The version of SI posted May 6, 2004 contained errors. The correct version was posted October 21, 2004.

Sterically Bulky Thioureas as Air and Moisture Stable Ligands for Pd-Catalyzed Heck Reactions of Aryl Halides

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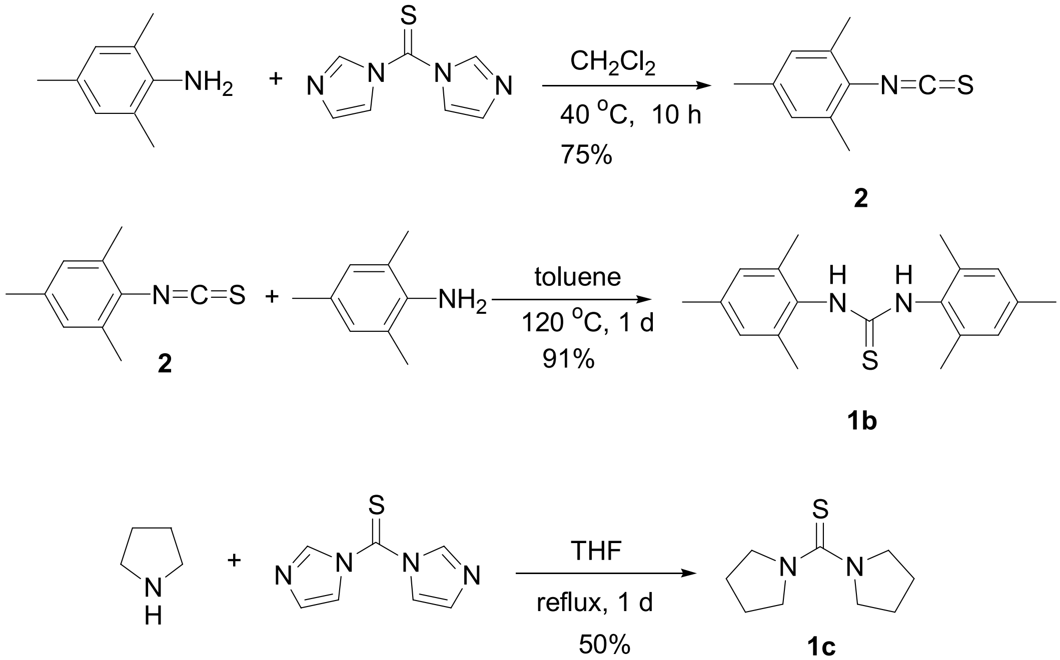
Supporting Information

1. Synthesis of acyclic thiourea ligands:



Scheme 1

Preparation of 1b:

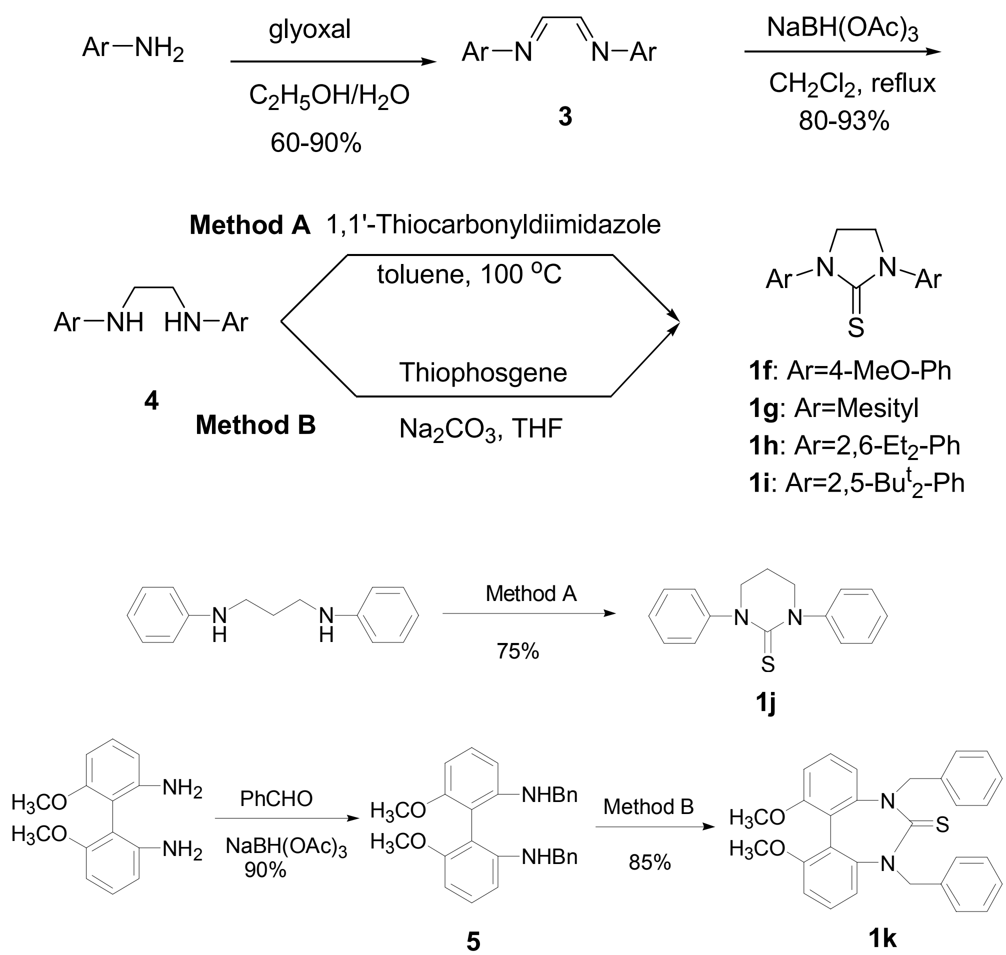
2,4,6-Trimethylaniline (0.16 mL, 1.2 mmol) and 1,1'-thiocarbonyl diimidazole (210 mg, 1.06 mmol) were stirred in dichloromethane (5 mL) at 40 °C for 10 h. 2-Mesityl isothiocyanate **2** was obtained (150 mg, 75%) after flash chromatography on silica gel. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (s, 2H), 2.32 (s, 6H), 2.26 (s, 3H); EI-MS: 177 (M^+, 100).

2-Mesityl isothiocyanate **2** (140 mg, 0.79 mmol) was heated with 2,4,6-trimethyl- aniline (128 mg, 0.95 mmol) in toluene (1 mL) at 120 °C for one day, and TLC analysis indicated that all isothiocyanate had been consumed. Toluene was removed under vacuum, and the residue was recrystalized from hexane to give **1b** as a white solid (223 mg, 91%). M.p. 202-203 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (s, 1H, NH), 6.99 (s, 2H), 6.85 (s, 2H), 6.48 (s, 1H, NH), 2.38 (s, 6H), 2.30 (s, 3H), 2.24 (s, 3H), 2.19 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 181.3, 139.1, 137.7, 137.2, 136.0, 133.1, 130.5, 129.7, 129.0, 21.0, 18.5, 18.0; IR (cm^{-1}): 3405, 3343, 1511, 1420, 1245; LRMS (EI): 312 (M^+, 44), 278 (100); HRMS (EI): calcd for $C_{19}H_{24}N_2S$ 312.1660, found 312.1650.

Preparation of 1c:

Pyrrolidine (0.4 g, 5.6 mmol) and 1,1'-thiocarbonyl diimidazole (0.3 g, 1.7 mmol) were refluxed in THF (5 mL) for 10 h. The crude reaction mixture was concentrated, and flash chromatography on silica gel gave thiourea **1c** as a white solid (160 mg, 50%). M.p. 125−125.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.62−3.59 (m, 4H), 1.92−1.88 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.1, 52.9, 25.6; IR (cm^{-1}): 1436, 1361, 1282, 1271; LRMS (EI): 184 (M^+, 100); HRMS (EI): calcd for $C_9H_{16}N_2S$ 184.1034, found 184.1032.

