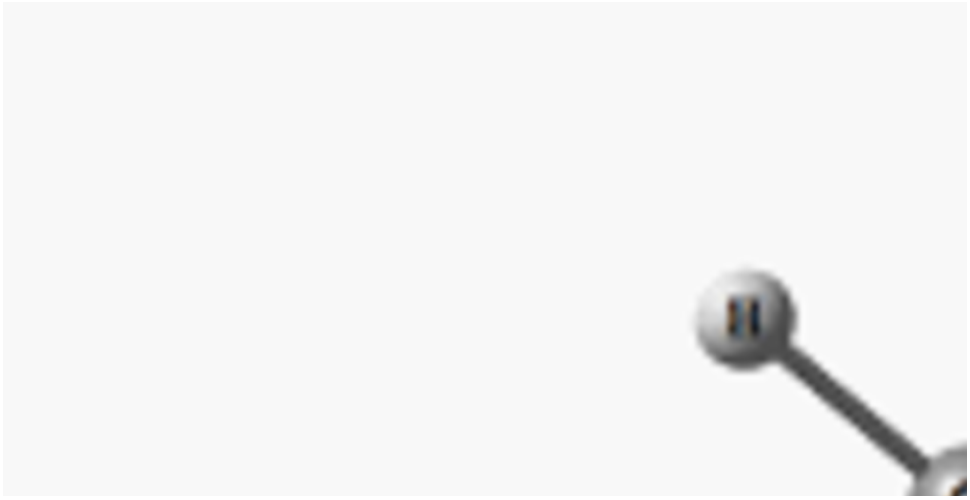


Figure S2. Optimized geometries of the C(sp^2)-C(sp^2) coupling reaction affording **Prod_1** complex calculated at B3LYP/*mix-basis* level. Bonding distances are given in angstroms.

Figure S3. Optimized geometries of the C(sp^2)-C(sp^3) coupling reaction affording **Prod_2** species calculated at B3LYP/*mix-basis* level. Bonding distances are given in angstroms.

Table S1. Cartesian coordinates (in Å) of all stationary points in the gas phase computed at B3LYP/*mix-basis* level.

Reactant

46	-2.369631000	-1.123709000	0.264146000
6	-3.040503000	-1.303050000	-1.679614000
1	-3.782448000	-2.109853000	-1.618581000
1	-3.554557000	-0.379130000	-1.975540000
6	-1.917600000	-1.681585000	-2.670207000
6	-1.146653000	-0.412217000	-3.101792000
1	-0.316195000	-0.663532000	-3.771547000
1	-1.811014000	0.281062000	-3.632533000

1	-0.740315000	0.106450000	-2.228330000
6	-2.521204000	-2.345521000	-3.925846000
1	-3.261556000	-1.680718000	-4.385595000
1	-1.760052000	-2.559620000	-4.685760000
1	-3.020189000	-3.286984000	-3.673722000
6	-0.980713000	-2.595548000	-1.896781000
6	-0.129944000	-3.540425000	-2.482957000
6	-0.994282000	-2.427329000	-0.491589000
6	0.718578000	-4.321038000	-1.691170000
1	-0.136022000	-3.684972000	-3.561316000
6	-0.130265000	-3.212960000	0.285123000
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1	-0.114751000	-3.109825000	1.368069000
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1	-1.142917000	1.513175000	3.261903000
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6	2.333836000	1.427754000	0.750165000
6	2.745481000	0.797944000	2.760998000
6	3.548647000	-0.016519000	1.929382000
7	3.279675000	0.406153000	0.631915000
7	2.005425000	1.679562000	1.999310000
6	2.784166000	0.628505000	4.153496000
1	2.175497000	1.255985000	4.796449000
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TS1

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1	-6.805062000	-3.535601000	-2.231104000
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Int1

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6	1.329489000	3.757946000	-2.077494000
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6	1.523804000	1.825647000	-3.521009000
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6	1.473886000	-3.312344000	-0.530654000
6	2.654468000	-2.601090000	-0.846306000
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1	4.340635000	-2.347449000	-2.194095000
6	1.862599000	-4.718615000	-2.427361000
1	1.578076000	-5.550377000	-3.064834000
6	3.029471000	-3.986357000	-2.735801000
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1	3.490570000	-0.637201000	2.685257000
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6	3.309045000	0.749410000	-0.214960000
6	5.066812000	-0.834391000	0.341054000
6	4.257011000	1.772775000	-0.255028000
1	2.266339000	0.952892000	-0.436389000

6	6.007889000	0.194589000	0.288294000
1	5.364636000	-1.851799000	0.575580000
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6	-4.946062000	-2.869180000	-1.405787000
1	-5.603801000	-3.476370000	-2.027844000
6	-4.071182000	-3.532510000	-0.638983000
1	-4.116253000	-4.621406000	-0.692416000
6	-2.674044000	-0.805151000	-2.261609000
1	-2.054467000	-0.693282000	-3.149857000
6	-2.023294000	-1.161699000	-1.115609000
1	-0.953541000	-1.341702000	-1.202653000
6	-3.017099000	-3.026783000	0.313813000
6	-2.605721000	-1.541032000	0.231221000
6	-5.137206000	-1.374948000	-1.558212000
6	-4.159907000	-0.720293000	-2.559071000
1	-2.111239000	-3.632912000	0.180675000
1	-1.834168000	-1.374698000	0.987478000
1	-4.307229000	-1.192872000	-3.540066000
1	-5.087692000	-0.865433000	-0.593227000
1	-4.444672000	0.331806000	-2.706016000
1	-6.151154000	-1.192965000	-1.933451000
1	-3.450267000	-0.903078000	0.505107000
1	-3.342066000	-3.234790000	1.344685000

TS2

46	2.049208000	-0.352589000	0.086237000
6	3.481121000	-1.842752000	0.213022000
1	4.291459000	-1.400851000	-0.377944000
1	3.792048000	-1.905536000	1.259880000
6	3.030477000	-3.197285000	-0.377447000
6	2.346485000	-4.059241000	0.707582000
1	2.013248000	-5.015779000	0.291073000
1	3.042448000	-4.271894000	1.528467000
1	1.471948000	-3.547544000	1.117812000
6	4.268574000	-3.952573000	-0.909345000
1	5.005663000	-4.089753000	-0.109986000
1	4.004045000	-4.947852000	-1.284345000
1	4.748070000	-3.400692000	-1.724289000
6	2.022594000	-2.871739000	-1.463914000
6	1.619957000	-3.752977000	-2.474509000
6	1.434349000	-1.593945000	-1.385639000
6	0.637701000	-3.377481000	-3.394165000
1	2.073409000	-4.738905000	-2.548385000
6	0.456781000	-1.217829000	-2.313721000
6	0.053809000	-2.111422000	-3.314353000

