Supporting Information 1

Enantioselective Pd-Catalyzed Allylic Alkylation of Indoles by a New Class of Chiral Ferrocenyl P/S Ligands

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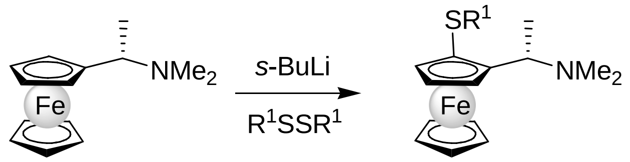
1. General Considerations

All reactions were carried out under a nitrogen atmosphere in an oven-dried glassware. Unless otherwise noted, commercial reagents were used as received without further purification. Toluene was distilled from sodium under a nitrogen atmosphere. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were distilled from sodium/benzophenone ketyl under a nitrogen atmosphere. Acetonitrile (CH_3CN), dichloromethane (CH_2Cl_2), 1,2-dichloroethane (DCE), 1,2-dimethoxyethane (DME), ethyl acetate (EtOAc) and hexane were distilled from CaH_2 under a nitrogen atmosphere. Thin layer chromatography was performed on silica gel plates. Silica gel (Merck, 230-400 mesh) was used for flash column chromatography. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on a Varian (500 MHz) or Bruker (400 MHz) spectrometer. Chemical shift (δ) are given in ppm and are referenced to residual solvent peaks (^{1}H NMR and ^{13}C NMR) or to an 85% H_3PO_4 in D_2O externally (^{31}P NMR). Coupling constants (*J*) were reported in hertz (Hz). Mass spectra and high resolution mass spectra (HRMS) were obtained on a VG MICROMASS, Fison VG platform, Finnigan Model Mat 95 ST instrument, or Brüker APEX 47e FT-ICR mass spectrometer. Optical rotations were recorded on a Perkin-Elmer 341 polarimeter in a 10 mm cell. Melting points were measured on a BUCHI Melting Point B-545 machine. X-ray crystal structure was determined by Brüker CCD area detector diffractometer. HPLC analyses were performed on a HP 1100 or HP1050 instrument using Chiralcel® OD-H, AD-H and OJ-H columns (0.46 cm diameter × 25 cm length). Authentic samples were prepared according to the reported procedures.[1] (*S*)-Ugi's amine was prepared according to the reported procedure.[2]

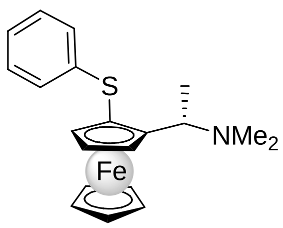
2. Preparation of P/S ligands L1-L8

2.1 Synthesis of thioether 3[3]

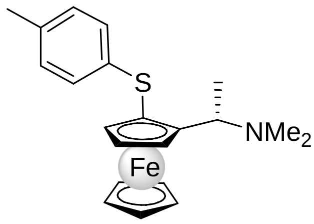


3

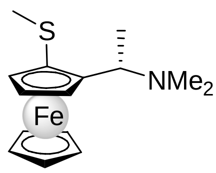
General procedure for the preparation of thioether ***3****:* To a solution of (*S*)-Ugi's amine (3.0 g, 11.7 mmol) in Et_2O (45 mL) was added dropwise *sec*-BuLi (11.2 mL, 14.6 mmol, 1.3 M solution in cyclohexane/hexane) at 0 °C under a nitrogen atmosphere. The reaction mixture was then warmed to room temperature and stirred for 4 h. The mixture was then cooled to 0 °C, followed by dropwise addition of the corresponding aryl or alkyl disulfide (15.2 mmol) dissolved in Et_2O (10 mL). After warming to room temperature, the mixture was refluxed for 24 h. The reaction was cooled in a ice-water bath and quenched with a saturated $NaHCO_3$ solution (~60 mL). The organic layer was separated and washed with ice water, and extracted with 8.5% H_3PO_4 solution to eliminate the odor of the thiol side products. The aqueous layer was separated and neutralized with 3 M NaOH solution. The aqueous layer was then extracted with EtOAc. The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by flash column chromatography to afford corresponding (*S*, R_p)-**3**.



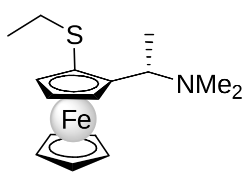
(*S*)-*N,N*-Dimethyl-1-[(*R*)-2-(phenylthio)ferrocenyl]ethyl-amine (**3a**). Yield: 90%, orange solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/5/0.01). $[\alpha]_D^{20}$ +144.1° (c 1.0, CH_2Cl_2); m.p.= 60-61 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.17-7.13 (m, 4H), 7.06-7.02 (m, 1H), 4.53 (s, 1H), 4.35 (s, 1H), 4.33 (s, 1H), 4.19 (s, 5H), 3.87 (q, 1H, *J* = 7.0 Hz), 1.92 (s, 6H), 1.46 (d, 3H, *J* = 6.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 140.3, 128.1, 126.5, 124.6, 92.8, 75.9, 75.5, 70.3, 68.3, 68.2, 55.7, 40.6, 15.8; IR (cm^{-1}) 3089, 3012, 2966, 2920, 2815, 2769, 1650, 1490, 1453, 1190, 1087, 1049, 1004, 820, 797; MS(EI): 365.13 $[M]^+$.



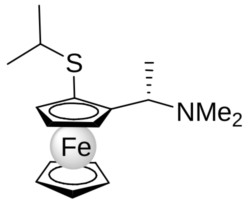
(*S*)-*N,N*-Dimethyl-1-[(*R*)-2-(*p*-tolylthio)ferrocenyl]ethyl amine (**3b**). Yield: 92%, orange solid. R_f = 0.2 (EtOAc/hexane/Et_3N = 1/5/0.01). $[\alpha]_D^{20}$ +174.2° (c 1.0, CH_2Cl_2); m.p.= 63-65 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.09 (d, 2H, *J* = 8.5 Hz), 6.97 (d, 2H, *J* = 8.0 Hz), 4.5 (s, 1H), 4.33-4.31 (m, 2H), 4.17 (s, 5H), 3.87 (q, 1H, *J* = 7.0 Hz), 2.25 (s, 3H), 1.94 (s, 6H), 1.47 (d, 3H, *J* = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.5, 134.5, 128.9, 126.9, 92.4, 76.8, 75.3, 70.3, 68.1, 68.0, 55.7, 40.7, 20.9, 16.0; IR (cm^{-1}) 3094, 2966, 2925, 2809, 2765, 1577, 1474, 1436, 1094, 1059, 1003, 930, 825, 741, 689; MS(ESI): 380.14 $[M+H]^+$.



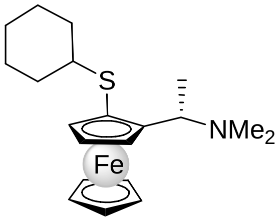
(*S*)-*N,N*-Dimethyl-1-[(*R*)-2-(methylthio)ferrocenyl]ethylamine (**3c**). Yield: 84%, orange solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/5/0.01). $[\alpha]_D^{20}$ +118.9° (c 1.0, CH_2Cl_2); m.p.= 78-80 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.31-4.30 (m, 1H), 4.18 (s, 1H), 4.16-4.15 (m, 1H), 4.10 (s, 5H), 3.93 (q, 1H, *J* = 7.0 Hz), 2.26 (s, 3H), 2.12 (s, 6H), 1.39 (d, 3H, *J* = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 92.0, 83.3, 70.9, 69.9, 67.2, 66.4, 56.0, 40.4, 19.8, 13.1; IR (cm^{-1}) 3078, 2969, 2928, 2809, 2765, 1656, 1445, 1361, 1259, 1186, 1095, 1055, 1003, 966, 929, 813; MS(ESI): 304.15 $[M+H]^+$.



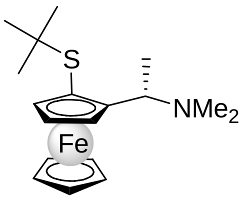
(*S*)-N,N-Dimethyl-1-[(*R*)-2-(ethylthio)ferrocenyl]ethylamine (**3d**). Yield: 87%, red oil. R_f = 0.5 (EtOAc/hexane/Et_3N = 1/3/0.01). $[\alpha]_D^{20}$ +38.5° (c 1.0, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.32 (s, 1H), 4.2 (s, 1H), 4.16-4.15 (m, 1H), 4.08 (s, 5H), 3.94 (q, 1H, *J* = 7.0 Hz), 2.80-2.73 (m, 1H), 2.65-2.58 (m, 1H), 2.11 (s, 6H), 1.35 (d, 3H, *J* = 7.0 Hz), 1.18 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 93.2, 80.1, 73.4, 69.9, 67.5, 66.6, 55.9, 40.2, 30.5, 14.7, 12.0; IR (cm^{-1}) 3093, 2968, 2927, 2864, 2815, 2772, 1673, 1452, 1365, 1260, 1155, 1096, 1060, 1002, 971, 931, 817; MS(ESI): 318.12 $[M+H]^+$.



(*S*)-N,N-Dimethyl-1-[(*R*)-2-(*iso*-propylthio)ferrocenyl]ethyl-amine (**3e**). Yield: 94%, red oil. R_f = 0.4 (EtOAc/hexane/Et_3N = 1/20/0.01). $[\alpha]_D^{20}$ –26.6° (c 1.0, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.33 (s, 1H), 4.21 (s, 1H), 4.17 (s, 1H), 4.09 (s, 5H), 3.98 (q, 1H, *J* = 7.0 Hz), 3.23-3.17 (m, 1H), 2.11 (s, 6H), 1.33 (d, 3H, *J* = 7.0 Hz), 1.20 (d, 3H, *J* = 7.0 Hz), 1.13 (d, 3H, *J* = 6.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 94.5, 78.3, 75.2, 69.9, 67.9, 66.8, 55.8, 39.9, 39.2, 23.8, 22.6, 10.8; IR (cm^{-1}) 3097, 2967, 2925, 2857, 2815, 2771, 1672, 1451, 1361, 1244, 1187, 1153, 1095, 1051, 1001, 971, 929, 821; MS(EI): 331.18 $[M]^+$.