2. Synthesis of cyclic thioureas



Scheme 2

The *N,N'*-diaryl diamines were prepared following literature procedures.[1] Two methods were used for the synthesis of cyclic thiourea ligands (Scheme 2).

Method A:

To a *N,N'*-diaryl diamine solution in dry toluene was added 1,1'-thiocarbonyl diimidazole (1.2 equiv). Then the solution was stirred at 100°C and the reaction was monitored by TLC. After completion, the solution was diluted with ethyl acetate and washed with dilute HCl and brine. The organic layer was concentrated under vacuum. The pure thiourea was obtained through flash chromatography or recrystallization from 95% ethanol.

Method B:

To a stirred mixture of *N,N'*-diaryl diamine and Na_2CO_3 (1.5 equiv) in dry THF was added a solution of thiophosgene (1.2 equiv) in THF dropwise at room temperature. After stirred at room temperature overnight, water and ethyl acetate were added. The organic layer was washed with dilute HCl and brine, dried and concentrated. The pure thiourea was obtained through flash chromatography or recrystallization from 95% ethanol.

Preparation of 1f:

Using method A; 75% yield. M.p. 167−168 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (d, J = 9.0 Hz, 4H), 6.95 (d, J = 9.0 Hz, 4H), 4.08 (s, 4H), 3.81 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 182.2, 158.1, 138.8, 127.5, 114.2, 55.4, 49.8; IR (cm^{-1}): 1511, 1443, 1285; LRMS (EI): 314 (M^+, 100); HRMS (EI): calcd for $C_{17}H_{18}N_2O_2S$ (M^+) 314.1089, found 314.1088.

Preparation of 1g:

Using method B; 85% yield. M.p. 218−218.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.91 (s, 4H), 3.94 (s, 4H), 2.26 (s, 6H), 2.24 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 181.1, 138.2, 136.6, 134.5, 129.5, 47.6, 21.1, 17.8; IR (cm^{-1}): 1488, 1331, 1271; LRMS (FAB): 339 (M^++1, 100); HRMS (FAB): calcd for $C_{21}H_{26}N_2S$ (M^++1) 339.1894, found 339.1879.

Preparation of 1h:

Using method B; 70% yield. M.p. 152−153 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (t, J = 6.6 Hz, 2H), 7.20 (d, J = 7.5 Hz, 4H), 4.02 (s, 4H), 2.80−2.70 (m, 4H), 2.69−2.60 (m, 4H), 1.33 (t, J = 7.5 Hz, 12H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 182.6, 142.5, 136.1, 128.8, 126.5, 49.1, 24.0, 14.4; IR (cm^{-1}): 1484, 1285; LRMS (EI): 366 (M^+, 39), 337 (100); HRMS (EI): calcd for $C_{23}H_{30}N_2S$ (M^+) 366.2130, found 366.2120.

Preparation of 1i:

Diimine **3i**: 92% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (s, 2H), 7.35 (d, J = 8.3 Hz, 2H), 7.25 (d, J = 8.3 Hz, 2H), 6.86 (s, 2H), 1.43 (s, 18H), 1.34 (s, 18H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6, 150.1, 150.0, 140.4, 126.0, 123.8, 116.0, 35.3, 34.4, 31.3, 30.5; IR (cm^{-1}): 1609, 1492, 1265; LRMS (EI): 432 (M^+, 100); HRMS (EI): calcd for $C_{30}H_{44}N_2$ (M^+) 432.3504, found

432.3504.

Diamine **4i**: 90% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.18 (d, *J* = 6.1 Hz, 2H), 6.80 (s, 2H), 6.75 (d, *J* = 6.1 Hz, 2H), 4.18 (br s, 2H, NH), 3.57 (s, 4H), 1.39 (s, 18H), 1.32 (s, 18H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.9, 146.2, 131.2, 126.0, 114.6, 110.0, 45.0, 34.4, 33.8, 31.4, 30.2; IR (cm^{-1}): 3688, 3601, 1561, 1265; LRMS (EI): 436 (M^+, 20), 219 (100); HRMS (EI): calcd for $C_{30}H_{48}N_2$ (M^+) 436.3817, found 436.3817.

Thiourea **li** was prepared using method B. *A solution of Thiophosgene in dilute THF must be dropped very slowly*. **1i** was isolated as a white solid (75% yield) after flash chromatography on silica gel. M.p. 212–214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.02 (s, 2H), 4.06–4.03 (m, 2H), 3.93–3.91 (m, 2H), 1.50 (s, 18H), 1.30 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.5, 150.4, 145.0, 140.8, 128.0, 127.8, 125.3, 53.4, 35.4, 34.3, 32.1, 31.3; IR (cm^{-1}): 1418, 1275; LRMS (FAB): 479 (M^+ + H); FAB-HRMS: calcd for $C_{31}H_{46}N_2S$ (M^+ + H) 479.3460, found 479.3460.

Preparation of 1j:

Using method A, 75% yield. M.p. 173−174 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41–7.15 (m, 10H), 3.82–3.77 (m, 4H), 2.32–2.24 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 180.7, 147.4, 129.2, 127.4, 125.8, 51.4, 22.3; IR (cm^{-1}): 1494, 1285; LRMS (EI): 268 (M^+, 73); EI-HRMS: calcd for $C_{16}H_{16}N_2S$ (M^+) 268.1034, found 268.1015.

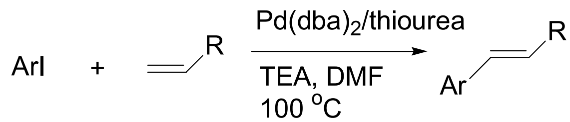
Preparation of 1k:

To a stirred suspension of racemic 2,2’-diamino-6,6’-dimethoxy-biphenyl[2] (60mg, 0.25 mmol) and $NaBH(OAc)_3$ (212 mg, 1 mmol) in dichloromethane (10 mL) was added a solution of benzaldehyde (0.06 ml, 0.58 mmol) in dichloromethane (2 mL) dropwise at room temperature. Then the mixture was stirred overnight. Flash chromatography on silica gel gave *N,N’*-dibenzyl diamine **5** as a white solid (94 mg, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.26–7.11 (m, 12H), 6.38 (d, *J* = 8.2 Hz, 2H), 6.32 (d, *J* = 7.7 Hz, 2H), 4.32 (s, 4H), 4.17 (br s 2H), 3.70 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1, 147.3, 139.9, 129.6, 128.4, 126.7, 126.6, 107.2, 104.2, 100.6, 55.7, 47.5; IR (cm^{-1}): 3432, 3086, 3051, 2938, 1586, 496, 1472, 1422, 1282, 1131; LRMS (EI): 424 (M^+, 33), 333 (100); HRMS (EI): calcd for $C_{28}H_{28}N_2O_2S$ (M^+) 424.2151, found 424.2138.

Thiourea **1k** was prepared using method B, 85% yield. M.p. 179−180 °C; ^{1}H NMR (400 MHz,

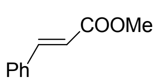
$CDCl_3$) δ 7.27 (t, *J* = 8.2 Hz, 2H), 7.04−7.00 (m, 6H), 6.88 (d, *J* = 8.2 Hz, 2H), 6.83−6.80 (m, 6H), 5.72 (d, *J* = 15.3 Hz, 2H), 4.81 (d, *J* = 15.3 Hz, 2H), 3.75 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.6, 157.2, 147.7, 137.1, 128.7, 127.9, 127.5, 126.7, 121.8, 113.9, 108.8, 56.8, 55.9; IR (cm^{-1}): 3051, 1592, 1579, 1464, 1420, 1245, 1190; LRMS (EI): 466 (M^+, 100), 375 (86); HRMS (EI): calcd for $C_{29}H_{26}N_2O_2S$ (M^+) 466.1715, found 466.1718.