1	0.334613000	-4.068648000	-4.176131000
1	0.004119000	-0.230380000	-2.269026000
1	-0.706163000	-1.813206000	-4.032309000
6	-2.553381000	0.643543000	0.940009000
6	-3.753152000	2.274637000	0.228535000
6	-4.487563000	1.101506000	-0.061719000
7	-3.701735000	0.051318000	0.408574000
7	-2.559829000	1.954266000	0.846440000
6	-4.270475000	3.530239000	-0.121668000
1	-3.711584000	4.432362000	0.104751000
6	-5.719414000	1.132822000	-0.720580000
1	-6.265184000	0.225594000	-0.956667000
6	-5.501481000	3.570682000	-0.764638000
1	-5.927219000	4.528288000	-1.048999000
6	-6.212612000	2.388785000	-1.062405000
1	-7.168916000	2.460210000	-1.572069000
6	-1.475055000	-0.124362000	1.592385000
6	-1.712048000	-1.238810000	2.399286000
7	-0.217899000	0.338699000	1.406355000
6	-0.618840000	-1.884200000	2.995883000
1	-2.722908000	-1.580999000	2.582531000
6	0.782600000	-0.321837000	1.911613000
6	0.672657000	-1.432660000	2.768490000
1	-0.782783000	-2.741182000	3.642869000
1	1.544552000	-1.906839000	3.198333000
6	-3.949193000	-1.333436000	0.149565000
6	-3.052941000	-2.071616000	-0.631145000
6	-5.104324000	-1.934943000	0.660792000
6	-3.309113000	-3.418723000	-0.884593000
1	-2.164687000	-1.598061000	-1.036435000
6	-5.359477000	-3.280066000	0.388644000
1	-5.787243000	-1.351412000	1.270226000
6	-4.461832000	-4.024696000	-0.379084000
1	-2.607041000	-3.986195000	-1.487831000
1	-6.257017000	-3.746008000	0.784379000
1	-4.660846000	-5.072277000	-0.584266000
35	2.579589000	0.937226000	2.356085000
6	2.913364000	5.106361000	-1.575194000
1	3.503206000	5.709784000	-2.265577000
6	1.619439000	5.431666000	-1.461266000
1	1.284792000	6.284795000	-2.053757000
6	2.145715000	2.020180000	-1.688861000
1	2.064264000	1.240585000	-2.445763000
6	1.008923000	2.346681000	-1.041911000
1	0.110325000	1.807914000	-1.340660000
6	0.518458000	4.813372000	-0.634739000
6	0.764977000	3.423367000	-0.009787000
6	3.679873000	3.989738000	-0.898520000
6	3.531097000	2.618219000	-1.591867000
1	-0.378984000	4.757296000	-1.267873000
1	-0.129020000	3.145070000	0.556119000

1	3.917399000	2.701988000	-2.617473000
1	3.412953000	3.902047000	0.156234000
1	4.195672000	1.897152000	-1.093413000
1	4.745905000	4.246345000	-0.912549000
1	1.579357000	3.472197000	0.713676000
1	0.248873000	5.513349000	0.171493000

Int2

46	-1.791550000	-0.489510000	-0.295877000
6	-2.869869000	-2.248834000	-0.465762000
1	-3.868688000	-1.808598000	-0.404664000
1	-2.698918000	-2.620110000	-1.476306000
6	-2.599603000	-3.276223000	0.656222000
6	-1.672120000	-4.403853000	0.147245000
1	-1.494610000	-5.141451000	0.936314000
1	-2.123744000	-4.923081000	-0.706518000
1	-0.701528000	-4.006696000	-0.161055000
6	-3.959278000	-3.891902000	1.064931000
1	-4.456400000	-4.342013000	0.198548000
1	-3.826685000	-4.680237000	1.813219000
1	-4.625943000	-3.133439000	1.487304000
6	-1.919318000	-2.550738000	1.804931000
6	-1.756207000	-3.086275000	3.090238000
6	-1.358372000	-1.297424000	1.520272000
6	-1.028135000	-2.393079000	4.058176000
1	-2.189685000	-4.052723000	3.336608000
6	-0.599500000	-0.614628000	2.471585000
6	-0.441255000	-1.163346000	3.748690000
1	-0.908075000	-2.818111000	5.050850000
1	-0.119807000	0.327288000	2.218786000
1	0.142772000	-0.633004000	4.496298000
6	2.970490000	0.818791000	-0.336620000
6	3.621755000	2.709390000	0.446208000
6	4.786248000	1.912925000	0.351004000
7	4.353470000	0.691832000	-0.160882000
7	2.518494000	2.001851000	0.014912000
6	3.708716000	4.020531000	0.936805000
1	2.818221000	4.636792000	1.005056000
6	6.043215000	2.370224000	0.755122000
1	6.927074000	1.744147000	0.694029000
6	4.956923000	4.487510000	1.329324000
1	5.055248000	5.498425000	1.713464000
6	6.105829000	3.672556000	1.242635000
1	7.063539000	4.071074000	1.564185000
6	2.110349000	-0.231820000	-0.912924000
6	2.540175000	-1.168168000	-1.860034000
7	0.823801000	-0.232159000	-0.501357000
6	1.619690000	-2.092848000	-2.361701000
1	3.562914000	-1.165870000	-2.215405000

6	-0.021858000	-1.095674000	-0.984209000
6	0.296752000	-2.078068000	-1.925193000
1	1.933170000	-2.812736000	-3.112496000
1	-0.446455000	-2.754636000	-2.324933000
6	5.170738000	-0.476094000	-0.258634000
6	4.898311000	-1.594132000	0.537207000
6	6.261014000	-0.482420000	-1.135654000
6	5.709061000	-2.724362000	0.438479000
1	4.059544000	-1.569553000	1.225338000
6	7.075677000	-1.612780000	-1.216974000
1	6.456778000	0.390896000	-1.749717000
6	6.798953000	-2.736080000	-0.435237000
1	5.493830000	-3.592969000	1.053465000
1	7.921661000	-1.616190000	-1.897707000
1	7.431095000	-3.616147000	-0.504604000
35	-2.455085000	0.403270000	-2.648169000
6	-5.720762000	3.486896000	0.228828000
1	-6.765888000	3.693568000	0.460450000
6	-4.815274000	4.258907000	0.842775000
1	-5.207871000	5.036737000	1.499230000
6	-4.011370000	0.907236000	0.865600000
1	-4.058787000	0.093301000	1.590031000
6	-2.941535000	1.727804000	0.979418000
1	-2.262424000	1.504554000	1.801650000
6	-3.306956000	4.240463000	0.778916000
6	-2.620019000	2.982311000	0.201396000
6	-5.496721000	2.342039000	-0.735114000
6	-5.209978000	0.988514000	-0.049157000
1	-2.930322000	4.409707000	1.797952000
1	-1.537311000	3.145821000	0.245353000
1	-6.085410000	0.700007000	0.549272000
1	-4.703450000	2.560008000	-1.450914000
1	-5.114579000	0.223265000	-0.832306000
1	-6.405125000	2.211247000	-1.334561000
1	-2.856436000	2.855768000	-0.854373000
1	-2.963400000	5.113217000	0.202968000