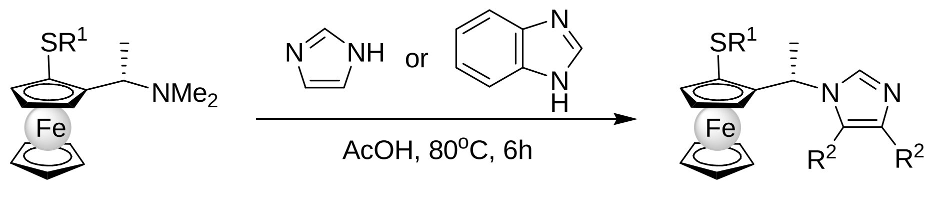


(*S*)-N,N-Dimethyl-1-[(*R*)-2-(cyclohexylthio)ferrocenyl]-ethylamine (**3f**). Yield: 90%, orange solid. R_f = 0.4 (EtOAc/hexane/Et_3N = 1/20/0.01). $[\alpha]_D^{20}$ –32.7° (c 1.0, CH_2Cl_2); m.p.= 66-67 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 4.30 (s, 1H), 4.20 (s, 1H), 4.16 (s, 1H), 4.08 (s, 5H), 3.97 (q, 1H, J = 7.0 Hz), 2.11 (s, 6H), 1.92-1.54 (m, 6H), 1.33 (d, 3H, J = 7.0 Hz), 1.29-1.09 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 94.4, 78.2, 75.1, 69.9, 67.8, 66.6, 55.9, 47.8, 40.0, 34.1, 33.0, 26.4, 25.9, 11.1; IR (cm^{-1}) 3091, 2969, 2932, 2848, 2815, 2772, 1649, 1468, 1449, 1362, 1263, 1188, 1096, 1060, 1048, 999, 930, 817; MS(EI): 371.16 $[M]^+$.



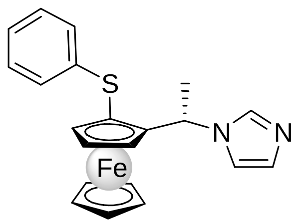
(*S*)-N,N-Dimethyl-1-[(*R*)-2-(*tert*-butylthio)ferrocenyl]ethyl-amine (**3g**). Yield: 38%, red oil. R_f = 0.6 (EtOAc/hexane/Et_3N = 1/15/0.01). $[\alpha]_D^{20}$ +169.1° (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 4.42-4.41 (m, 1H), 4.26-4.25 (m, 1H), 4.22-4.21 (m, 1H), 4.10 (s, 5H), 3.86 (q, 1H, J = 7.0 Hz), 2.13 (s, 6H), 1.31 (d, 3H, J = 7.0 Hz), 1.24 (s, 9H); ^{13}C NMR(125 MHz, $CDCl_3$): δ 95.0, 76.8, 70.1, 68.1, 67.3, 55.3, 46.0, 39.9, 31.3, 10.1; IR (cm^{-1}) 3094, 2963, 2935, 2894, 2859, 2814, 2771, 1673, 1454, 1363, 1264, 1243, 1169, 1095, 1061, 1002, 931, 818; MS(EI): 345.14 $[M]^+$.

2.2 Synthesis of 4

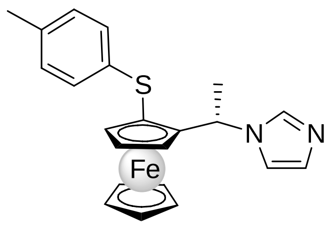


3 **4**

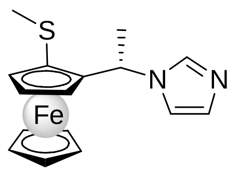
General procedure for the preparation of ***4****:* A mixture of thioether **3** and imidazole or benzimidazole (8 equiv.) in degassed glacial AcOH was stirred at 80 °C for 6 h. The reaction mixture was quenched with an excess saturated $NaHCO_3$ solution and extracted with CH_2Cl_2 (15 mL × 3). The combined organic extracts were washed with brine and dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure. The crude product was purified by flash column chromatography to afford the corresponding (S, R_p)-**4**.



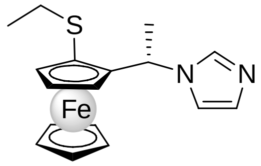
1-{(*S*)-1-[(*R*)-2-(Phenylthio)ferrocenyl]ethyl}-imidazole (4a). **3a** (1 g, 2.74 mmol) and imidazole (1.49 g, 21.92 mmol) in glacial AcOH (10 mL) were used with reference to the general procedure. Yield: 60%, yellow solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 3/1/0.01). $[\alpha]_D^{20}$ +114.5^o (c 1.0, CH_2Cl_2); m.p.= 177-178 ^oC; ^1H NMR (500 MHz, $CDCl_3$): δ 7.15 (s, 1H), 6.98-6.94 (m, 3H), 6.66 (s, 1H), 6.62 (s, 1H), 6.57-6.56 (m, 4H), 5.48 (q, 1H, *J* = 7.0 Hz), 4.59 (s, 1H), 4.52 (s, 1H), 4.44 (s, 1H), 4.26 (s, 5H), 1.84 (d, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.6, 135.2, 128.5, 128.4, 125.2, 125.0, 116.4, 91.3, 76.5, 75.4, 70.5, 69.2, 67.6, 50.4, 22.2; IR (cm^{-1}) 3073, 2980, 2935, 1581, 1493, 1476, 1449, 1398, 1246, 1218, 1107, 1080, 1026, 902, 814, 736, 692; MS(ESI): 389.06 $[M+H]^+$; HRMS(ESI): calcd for $C_{21}H_{21}N_2SFe$ $[M+H]^+$: 389.0775, found 389.0795.



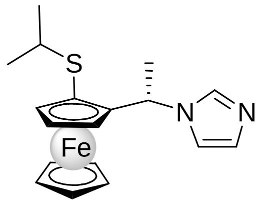
1-{(*S*)-1-[(*R*)-2-(*p*-Tolylthio)ferrocenyl]ethyl}-imidazole (4b). **3b** (1 g, 2.64 mmol) and imidazole (1.44 g, 21.12 mmol) in glacial AcOH (10 mL) were used with reference to the general procedure. Yield: 38%, yellow solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 3/1/0.01). $[\alpha]_D^{20}$ +145.5^o (c 1.0, CH_2Cl_2); m.p.= 152-154 ^oC; ^1H NMR (500 MHz, $CDCl_3$): δ 7.21 (s, 1H), 6.79 (d, 2H, *J* = 8.5 Hz), 6.70 (s, 1H), 6.64 (s, 1H), 6.48 (d, 2H, *J* = 7.5 Hz), 5.49 (q, 1H, *J* = 7.0 Hz), 4.56 (s, 1H), 4.51 (s, 1H), 4.42-4.41 (m, 1H), 4.26 (s, 5H), 2.18 (s, 3H), 1.86 (d, 3H, *J* = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.3, 135.01, 135.00, 129.3, 128.5, 125.9, 116.6, 91.0, 76.5, 76.4, 70.6, 69.1, 67.5, 50.5, 22.4, 20.8; IR (cm^{-1}) 3104, 3074, 1654, 1493, 1455, 1395, 1222, 1105, 1079, 1002, 810, 739, 664; MS(ESI): 403.10 $[M+H]^+$; HRMS(ESI): calcd for $C_{22}H_{23}N_2SFe$ $[M+H]^+$: 403.0931; found 403.0921.



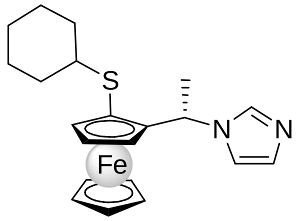
1-{(*S*)-1-[(*R*)-2-(Methylthio)ferrocenyl]ethyl}-imidazole (4c). **3c** (1 g, 3.30 mmol) and imidazole (1.80 g, 26.4 mmol) in glacial AcOH (12 mL) were used with reference to the general procedure. Yield: 72%, orange solid. R_f = 0.2 (EtOAc/hexane/Et_3N = 2/1/0.01). $[\alpha]_D^{20}$ +188.9^o (c 1.0, CH_2Cl_2); m.p.= 94-96 ^oC; ^1H NMR (500 MHz, $CDCl_3$): δ 7.49 (s, 1H), 6.94 (s, 1H), 6.81 (s, 1H), 5.58 (q, 1H, *J* = 7.0 Hz), 4.46 (s, 1H), 4.42 (s, 1H), 4.29-4.28 (m, 1H), 4.17 (s, 5H), 1.82 (d, 3H, *J* = 7.0 Hz), 1.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.7, 128.6, 116.9, 89.5, 81.2, 75.0, 70.2, 68.2, 66.9, 51.1, 21.8, 20.5; IR (cm^{-1}) 3089, 2983, 2915, 1653, 1485, 1452, 1394, 1313, 1284, 1245, 1214, 1105, 1077, 1056, 1003, 953, 904, 810, 751, 662; MS(ESI): 327.13 $[M+H]^+$; HRMS(ESI): calcd for $C_{16}H_{19}N_2SFe$ $[M+H]^+$: 327.0618, found 327.0605.



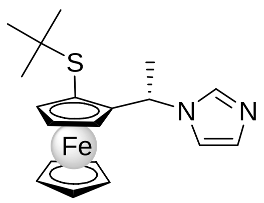
1-{(*S*)-1-[(*R*)-2-(Ethylthio)ferrocenyl]ethyl}-imidazole (**4d**). **3d** (1 g, 3.15 mmol) and imidazole (1.72 g, 25.2 mmol) in glacial AcOH (11 mL) were used with reference to the general procedure. Yield: 95%, red oil. R_f = 0.3 (EtOAc/hexane/Et_3N = 2/1/0.01). $[\alpha]_D^{20}$ +140.2° (c 1.0, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 (s, 1H), 6.90 (s, 1H), 6.77 (s, 1H), 5.56 (q, 1H, J = 7.0 Hz), 4.45 (s, 1H), 4.42 (s, 1H), 4.30 (s, 1H), 4.16 (s, 5H), 1.91-1.84 (m, 1H), 1.80 (d, 3H, J = 7.0 Hz), 1.73-1.66 (m, 1H), 0.87 (t, 3H, J = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.6, 128.5, 116.8, 89.6, 78.8, 76.3, 70.2, 68.2, 67.1, 50.9, 30.7, 22.0, 14.5; IR (cm^{-1}) 3103, 2975, 2926, 2869, 1646, 1496, 1451, 1402, 1375, 1251, 1219, 1108, 1077, 1001, 910, 820, 737, 664; MS(ESI): 341.11 $[M+H]^+$; HRMS(ESI): calcd for $C_{17}H_{21}N_2SFe$ $[M+H]^+$: 341.0775; found 341.0759.



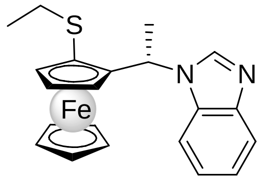
1-{(*S*)-1-[(*R*)-2-(*iso*-Propylthio)ferrocenyl]ethyl}-imidazole (**4e**). **3e** (1 g, 3.02 mmol) and imidazole (1.64 g, 24.16 mmol) in glacial AcOH (11 mL) were used with reference to the general procedure. Yield: 90%, orange solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +131.6° (c 1.0, CH_2Cl_2); m.p.= 112-115 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (s, 1H), 6.90 (s, 1H), 6.76 (s, 1H), 5.56 (q, 1H, J = 7.0 Hz), 4.48 (s, 1H), 4.42 (s, 1H), 4.32 (s, 1H), 4.16 (s, 5H), 1.80 (d, 3H, J = 7.0 Hz), 1.78-1.74 (m, 1H), 0.89 (d, 6H, J = 5.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.6, 128.8, 116.8, 89.9, 78.2, 76.9, 70.3, 68.3, 67.3, 50.9, 39.3, 23.4, 22.3, 22.2; IR (cm^{-1}) 3087, 2951, 2919, 2858, 1638, 1496, 1449, 1407, 1251, 1219, 1151, 1108, 1069, 1031, 907, 819, 740, 661; MS(EI): 354.13 $[M]^+$; HRMS(EI): calcd for $C_{18}H_{22}FeN_2S$ $[M]^+$: 354.0853; found 354.0862.