General procedure for Heck reaction of aryl iodides and olefins

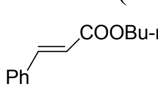


$Pd(dba)_2$ (1.5 mg, 0. 0025 mmol) and thiourea (4 equiv) were stirred in DMF (0.5 mL) for 0.5 h at rt. Iodobenzene (0.28 mL, 2.5 mmol, substrate/catalyst ratio = 1000:1) and methyl acrylate (0.27 mL, 3.0 mmol) and TEA (0.42 mL, 3.0 mmol) were then added. The flask was sealed with rubber septa and heated at 100°C (the same result was obtained when the reaction was conducted with a condenser in open air). After the indicated time, the solution was diluted with ethyl acetate (20 mL) and washed with water and brine. Ethyl acetate was removed under vacuum and nitrobenzene (0.128 mL) was added as an internal standard. The yield of coupling product was determined by ^1H NMR (400 MHz or 300 MHz) analysis, by comparing the peak intensities of the α/β-H of the product and the *ortho*-H of nitrobenzene (internal standard).

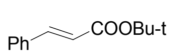
When the reactions were conducted at a lower catalyst loading, the calculated amount of the solution of $Pd(dba)_2$ and thiourea in DMF (0.0025M) was used.



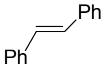
^1H NMR (300 MHz, $CDCl_3$) δ 7.67−7.63 (m, 2H), 7.54 (d, *J* = 4.1 Hz, 2H), 7.38 (d, *J* = 3.3 Hz, 1H), 7.10 (t, *J* = 6.5 Hz, 1H), 6.44 (d, *J* = 16.1 Hz, 1H), 3.81 (s, 3H). To determine the reaction yield, the product peak at 6.44 ppm was selected for comparison with that of the *ortho*-H (at 8.20 ppm) of nitrobenzene (internal standard).



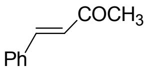
^1H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 16.0 Hz, 1H), 7.52−7.57 (m, 2H), 7.40−7.45 (m, 3H), 6.49 (d, *J* = 16.0 Hz, 1H), 4.26 (t, *J* = 6.9 Hz, 2H), 1.71−1.78 (m, 2H), 1.54−1.45 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).



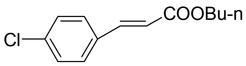
^1H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 16.0 Hz, 1H), 7.53−7.57 (m, 2H), 7.40–7.45 (m, 3H), 6.49 (d, *J* = 16.0 Hz, 1H), 1.34 (s, 9H).



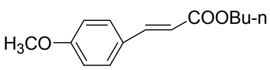
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.2 Hz, 4H), 7.38 (dd, *J* = 7.1, 1.5 Hz, 4H), 7.28 (d, *J* = 7.2 Hz, 2H), 7.13 (s, 2H).



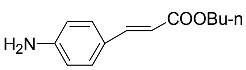
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 9.4 Hz, 2H), 7.52 (d, *J* = 16.0 Hz, 1H), 7.40 (t, *J* = 3.5 Hz, 3H), 6.72 (d, *J* = 16.0 Hz, 1H), 2.39 (s, 3H).



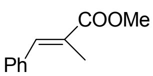
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 16.2 Hz, 1H), 7.43 (d, *J* = 6.2 Hz, 2H), 7.35 (d, *J* = 6.2 Hz, 2H), 6.40 (d, *J* = 16.2 Hz, 1H), 4.26 (t, *J* = 6.9 Hz, 2H), 1.78–1.71 (m, 2H), 1.54–1.45 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).



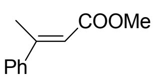
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 16.0 Hz, 1H), 7.51 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 6.36 (d, *J* = 16.0 Hz, 1H), 4.25 (t, *J* = 6.8 Hz, 2H), 3.87 (s, 3H), 1.76–1.70 (m, 2H), 1.52–1.46 (m, 2H), 1.02 (t, *J* = 7.5 Hz, 3H).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 15.7 Hz, 1H), 6.62 (d, *J* = 8.4 Hz, 2H), 6.51 (d, *J* = 15.7 Hz, 1H), 6.17 (s, 2H), 4.26 (t, *J* = 6.9 Hz, 2H), 1.78–1.77 (m, 2H), 1.54–1.45 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H).

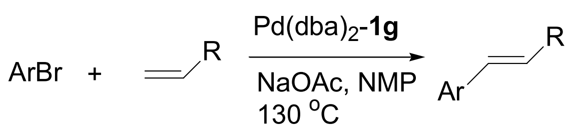


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 6.9 Hz, 2H), 7.40–7.19 (m, 4H), 3.82 (s, 3H), 2.13 (s, 3H).

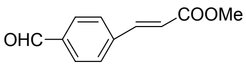


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53–7.45 (m, 3H), 7.37–7.35 (m, 2H), 6.13 (q, *J* = 1.2 Hz, 1H), 3.75 (s, 3H), 2.58 (d, *J* = 1.3 Hz, 3H).

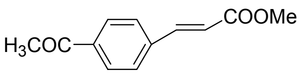
General procedure for Heck reaction of aryl bromides and olefins



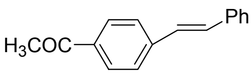
$Pd(dba)_2$ (1.5 mg, 0. 0025 mmol) and thiourea **1g** (3.4 mg, 0.01mmol) were stirred in NMP (0.5 mL) for 0.5 h at rt. Aryl bromide (2.5 mmol, *S/C* = 1000), olefin (3.8 mmol) and sodium acetate 330 mg (3.8 mmol) were added in turn. Then the flask was sealed with a septa and heated at 130°C. After indicated time, the solution was dilute with ethyl acetate (20 mL) and washed with water and brine. Ethyl acetate was removed under vacuum and nitrobenzene (0.128 mL) was added as internal standard. The yield of coupling product was determined by ^{1}H NMR (400 MHz or 300 MHz) analysis, by comparing the peak intensities of the α/β-H of the product and the *ortho*-H of nitrobenzene (internal standard).



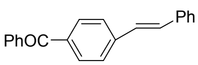
^{1}H NMR (300 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.87 (d, *J* = 8.1 Hz, 2H), 7.70−7.62 (m, 3H), 6.52 (d, *J* = 15.9 Hz, 1H), 3.79 (s, 3H).



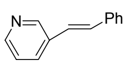
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80−7.75 (m, 3H), 7.42 (d, *J* = 6.8 Hz, 2H), 6.34 (d, *J* = 16.1Hz, 1H), 3.63 (s, 3H), 2.42 (s, 3H).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53−7.45 (m, 4H), 7.36−7.32 (m, 4H), 7.28−7.26 (m, 2H), 7.17 (d, *J* = 12.3 Hz, 1H), 7.07 (d, *J* = 12.3 Hz, 1H), 2.55 (s, 3H).

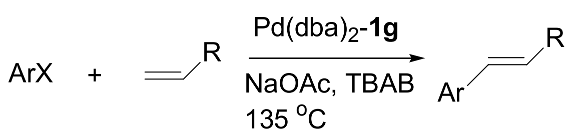


^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85−7.32 (m, 15H), 6.24 (d, *J* = 16.2 Hz, 1H).

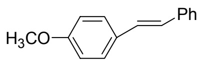


^{1}H NMR (300 MHz, $CDCl_3$) δ 8.70 (d, *J* = 1.3 Hz, 1H), 8.45 (d, *J* = 3.5 Hz, 1H), 7.52 (d, *J* = 9.0 Hz, 1H), 7.36−7.33 (m, 2H), 7.30−7.25 (m, 4H), 7.10 (d, *J* = 16.2 Hz, 1H), 7.00 (d, *J* = 16.2 Hz, 1H).