TS3

46	-2.157027000	-0.316996000	-0.471946000
6	-3.278022000	-1.900921000	-1.187676000
1	-4.154073000	-1.452140000	-1.651074000
1	-2.662629000	-2.355118000	-1.963393000
6	-3.641406000	-2.841823000	-0.019818000
6	-3.730899000	-4.292314000	-0.550051000
1	-4.088343000	-4.979636000	0.224138000
1	-4.432896000	-4.347612000	-1.389009000
1	-2.758522000	-4.657376000	-0.896627000
6	-5.030038000	-2.422563000	0.528022000
1	-5.791521000	-2.523239000	-0.252847000

1	-5.328688000	-3.045343000	1.376702000
1	-5.018488000	-1.379835000	0.859077000
6	-2.620245000	-2.701096000	1.107443000
6	-2.707719000	-3.469851000	2.277213000
6	-1.653654000	-1.675714000	1.059319000
6	-1.884149000	-3.219549000	3.373759000
1	-3.451216000	-4.259923000	2.342002000
6	-0.836495000	-1.412077000	2.165775000
6	-0.958624000	-2.174202000	3.325991000
1	-1.970445000	-3.833129000	4.265961000
1	-0.083104000	-0.633773000	2.100184000
1	-0.322716000	-1.962955000	4.181070000
6	2.823070000	0.281492000	-0.439925000
6	3.712712000	2.211689000	-0.122695000
6	4.775941000	1.283072000	-0.048956000
7	4.189028000	0.036842000	-0.260215000
7	2.520684000	1.558045000	-0.364245000
6	3.964053000	3.580639000	0.049978000
1	3.151473000	4.296939000	-0.013484000
6	6.091307000	1.669551000	0.221439000
1	6.897078000	0.946969000	0.294793000
6	5.271503000	3.974673000	0.305902000
1	5.497035000	5.027708000	0.444668000
6	6.317961000	3.032088000	0.393827000
1	7.326276000	3.377840000	0.601428000
6	1.832031000	-0.768042000	-0.755595000
6	2.133489000	-1.891994000	-1.532070000
7	0.588149000	-0.564762000	-0.278882000
6	1.116843000	-2.816888000	-1.777341000
1	3.128186000	-2.042471000	-1.932165000
6	-0.377293000	-1.416519000	-0.548948000
6	-0.161273000	-2.599768000	-1.276834000
1	1.322239000	-3.707455000	-2.364528000
1	-0.949082000	-3.319665000	-1.445253000
6	4.866520000	-1.211968000	-0.110697000
6	4.489794000	-2.101100000	0.901721000
6	5.926718000	-1.527290000	-0.967841000
6	5.164562000	-3.313395000	1.041392000
1	3.677335000	-1.837265000	1.570880000
6	6.606406000	-2.736099000	-0.810624000
1	6.204758000	-0.830015000	-1.751752000
6	6.224316000	-3.632589000	0.189269000
1	4.867869000	-4.004161000	1.824849000
1	7.429502000	-2.978712000	-1.475993000
1	6.751420000	-4.574628000	0.305808000
35	-3.423356000	1.187951000	-2.063200000
6	-2.591411000	5.038969000	1.493549000
1	-3.061100000	5.668795000	2.249778000
6	-1.281360000	5.231286000	1.294189000
1	-0.812388000	6.015648000	1.890780000
6	-2.162109000	1.899757000	1.456174000

1	-2.110062000	1.099730000	2.194632000
6	-1.035858000	2.124105000	0.743498000
1	-0.175450000	1.501553000	0.974626000
6	-0.318661000	4.535611000	0.362463000
6	-0.755083000	3.200070000	-0.278926000
6	-3.518712000	4.043749000	0.830306000
6	-3.481967000	2.634043000	1.458103000
1	0.614085000	4.363684000	0.919386000
1	0.074218000	2.850662000	-0.901504000
1	-3.807744000	2.703724000	2.505787000
1	-3.332980000	3.966975000	-0.241548000
1	-4.233703000	2.012041000	0.953093000
1	-4.546793000	4.413111000	0.925725000
1	-1.604528000	3.348450000	-0.945096000
1	-0.042819000	5.233082000	-0.444192000

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46	1.595120000	-0.843153000	-0.831298000
6	3.489557000	-0.244984000	-1.271336000
1	3.924580000	-1.045649000	-1.870645000
1	3.344626000	0.626669000	-1.923043000
6	4.425492000	0.076612000	-0.106394000
6	5.789148000	0.491650000	-0.736341000
1	6.543784000	0.701107000	0.028941000
1	6.166618000	-0.316376000	-1.371244000
1	5.681115000	1.389104000	-1.354967000
6	4.637054000	-1.215723000	0.723499000
1	4.844854000	-2.050019000	0.048589000
1	5.473942000	-1.134925000	1.423632000
1	3.735113000	-1.473362000	1.284577000
6	3.973533000	1.236248000	0.810228000
6	4.762079000	1.440620000	1.961208000
6	2.924766000	2.165673000	0.588314000
6	4.559985000	2.475460000	2.865190000
1	5.580669000	0.756361000	2.149613000
6	2.736007000	3.220549000	1.515220000
6	3.529146000	3.383996000	2.641516000
1	5.204801000	2.568353000	3.734418000
1	1.913650000	3.910292000	1.353560000
1	3.337617000	4.200820000	3.330733000
6	-1.101114000	0.247386000	-1.190541000
6	-1.721961000	-1.811560000	-0.894166000
6	-2.878181000	-1.090295000	-1.264190000
7	-2.460391000	0.228106000	-1.455394000
7	-0.650258000	-0.947897000	-0.846846000
6	-1.787395000	-3.188302000	-0.634366000
1	-0.886897000	-3.736552000	-0.379362000
6	-4.134666000	-1.694523000	-1.359607000
1	-5.021154000	-1.131502000	-1.630421000