1-{(*S*)-1-[(*R*)-2-(Cyclohexylthio)ferrocenyl]ethyl}-imidazole (**4f**). **3f** (1 g, 2.69 mmol) and imidazole (1.46 g, 21.52 mmol) in glacial AcOH (10 mL) were used with reference to the general procedure. Yield: 92%, orange solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +95.6° (c 1.0, CH_2Cl_2); m.p.= 153-155 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40 (s, 1H), 6.91 (s, 1H), 6.75 (s, 1H), 5.57 (q, 1H, J = 7.0 Hz), 4.47 (s, 1H), 4.39 (s, 1H), 4.30 (s, 1H), 4.16 (s, 5H), 1.80 (d, 3H, J = 7.0 Hz), 1.55-1.32 (m, 6H), 1.03-0.80 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.6, 128.7, 116.8, 90.1, 77.7, 76.9, 70.3, 68.2, 67.3, 50.9, 47.6, 33.7, 32.6, 25.9, 25.5, 22.3; IR (cm^{-1}) 3066, 2977, 2924, 2849, 1653, 1492, 1449, 1400, 1338, 1249, 1216, 1107, 1069, 1033, 999, 906, 817, 734, 662; MS(EI): 394.13 $[M]^+$; HRMS(EI): calcd for $C_{21}H_{26}FeN_2S$ $[M]^+$: 394.1166; found 394.1181.

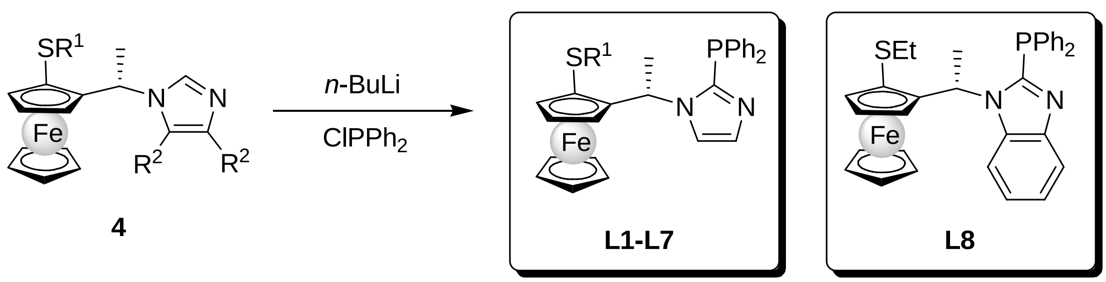


1-{(*S*)-1-[(*R*)-2-(*tert*-Butylthio)ferrocenyl]ethyl}-imidazole (**4g**). **3g** (1 g, 2.90 mmol) and imidazole (1.58 g, 23.2 mmol) in glacial AcOH (11 mL) were used with reference to the general procedure. Yield: 92%, yellow solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +231.9° (c 1.0, CH_2Cl_2); m.p.= 110-113 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.43 (s, 1H), 6.89 (s, 1H), 6.79 (s, 1H), 5.47 (q, 1H, *J* = 7.0 Hz), 4.55 (s, 1H), 4.50 (s, 1H), 4.39 (s, 1H), 4.17 (s, 5H), 1.81 (d, 3H, *J* = 6.5 Hz), 0.85 (s 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.7, 128.8, 117.1, 89.4, 77.3, 77.2, 70.6, 68.8, 67.6, 50.5, 46.2, 30.3, 23.8; IR (cm^{-1}) 3076, 2957, 2932, 2771, 1652, 1493, 1453, 1406, 1362, 1248, 1218, 1170, 1107, 1071, 1000, 814, 730, 661; MS(EI): 368.10 $[M]^+$; HRMS(EI): calcd for $C_{19}H_{24}FeN_2S$ $[M]^+$: 368.1010; found 368.1005.

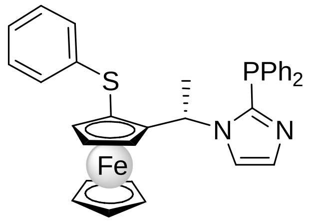


1-{(*S*)-1-[(*R*)-2-(Ethylthio)ferrocenyl]ethyl}-benzimidazole (**4h**). **3d** (1 g, 3.15 mmol) and benzimidazole (2.98 g, 25.20 mmol) in glacial AcOH (11 mL) were used with reference to the general procedure. Yield: 95%, red oil. R_f = 0.35 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +98.7° (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 7.74-7.72 (m, 2H), 7.53-7.50 (m, 1H), 7.25-7.19 (m, 2H), 5.86 (q, 1H, *J* = 7.0 Hz), 4.61 (s, 1H), 4.44 (s, 1H), 4.35 (s, 1H), 4.21 (s, 5H), 1.90 (d, 3H, *J* = 6.5 Hz), 1.59-1.52 (m, 1H), 1.50-1.41 (m, 1H), 0.63 (t, 3H, *J* = 7.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.7, 141.4, 132.5, 122.4, 121.7, 120.1, 110.2, 89.4, 79.0, 76.4, 70.3, 68.3, 67.6, 49.6, 30.6, 20.3, 14.1. IR (cm^{-1}) 3090, 2975, 2926, 2868, 1662, 1613, 1487, 1454, 1391, 1280, 1208, 1105, 1033, 1002, 822, 742; MS(ESI): 391.12 $[M+H]^+$; HRMS(ESI): calcd for $C_{21}H_{23}N_2SFe$ $[M+H]^+$: 391.0931, found 391.0937.

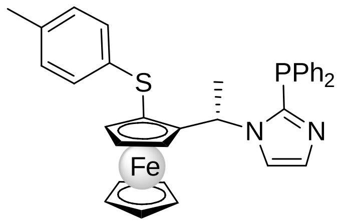
2.3 Preparation of P/S ligands L1-L8



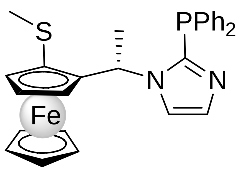
*General procedure for the preparation of P/S ligands **L1-L8**:* To a solution of **4** in THF was added dropwise *n*-BuLi (1 equiv., 1.6 M solution in hexane) at -78 °C, and the mixture was stirred for 30 min under a nitrogen atmosphere. Afterwards, chlorodiphenylphosphine (1.1 equiv.) was then added dropwise to the reaction mixture at 0 °C. The reaction mixture was stirred for further 4 h at room temperature, and then evaporated under reduced pressure. The residue was purified by flash chromatography to afford **L1-L8**.



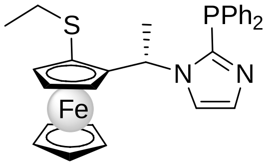
1-{(*S*)-1-[(*R*)-2-(Phenylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (**L1**). **4a** (0.5 g, 1.29 mmol), *n*-BuLi (0.81 mL, 1.6 M solution in hexane) and $ClPPh_2$ (255 μL, 1.42 mmol) in THF (16 mL) were used with reference to the general procedure. Yield: 76%, yellow solid. R_f = 0.42 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +10.6° (c 1.0, CH_2Cl_2); m.p.= 127-129 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52-7.49 (m, 2H), 7.34-7.33 (m, 3H), 7.19 (t, 1H, *J* = 7.0 Hz), 7.12-7.09 (m, 2H), 7.02 (s, 1H), 6.98 (t, 2H, *J* = 7.5 Hz), 6.92-6.86 (m, 3H), 6.84 (s, 1H), 6.43-6.42 (m, 2H), 6.32 (t, 1H, *J* = 7.5 Hz), 4.65 (s, 1H), 4.54-4.53 (s, 1H), 4.47-4.46 (m, 1H), 4.30 (s, 5H), 1.62 (d, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.2, 139.2, 135.9, 135.3, 134.3, 134.1, 133.1, 132.9, 130.8, 129.0, 128.5, 128.4, 128.3, 128.1, 127.9, 127.8, 125.2, 124.7, 118.7, 118.6, 91.4, 75.8, 70.6, 69.4, 68.2, 68.2, 67.0, 50.4, 50.2, 22.5; ^{31}P NMR (202 MHz, $CDCl_3$): δ –30.5; IR (cm^{-1}) 3052, 2362, 1649, 1578, 1476, 1431, 1376, 1245, 1104, 1027, 999, 827, 739, 692; MS(EI): 572.15 [M]$^+$; HRMS(EI): calcd for $C_{33}H_{29}N_2PSFe$ [M]$^+$: 572.1138; found 572.1135.



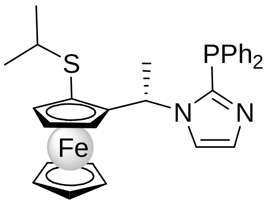
1-{(*S*)-1-[(*R*)-2-(*p*-Tolylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (**L2**). **4b** (0.5 g, 1.24 mmol), *n*-BuLi (0.78 mL, 1.6 M solution in hexane) and $ClPPh_2$ (245 μL, 1.36 mmol) in THF (15 mL) were used with reference to the general procedure. Yield: 63%, yellow solid. R_f = 0.45 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +21.3° (c 1.0, CH_2Cl_2); m.p.= 128-129 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.53-7.49 (m, 2H), 7.34-7.33 (m, 3H), 7.20-7.17 (m, 1H), 7.11-7.08 (m, 2H), 7.03 (s, 1H), 7.00-6.96 (m, 2H), 6.83 (s, 1H), 6.70 (d, 2H, *J* = 8.5 Hz), 6.36-6.31 (m, 3H), 4.63 (s, 1H), 4.52-4.51 (m, 1H), 4.45-4.44 (m, 1H), 4.29 (s, 5H), 2.17 (s, 3H), 1.62 (d, 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.3, 136.0, 135.9, 135.6, 135.4, 134.5, 134.3, 134.2, 133.1, 133.0, 130.8, 129.1, 129.0, 128.5, 128.4, 128.1, 127.9, 127.8, 125.6, 118.7, 91.3, 76.6, 76.5, 70.6, 69.3, 68.0, 50.4, 50.3, 22.5, 20.8; ^{31}P NMR (202 MHz, $CDCl_3$): δ –33.6; IR (cm^{-1}) 3052, 2976, 2924, 1637, 1490, 1431, 1376, 1246, 1104, 1066, 1029, 999, 827, 801, 743, 694; MS(ESI): 587.19 [M+H]$^+$; HRMS(ESI): calcd for $C_{34}H_{32}N_2PSFe$ [M+H]$^+$: 587.1373, found 587.1401.