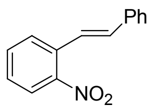
General procedure for Heck reaction of deactivated aryl bromides and activated chlorides with olefins[3]



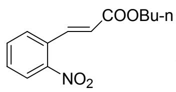
Pd(dba)$_2$ (1.5 mg, 0. 0025 mmol), thiourea **1g** (3.4mg, 0.01mmol) and sodium acetate (33 mg, 3.8 mmol) were stirred in molten TBAB (0.5 g) for 10 min at 100°C. Aryl halide (0.25 mmol, *S/C*=100) and olefin (0.38 mmol) were added in turn. Then the flask was sealed with a septa and heated at 135°C. After indicated time, the solution was dilute with ethyl acetate (20 mL) and washed with water and brine. Ethyl acetate was removed under vacuum and nitrobenzene (0.0128 mL) was added as internal standard. The yield of coupling product was determined by ^{1}H NMR (400 MHz or 300 MHz) analysis, by comparing the peak intensities of the α/β-H of the product and the *ortho*-H of nitrobenzene (internal standard).



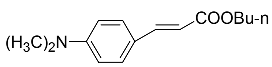
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64−7.52 (m, 4H), 7.45−7.40 (m, 3H), 7.33 (d, *J* = 12.1 Hz, 1H), 7.10 (d, *J* = 12.1 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 2H), 3.88 (s, 3H).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.0 Hz, 1H), 7.74 (d, *J* = 7.0 Hz, 1H), 7.60−7.51 (m, 5H), 7.39−7.30 (m, 3H), 7.07 (d, *J* = 16.1 Hz, 1H).



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 17.3 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 6.8 Hz, 1H), 7.27−7.24 (m, 2H), 6.36 (d, *J* = 17.3 Hz, 1H), 4.22 (t, *J* = 5.0 Hz, 2H), 1.71−1.67 (m, 2H), 1.32−1.28 (m, 2H), 0.96 (t, *J* = 6.8 Hz, 3H).



^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 15.6 Hz, 1H), 7.41 (d, *J* = 7.1 Hz, 2H), 6.66 (d, *J* = 7.1 Hz, 2H), 6.22 (d, *J* = 15.6 Hz, 1H), 4.18 (t, *J* = 6.7 Hz, 2H), 3.00 (s, 6H), 1.71−1.66 (m, 2H), 1.47−1.40 (m, 2H), 0.96 (t, *J* = 8.2 Hz, 3H).

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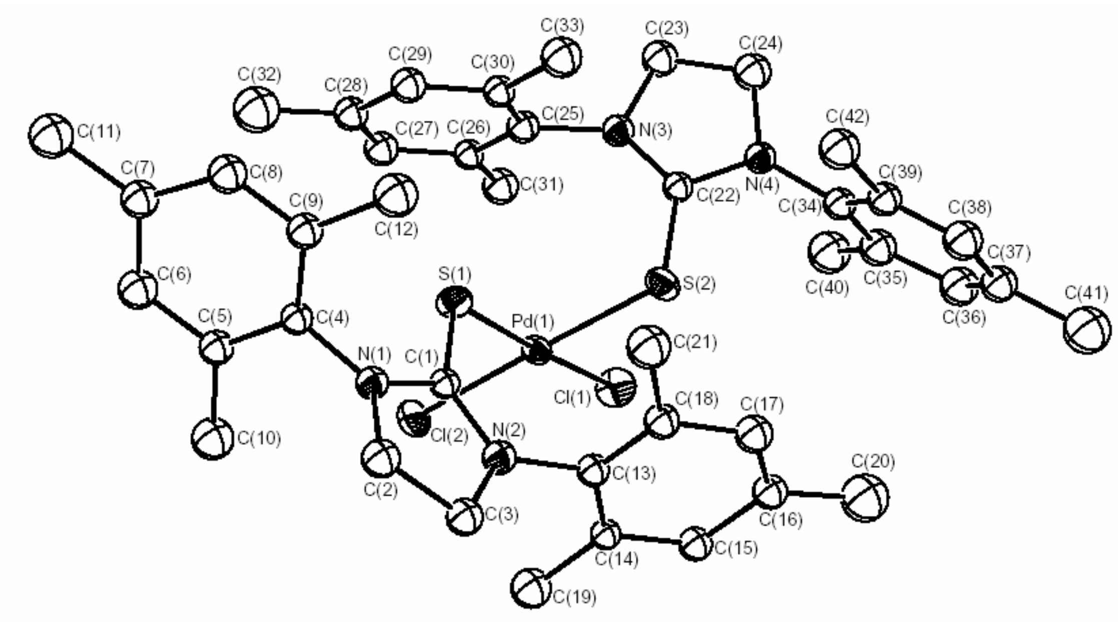
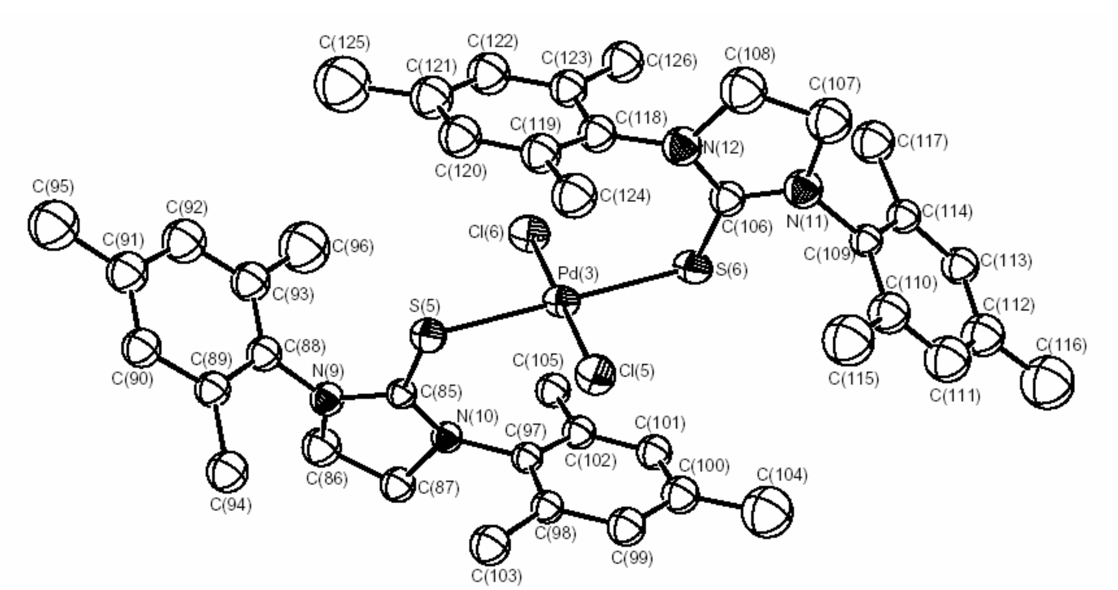
X-Ray Structures of Cis- and Trans- $PdCl_2 \cdot (1g)_2$



Cis- $PdCl_2 \cdot (1g)_2$



Trans- $PdCl_2 \cdot (1g)_2$

Table 1. Crystal data and structure refinement for $PdCl_2$-(**1g**)$_2$.

Identification code	$PdCl_2$-(**1g**)$_2$.	
Empirical formula	$C_{42.50} H_{53.50} Cl_3 N_4 O_{0.25} Pd S_2$	
Formula weight	901.26	
Temperature	253(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/a	
Unit cell dimensions	a = 21.560(4) Å	α= 90°.
	b = 31.285(6) Å	β= 97.14(3)°.
	c = 27.132(5) Å	γ = 90°.
Volume	18159(6) Å^3	
Z	16	
Density (calculated)	1.319 Mg/m^3	
Absorption coefficient	0.711 mm^{-1}	
F(000)	7480	
Crystal size	0.4 x 0.2 x 0.15 mm^3	
Theta range for data collection	1.00 to 25.57°.	
Index ranges	-24<=h<=24, -35<=k<=35, -32<=l<=32	
Reflections collected	60980	
Independent reflections	23410 [R(int) = 0.0672]	
Completeness to theta = 25.57°	68.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23410 / 18 / 956	
Goodness-of-fit on F^2	0.879	
Final R indices [I>2sigma(I)]	R1 = 0.0806, wR2 = 0.2247	
R indices (all data)	R1 = 0.1884, wR2 = 0.2675	
Largest diff. peak and hole	2.155 and -1.090 e.Å^{-3}	

Table 3. Bond lengths [Å] and angles [°] for $PdCl_2$-(**1g**)$_2$..