6	-3.032314000	-3.794064000	-0.740698000
1	-3.124954000	-4.858713000	-0.550340000
6	-4.186276000	-3.059017000	-1.092490000
1	-5.140234000	-3.573443000	-1.159228000
6	-0.186532000	1.399529000	-1.269761000
6	-0.476867000	2.603661000	-1.913442000
7	1.009585000	1.192390000	-0.650761000
6	0.484252000	3.612806000	-1.893194000
1	-1.412697000	2.738333000	-2.437904000
6	1.871499000	2.217120000	-0.482097000
6	1.642286000	3.436940000	-1.147023000
1	0.310494000	4.541083000	-2.428663000
1	2.372929000	4.231939000	-1.055869000
6	-3.354513000	1.326679000	-1.673285000
6	-3.616097000	2.224439000	-0.633516000
6	-3.980891000	1.466063000	-2.915509000
6	-4.498227000	3.282652000	-0.852484000
1	-3.136714000	2.080435000	0.330452000
6	-4.869720000	2.523045000	-3.120052000
1	-3.763171000	0.756473000	-3.707466000
6	-5.124553000	3.433460000	-2.092344000
1	-4.703815000	3.983903000	-0.049442000
1	-5.357245000	2.636034000	-4.083509000
1	-5.813873000	4.256380000	-2.255574000
35	2.137530000	-3.230625000	-1.324656000
6	-2.160578000	-1.815132000	4.583509000
1	-1.601747000	-2.345334000	5.354943000
6	-3.351812000	-1.328277000	4.952244000
1	-3.656428000	-1.526725000	5.980907000
6	-1.512008000	0.891185000	3.015456000
1	-0.893748000	1.786308000	3.101375000
6	-2.835696000	1.091854000	2.934177000
1	-3.171115000	2.129007000	2.997153000
6	-4.377024000	-0.536635000	4.177096000
6	-3.949854000	0.071980000	2.824855000
6	-1.450557000	-1.716566000	3.249512000
6	-0.705247000	-0.382696000	3.029356000
1	-4.731239000	0.275045000	4.829219000
1	-4.829160000	0.567560000	2.395761000
1	0.055525000	-0.275195000	3.815896000
1	-2.131068000	-1.907386000	2.416535000
1	-0.134920000	-0.449430000	2.090924000
1	-0.702449000	-2.515645000	3.198771000
1	-3.694974000	-0.724567000	2.122466000
1	-5.260674000	-1.172655000	4.011618000

TS4

46	-2.045353000	-0.297868000	0.331814000
6	-1.010443000	-1.759267000	1.736889000

1	-1.697456000	-2.574296000	1.506622000
1	0.001068000	-2.151616000	1.783034000
6	-1.316497000	-0.998858000	3.058598000
6	-0.474221000	-1.666938000	4.168388000
1	-0.736643000	-1.276861000	5.157006000
1	-0.661319000	-2.746058000	4.186944000
1	0.596273000	-1.503218000	4.009349000
6	-2.813615000	-1.149666000	3.427431000
1	-3.076023000	-2.204726000	3.563013000
1	-3.026628000	-0.617812000	4.360466000
1	-3.465017000	-0.745608000	2.647763000
6	-0.974700000	0.476082000	2.870377000
6	-0.481307000	1.297120000	3.892102000
6	-1.191020000	1.039600000	1.602273000
6	-0.190084000	2.641004000	3.651477000
1	-0.309118000	0.885018000	4.882310000
6	-0.875984000	2.370692000	1.347405000
6	-0.380376000	3.175978000	2.379218000
1	0.197527000	3.262250000	4.453821000
1	-0.988837000	2.802072000	0.358574000
1	-0.136921000	4.215545000	2.177687000
6	3.050213000	0.507565000	-0.536396000
6	4.070367000	2.386868000	-0.358088000
6	5.085969000	1.413749000	-0.503880000
7	4.412086000	0.199573000	-0.624228000
7	2.823497000	1.791298000	-0.384631000
6	4.412734000	3.738419000	-0.210812000
1	3.635608000	4.487864000	-0.102026000
6	6.444530000	1.739067000	-0.480468000
1	7.216347000	0.982323000	-0.572795000
6	5.761700000	4.072695000	-0.201380000
1	6.056588000	5.111681000	-0.088018000
6	6.761930000	3.086458000	-0.330562000
1	7.806100000	3.384515000	-0.311640000
6	1.973733000	-0.494573000	-0.699622000
6	2.023747000	-1.487479000	-1.685472000
7	0.911887000	-0.361111000	0.117753000
6	0.934945000	-2.350947000	-1.812313000
1	2.886395000	-1.578581000	-2.335110000
6	-0.126506000	-1.151892000	-0.044112000
6	-0.170636000	-2.203405000	-0.979445000
1	0.940967000	-3.133621000	-2.565618000
1	-1.040788000	-2.842317000	-1.059362000
6	5.032537000	-1.085183000	-0.649164000
6	4.764264000	-2.017082000	0.359502000
6	5.926126000	-1.400016000	-1.679380000
6	5.379603000	-3.267993000	0.324655000
1	4.083581000	-1.753855000	1.162501000
6	6.549266000	-2.648411000	-1.697122000
1	6.119523000	-0.670806000	-2.459704000
6	6.274526000	-3.585776000	-0.699584000

1	5.167181000	-3.991044000	1.106427000
1	7.243051000	-2.889835000	-2.496847000
1	6.756465000	-4.558509000	-0.718850000
35	-3.632068000	-2.235095000	-0.641528000
6	-5.942153000	2.029304000	-2.366744000
1	-6.818845000	2.669006000	-2.264047000
6	-5.010094000	2.438413000	-3.237194000
1	-5.223853000	3.359541000	-3.780582000
6	-3.747335000	1.441291000	-0.222069000
1	-3.431476000	2.061745000	0.613800000
6	-2.855454000	1.357334000	-1.261436000
1	-1.946242000	1.946679000	-1.162684000
6	-3.681185000	1.822032000	-3.607141000
6	-3.073914000	0.779740000	-2.638761000
6	-5.940382000	0.800441000	-1.484438000
6	-5.188079000	0.985539000	-0.146893000
1	-2.960213000	2.641168000	-3.739430000
1	-2.101850000	0.475483000	-3.042446000
1	-5.714144000	1.734863000	0.459311000
1	-5.545602000	-0.074597000	-2.001491000
1	-5.244430000	0.043319000	0.411215000
1	-6.977351000	0.550135000	-1.232844000
1	-3.677347000	-0.123905000	-2.593714000
1	-3.763469000	1.354522000	-4.599911000

Prod_2

46	-0.279697000	0.281422000	-0.851641000
6	-0.574440000	3.310719000	-1.667778000
1	-0.230566000	2.449209000	-2.249112000
1	-0.845845000	4.098465000	-2.380153000
6	0.607875000	3.852964000	-0.821124000
6	0.141109000	5.174695000	-0.163135000
1	0.968991000	5.737031000	0.272953000
1	-0.315981000	5.826526000	-0.916949000
1	-0.592771000	4.996014000	0.629014000
6	1.748469000	4.166376000	-1.821397000
1	1.421224000	4.888682000	-2.579591000
1	2.611239000	4.588910000	-1.298714000
1	2.079504000	3.255583000	-2.329356000
6	1.148705000	2.851243000	0.225251000
6	1.964318000	3.395766000	1.242529000
6	0.978882000	1.449615000	0.212598000
6	2.573179000	2.621374000	2.222124000
1	2.136681000	4.466481000	1.264977000
6	1.604736000	0.671036000	1.206580000
6	2.386557000	1.241282000	2.209314000
1	3.189683000	3.094232000	2.981741000
1	1.491959000	-0.406063000	1.187254000
1	2.858177000	0.604899000	2.952917000