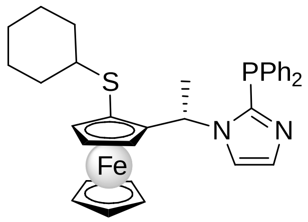
1-{(*S*)-1-[(*R*)-2-(Methylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (L3). **4c** (0.5 g, 1.53 mmol), *n*-BuLi (0.96 mL, 1.6 M solution in hexane) and $ClPPh_2$ (302 μL, 1.68 mmol) in THF (19 mL) were used with reference to the general procedure. Yield: 70%, yellow solid. R_f = 0.5 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +126.3° (c 1.0, CH_2Cl_2); m.p.= 153-154 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.68-7.64 (m, 2H), 7.51-7.48 (m, 2H), 7.37-7.33 (m, 6H), 7.13 (s, 1H), 6.76-6.75 (m, 1H), 6.41 (p, 1H, *J* = 7.0 Hz), 4.50-4.49 (m, 1H), 4.41-4.40 (m, 1H), 4.31-4.30 (m, 1H), 4.22 (s, 5H), 1.67 (d, 3H, *J* = 7.0 Hz), 1.26 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.6, 136.4, 136.3, 135.4, 135.3, 134.2, 134.1, 133.6, 133.4, 131.1, 131.0, 128.9, 128.7, 128.5, 128.4, 128.2, 128.1, 119.0, 90.3, 81.4, 75.1, 70.3, 68.1, 67.3, 67.2, 51.0, 50.8, 22.0, 20.2; ^{31}P NMR (202 MHz, $CDCl_3$): δ –35.1; IR (cm^{-1}) 3064, 2988, 2925, 1649, 1476, 1432, 1376, 1103, 1029, 999, 950, 819, 752, 694; MS (ESI): 511.1 $[M+H]^+$; HRMS(ESI): calcd for $C_{28}H_{28}N_2PSFe$ $[M+H]^+$: 511.1060, found 511.1056.



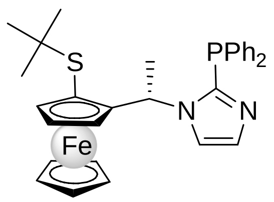
1-{(*S*)-1-[(*R*)-2-(Ethylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (L4). **4d** (0.5 g, 1.47 mmol), *n*-BuLi (0.92 mL, 1.6 M solution in hexane) and $ClPPh_2$ (290 μL, 1.62 mmol) in THF (18 mL) were used with reference to the general procedure. Yield: 48%, yellow solid. R_f = 0.36 (EtOAc/hexane/Et_3N = 1/1/0.01). $[\alpha]_D^{20}$ +94.4° (c 1.0, CH_2Cl_2); m.p.= 147-149 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.66-7.63 (m, 2H), 7.50-7.47 (m, 2H), 7.35-7.32 (m, 6H), 7.12 (s, 1H), 6.74 (s, 1H), 6.38 (p, 1H, *J* = 7.0 Hz), 4.50 (s, 1H), 4.42 (s, 1H), 4.33-4.32 (m, 1H), 4.22 (s, 5H), 1.69-1.62 (m, 4H), 1.39-1.32 (m, 1H), 0.72 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.5, 136.3, 136.3, 135.4, 135.3, 134.2, 134.0, 133.6, 133.5, 131.0, 130.9, 128.9, 128.7, 128.5, 128.4, 128.2, 128.1, 118.9, 90.5, 79.0, 76.4, 70.3, 68.2, 67.6, 50.9, 50.8, 30.1, 22.2, 14.5; ^{31}P NMR (202 MHz, $CDCl_3$): δ –34.9; IR (cm^{-1}) 3073, 2968, 2921, 1650, 1477, 1431, 1373, 1260, 1101, 1064, 1028, 1003, 920, 818, 745, 696; MS(ESI): 525.17 $[M+H]^+$; HRMS(ESI): calcd for $C_{29}H_{30}N_2PSFe$ $[M+H]^+$: 525.1217, found 525.1192.



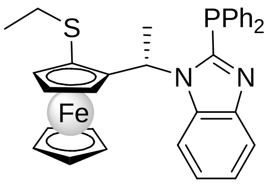
1-{(*S*)-1-[(*R*)-2-(*iso*-Propylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (L5). **4e** (0.5 g, 1.41 mmol), *n*-BuLi (0.88 mL, 1.6 M solution in hexane) and $ClPPh_2$ (278 μL, 1.55 mmol) in THF (17 mL) were used with reference to the general procedure. Yield: 55%, yellow solid. R_f = 0.4 (EtOAc/hexane/Et_3N = 1/2/0.01). $[\alpha]_D^{20}$ +69.1° (c 1.0, CH_2Cl_2); m.p.= 150-153 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.66-7.63 (m, 2H), 7.52-7.56 (m, 2H), 7.35-7.31 (m, 6H), 7.11 (s, 1H), 6.74-6.72 (m, 1H), 6.32 (p, 1H, J = 6.5 Hz), 4.51-4.50 (m, 1H), 4.44-4.43 (m, 1H), 4.34-4.44 (m, 1H), 4.21 (s, 5H), 1.81-1.74 (m, 1H), 1.62 (d, 3H, J = 7.0 Hz), 0.76 (d, 3H, J = 6.5 Hz), 0.67 (d, 3H, J = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.3, 136.4, 135.2, 134.2, 134.0, 133.8, 133.6, 130.7, 128.9, 128.8, 128.5, 128.4, 128.3, 128.2, 119.2, 90.6, 78.4, 77.0, 70.4, 68.3, 67.8, 50.9, 50.7, 38.4, 23.1, 22.4, 22.0; ^{31}P NMR (202 MHz, $CDCl_3$): δ –34.6; IR (cm^{-1}) 3076, 2959, 2919, 2859, 1649, 1476, 1431, 1374, 1245, 1103, 1052, 1028, 1002, 821, 744, 697; MS(EI): 538.20 $[M]^+$; HRMS(EI): calcd for $C_{30}H_{31}N_2PSFe$ $[M]^+$: 538.1295; found 538.1283.



1-{(*S*)-1-[(*R*)-2-(Cyclohexylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (**L6**). **4f** (0.5 g, 1.27 mmol), *n*-BuLi (0.79 mL, 1.6 M solution in hexane) and $ClPPh_2$ (251 μL, 1.40 mmol) in THF (16 mL) were used, with reference to the general procedure. Yield: 55%, yellow solid. R_f = 0.4 (EtOAc/hexane/Et_3N = 1/2/0.01). $[\alpha]_D^{20}$ +38.3° (c 1.0, CH_2Cl_2); m.p.= 133-134 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.70-7.69 (m, 2H), 7.51-7.48 (m, 2H), 7.34-7.29 (m, 6H), 7.12 (s, 1H), 6.69-6.68 (m, 1H), 6.33 (p, 1H, J = 7.0 Hz), 4.50 (s, 1H), 4.40 (s, 1H), 4.33-4.32 (m, 1H), 4.21 (s, 5H), 1.63 (d, 3H, J = 7.0 Hz), 1.46-1.23 (m, 6H), 0.96-0.70 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.3, 144.2, 136.6, 136.5, 136.3, 134.3, 134.1, 133.7, 133.5, 130.6, 130.5, 128.9, 128.7, 128.4, 128.3, 128.2, 128.1, 119.2, 90.7, 77.6, 77.2, 70.4, 68.2, 67.8, 50.9, 50.8, 46.4, 32.4, 32.3, 25.9, 25.5, 22.4, 22.3; ^{31}P NMR(202 MHz, $CDCl_3$): δ –35.2; IR (cm^{-1}) 3049, 2978, 2925, 2849, 1651, 1479, 1432, 1373, 1247, 1100, 1029, 999, 810, 742, 695; MS(ESI): 579.29 $[M+H]^+$; HRMS(ESI): calcd for $C_{33}H_{36}N_2PSFe$ $[M+H]^+$: 579.1686, found 579.1683.

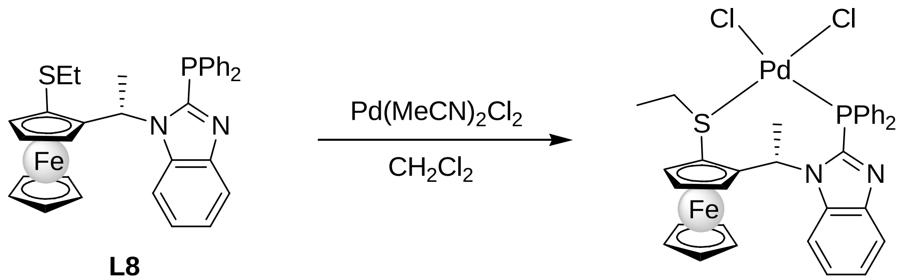


1-{(*S*)-1-[(*R*)-2-(*tert*-Butylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)imidazole (**L7**). **4g** (0.5 g, 1.36 mmol), *n*-BuLi (0.85 mL, 1.6 M solution in hexane) and $ClPPh_2$ (269 μL, 1.50 mmol) in THF (17 mL) were used with reference to the general procedure. Yield: 50%, yellow solid. R_f = 0.3 (EtOAc/hexane/Et_3N = 1/3/0.01). $[\alpha]_D^{20}$ +142.7° (c 1.0, CH_2Cl_2); m.p.= 64-67 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.71-7.67 (m, 2H), 7.50-7.46 (m, 2H), 7.34-7.30 (m, 6H), 7.12 (s, 1H), 6.86 (s, 1H), 6.26 (p, 1H, J = 7.0 Hz), 4.57 (s, 1H), 4.49 (s, 1H), 4.40-4.39 (m, 1H), 4.20 (s, 5H), 1.64 (d, 3H, J = 7.0 Hz), 0.76 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.1, 136.6, 136.5, 135.0, 134.5, 134.3, 133.7, 133.5, 130.7, 130.6, 128.9, 128.7, 128.5, 128.4, 128.3, 128.2, 119.3, 90.1, 77.6, 77.3, 70.7, 68.8, 68.1, 50.3, 50.2, 46.1, 30.2, 23.7; ^{31}P NMR (202 MHz, $CDCl_3$): δ –34.7; IR (cm^{-1}) 3052, 2965, 1649, 1476, 1453, 1432, 1365, 1244, 1153, 1102, 1066, 1027, 1001, 823, 745, 696; MS(ESI): 553.11 $[M+H]^+$; HRMS(ESI): calcd for $C_{31}H_{34}N_2PSFe$ $[M+H]^+$: 553.1530, found 553.1525.