Pd(1)-S(1)	2.279(4)	N(4)-C(34)	1.437(15)
Pd(1)-S(2)	2.310(4)	N(4)-C(24)	1.461(13)
Pd(1)-Cl(2)	2.337(4)	N(5)-C(43)	1.354(14)
Pd(1)-Cl(1)	2.362(4)	N(5)-C(46)	1.442(15)
Pd(2)-S(3)	2.282(4)	N(5)-C(44)	1.484(14)
Pd(2)-S(4)	2.297(4)	N(6)-C(43)	1.324(14)
Pd(2)-Cl(3)	2.346(5)	N(6)-C(55)	1.401(15)
Pd(2)-Cl(4)	2.358(5)	N(6)-C(45)	1.472(13)
Pd(3)-S(6)	2.310(4)	N(7)-C(64)	1.309(14)
Pd(3)-S(5)	2.311(4)	N(7)-C(67)	1.409(15)
Pd(3)-Cl(5)	2.318(4)	N(7)-C(65)	1.498(14)
Pd(3)-Cl(6)	2.320(4)	N(8)-C(64)	1.385(14)
Pd(4)-S(8)	2.317(4)	N(8)-C(76)	1.440(16)
Pd(4)-Cl(8)	2.323(4)	N(8)-C(66)	1.507(14)
Pd(4)-S(7)	2.325(4)	N(9)-C(85)	1.343(15)
Pd(4)-Cl(7)	2.325(4)	N(9)-C(88)	1.401(14)
S(1)-C(1)	1.662(10)	N(9)-C(86)	1.454(15)
S(2)-C(22)	1.703(10)	N(10)-C(85)	1.359(12)
S(3)-C(43)	1.708(10)	N(10)-C(97)	1.446(15)
S(4)-C(64)	1.693(10)	N(10)-C(87)	1.483(15)
S(5)-C(85)	1.676(12)	N(11)-C(106)	1.266(16)
S(6)-C(106)	1.726(13)	N(11)-C(109)	1.461(14)
S(7)-C(127)	1.685(12)	N(11)-C(107)	1.520(17)
S(8)-C(148)	1.662(13)	N(12)-C(106)	1.376(14)
N(1)-C(1)	1.343(13)	N(12)-C(118)	1.401(17)
N(1)-C(4)	1.407(14)	N(12)-C(108)	1.490(17)
N(1)-C(2)	1.512(13)	N(13)-C(127)	1.354(15)
N(2)-C(1)	1.353(13)	N(13)-C(130)	1.490(15)
N(2)-C(13)	1.448(15)	N(13)-C(128)	1.536(15)
N(2)-C(3)	1.459(13)	N(14)-C(127)	1.303(12)
N(3)-C(22)	1.368(14)	N(14)-C(139)	1.446(15)
N(3)-C(23)	1.469(13)	N(14)-C(129)	1.500(15)
N(3)-C(25)	1.500(16)	N(15)-C(151)	1.373(16)
N(4)-C(22)	1.356(14)	N(15)-C(148)	1.407(14)

N(15)-C(149)	1.436(18)	C(35)-C(40)	1.55(2)
N(16)-C(148)	1.302(17)	C(36)-C(37)	1.353(19)
N(16)-C(160)	1.447(15)	C(37)-C(38)	1.369(19)
N(16)-C(150)	1.472(18)	C(37)-C(41)	1.49(2)
C(2)-C(3)	1.531(17)	C(38)-C(39)	1.318(18)
C(4)-C(9)	1.365(17)	C(39)-C(42)	1.509(18)
C(4)-C(5)	1.370(17)	C(44)-C(45)	1.545(18)
C(5)-C(6)	1.394(18)	C(46)-C(51)	1.373(18)
C(5)-C(10)	1.491(18)	C(46)-C(47)	1.434(19)
C(6)-C(7)	1.397(19)	C(47)-C(48)	1.354(18)
C(7)-C(8)	1.414(18)	C(47)-C(52)	1.474(19)
C(7)-C(11)	1.529(19)	C(48)-C(49)	1.358(19)
C(8)-C(9)	1.344(17)	C(49)-C(50)	1.282(19)
C(9)-C(12)	1.492(18)	C(49)-C(53)	1.54(2)
C(13)-C(18)	1.349(18)	C(50)-C(51)	1.297(17)
C(13)-C(14)	1.397(18)	C(51)-C(54)	1.48(2)
C(14)-C(15)	1.423(16)	C(55)-C(56)	1.401(18)
C(14)-C(19)	1.511(18)	C(55)-C(60)	1.405(18)
C(15)-C(16)	1.451(18)	C(56)-C(57)	1.434(19)
C(16)-C(17)	1.365(19)	C(56)-C(61)	1.48(2)
C(16)-C(20)	1.59(2)	C(57)-C(58)	1.35(2)
C(17)-C(18)	1.426(17)	C(58)-C(59)	1.391(19)
C(18)-C(21)	1.53(2)	C(58)-C(62)	1.47(2)
C(23)-C(24)	1.504(18)	C(59)-C(60)	1.415(17)
C(25)-C(30)	1.358(18)	C(60)-C(63)	1.508(19)
C(25)-C(26)	1.405(18)	C(65)-C(66)	1.484(18)
C(26)-C(27)	1.398(17)	C(67)-C(68)	1.373(18)
C(26)-C(31)	1.524(18)	C(67)-C(72)	1.442(17)
C(27)-C(28)	1.384(18)	C(68)-C(69)	1.398(19)
C(28)-C(29)	1.345(18)	C(68)-C(73)	1.536(19)
C(28)-C(32)	1.445(19)	C(69)-C(70)	1.390(19)
C(29)-C(30)	1.373(17)	C(70)-C(71)	1.351(19)
C(30)-C(33)	1.490(19)	C(70)-C(74)	1.51(2)
C(34)-C(39)	1.390(17)	C(71)-C(72)	1.432(18)
C(34)-C(35)	1.403(18)	C(72)-C(75)	1.472(18)
C(35)-C(36)	1.406(19)	C(76)-C(81)	1.384(17)