6	-3.104101000	-0.431600000	-0.298188000
6	-2.429525000	-2.409684000	-0.882372000
6	-3.628521000	-2.588844000	-0.157623000
7	-4.046862000	-1.307674000	0.208886000
7	-2.139830000	-1.063317000	-0.955709000
6	-1.726249000	-3.510925000	-1.390993000
1	-0.794691000	-3.358533000	-1.925318000
6	-4.165048000	-3.854492000	0.093305000
1	-5.079599000	-3.987094000	0.661018000
6	-2.261294000	-4.769128000	-1.150899000
1	-1.745306000	-5.648095000	-1.524367000
6	-3.459613000	-4.937411000	-0.421488000
1	-3.838824000	-5.940907000	-0.253249000
6	-3.118653000	1.037431000	-0.270187000
6	-4.238440000	1.842103000	-0.046551000
7	-1.933076000	1.582099000	-0.646116000
6	-4.118670000	3.216086000	-0.253710000
1	-5.184388000	1.405330000	0.244216000
6	-1.835284000	2.885242000	-0.960803000
6	-2.925617000	3.739284000	-0.741947000
1	-4.972374000	3.864933000	-0.083517000
1	-2.835853000	4.792569000	-0.982418000
6	-5.141590000	-1.029806000	1.088978000
6	-4.892606000	-0.553845000	2.380343000
6	-6.450033000	-1.265510000	0.655766000
6	-5.964689000	-0.296136000	3.234552000
1	-3.869302000	-0.393639000	2.704869000
6	-7.515349000	-1.015618000	1.522267000
1	-6.622409000	-1.633783000	-0.350557000
6	-7.274826000	-0.527675000	2.808525000
1	-5.774166000	0.076014000	4.236425000
1	-8.532336000	-1.197812000	1.188770000
1	-8.106138000	-0.331288000	3.478667000
35	1.534625000	-1.266695000	-1.616320000
6	8.187384000	-1.980916000	-0.332767000
1	8.511811000	-2.179688000	-1.354493000
6	8.823063000	-0.989922000	0.304219000
1	9.619713000	-0.493062000	-0.251954000
6	5.383303000	-0.933394000	0.796176000
1	4.474688000	-0.424625000	0.474734000
6	6.064566000	-0.362085000	1.797403000
1	5.658484000	0.574920000	2.179332000
6	8.628141000	-0.423563000	1.689269000
6	7.349073000	-0.813898000	2.460604000
6	7.045583000	-2.852090000	0.146126000
6	5.655082000	-2.193718000	0.013784000
1	8.660592000	0.672429000	1.604944000
1	7.409840000	-0.344796000	3.450419000
1	5.472972000	-1.966158000	-1.045577000
1	7.204305000	-3.187229000	1.173823000
1	4.885288000	-2.936634000	0.273113000

1	7.034778000	-3.765520000	-0.460666000
1	7.344913000	-1.889957000	2.649248000
1	9.505396000	-0.685928000	2.302311000

Crystallographic Structure Determination.

A suitable single crystal of **3a** was obtained by slow diffusion of CH_2Cl_2/hexanes at room temperature. The crystal was coated with dry perfluoropolyether and was mounted on a glass fiber under a cold nitrogen stream [100(2) K]. Intensity data were collected on a Bruker-Nonius X8Apex-II CCD diffractometer equipped with a Mo $K_{\alpha 1}$ radiation (λ= 0.71073Å) source and graphite monochromator. All structur was solved by direct methods with SHELXL-97[13] and refined by full-matrix least-squares procedures utilizing SHELXL-97.[14]

Table 1. Crystal data and structure refinement for CCDC 831992.

Empirical formula	C_{28} H_{24} Br N_3 Pd	
Formula weight	588.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.3675(7) Å	α= 90°.
	b = 8.5040(4) Å	β= 90.387(2)°.
	c = 21.0854(11) Å	γ = 90°.
Volume	2396.9(2) $Å^3$	
Z	4	
Density (calculated)	1.632 Mg/m^3	
Absorption coefficient	2.463 mm^{-1}	
F(000)	1176	
Crystal size	0.31 x 0.28 x 0.20 mm^3	
Theta range for data collection	2.45 to 30.48°.	
Index ranges	-17<=h<=19, -12<=k<=12, -19<=l<=30	
Reflections collected	49938	
Independent reflections	7288 [R(int) = 0.0241]	
Completeness to theta = 30.48°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6187 and 0.4857	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7288 / 0 / 300	
Goodness-of-fit on F^2	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.0229, wR2 = 0.0516	
R indices (all data)	R1 = 0.0294, wR2 = 0.0536	
Largest diff. peak and hole	0.875 and -0.632 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ea01107a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	7955(1)	10358(1)	3383(1)	12(1)
Br(1)	6955(1)	11855(1)	4136(1)	22(1)
N(3)	8761(1)	9265(2)	2656(1)	13(1)
N(1)	7329(1)	11462(2)	2542(1)	14(1)
N(2)	6745(1)	10670(2)	1595(1)	16(1)
C(23)	6499(1)	9644(2)	1073(1)	17(1)
C(5)	11277(1)	9277(2)	3120(1)	18(1)
C(4)	10324(1)	8674(2)	3252(1)	16(1)
C(13)	9541(1)	7816(2)	1575(1)	16(1)
C(15)	8280(1)	9345(2)	2080(1)	13(1)
C(3)	10080(1)	8216(2)	3876(1)	20(1)
C(2)	9047(1)	7588(2)	4062(1)	21(1)
C(16)	7426(1)	10430(2)	2075(1)	14(1)
C(11)	9665(1)	8559(2)	2679(1)	14(1)
C(6)	11992(1)	9491(2)	3594(1)	23(1)
C(27)	6327(2)	9193(2)	-43(1)	27(1)
C(24)	6189(1)	8117(2)	1201(1)	22(1)
C(17)	6556(1)	12457(2)	2363(1)	16(1)
C(28)	6563(1)	10205(2)	456(1)	22(1)
C(12)	10061(1)	7819(2)	2143(1)	15(1)
C(8)	10828(2)	8428(3)	4340(1)	28(1)
C(25)	5976(1)	7120(2)	700(1)	25(1)
C(14)	8644(1)	8628(2)	1537(1)	16(1)
C(18)	6184(1)	11977(2)	1769(1)	17(1)
C(1)	8344(1)	8999(2)	4132(1)	20(1)
C(26)	6054(1)	7648(2)	79(1)	26(1)
C(10)	8637(2)	6336(2)	3601(1)	26(1)
C(7)	11761(1)	9059(3)	4207(1)	29(1)
C(9)	9085(2)	6790(3)	4722(1)	35(1)
C(22)	6162(1)	13779(2)	2664(1)	23(1)
C(19)	5397(1)	12743(2)	1463(1)	24(1)
C(20)	5009(1)	14048(3)	1765(1)	30(1)
C(21)	5397(2)	14564(2)	2351(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for CCDC 831992.