1-{(*S*)-1-[(*R*)-2-(Ethylthio)ferrocenyl]ethyl}-2-(diphenylphosphino)benzimidazole (**L8**). **4h** (0.5 g, 1.28 mmol), *n*-BuLi (0.80 mL, 1.6 M solution in hexane) and $ClPPh_2$ (253 μL, 1.41 mmol) in THF (16 mL) were used with reference to the general procedure. Yield: 57%, yellow solid. R_f = 0.2 (EtOAc/hexane/Et_3N = 1/2/0.01). $[\alpha]_D^{20}$ +112.6° (c 1.0, CH_2Cl_2); m.p.= 72-75 °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.76-7.73 (m, 3H), 7.53 (bs, 2H), 7.41-7.36 (m, 6H), 7.25 (bs, 1H), 7.12 (t, 1H, *J* = 7.5 Hz), 7.04-7.01 (m, 1H), 6.78 (bs, 1H), 4.73 (s, 1H), 4.39 (s, 1H), 4.33-4.32 (m, 1H), 4.25 (s, 5H), 1.71 (d, 3H, *J* = 5.0 Hz), 1.33-1.22 (m, 1H), 1.07-1.00 (m, 1H), 0.44 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.8, 144.7, 135.3, 134.8, 134.4, 134.2, 134.1, 133.9, 129.2, 129.0, 128.6, 128.6, 128.3, 128.2, 122.3, 121.4, 120.5, 111.8, 88.9, 79.9, 76.8, 70.5, 69.1, 67.8, 51.5, 51.4, 29.9, 18.9, 13.9; ^{31}P NMR (202 MHz, $CDCl_3$): δ -28.6; IR (cm^{-1}) 3051, 2973, 2923, 2866, 1638, 1478, 1456, 1434, 1415, 1372, 1332, 1258, 1103, 1032, 1000, 824, 742, 695; MS(ESI): 575.10 $[M+H]^+$; HRMS(ESI): calcd for $C_{33}H_{32}N_2PSFe$ $[M+H]^+$: 575.1373, found 575.1345.

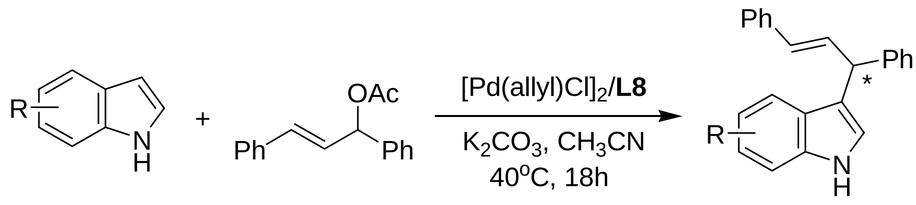
2.4 Synthesis of Pd(L8)Cl_2 complex



A mixture of **L8** (50 mg, 0.087 mmol) and $Pd(MeCN)_2Cl_2$ (22.6 mg, 0.087 mmol) in CH_2Cl_2 (2 mL) was stirred for 3 h at room temperature under a nitrogen atmosphere. Hexane (8 mL) was added to the resulting solution with stirring to precipitate the complex. The brick-red complex was filtered and dried under reduced pressure. A suitable crystal for X-ray analysis was grown by slow diffusion of hexane into a solution of Pd(**L8**)Cl_2 in CH_2Cl_2. Yield: 85%, brick-red solid. $[\alpha]_D^{20}$ –131.9° (c 1.06, CH_2Cl_2); m.p.= >250 °C; ^1H NMR (500 MHz, CD_2Cl_2): δ 8.30-8.22 (m, 2H), 7.86-7.82 (m, 2H), 7.68-7.56 (m, 7H), 7.23-7.12 (m, 3H), 6.48 (bs, 1H), 4.77 (s, 1H), 4.66 (s, 5H), 4.52 (bs, 1H), 4.36 (s, 1H), 2.33 (bs, 1H), 1.25 (bs, 1H), 1.13 (d, 3H, *J* =

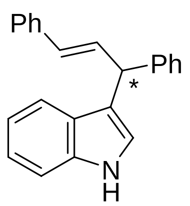
6.0 Hz), 0.93-0.85 (m, 3H); ^{13}C NMR (100 MHz, CD_2Cl_2): δ 144.6, 137.4, 137.3, 134.9, 134.8, 133.7, 133.4, 133.3, 132.3, 132.2, 129.9, 129.8, 128.9, 128.7, 127.5, 125.1, 123.7, 121.7, 112.7, 83.6, 72.6, 70.1, 68.2, 52.7, 15.5, 12.9; ^{31}P NMR (202 MHz, CD_2Cl_2): δ 7.8; IR (cm^{-1}) 3070, 2984, 1620, 1456, 1435, 1343, 1319, 1256, 1098, 1000, 826, 746, 693; HRMS(EI): calcd for $C_{33}H_{31}N_2Cl_2PSFePd$ $[M]^+$: 749.9707, found 749.9771.

3. Pd-catalyzed asymmetric allylic alkylation of indoles

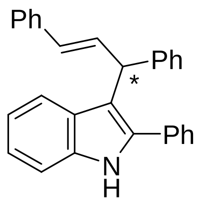


1 **2**

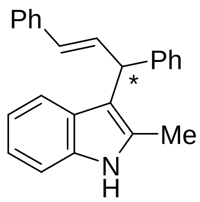
General procedure for the alkylation of indoles: A solution of $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (2.7 mg, 7.5 μmol) and **L8** (9.5 mg, 16.5 μmol) in CH_2Cl_2 (100 μL) was stirred for 15 min under a nitrogen atmosphere in a Teflon-lined screw-capped vial. 1,3-Diphenyl-2-propenyl acetate (90.8 mg, 0.36 mmol) in CH_3CN (2 mL) was then added, and the mixture was stirred for further 5 min. After addition of indole **1** (0.3 mmol) and K_2CO_3 (82.9 mg, 0.6 mmol), the reaction mixture was stirred at 40 °C for 18 h. The resulting mixture was quenched with water (4 mL) and extracted with EtOAc. The combined organic extracts were dried over anhydrous Na_2SO_4, filtered and evaporated under reduced pressure. The crude product was purified by flash column chromatography to afford the alkylated product **2**.



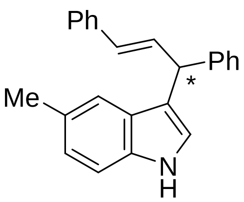
3-((*E*)-1,3-Diphenyl-2-propenyl)indole (**2a**).
Indole **1a** (35.1 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 74%, white solid. R_f = 0.24 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –45.8° (c 0.98, CH_2Cl_2); m.p.= 120-123 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.96 (bs, 1H), 7.46 (d, 1H, *J* = 8.0 Hz), 7.40-7.29 (m, 9H), 7.27-7.19 (m, 3H), 7.06 (t, 1H, *J* = 7.5 Hz), 6.91 (s, 1H), 6.76 (dd, 1H, *J* = 15.5, 7.0 Hz), 6.47 (d, 1H, *J* = 15.5 Hz), 5.15 (d, 1H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.3, 137.4, 136.6, 132.5, 130.5, 128.5, 128.4, 127.1, 126.7, 126.4, 126.3, 122.6, 122.0, 119.8, 119.4, 118.6, 111.1, 46.1; IR (cm^{-1}) 3425, 3055, 1701, 1599, 1492, 1453, 1417, 1336, 1094, 968, 739; HRMS(EI): calcd for $C_{23}H_{19}N$ $[M]^+$: 309.1517, found 309.1514.



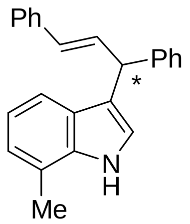
3-((*E*)-1,3-Diphenyl-2-propenyl)-2-phenylindole (**2b**).
2-Phenylindole **1b** (58.0 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 77%, pale yellow solid. R_f = 0.2 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –71.9° (c 1.0, CH_2Cl_2); m.p.= 40-42 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (bs, 1H), 7.58 (d, 2H, *J* = 6.5 Hz), 7.51-7.45 (m, 3H), 7.44-7.38 (m, 6H), 7.33-7.30 (m, 4H), 7.25-7.21 (m, 3H), 7.06 (t, 1H, *J* = 7.5 Hz), 6.95 (dd, 1H, *J* = 16.0, 7.5 Hz), 6.47 (d, 1H, *J* = 15.5 Hz), 5.34 (d, 1H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.4, 137.5, 136.2, 135.6, 132.9, 132.2, 131.0, 128.8, 128.6, 128.4, 128.3, 128.2, 127.9, 127.1, 126.3, 126.1, 122.1, 121.2, 119.7, 113.8, 110.9, 45.1; IR (cm^{-1}) 3416, 3055, 3027, 1600, 1491, 1450, 1306, 1264, 1156, 968; HRMS(EI): calcd for $C_{29}H_{23}N$ $[M]^+$: 385.1830, found 385.1828.



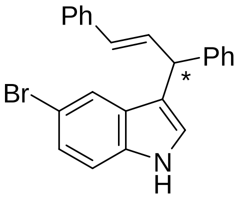
3-((*E*)-1,3-Diphenyl-2-propenyl)-2-methylindole (**2c**).
2-Methylindole **1c** (39.4 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 78%, yellow solid. R_f = 0.2 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ +3.4° (c 0.94, CH_2Cl_2); m.p.= 39-41 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.77 (bs, 1H), 7.43-7.39 (m, 4H), 7.34-7.29 (m, 4H), 7.26-7.23 (m, 4H), 7.14 (t, 1H, *J* = 7.5 Hz), 7.02 (t, 1H, *J* = 7.5 Hz), 6.88 (dd, 1H, *J* = 15.5, 7.5 Hz), 6.47 (d, 1H, *J* = 15.5 Hz), 5.19 (d, 1H, *J* = 7.0 Hz), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.4, 137.5, 135.3, 132.1, 131.6, 130.5, 128.5, 128.4, 128.3, 128.2, 127.9, 127.0, 126.2, 126.1, 120.9, 119.4, 119.2, 112.8, 110.2, 45.0, 12.3; IR (cm^{-1}) 3415, 3056, 3026, 1619, 1491, 1458, 968; HRMS(EI): calcd for $C_{24}H_{21}N$ $[M]^+$: 323.1674, found 323.1660.



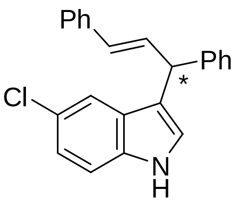
3-((*E*)-1,3-Diphenyl-2-propenyl)-5-methylindole (**2d**).
5-Methylindole **1d** (39.4 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 77%, pale yellow oil. R_f = 0.27 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –48.3° (c 1.01, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (bs, 1H), 7.42-7.31 (m, 8H), 7.29-7.23 (m, 3H), 7.06-7.04 (m, 1H), 6.87 (s, 1H), 6.76 (dd, 1H, *J* = 15.5, 7.5 Hz), 6.47 (d, 1H, *J* = 15.5 Hz), 5.14 (d, 1H, *J* = 7.0 Hz), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.4, 137.5, 134.9, 132.6, 130.4, 128.6, 128.5, 128.4, 128.3, 127.1, 126.9, 126.3, 123.7, 122.7, 119.3, 118.0, 110.7, 45.9, 21.5; IR (cm^{-1}) 3466, 2096, 1638, 1421; HRMS(EI): calcd for $C_{24}H_{21}N$ $[M]^+$: 323.1674, found 323.1646.