C(76)-C(77)	1.434(19)	C(114)-C(117)	1.538(18)
C(77)-C(78)	1.408(18)	C(118)-C(123)	1.410(18)
C(77)-C(82)	1.499(18)	C(118)-C(119)	1.428(15)
C(78)-C(79)	1.367(18)	C(119)-C(120)	1.332(19)
C(79)-C(80)	1.344(19)	C(119)-C(124)	1.528(18)
C(79)-C(83)	1.54(2)	C(120)-C(121)	1.35(2)
C(80)-C(81)	1.385(16)	C(121)-C(122)	1.424(17)
C(81)-C(84)	1.495(18)	C(121)-C(125)	1.50(2)
C(86)-C(87)	1.505(17)	C(122)-C(123)	1.360(19)
C(88)-C(89)	1.351(14)	C(123)-C(126)	1.511(16)
C(88)-C(93)	1.357(17)	C(128)-C(129)	1.515(16)
C(89)-C(90)	1.418(16)	C(130)-C(131)	1.304(14)
C(89)-C(94)	1.492(16)	C(130)-C(135)	1.422(18)
C(90)-C(91)	1.371(19)	C(131)-C(132)	1.411(17)
C(91)-C(92)	1.374(16)	C(131)-C(136)	1.557(16)
C(91)-C(95)	1.469(19)	C(132)-C(133)	1.359(18)
C(92)-C(93)	1.389(17)	C(133)-C(134)	1.406(16)
C(93)-C(96)	1.457(17)	C(133)-C(137)	1.493(19)
C(97)-C(98)	1.371(16)	C(134)-C(135)	1.412(17)
C(97)-C(102)	1.415(14)	C(135)-C(138)	1.552(16)
C(98)-C(99)	1.385(17)	C(139)-C(140)	1.393(16)
C(98)-C(103)	1.484(15)	C(139)-C(144)	1.396(14)
C(99)-C(100)	1.424(15)	C(140)-C(141)	1.360(17)
C(100)-C(101)	1.338(18)	C(140)-C(145)	1.514(15)
C(100)-C(104)	1.52(2)	C(141)-C(142)	1.418(15)
C(101)-C(102)	1.377(18)	C(142)-C(143)	1.338(18)
C(102)-C(105)	1.499(16)	C(142)-C(146)	1.50(2)
C(107)-C(108)	1.496(18)	C(143)-C(144)	1.389(18)
C(109)-C(114)	1.378(14)	C(144)-C(147)	1.472(17)
C(109)-C(110)	1.393(18)	C(149)-C(150)	1.57(2)
C(110)-C(111)	1.364(18)	C(151)-C(156)	1.362(18)
C(110)-C(115)	1.533(17)	C(151)-C(152)	1.429(15)
C(111)-C(112)	1.330(17)	C(152)-C(153)	1.37(2)
C(112)-C(113)	1.377(19)	C(152)-C(157)	1.495(19)
C(112)-C(116)	1.48(2)	C(153)-C(154)	1.36(2)
C(113)-C(114)	1.385(16)	C(154)-C(155)	1.415(17)

C(154)-C(158)	1.50(2)	S(3)-Pd(2)-Cl(4)	88.41(18)
C(155)-C(156)	1.338(19)	S(4)-Pd(2)-Cl(4)	176.90(14)
C(156)-C(159)	1.548(16)	Cl(3)-Pd(2)-Cl(4)	93.2(3)
C(160)-C(165)	1.356(14)	S(6)-Pd(3)-S(5)	179.80(17)
C(160)-C(161)	1.427(18)	S(6)-Pd(3)-Cl(5)	89.60(15)
C(161)-C(162)	1.376(18)	S(5)-Pd(3)-Cl(5)	90.42(14)
C(161)-C(166)	1.548(18)	S(6)-Pd(3)-Cl(6)	90.56(15)
C(162)-C(163)	1.389(17)	S(5)-Pd(3)-Cl(6)	89.42(15)
C(163)-C(164)	1.396(18)	Cl(5)-Pd(3)-Cl(6)	179.63(19)
C(163)-C(167)	1.49(2)	S(8)-Pd(4)-Cl(8)	89.19(15)
C(164)-C(165)	1.382(17)	S(8)-Pd(4)-S(7)	179.6(2)
C(165)-C(168)	1.502(18)	Cl(8)-Pd(4)-S(7)	91.18(15)
Cl(9)-C(169)	1.75(2)	S(8)-Pd(4)-Cl(7)	90.82(14)
Cl(10)-O(1)#1	1.50(3)	Cl(8)-Pd(4)-Cl(7)	179.59(17)
Cl(10)-C(169)	1.78(2)	S(7)-Pd(4)-Cl(7)	88.81(15)
Cl(11)-C(171)	1.21(4)	C(1)-S(1)-Pd(1)	111.1(4)
Cl(11)-Cl(13)	1.226(14)	C(22)-S(2)-Pd(1)	110.3(5)
Cl(11)-Cl(14)	1.71(2)	C(43)-S(3)-Pd(2)	111.1(4)
Cl(11)-C(170)	1.78(2)	C(64)-S(4)-Pd(2)	111.0(4)
Cl(12)-Cl(14)	1.201(15)	C(85)-S(5)-Pd(3)	110.6(4)
Cl(12)-C(170)	1.79(2)	C(106)-S(6)-Pd(3)	111.8(4)
Cl(13)-C(171)	1.76(2)	C(127)-S(7)-Pd(4)	110.6(4)
Cl(14)-C(170)	1.27(4)	C(148)-S(8)-Pd(4)	110.7(4)
Cl(14)-C(171)	1.77(2)	C(1)-N(1)-C(4)	126.4(9)
C(170)-C(171)	1.63(6)	C(1)-N(1)-C(2)	112.5(9)
O(1)-Cl(10)#2	1.50(3)	C(4)-N(1)-C(2)	121.0(9)
		C(1)-N(2)-C(13)	126.1(9)
S(1)-Pd(1)-S(2)	90.8(2)	C(1)-N(2)-C(3)	113.6(10)
S(1)-Pd(1)-Cl(2)	88.96(16)	C(13)-N(2)-C(3)	118.5(9)
S(2)-Pd(1)-Cl(2)	178.09(13)	C(22)-N(3)-C(23)	111.4(10)
S(1)-Pd(1)-Cl(1)	176.52(13)	C(22)-N(3)-C(25)	126.4(9)
S(2)-Pd(1)-Cl(1)	88.14(16)	C(23)-N(3)-C(25)	120.3(10)
Cl(2)-Pd(1)-Cl(1)	92.26(17)	C(22)-N(4)-C(34)	125.5(9)
S(3)-Pd(2)-S(4)	90.9(2)	C(22)-N(4)-C(24)	107.1(10)
S(3)-Pd(2)-Cl(3)	177.09(15)	C(34)-N(4)-C(24)	127.3(10)
S(4)-Pd(2)-Cl(3)	87.61(18)	C(43)-N(5)-C(46)	127.7(9)

C(43)-N(5)-C(44)	108.7(10)	N(1)-C(1)-S(1)	120.2(8)
C(46)-N(5)-C(44)	120.8(10)	N(2)-C(1)-S(1)	131.9(9)
C(43)-N(6)-C(55)	127.9(10)	N(1)-C(2)-C(3)	101.2(9)
C(43)-N(6)-C(45)	112.2(10)	N(2)-C(3)-C(2)	103.3(9)
C(55)-N(6)-C(45)	119.9(10)	C(9)-C(4)-C(5)	122.7(12)
C(64)-N(7)-C(67)	126.4(10)	C(9)-C(4)-N(1)	120.3(12)
C(64)-N(7)-C(65)	113.1(10)	C(5)-C(4)-N(1)	116.9(12)
C(67)-N(7)-C(65)	120.3(10)	C(4)-C(5)-C(6)	118.7(13)
C(64)-N(8)-C(76)	126.8(9)	C(4)-C(5)-C(10)	120.9(13)
C(64)-N(8)-C(66)	107.8(10)	C(6)-C(5)-C(10)	120.3(13)
C(76)-N(8)-C(66)	124.4(10)	C(5)-C(6)-C(7)	121.5(15)
C(85)-N(9)-C(88)	125.8(11)	C(6)-C(7)-C(8)	114.5(14)
C(85)-N(9)-C(86)	110.7(10)	C(6)-C(7)-C(11)	119.2(14)
C(88)-N(9)-C(86)	122.7(12)	C(8)-C(7)-C(11)	126.3(14)
C(85)-N(10)-C(97)	127.2(10)	C(9)-C(8)-C(7)	125.5(15)
C(85)-N(10)-C(87)	110.1(9)	C(8)-C(9)-C(4)	116.9(13)
C(97)-N(10)-C(87)	119.4(9)	C(8)-C(9)-C(12)	119.7(14)
C(106)-N(11)-C(109)	125.8(12)	C(4)-C(9)-C(12)	123.4(13)
C(106)-N(11)-C(107)	115.6(11)	C(18)-C(13)-C(14)	125.1(13)
C(109)-N(11)-C(107)	118.2(11)	C(18)-C(13)-N(2)	117.5(13)
C(106)-N(12)-C(118)	126.1(13)	C(14)-C(13)-N(2)	117.3(12)
C(106)-N(12)-C(108)	105.7(11)	C(13)-C(14)-C(15)	115.3(12)
C(118)-N(12)-C(108)	126.4(12)	C(13)-C(14)-C(19)	124.3(12)
C(127)-N(13)-C(130)	127.3(10)	C(15)-C(14)-C(19)	120.4(12)
C(127)-N(13)-C(128)	113.1(9)	C(14)-C(15)-C(16)	121.4(13)
C(130)-N(13)-C(128)	119.2(10)	C(17)-C(16)-C(15)	118.3(13)
C(127)-N(14)-C(139)	128.5(11)	C(17)-C(16)-C(20)	122.5(14)
C(127)-N(14)-C(129)	110.6(10)	C(15)-C(16)-C(20)	119.2(13)
C(139)-N(14)-C(129)	118.7(9)	C(16)-C(17)-C(18)	121.0(14)
C(151)-N(15)-C(148)	125.8(12)	C(13)-C(18)-C(17)	118.7(14)
C(151)-N(15)-C(149)	125.0(12)	C(13)-C(18)-C(21)	124.9(13)
C(148)-N(15)-C(149)	106.4(11)	C(17)-C(18)-C(21)	116.4(13)
C(148)-N(16)-C(160)	131.0(12)	N(4)-C(22)-N(3)	111.3(9)
C(148)-N(16)-C(150)	116.1(12)	N(4)-C(22)-S(2)	119.2(9)
C(160)-N(16)-C(150)	112.7(12)	N(3)-C(22)-S(2)	129.5(9)
N(1)-C(1)-N(2)	107.9(9)	N(3)-C(23)-C(24)	100.7(10)