Pd(1)-C(1)	2.0217(16)	N(1)-C(17)	1.386(2)
Pd(1)-N(3)	2.0972(13)	N(2)-C(16)	1.373(2)
Pd(1)-N(1)	2.1692(13)	N(2)-C(18)	1.391(2)
Pd(1)-Br(1)	2.4392(2)	N(2)-C(23)	1.440(2)
N(3)-C(11)	1.349(2)	C(23)-C(28)	1.389(2)
N(3)-C(15)	1.374(2)	C(23)-C(24)	1.390(2)
N(1)-C(16)	1.326(2)	C(5)-C(6)	1.390(2)

C(5)-C(4)	1.403(2)	C(1)-Pd(1)-N(1)	168.93(7)
C(5)-H(5)	0.9500	N(3)-Pd(1)-N(1)	77.97(5)
C(4)-C(3)	1.412(2)	C(1)-Pd(1)-Br(1)	85.95(5)
C(4)-C(11)	1.494(2)	N(3)-Pd(1)-Br(1)	173.27(4)
C(13)-C(12)	1.381(2)	N(1)-Pd(1)-Br(1)	95.50(4)
C(13)-C(14)	1.385(2)	C(11)-N(3)-C(15)	117.88(13)
C(13)-H(13)	0.9500	C(11)-N(3)-Pd(1)	129.46(11)
C(15)-C(14)	1.387(2)	C(15)-N(3)-Pd(1)	112.64(10)
C(15)-C(16)	1.467(2)	C(16)-N(1)-C(17)	106.18(13)
C(3)-C(8)	1.405(2)	C(16)-N(1)-Pd(1)	106.37(10)
C(3)-C(2)	1.534(3)	C(17)-N(1)-Pd(1)	140.31(11)
C(2)-C(1)	1.532(2)	C(16)-N(2)-C(18)	106.22(13)
C(2)-C(10)	1.540(3)	C(16)-N(2)-C(23)	128.37(14)
C(2)-C(9)	1.548(3)	C(18)-N(2)-C(23)	124.40(14)
C(11)-C(12)	1.400(2)	C(28)-C(23)-C(24)	121.50(16)
C(6)-C(7)	1.382(3)	C(28)-C(23)-N(2)	119.51(16)
C(6)-H(6)	0.9500	C(24)-C(23)-N(2)	118.98(15)
C(27)-C(26)	1.388(3)	C(6)-C(5)-C(4)	121.75(17)
C(27)-C(28)	1.393(3)	C(6)-C(5)-H(5)	119.1
C(27)-H(27)	0.9500	C(4)-C(5)-H(5)	119.1
C(24)-C(25)	1.384(3)	C(5)-C(4)-C(3)	120.10(15)
C(24)-H(24)	0.9500	C(5)-C(4)-C(11)	113.21(15)
C(17)-C(22)	1.395(2)	C(3)-C(4)-C(11)	126.68(16)
C(17)-C(18)	1.406(2)	C(12)-C(13)-C(14)	118.66(15)
C(28)-H(28)	0.9500	C(12)-C(13)-H(13)	120.7
C(12)-H(12)	0.9500	C(14)-C(13)-H(13)	120.7
C(8)-C(7)	1.388(3)	N(3)-C(15)-C(14)	122.88(14)
C(8)-H(8)	0.9500	N(3)-C(15)-C(16)	113.35(14)
C(25)-C(26)	1.387(3)	C(14)-C(15)-C(16)	123.27(14)
C(25)-H(25)	0.9500	C(8)-C(3)-C(4)	116.44(17)
C(14)-H(14)	0.9500	C(8)-C(3)-C(2)	120.30(16)
C(18)-C(19)	1.393(2)	C(4)-C(3)-C(2)	123.21(15)
C(1)-H(1A)	0.9900	C(1)-C(2)-C(3)	107.83(15)
C(1)-H(1B)	0.9900	C(1)-C(2)-C(10)	112.70(15)
C(26)-H(26)	0.9500	C(3)-C(2)-C(10)	113.41(15)
C(10)-H(10A)	0.9800	C(1)-C(2)-C(9)	105.85(15)
C(10)-H(10B)	0.9800	C(3)-C(2)-C(9)	110.98(15)
C(10)-H(10C)	0.9800	C(10)-C(2)-C(9)	105.84(16)
C(7)-H(7)	0.9500	N(1)-C(16)-N(2)	112.47(14)
C(9)-H(9A)	0.9800	N(1)-C(16)-C(15)	119.45(14)
C(9)-H(9B)	0.9800	N(2)-C(16)-C(15)	127.56(14)
C(9)-H(9C)	0.9800	N(3)-C(11)-C(12)	120.95(14)
C(22)-C(21)	1.385(3)	N(3)-C(11)-C(4)	121.48(14)
C(22)-H(22)	0.9500	C(12)-C(11)-C(4)	117.30(14)
C(19)-C(20)	1.383(3)	C(7)-C(6)-C(5)	118.74(18)
C(19)-H(19)	0.9500	C(7)-C(6)-H(6)	120.6
C(20)-C(21)	1.407(3)	C(5)-C(6)-H(6)	120.6
C(20)-H(20)	0.9500	C(26)-C(27)-C(28)	120.24(17)
C(21)-H(21)	0.9500	C(26)-C(27)-H(27)	119.9
		C(28)-C(27)-H(27)	119.9
C(1)-Pd(1)-N(3)	100.77(6)	C(25)-C(24)-C(23)	118.96(17)