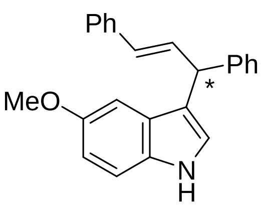
3-((*E*)-1,3-Diphenyl-2-propenyl)-7-methylindole (**2e**). 7-Methylindole **1e** (39.4 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 75%, yellow oil. R_f = 0.3 (EtOAc/hexane = 1/12). $[\alpha]_D^{20}$ –40.7° (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 7.85 (bs, 1H), 7.48-7.29 (m, 11H), 7.09-7.07 (m, 2H), 6.92 (d, 1H, *J* = 2.5 Hz), 6.85 (dd, 1H, *J* = 15.5, 8.0 Hz), 6.56 (d, 1H, *J* = 15.5 Hz), 5.23 (d, 1H, *J* = 7.0 Hz), 2.54 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.4, 137.4, 136.1, 132.5, 130.5, 128.4, 128.3, 127.1, 126.3, 126.2, 122.6, 122.3, 120.2, 119.6, 119.0, 117.6, 46.2, 16.5; IR (cm^{-1}) 3462, 3054, 1633, 1439, 1450, 1341, 968; HRMS(EI): calcd for $C_{24}H_{21}N$ $[M]^+$: 323.1674, found 323.1654.



5-Bromo-3-((*E*)-1,3-diphenyl-2-propenyl)indole (**2f**). 5-Bromoindole **1f** (58.8 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 66%, colorless oil. R_f = 0.12 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –35.1° (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 7.99 (bs, 1H), 7.57 (s, 1H), 7.40-7.21 (m, 12H), 6.91-6.90 (m, 1H), 6.71 (dd, 1H, *J* = 16.0, 7.0 Hz), 6.44 (d, 1H, *J* = 15.5 Hz), 5.08 (d, 1H, *J* = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.8, 137.2, 135.2, 132.0, 130.7, 128.5, 128.3, 127.2, 126.5, 126.3, 124.9, 123.8, 122.2, 118.3, 112.7, 112.6, 45.8; IR (cm^{-1}) 3457, 3055, 2983, 1726, 1643, 1493, 1454, 1417, 1096, 969; HRMS(EI): calcd for $C_{23}H_{18}BrN$ $[M]^+$: 387.0623, found 387.0617.

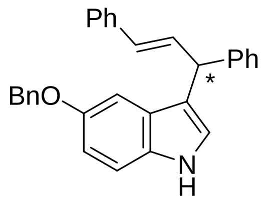


5-Chloro-3-((*E*)-1,3-diphenyl-2-propenyl)indole (**2g**). 5-Chloroindole **1g** (45.5 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 61%, pale yellow oil. R_f = 0.12 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –37.0° (c 0.94, CH_2Cl_2); ^1H NMR (500 MHz, $CDCl_3$): δ 7.97 (bs, 1H), 7.43-7.24 (m, 12H), 7.16-7.14 (m, 1H), 6.93 (s, 1H), 6.72 (dd, 1H, *J* = 15.5, 7.5 Hz), 6.45 (d, 1H, *J* = 16.0 Hz), 5.09 (d, 1H, *J* = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.9, 137.3, 134.9, 132.0, 130.8, 128.5, 128.4, 127.8, 127.2, 127.3, 126.5, 126.3, 125.1, 123.9, 122.4, 119.2, 118.4, 112.1, 45.9; IR (cm^{-1}) 3455, 3055, 3027, 1725, 1599, 1493, 1459, 1418, 1097, 968, 894, 798; HRMS(EI): calcd for $C_{23}H_{18}ClN$ $[M]^+$: 343.1128, found 343.1134.



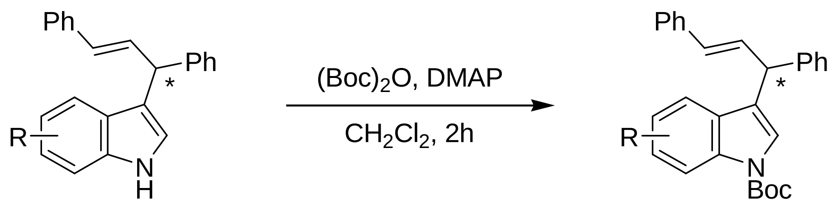
3-((*E*)-1,3-diphenyl-2-propenyl)-5-methoxyindole (**2h**). 5-Methoxyindole **1h** (44.2 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 85%, colorless oil. R_f = 0.15 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –38.5° (c 0.96, CH_2Cl_2);

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (bs, 1H), 7.38-7.19 (m, 12H), 6.89-6.83 (m, 2H), 6.72 (dd, 1H, *J* = 15.5, 7.0 Hz), 6.45 (d, 1H, *J* = 16.5 Hz), 5.08 (d, 1H, *J* = 7.5 Hz), 3.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.7, 143.3, 137.4, 132.5, 131.7, 130.5, 128.5, 128.4, 128.3, 127.2, 127.1, 126.4, 126.3, 123.4, 118.2, 112.1, 111.8, 101.7, 55.7, 46.2; IR (cm^{-1}) 3427, 3055, 3027, 2942, 2831, 1623, 1582, 1484, 1451, 1214, 1172, 1030, 968, 799; HRMS(EI): calcd for $C_{24}H_{21}NO$ $[M]^+$: 339.1623, found 339.1628.



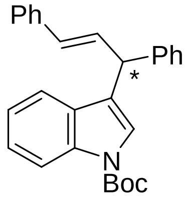
5-Benzyloxy-3-((*E*)-1,3-diphenyl-2-propenyl)indole (**2i**). 5-Benzyloxyindole **1i** (67.0 mg, 0.3 mmol) was used with reference to the general procedure. Yield: 56%, colorless oil. R_f = 0.12 (EtOAc/hexane = 1/9). $[\alpha]_D^{20}$ –30.2° (c 1.0, CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (bs, 1H), 7.39-7.19 (m, 16H), 6.94-6.89 (m, 3H), 6.70 (dd, 1H, *J* = 15.5, 7.0 Hz), 6.44 (d, 1H, *J* = 16.0 Hz), 5.06 (d, 1H, *J* = 7.0 Hz), 4.96 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.9, 143.2, 137.6, 132.4, 131.9, 130.5, 128.4, 128.3, 127.7, 127.6, 127.1, 126.3, 126.2, 123.4, 118.3, 112.9, 111.8, 103.4, 70.8, 46.2; IR (cm^{-1}) 3431, 3055, 2303, 1623, 1481, 1452, 1183, 1025, 969, 798; HRMS(EI): calcd for $C_{30}H_{25}NO$ $[M]^+$: 415.1936, found 415.1940.

4. Boc-derivatization of indoles 2 for HPLC determinations



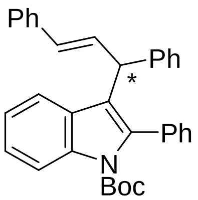
2 **5**

General procedure for the N-Boc protection of alkylated indoles: To a solution of **2** (0.1 mmol) and DMAP (0.6 mg, 0.005 mmol) in CH_2Cl_2 (2 mL) was added $(Boc)_2O$ (32.7 mg, 0.15 mmol), and the solution was stirred for 2 h at room temperature. The resulting mixture was evaporated under reduced pressure and purified by flash column chromatography to afford the *N*-Boc-protected alkylated indole **5**.

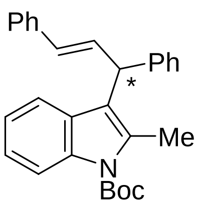


***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)indole carboxylate** (**5a**). **2a** (31 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 99%, colorless oil. R_f = 0.3 (EtOAc/hexane = 1/20). $[\alpha]_D^{20}$ –38.8° (c 1.01, CH_2Cl_2), 95% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 8.1 min and 9.7

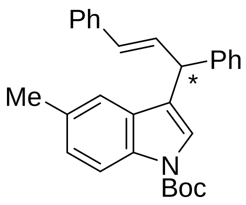
min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (bs, 1H), 7.43-7.24 (m, 13H), 7.18 (t, 1H, *J* = 7.5 Hz), 6.74 (dd, 1H, *J* = 16.0, 7.5 Hz), 6.49 (d, 1H, *J* = 16.5 Hz), 5.09 (d, 1H, *J* = 7.5 Hz), 1.72 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.9, 142.0, 137.2, 135.6, 131.3, 131.2, 129.8, 128.5, 128.4, 128.3, 127.3, 126.7, 126.4, 124.3, 123.8, 122.9, 122.4, 120.1, 115.2, 83.6, 45.9, 28.2; IR (cm^{-1}) 3057, 2982, 1808, 1730, 1645, 1452, 1372, 1308, 1213, 1156, 1119, 1075, 844; HRMS(EI): calcd for $C_{28}H_{27}NO_2$ $[M]^+$: 409.2042, found 409.2056.



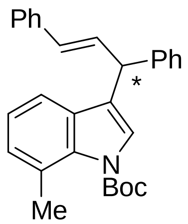
***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)-2-phenylindole carboxylate (5b)**. **2b** (39 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 99%, white solid. R_f = 0.3 (EtOAc/hexane = 1/20). m.p.= 154-155 °C. $[\alpha]_D^{20}$ –39.6° (c 1.0, CH_2Cl_2), 92% ee by HPLC (Chiralcel AD-H, *i*-PrOH/hexane = 1/99, 1.0 mL/min, 254 nm, t_R = 4.1 min and 10.1 min). Recrystallization from CH_2Cl_2/hexane gave the product with 99.5% ee {$[\alpha]_D^{20}$ –46.5° (c 1.0, CH_2Cl_2)}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.36 (d, 1H, *J* = 8.5 Hz), 7.50-7.20 (m, 17H), 7.17 (t, 1H, *J* = 7.5 Hz), 6.82 (dd, 1H, *J* = 15.5, 8.0 Hz), 6.37 (d, 1H, *J* = 16.0 Hz), 4.92 (d, 8.0 Hz), 1.29 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.1, 142.5, 137.3, 136.9, 136.6, 134.2, 131.6, 130.6, 129.9, 128.4, 128.2, 127.9, 127.8, 127.2, 126.3, 126.2, 124.2, 122.5, 121.2, 120.9, 115.3, 82.9, 44.8, 27.5; IR (cm^{-1}) 3026, 2978, 1721, 1600, 1493, 1452, 1364, 1326, 1253, 1227, 1153, 1073, 767, 748, 697; HRMS(EI): calcd for $C_{34}H_{31}NO_2$ $[M]^+$: 485.2355, found 485.2361.