N(4)-C(24)-C(23)	108.0(10)	C(47)-C(46)-N(5)	117.4(13)
C(30)-C(25)-C(26)	127.5(13)	C(48)-C(47)-C(46)	114.9(14)
C(30)-C(25)-N(3)	116.2(12)	C(48)-C(47)-C(52)	121.7(15)
C(26)-C(25)-N(3)	116.2(12)	C(46)-C(47)-C(52)	123.4(13)
C(27)-C(26)-C(25)	114.6(13)	C(47)-C(48)-C(49)	121.9(16)
C(27)-C(26)-C(31)	121.2(13)	C(50)-C(49)-C(48)	121.5(16)
C(25)-C(26)-C(31)	124.3(12)	C(50)-C(49)-C(53)	119.6(16)
C(28)-C(27)-C(26)	119.7(14)	C(48)-C(49)-C(53)	118.9(15)
C(29)-C(28)-C(27)	120.6(14)	C(49)-C(50)-C(51)	121.4(17)
C(29)-C(28)-C(32)	121.1(14)	C(50)-C(51)-C(46)	121.2(15)
C(27)-C(28)-C(32)	118.2(14)	C(50)-C(51)-C(54)	122.8(15)
C(28)-C(29)-C(30)	124.2(14)	C(46)-C(51)-C(54)	115.9(13)
C(25)-C(30)-C(29)	113.3(13)	N(6)-C(55)-C(56)	119.1(13)
C(25)-C(30)-C(33)	126.5(13)	N(6)-C(55)-C(60)	118.9(13)
C(29)-C(30)-C(33)	120.2(13)	C(56)-C(55)-C(60)	121.9(13)
C(39)-C(34)-C(35)	119.6(13)	C(55)-C(56)-C(57)	116.5(15)
C(39)-C(34)-N(4)	123.4(13)	C(55)-C(56)-C(61)	121.7(14)
C(35)-C(34)-N(4)	116.7(13)	C(57)-C(56)-C(61)	121.6(15)
C(34)-C(35)-C(36)	118.1(15)	C(58)-C(57)-C(56)	123.9(17)
C(34)-C(35)-C(40)	119.3(14)	C(57)-C(58)-C(59)	117.3(15)
C(36)-C(35)-C(40)	122.6(15)	C(57)-C(58)-C(62)	123.4(16)
C(37)-C(36)-C(35)	118.3(16)	C(59)-C(58)-C(62)	119.1(15)
C(36)-C(37)-C(38)	123.3(16)	C(58)-C(59)-C(60)	123.3(14)
C(36)-C(37)-C(41)	113.3(15)	C(55)-C(60)-C(59)	116.9(13)
C(38)-C(37)-C(41)	123.4(16)	C(55)-C(60)-C(63)	118.6(13)
C(39)-C(38)-C(37)	119.2(16)	C(59)-C(60)-C(63)	124.4(14)
C(38)-C(39)-C(34)	121.4(14)	N(7)-C(64)-N(8)	110.3(9)
C(38)-C(39)-C(42)	120.0(14)	N(7)-C(64)-S(4)	120.1(9)
C(34)-C(39)-C(42)	118.5(13)	N(8)-C(64)-S(4)	129.0(9)
N(6)-C(43)-N(5)	112.1(9)	C(66)-C(65)-N(7)	101.9(11)
N(6)-C(43)-S(3)	119.7(9)	C(65)-C(66)-N(8)	105.3(10)
N(5)-C(43)-S(3)	128.1(9)	C(68)-C(67)-N(7)	121.3(13)
N(5)-C(44)-C(45)	104.4(10)	C(68)-C(67)-C(72)	121.3(13)
N(6)-C(45)-C(44)	101.4(10)	N(7)-C(67)-C(72)	117.4(12)
C(51)-C(46)-C(47)	118.9(13)	C(67)-C(68)-C(69)	120.3(14)
C(51)-C(46)-N(5)	123.5(13)	C(67)-C(68)-C(73)	120.3(13)

C(69)-C(68)-C(73)	119.4(14)	C(90)-C(91)-C(95)	123.4(13)
C(70)-C(69)-C(68)	120.7(15)	C(92)-C(91)-C(95)	119.0(15)
C(71)-C(70)-C(69)	118.8(15)	C(91)-C(92)-C(93)	123.0(15)
C(71)-C(70)-C(74)	121.1(16)	C(88)-C(93)-C(92)	117.9(13)
C(69)-C(70)-C(74)	120.1(15)	C(88)-C(93)-C(96)	120.9(14)
C(70)-C(71)-C(72)	124.3(15)	C(92)-C(93)-C(96)	121.2(15)
C(71)-C(72)-C(67)	114.6(12)	C(98)-C(97)-C(102)	123.6(12)
C(71)-C(72)-C(75)	123.6(13)	C(98)-C(97)-N(10)	117.5(10)
C(67)-C(72)-C(75)	121.8(13)	C(102)-C(97)-N(10)	118.6(11)
C(81)-C(76)-C(77)	120.5(13)	C(97)-C(98)-C(99)	116.2(11)
C(81)-C(76)-N(8)	121.5(13)	C(97)-C(98)-C(103)	125.0(12)
C(77)-C(76)-N(8)	117.5(13)	C(99)-C(98)-C(103)	118.7(12)
C(78)-C(77)-C(76)	116.8(13)	C(98)-C(99)-C(100)	121.1(14)
C(78)-C(77)-C(82)	123.2(14)	C(101)-C(100)-C(99)	119.8(15)
C(76)-C(77)-C(82)	120.0(13)	C(101)-C(100)-C(104)	119.4(13)
C(79)-C(78)-C(77)	122.0(14)	C(99)-C(100)-C(104)	120.7(14)
C(80)-C(79)-C(78)	118.7(14)	C(100)-C(101)-C(102)	121.5(13)
C(80)-C(79)-C(83)	118.5(14)	C(101)-C(102)-C(97)	117.3(12)
C(78)-C(79)-C(83)	122.4(15)	C(101)-C(102)-C(105)	120.7(10)
C(79)-C(80)-C(81)	123.9(14)	C(97)-C(102)-C(105)	121.9(12)
C(76)-C(81)-C(80)	117.9(13)	N(11)-C(106)-N(12)	111.7(12)
C(76)-C(81)-C(84)	117.2(12)	N(11)-C(106)-S(6)	120.4(10)
C(80)-C(81)-C(84)	124.9(13)	N(12)-C(106)-S(6)	128.0(11)
N(9)-C(85)-N(10)	109.8(10)	C(108)-C(107)-N(11)	97.4(12)
N(9)-C(85)-S(5)	120.8(8)	N(12)-C(108)-C(107)	109.2(12)
N(10)-C(85)-S(5)	129.4(9)	C(114)-C(109)-C(110)	120.5(12)
N(9)-C(86)-C(87)	104.5(11)	C(114)-C(109)-N(11)	119.3(11)
N(10)-C(87)-C(86)	101.9(10)	C(110)-C(109)-N(11)	120.1(10)
C(89)-C(88)-C(93)	121.7(13)	C(111)-C(110)-C(109)	119.1(13)
C(89)-C(88)-N(9)	116.5(12)	C(111)-C(110)-C(115)	120.8(15)
C(93)-C(88)-N(9)	121.6(11)	C(109)-C(110)-C(115)	120.1(13)
C(88)-C(89)-C(90)	119.7(13)	C(112)-C(111)-C(110)	121.7(17)
C(88)-C(89)-C(94)	121.9(12)	C(111)-C(112)-C(113)	119.6(16)
C(90)-C(89)-C(94)	118.3(11)	C(111)-C(112)-C(116)	120.3(16)
C(91)-C(90)-C(89)	120.0(12)	C(113)-C(112)-C(116)	120.1(14)
C(90)-C(91)-C(92)	117.6(14)	C(112)-C(113)-C(114)	121.4(13)