C(25)-C(24)-H(24)	120.5	C(20)-C(19)-H(19)	121.8
C(23)-C(24)-H(24)	120.5	C(18)-C(19)-H(19)	121.8
N(1)-C(17)-C(22)	130.63(16)	C(19)-C(20)-C(21)	121.24(17)
N(1)-C(17)-C(18)	108.87(14)	C(19)-C(20)-H(20)	119.4
C(22)-C(17)-C(18)	120.47(15)	C(21)-C(20)-H(20)	119.4
C(23)-C(28)-C(27)	118.69(17)	C(22)-C(21)-C(20)	122.33(18)
C(23)-C(28)-H(28)	120.7	C(22)-C(21)-H(21)	118.8
C(27)-C(28)-H(28)	120.7	C(20)-C(21)-H(21)	118.8
C(13)-C(12)-C(11)	120.67(15)		
C(13)-C(12)-H(12)	119.7		
C(11)-C(12)-H(12)	119.7		
C(7)-C(8)-C(3)	123.08(18)		
C(7)-C(8)-H(8)	118.5		
C(3)-C(8)-H(8)	118.5		
C(24)-C(25)-C(26)	120.41(18)		
C(24)-C(25)-H(25)	119.8		
C(26)-C(25)-H(25)	119.8		
C(13)-C(14)-C(15)	118.68(15)		
C(13)-C(14)-H(14)	120.7		
C(15)-C(14)-H(14)	120.7		
N(2)-C(18)-C(19)	131.12(17)		
N(2)-C(18)-C(17)	106.25(14)		
C(19)-C(18)-C(17)	122.62(17)		
C(2)-C(1)-Pd(1)	121.80(11)		
C(2)-C(1)-H(1A)	106.9		
Pd(1)-C(1)-H(1A)	106.9		
C(2)-C(1)-H(1B)	106.9		
Pd(1)-C(1)-H(1B)	106.9		
H(1A)-C(1)-H(1B)	106.7		
C(25)-C(26)-C(27)	120.12(18)		
C(25)-C(26)-H(26)	119.9		
C(27)-C(26)-H(26)	119.9		
C(2)-C(10)-H(10A)	109.5		
C(2)-C(10)-H(10B)	109.5		
H(10A)-C(10)-H(10B)	109.5		
C(2)-C(10)-H(10C)	109.5		
H(10A)-C(10)-H(10C)	109.5		
H(10B)-C(10)-H(10C)	109.5		
C(6)-C(7)-C(8)	119.87(17)		
C(6)-C(7)-H(7)	120.1		
C(8)-C(7)-H(7)	120.1		
C(2)-C(9)-H(9A)	109.5		
C(2)-C(9)-H(9B)	109.5		
H(9A)-C(9)-H(9B)	109.5		
C(2)-C(9)-H(9C)	109.5		
H(9A)-C(9)-H(9C)	109.5		
H(9B)-C(9)-H(9C)	109.5		
C(21)-C(22)-C(17)	116.83(18)		
C(21)-C(22)-H(22)	121.6		
C(17)-C(22)-H(22)	121.6		
C(20)-C(19)-C(18)	116.46(18)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for CCDC 831992. 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)	12(1)	13(1)	11(1)	-1(1)	0(1)	1(1)
Br(1)	25(1)	27(1)	15(1)	-5(1)	1(1)	9(1)
N(3)	15(1)	12(1)	12(1)	0(1)	-1(1)	0(1)
N(1)	14(1)	15(1)	14(1)	2(1)	2(1)	2(1)
N(2)	16(1)	17(1)	15(1)	3(1)	-3(1)	1(1)
C(23)	15(1)	20(1)	16(1)	1(1)	-5(1)	0(1)
C(5)	17(1)	18(1)	18(1)	-3(1)	-3(1)	5(1)
C(4)	19(1)	15(1)	15(1)	-3(1)	-3(1)	6(1)
C(13)	19(1)	15(1)	15(1)	-3(1)	1(1)	0(1)
C(15)	14(1)	13(1)	13(1)	0(1)	-1(1)	-1(1)
C(3)	23(1)	22(1)	15(1)	-1(1)	-2(1)	9(1)
C(2)	26(1)	24(1)	14(1)	6(1)	1(1)	7(1)
C(16)	14(1)	15(1)	12(1)	3(1)	-1(1)	-1(1)
C(11)	16(1)	12(1)	14(1)	1(1)	-1(1)	1(1)
C(6)	17(1)	26(1)	26(1)	-10(1)	-5(1)	7(1)
C(27)	33(1)	32(1)	16(1)	3(1)	-7(1)	0(1)
C(24)	22(1)	24(1)	19(1)	5(1)	-4(1)	-3(1)
C(17)	14(1)	18(1)	17(1)	6(1)	2(1)	3(1)
C(28)	26(1)	22(1)	18(1)	5(1)	-3(1)	-1(1)
C(12)	15(1)	14(1)	17(1)	0(1)	1(1)	2(1)
C(8)	28(1)	40(1)	14(1)	-2(1)	-5(1)	12(1)
C(25)	23(1)	23(1)	30(1)	2(1)	-9(1)	-4(1)
C(14)	18(1)	18(1)	13(1)	-1(1)	-2(1)	0(1)
C(18)	14(1)	18(1)	19(1)	6(1)	2(1)	2(1)
C(1)	23(1)	25(1)	12(1)	4(1)	1(1)	6(1)
C(26)	26(1)	30(1)	23(1)	-4(1)	-10(1)	1(1)
C(10)	33(1)	18(1)	28(1)	6(1)	4(1)	3(1)
C(7)	24(1)	39(1)	22(1)	-10(1)	-10(1)	13(1)
C(9)	38(1)	43(1)	24(1)	17(1)	3(1)	12(1)
C(22)	25(1)	23(1)	20(1)	4(1)	6(1)	9(1)
C(19)	18(1)	31(1)	24(1)	10(1)	-2(1)	5(1)
C(20)	22(1)	37(1)	30(1)	15(1)	4(1)	14(1)
C(21)	32(1)	29(1)	29(1)	8(1)	10(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 831992.

	x	y	z	U(eq)
H(5)	11438	9546	2696	21
H(13)	9793	7268	1218	19
H(6)	12628	9927	3497	28
H(27)	6353	9562	-467	32
H(24)	6124	7764	1626	26
H(28)	6763	11257	375	26
H(12)	10693	7314	2171	18
H(8)	10688	8126	4764	33
H(25)	5776	6068	780	30
H(14)	8285	8693	1148	20
H(1A)	8648	9704	4453	24
H(1B)	7715	8596	4317	24
H(26)	5919	6950	-263	32
H(10A)	8029	5869	3778	39
H(10B)	9141	5514	3540	39
H(10C)	8479	6828	3192	39
H(7)	12240	9192	4538	34
H(9A)	9244	7578	5046	52
H(9B)	9601	5972	4723	52
H(9C)	8434	6315	4813	52
H(22)	6408	14124	3065	27
H(19)	5140	12388	1066	29
H(20)	4470	14606	1574	36
H(21)	5124	15483	2539	36

Table 6. Torsion angles [°] for CCDC 831992.

C(1)-Pd(1)-N(3)-C(11)	-34.38(15)
N(1)-Pd(1)-N(3)-C(11)	156.84(15)
C(1)-Pd(1)-N(3)-C(15)	147.42(11)
N(1)-Pd(1)-N(3)-C(15)	-21.36(11)
C(1)-Pd(1)-N(1)-C(16)	-56.9(3)
N(3)-Pd(1)-N(1)-C(16)	27.69(10)
Br(1)-Pd(1)-N(1)-C(16)	-153.95(10)
C(1)-Pd(1)-N(1)-C(17)	87.1(4)
N(3)-Pd(1)-N(1)-C(17)	171.65(18)
Br(1)-Pd(1)-N(1)-C(17)	-9.99(18)
C(16)-N(2)-C(23)-C(28)	-125.06(19)
C(18)-N(2)-C(23)-C(28)	68.0(2)
C(16)-N(2)-C(23)-C(24)	55.8(2)
C(18)-N(2)-C(23)-C(24)	-111.09(19)
C(6)-C(5)-C(4)-C(3)	-2.2(3)
C(6)-C(5)-C(4)-C(11)	179.19(15)
C(11)-N(3)-C(15)-C(14)	5.2(2)
Pd(1)-N(3)-C(15)-C(14)	-176.33(13)
C(11)-N(3)-C(15)-C(16)	-166.87(14)
Pd(1)-N(3)-C(15)-C(16)	11.55(16)
C(5)-C(4)-C(3)-C(8)	1.1(2)
C(11)-C(4)-C(3)-C(8)	179.58(16)
C(5)-C(4)-C(3)-C(2)	178.34(16)
C(11)-C(4)-C(3)-C(2)	-3.2(3)
C(8)-C(3)-C(2)-C(1)	97.84(19)
C(4)-C(3)-C(2)-C(1)	-79.3(2)
C(8)-C(3)-C(2)-C(10)	-136.64(18)
C(4)-C(3)-C(2)-C(10)	46.3(2)
C(8)-C(3)-C(2)-C(9)	-17.7(2)
C(4)-C(3)-C(2)-C(9)	165.24(17)
C(17)-N(1)-C(16)-N(2)	-0.95(18)
Pd(1)-N(1)-C(16)-N(2)	156.02(11)
C(17)-N(1)-C(16)-C(15)	171.40(14)
Pd(1)-N(1)-C(16)-C(15)	-31.63(17)
C(18)-N(2)-C(16)-N(1)	1.10(18)
C(23)-N(2)-C(16)-N(1)	-167.66(15)
C(18)-N(2)-C(16)-C(15)	-170.49(15)
C(23)-N(2)-C(16)-C(15)	20.7(3)
N(3)-C(15)-C(16)-N(1)	15.1(2)
C(14)-C(15)-C(16)-N(1)	-156.98(16)
N(3)-C(15)-C(16)-N(2)	-173.83(15)
C(14)-C(15)-C(16)-N(2)	14.1(3)
C(15)-N(3)-C(11)-C(12)	-5.2(2)
Pd(1)-N(3)-C(11)-C(12)	176.73(11)
C(15)-N(3)-C(11)-C(4)	168.61(15)
Pd(1)-N(3)-C(11)-C(4)	-9.5(2)
C(5)-C(4)-C(11)-N(3)	-124.02(17)
C(3)-C(4)-C(11)-N(3)	57.4(2)
C(5)-C(4)-C(11)-C(12)	50.0(2)