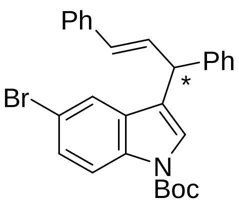
***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)-2-methylindole carboxylate (5c)**. **2c** (32 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 99%, colorless oil. R_f = 0.3 (EtOAc/hexane = 1/20). $[\alpha]_D^{20}$ +1.2° (c 0.89, CH_2Cl_2), 95% ee by HPLC (Chiralcel OJ-H, *i*-PrOH/hexane = 20/80, 0.3 mL/min, 254 nm, t_R = 17.4 min and 22.2 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.20 (d, 1H, *J* = 8.5 Hz), 7.44-7.24 (m, 12H), 7.13 (t, 1H, *J* = 8.0 Hz), 6.87 (dd, 1H, *J* = 16.0, 7.5 Hz), 6.53 (d, 1H, *J* = 16.0 Hz), 5.25 (d, 1H, *J* = 7.5 Hz), 1.75 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.7, 142.3, 137.2, 136.0, 133.9, 131.5, 130.6, 128.9, 128.5, 128.3, 128.0, 127.3, 126.3, 126.2, 123.2,122.2, 119.5, 119.2, 115.3, 83.6, 44.5, 28.3, 14.3; IR (cm^{-1}) 3056, 3026, 2979, 2932, 1807, 1730, 1455, 1358, 1322, 1260, 1221, 1158, 1118, 1071, 966, 845; HRMS(EI): calcd for $C_{29}H_{29}NO_2$ $[M]^+$: 423.2198, found 423.2203.



***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)-5-methylindole carboxylate** (**5d**). **2d** (32 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 92%, colorless oil. R_f = 0.3 (EtOAc/hexane = 1/20). $[\alpha]_D^{20}$ –41.2° (c 1.05, CH_2Cl_2), 96% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 9.0 min and 10.9 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01 (bs, 1H), 7.40-7.22 (m, 11H), 7.16-7.12 (m, 2H), 6.71 (dd, 1H, J = 16.0, 7.0 Hz), 6.44 (d, 1H, J = 16.0 Hz), 5.04 (d, 1H, J = 7.5 Hz), 2.38 (s, 3H), 1.68 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.9, 142.1, 137.2, 133.9, 131.8, 131.3, 131.1, 130.0, 128.5, 128.4, 128.3, 127.3, 126.6, 126.3, 125.7, 123.8, 122.7, 119.8, 114.8, 83.4, 45.7, 28.2, 21.4; IR (cm^{-1}) 3026, 2980, 2931, 1730, 1598, 1473, 1453, 1374, 1291, 1217, 1157, 1075, 968, 854, 804; HRMS(EI): calcd for $C_{29}H_{29}NO_2$ $[M]^+$: 423.2198, found 423.2210.

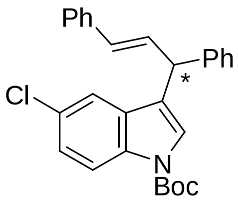


***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)-5-methylindole carboxylate** (**5e**). **2e** (32 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 97%, white solid. R_f = 0.3 (EtOAc/hexane = 1/20). m.p.= 124-126°C. $[\alpha]_D^{20}$ –44.8° (c 1.05, CH_2Cl_2), 96% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 3/97, 0.7 mL/min, 254 nm, t_R = 6.1 min and 6.6 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.47-7.36 (m, 9H), 7.34-7.27 (m, 3H), 7.18-7.12 (m, 2H), 6.78 (dd, 1H, J = 16.0, 7.5 Hz), 6.53 (d, 1H, J = 16.5 Hz), 5.11 (d, 1H, J = 7.0 Hz), 2.73 (s, 3H), 1.70 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.6, 142.1, 137.2, 135.4, 131.3, 131.2, 131.1, 128.5, 128.4, 128.3, 127.7, 127.3, 126.6, 126.3, 125.9, 125.3, 122.9, 122.5, 117.6, 83.3, 45.8, 28.0, 22.2; IR (cm^{-1}) 3027, 2973, 2930, 1743, 1489, 1452, 1347, 1254, 1221, 1159, 1046, 1031, 975, 794, 765, 747, 700; HRMS(EI): calcd for $C_{29}H_{29}NO_2$ $[M]^+$: 423.2198, found 423.2212.

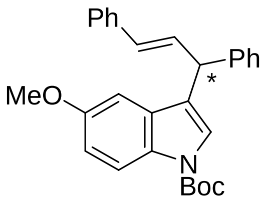


***N-tert*-Butyl 5-bromo-3-((*E*)-1,3-diphenyl-2-propenyl)indole carboxylate** (**5f**). **2f** (39 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 94%, white waxy solid. R_f = 0.3 (EtOAc/hexane = 1/20). m.p.= 71-74°C. $[\alpha]_D^{20}$ –32.9° (c 1.0, CH_2Cl_2), 94% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 7.8 min and 8.6 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07 (bs, 1H), 7.53 (s, 1H), 7.44-7.25 (m, 12H), 6.71 (dd, 1H, J = 16.0, 7.0 Hz), 6.48 (d, 1H, J = 15.5 Hz), 5.04 (d, 1H, J = 7.5 Hz), 1.71 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.4, 141.5, 136.9, 134.5, 131.5, 131.4, 130.7, 128.6, 128.5, 128.3, 127.4, 127.2, 126.9, 126.3, 124.8, 122.6, 122.3, 116.7, 115.8, 84.1, 45.6, 28.1; IR (cm^{-1}) 3058, 3027, 2980, 2933, 1734, 1450, 1372, 1154, 1055, 967, 842, 805; HRMS(EI):

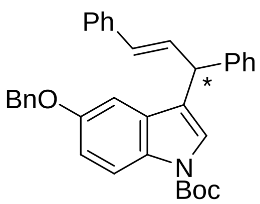
calcd for $C_{28}H_{26}BrNO_2$ $[M]^+$: 487.1147, found 487.1151.



***N-tert*-Butyl 5-chloro-3-((*E*)-1,3-diphenyl-2-propenyl)indole carboxylate** (**5g**). **2g** (34 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 94%, white waxy solid. R_f = 0.3 (EtOAc/hexane = 1/20). m.p.= 53-56°C. $[\alpha]_D^{20}$ –36.1° (c 0.95, CH_2Cl_2), 96% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 8.2 min and 9.1 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (bs, 1H), 7.46-7.27 (m, 13H), 6.72 (dd, 1H, *J* = 15.5, 7.5 Hz), 6.49 (d, 1H, *J* = 16.0 Hz), 5.04 (d, 1H, *J* = 7.5 Hz), 1.71 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.4, 141.6, 136.9, 134.2, 131.5, 131.0, 130.7, 128.6, 128.5, 128.3, 128.1, 127.4, 126.8, 126.3, 124.9, 124.5, 122.4, 119.5, 116.3, 84.1, 45.7, 28.1; IR (cm^{-1}) 3056, 3028, 2981, 2934, 1733, 1601, 1452, 1373, 1155, 1062, 968, 846, 808; HRMS(EI): calcd for $C_{28}H_{26}ClNO_2$ $[M]^+$: 443.1652, found 443.1662.



***N-tert*-Butyl 3-((*E*)-1,3-diphenyl-2-propenyl)-2-methoxy-indole carboxylate** (**5h**). **2h** (34 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 88%, pale yellow oil. R_f = 0.3 (EtOAc/hexane = 1/20). $[\alpha]_D^{20}$ –37.6° (c 0.95, CH_2Cl_2), 94% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 10.8 min and 12.9 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.02 (bs, 1H), 7.40-7.22 (m, 11H), 6.93-6.89 (m, 1H), 6.79 (d, 1H, *J* = 3.0 Hz), 6.69 (dd, 1H, *J* = 15.5, 7.0 Hz), 6.46 (d, 1H, *J* = 16.0 Hz), 5.01 (d, 1H, *J* = 7.0 Hz), 3.73 (s, 3H), 1.68 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.5, 149.8, 141.9, 137.2, 131.3, 131.1, 130.7, 128.6, 128.5, 128.4, 127.3, 126.7, 126.3, 124.4, 122.7, 115.9, 112.7, 102.9, 83.5, 55.5, 45.9, 28.2; IR (cm^{-1}) 3061, 3031, 2985, 2837, 1732, 1619, 1480, 1452, 1384, 1343, 1269, 1160, 1080, 972, 855; HRMS(EI): calcd for $C_{29}H_{29}NO_3$ $[M]^+$: 439.2147, found 439.2145.



***N-tert*-Butyl 5-benzyloxy-3-((*E*)-1,3-diphenyl-2-propenyl) indole carboxylate** (**5i**). **2i** (42 mg, 0.1 mmol) was used with reference to the general procedure. Yield: 94%, colorless oil. R_f = 0.3 (EtOAc/hexane = 1/20). $[\alpha]_D^{20}$ –28.2° (c 0.97, CH_2Cl_2), 94% ee by HPLC (Chiralcel OD-H, *i*-PrOH/hexane = 1/99, 0.7 mL/min, 254 nm, t_R = 15.7 min and 17.8 min); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (bs, 1H), 7.43-7.25 (m, 17H), 7.05-7.03 (m, 1H), 6.92 (d, 1H, *J* = 2.0 Hz), 6.72 (dd, 1H, *J* = 15.5, 7.5 Hz), 6.48 (d, 1H, *J* = 16.0 Hz), 5.03-4.99 (m, 3H), 1.71 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.6, 149.7, 141.9, 137.1, 131.2, 130.9, 130.6, 128.5, 128.4, 128.3, 127.8, 127.5, 127.3, 126.7, 126.3, 124.4, 122.7, 115.9, 113.6, 104.4, 83.4, 70.4, 45.9, 28.1; IR (cm^{-1}) 3059, 3028, 2979, 2932, 1729, 1613, 1472, 1451, 1379, 1266, 1156, 1074, 1025, 968, 852, 800; HRMS(EI): calcd for $C_{35}H_{33}NO_3$ $[M]^+$: 515.2460, found 515.2482.

5. References

[1] Bandini, M.; Melloni, A.; Umani-Ronchi, A. *Org. Lett.* **2004**, *6*, 3199.

[2] Lam, W. S.; Kok, S. H. L.; Au-Yeung, T. T.-L.; Wu, J.; Cheung, H. Y.; Lam, F. L.; Yeung, C.-H.; Chan, A. S. C. *Adv. Synth. Catal.* **2006**, *348*, 370.

[3] Okoroator, M. O.; Ward, D. L.; Brubaker, C. H. *Organometallics* **1988**, *7*, 1504.