C(109)-C(114)-C(113)	117.6(12)
C(109)-C(114)-C(117)	117.6(11)
C(113)-C(114)-C(117)	124.4(11)
N(12)-C(118)-C(123)	119.2(12)
N(12)-C(118)-C(119)	120.9(13)
C(123)-C(118)-C(119)	118.8(13)
C(120)-C(119)-C(118)	119.4(14)
C(120)-C(119)-C(124)	121.3(12)
C(118)-C(119)-C(124)	119.3(13)
C(119)-C(120)-C(121)	123.0(15)
C(120)-C(121)-C(122)	118.5(16)
C(120)-C(121)-C(125)	123.1(15)
C(122)-C(121)-C(125)	118.3(16)
C(123)-C(122)-C(121)	120.8(16)
C(122)-C(123)-C(118)	118.9(13)
C(122)-C(123)-C(126)	118.9(14)
C(118)-C(123)-C(126)	122.1(13)
N(14)-C(127)-N(13)	110.5(11)
N(14)-C(127)-S(7)	131.9(10)
N(13)-C(127)-S(7)	117.6(8)
C(129)-C(128)-N(13)	98.6(10)
N(14)-C(129)-C(128)	106.8(10)
C(131)-C(130)-C(135)	122.3(13)
C(131)-C(130)-N(13)	123.0(12)
C(135)-C(130)-N(13)	114.7(11)
C(130)-C(131)-C(132)	121.4(13)
C(130)-C(131)-C(136)	118.5(12)
C(132)-C(131)-C(136)	120.1(10)
C(133)-C(132)-C(131)	119.4(13)
C(132)-C(133)-C(134)	120.0(14)
C(132)-C(133)-C(137)	119.8(13)
C(134)-C(133)-C(137)	120.1(14)
C(133)-C(134)-C(135)	120.2(14)
C(134)-C(135)-C(130)	116.6(12)
C(134)-C(135)-C(138)	119.9(13)
C(130)-C(135)-C(138)	123.3(13)
C(140)-C(139)-C(144)	121.2(12)
C(140)-C(139)-N(14)	119.7(10)
C(144)-C(139)-N(14)	119.0(12)
C(141)-C(140)-C(139)	117.9(11)
C(141)-C(140)-C(145)	119.4(13)
C(139)-C(140)-C(145)	122.6(12)
C(140)-C(141)-C(142)	122.6(14)
C(143)-C(142)-C(141)	117.0(14)
C(143)-C(142)-C(146)	123.9(13)
C(141)-C(142)-C(146)	119.0(14)
C(142)-C(143)-C(144)	123.6(13)
C(143)-C(144)-C(139)	117.5(13)
C(143)-C(144)-C(147)	119.3(11)
C(139)-C(144)-C(147)	123.2(13)
N(16)-C(148)-N(15)	110.6(12)
N(16)-C(148)-S(8)	119.8(10)
N(15)-C(148)-S(8)	129.5(11)
N(15)-C(149)-C(150)	108.9(13)
N(16)-C(150)-C(149)	97.2(13)
C(156)-C(151)-N(15)	123.7(12)
C(156)-C(151)-C(152)	118.1(13)
N(15)-C(151)-C(152)	118.0(13)
C(153)-C(152)-C(151)	119.2(14)
C(153)-C(152)-C(157)	119.2(13)
C(151)-C(152)-C(157)	121.6(14)
C(154)-C(153)-C(152)	120.7(15)
C(153)-C(154)-C(155)	119.9(17)
C(153)-C(154)-C(158)	121.4(15)
C(155)-C(154)-C(158)	118.7(17)
C(156)-C(155)-C(154)	119.0(16)
C(155)-C(156)-C(151)	123.0(13)
C(155)-C(156)-C(159)	118.7(14)
C(151)-C(156)-C(159)	118.3(13)
C(165)-C(160)-C(161)	121.2(12)
C(165)-C(160)-N(16)	121.3(12)
C(161)-C(160)-N(16)	117.3(11)

C(162)-C(161)-C(160)	119.0(13)
C(162)-C(161)-C(166)	118.8(15)
C(160)-C(161)-C(166)	122.1(14)
C(161)-C(162)-C(163)	121.0(16)
C(162)-C(163)-C(164)	117.3(14)
C(162)-C(163)-C(167)	120.8(15)
C(164)-C(163)-C(167)	121.9(13)
C(165)-C(164)-C(163)	123.5(12)
C(160)-C(165)-C(164)	117.7(13)
C(160)-C(165)-C(168)	118.2(12)
C(164)-C(165)-C(168)	124.0(12)
O(1)#1-Cl(10)-C(169)	111.4(18)
C(171)-Cl(11)-Cl(13)	92.9(14)
C(171)-Cl(11)-Cl(14)	72.3(11)
Cl(13)-Cl(11)-Cl(14)	156.5(13)
C(171)-Cl(11)-C(170)	63(3)
Cl(13)-Cl(11)-C(170)	114.5(16)
Cl(14)-Cl(11)-C(170)	42.6(11)
Cl(14)-Cl(12)-C(170)	45.1(12)
Cl(11)-Cl(13)-C(171)	43.1(12)
Cl(12)-Cl(14)-C(170)	92.9(14)
Cl(12)-Cl(14)-Cl(11)	159.4(14)
C(170)-Cl(14)-Cl(11)	71.5(11)
Cl(12)-Cl(14)-C(171)	120.5(17)
C(170)-Cl(14)-C(171)	62(3)
Cl(11)-Cl(14)-C(171)	40.4(11)
Cl(9)-C(169)-Cl(10)	103.3(17)
Cl(14)-C(170)-C(171)	74(2)
Cl(14)-C(170)-Cl(11)	66.0(16)
C(171)-C(170)-Cl(11)	41.2(12)
Cl(14)-C(170)-Cl(12)	42.0(9)
C(171)-C(170)-Cl(12)	99(2)
Cl(11)-C(170)-Cl(12)	106.9(19)
Cl(11)-C(171)-C(170)	76(2)
Cl(11)-C(171)-Cl(13)	44.0(9)
C(170)-C(171)-Cl(13)	97(2)
Cl(11)-C(171)-Cl(14)	67.3(17)
C(170)-C(171)-Cl(14)	43.7(12)
Cl(13)-C(171)-Cl(14)	109(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y-1/2,-z #2 -x+3/2,y+1/2,-z