C(3)-C(4)-C(11)-C(12)	-128.57(18)
C(4)-C(5)-C(6)-C(7)	1.7(3)
C(28)-C(23)-C(24)-C(25)	2.5(3)
N(2)-C(23)-C(24)-C(25)	-178.43(16)
C(16)-N(1)-C(17)-C(22)	-177.53(18)
Pd(1)-N(1)-C(17)-C(22)	38.5(3)
C(16)-N(1)-C(17)-C(18)	0.41(18)
Pd(1)-N(1)-C(17)-C(18)	-143.59(14)
C(24)-C(23)-C(28)-C(27)	-1.2(3)
N(2)-C(23)-C(28)-C(27)	179.65(16)
C(26)-C(27)-C(28)-C(23)	-1.3(3)
C(14)-C(13)-C(12)-C(11)	3.2(2)
N(3)-C(11)-C(12)-C(13)	1.0(2)
C(4)-C(11)-C(12)-C(13)	-172.98(15)
C(4)-C(3)-C(8)-C(7)	0.3(3)
C(2)-C(3)-C(8)-C(7)	-176.96(18)
C(23)-C(24)-C(25)-C(26)	-1.2(3)
C(12)-C(13)-C(14)-C(15)	-3.2(2)
N(3)-C(15)-C(14)-C(13)	-1.0(2)
C(16)-C(15)-C(14)-C(13)	170.29(15)
C(16)-N(2)-C(18)-C(19)	179.88(18)
C(23)-N(2)-C(18)-C(19)	-10.8(3)
C(16)-N(2)-C(18)-C(17)	-0.78(17)
C(23)-N(2)-C(18)-C(17)	168.55(15)
N(1)-C(17)-C(18)-N(2)	0.24(18)
C(22)-C(17)-C(18)-N(2)	178.43(15)
N(1)-C(17)-C(18)-C(19)	179.65(16)
C(22)-C(17)-C(18)-C(19)	-2.2(3)
C(3)-C(2)-C(1)-Pd(1)	65.71(18)
C(10)-C(2)-C(1)-Pd(1)	-60.2(2)
C(9)-C(2)-C(1)-Pd(1)	-175.46(14)
N(3)-Pd(1)-C(1)-C(2)	-0.67(16)
N(1)-Pd(1)-C(1)-C(2)	81.7(4)
Br(1)-Pd(1)-C(1)-C(2)	179.66(15)
C(24)-C(25)-C(26)-C(27)	-1.3(3)
C(28)-C(27)-C(26)-C(25)	2.5(3)
C(5)-C(6)-C(7)-C(8)	-0.2(3)
C(3)-C(8)-C(7)-C(6)	-0.8(3)
N(1)-C(17)-C(22)-C(21)	178.15(18)
C(18)-C(17)-C(22)-C(21)	0.4(3)
N(2)-C(18)-C(19)-C(20)	-178.92(17)
C(17)-C(18)-C(19)-C(20)	1.8(3)
C(18)-C(19)-C(20)-C(21)	0.1(3)
C(17)-C(22)-C(21)-C(20)	1.5(3)
C(19)-C(20)-C(21)-C(22)	-1.8(3)

Symmetry transformations used to generate equivalent atoms:

References

1. Cámpora J.; López J. A.; Palma P.; Valerga P.; Spillner E.; Carmona E., *Angew. Chem. Int. Ed. Engl.* **1999**, *38*, 147.
2. Jovic F, Louise L, Mioskowski C, Renard P. *Tetrahedron Letters* **2005**, *46*, 6809-6814.
3. S. Haneda, Z. Gan, K. Eda, M. Hayashi, *Org. Lett.* **2003**, *5*, 3713.
4. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Gaussian 03, Revision D.01 ed.; Gaussian, Inc.: Wallingford CT, 2004.
5. Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652; Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter* **1998**, *37*, 785-789; Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627; Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Chem.* **1980**, *58*, 1200-1211.
6. Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270-283; Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 284-298.
7. Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213-222; Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257-2261.
8. Roy, L. E.; Hay, P. J.; Martin, R. L. *J. Chem. Theory Comput.* **2008**, *4*, 1029-1031.
9. Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. v. R. *J. Comput. Chem.* **1983**, *4*, 294-301; Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265-3269; Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650-654.
10. Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363-368; Hratchian, H. P.; Schlegel, H. B. In *Theory and Applications of Computational Chemistry: The First 40 Years*; Dykstra, C. E., Frenking, G., Kim, K. S., Scuseria, G., Eds.; Elsevier: Amsterdam, 2005, p 195-249.

11. Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995-2001; Cammi, R.; Mennucci, B.; Tomasi, J. *J. Phys. Chem. A* **1999**, *103*, 9100-9108; Klamt, A.; Schüürmann, G. *J. Chem. Soc. Perkin. Trans 2* **1993**, *2*, 799-805; Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999-3094.
12. Grimme, S.; *J. Comput. Chem.* **2006**, *27*, 1787-1799.
13. Burla, M. C.; Caliandro, R.; Camalli, M.; Carrozzini, B.; Cascarano, G. L.; De Caro, L.; Gaicovazzo, C.; Polidori, G.; Spagna, R.; *J. Appl. Crystallogr*., **2005**, *38*, 381–388.
14. Sheldrick, G. M.; *Acta Crystallogr*., **2008**, *A64*, 112–12.