6. X-ray crystallographic data of $Pd(L8)Cl_2$

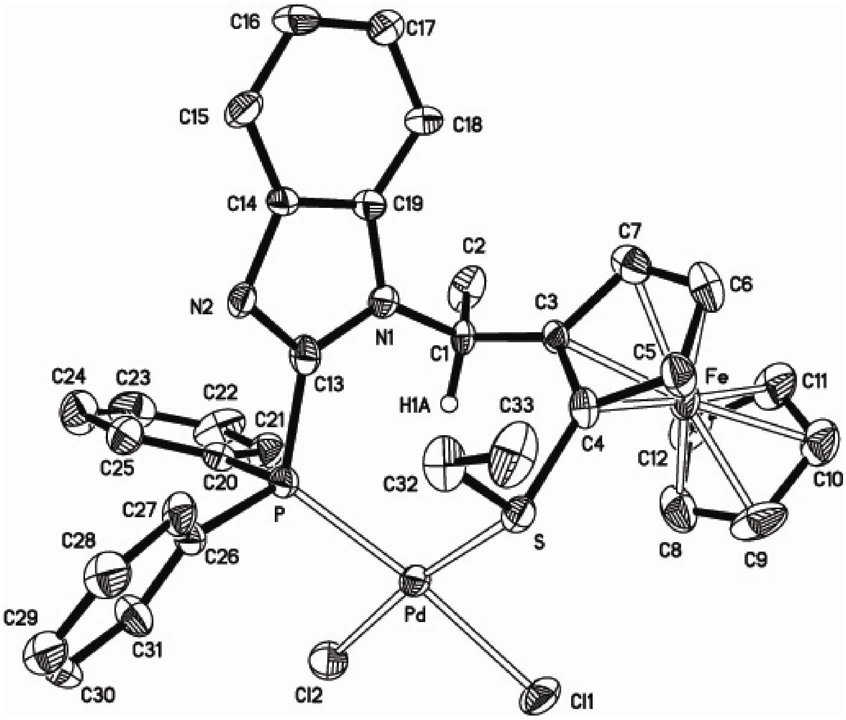


Fig. 1 The molecular structure of [Pd(**L8**)Cl_2] (hydrogen atoms omitted)

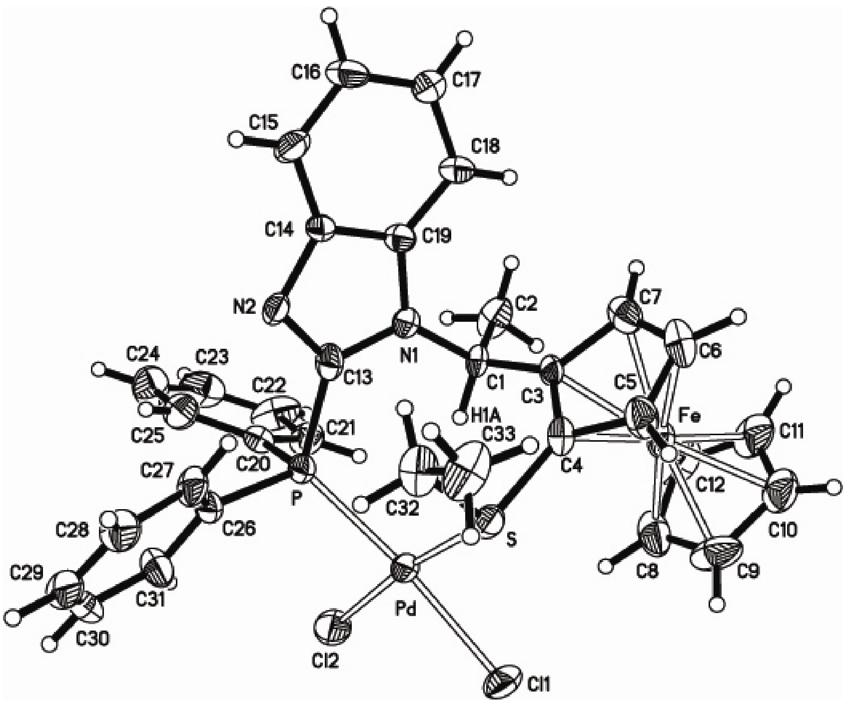


Fig. 2 The molecular structure of [Pd(**L8**)Cl_2] with hydrogen atoms

Table 1. Crystal data and structure refinement for Pd(**L8**)Cl_2

Identification code	gama15	
Empirical formula	$Pd(Cl)_2[FePSC_{33}H_{31}N_2]$ .I/2(CH_2Cl_2)	
Formula weight	794.24	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.865(2) Å	= 90°.
	b = 20.931(5) Å	= 90°.
	c = 31.720(8) Å	= 90°.
Volume	6550(3) $Å^3$	
Z	8	
Density (calculated)	1.611 Mg/m^3	
Absorption coefficient	1.377 mm^{-1}	
F(000)	3208	
Crystal size	0.14 x 0.10 x 0.06 mm^3	
Theta range for data collection	1.95 to 27.59°.	
Index ranges	-12<=h<=12, -26<=k<=27, -40<=l<=41	
Reflections collected	60695	
Independent reflections	15099 [R(int) = 0.1312]	
Completeness to theta = 27.59°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.700	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15099 / 0 / 770	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0687, wR2 = 0.1544	
R indices (all data)	R1 = 0.1381, wR2 = 0.1943	
Absolute structure parameter	-0.01(3)	
Largest diff. peak and hole	0.901 and -0.678 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gama15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd	3400(1)	7611(1)	6862(1)	34(1)
Fe	668(1)	6131(1)	7444(1)	42(1)
Cl(1)	3102(1)	6851(1)	6323(1)	56(1)
Cl(2)	5662(1)	7660(1)	6705(1)	57(1)
S	1052(1)	7546(1)	6923(1)	38(1)
P	3820(1)	8392(1)	7336(1)	32(1)
N(1)	2254(3)	7904(1)	8009(1)	38(1)
N(2)	2276(3)	8989(1)	7951(1)	35(1)
C(1)	2442(3)	7227(1)	7904(1)	34(1)
C(2)	3155(4)	6858(2)	8256(1)	55(1)
C(3)	1109(4)	6962(2)	7755(1)	32(1)
C(4)	485(4)	7083(2)	7346(1)	39(1)
C(5)	-797(4)	6789(2)	7356(1)	50(1)
C(6)	-997(4)	6494(2)	7744(1)	56(1)
C(7)	163(4)	6586(2)	7996(1)	51(1)
C(8)	2186(5)	5716(2)	7115(2)	66(2)
C(9)	899(6)	5582(2)	6927(1)	80(2)
C(10)	111(5)	5237(2)	7220(1)	65(2)
C(11)	881(5)	5178(2)	7581(2)	69(2)
C(12)	2160(5)	5460(2)	7523(2)	71(2)
C(13)	2682(4)	8444(2)	7782(1)	38(1)
C(14)	1545(4)	8808(2)	8315(1)	36(1)
C(15)	930(4)	9195(2)	8612(1)	45(1)
C(16)	302(4)	8905(2)	8956(1)	51(1)
C(17)	252(4)	8241(2)	8987(1)	49(1)
C(18)	856(4)	7837(2)	8679(1)	45(1)
C(19)	1531(4)	8148(2)	8349(1)	35(1)
C(20)	5399(4)	8393(2)	7626(1)	38(1)
C(21)	6011(4)	7825(2)	7741(1)	51(1)
C(22)	7193(4)	7832(2)	7991(1)	66(1)
C(23)	7699(4)	8400(3)	8114(1)	69(2)
C(24)	7128(5)	8977(2)	8014(1)	67(2)
C(25)	5953(4)	8951(2)	7769(1)	55(1)

C(26)	3775(4)	9160(2)	7062(1)	35(1)
C(27)	2616(4)	9541(2)	7034(1)	42(1)
C(28)	2632(5)	10072(2)	6773(1)	55(1)
C(29)	3769(5)	10248(2)	6562(1)	61(1)
C(30)	4903(5)	9876(2)	6589(1)	61(1)
C(31)	4899(4)	9325(2)	6828(1)	50(1)
C(32)	292(4)	8327(2)	7034(1)	56(1)
C(33)	-1162(4)	8350(2)	6909(2)	70(2)
Pd(2)	5492(1)	4638(1)	4288(1)	43(1)
Fe(2)	2984(1)	6374(1)	4672(1)	41(1)
Cl(3)	4030(1)	4757(1)	3707(1)	70(1)
Cl(4)	5404(2)	3545(1)	4217(1)	81(1)
S(2)	5808(1)	5736(1)	4231(1)	42(1)
P(2)	6652(1)	4383(1)	4879(1)	40(1)
N(3)	6373(3)	5508(1)	5357(1)	33(1)
N(4)	8509(3)	5100(1)	5338(1)	37(1)
C(34)	4924(3)	5558(2)	5275(1)	36(1)
C(35)	4081(4)	5479(2)	5675(1)	47(1)
C(36)	4610(4)	6149(2)	5027(1)	41(1)
C(37)	4973(4)	6241(2)	4595(1)	39(1)
C(38)	4607(4)	6867(2)	4472(1)	50(1)
C(39)	4034(4)	7174(2)	4830(1)	52(1)
C(40)	4047(4)	6739(2)	5169(1)	45(1)
C(41)	1425(5)	5757(2)	4806(1)	67(2)
C(42)	1880(4)	5691(3)	4382(2)	89(2)
C(43)	1687(4)	6280(3)	4172(2)	98(2)
C(44)	1167(4)	6709(3)	4483(2)	86(2)
C(45)	993(5)	6372(2)	4840(2)	69(2)
C(46)	7257(4)	5037(2)	5212(1)	35(1)
C(47)	8472(3)	5650(2)	5591(1)	33(1)
C(48)	9540(4)	5935(2)	5812(1)	42(1)
C(49)	9248(4)	6485(2)	6031(1)	46(1)
C(50)	7931(4)	6745(2)	6041(1)	40(1)
C(51)	6868(4)	6465(2)	5828(1)	43(1)
C(52)	7172(3)	5914(2)	5602(1)	32(1)
C(53)	8200(4)	3950(2)	4784(1)	45(1)
C(54)	9273(4)	4222(2)	4586(1)	58(1)
C(55)	10437(5)	3909(2)	4474(2)	73(2)

C(56)	10595(6)	3270(2)	4602(2)	84(2)
C(57)	9534(6)	2979(2)	4818(2)	89(2)
C(58)	8295(6)	3307(2)	4904(2)	79(2)
C(59)	5607(4)	3962(2)	5256(1)	46(1)
C(60)	6058(5)	3812(2)	5656(1)	58(1)
C(61)	5226(6)	3549(3)	5951(2)	89(2)
C(62)	3883(6)	3441(3)	5872(2)	89(2)
C(63)	3392(6)	3615(2)	5478(2)	81(2)
C(64)	4210(4)	3868(2)	5167(1)	57(1)
C(65)	7575(4)	5938(2)	4320(1)	48(1)
C(66)	7847(5)	6610(2)	4152(2)	94(2)
Cl(5)	3955(3)	10228(1)	8350(1)	171(1)
Cl(6)	4311(2)	10997(1)	7609(1)	123(1)
C(67)	4005(6)	10959(3)	8144(2)	105(2)

Table 3. Bond lengths [Å] and angles [°] for gama15.

Pd-P	2.2591(10)
Pd-Cl(2)	2.2893(12)
Pd-S	2.3281(11)
Pd-Cl(1)	2.3531(11)
Fe-C(9)	2.015(4)
Fe-C(5)	2.017(4)
Fe-C(8)	2.022(5)
Fe-C(4)	2.025(3)
Fe-C(6)	2.044(4)
Fe-C(3)	2.045(3)
Fe-C(12)	2.050(5)
Fe-C(11)	2.051(4)
Fe-C(7)	2.054(4)
Fe-C(10)	2.075(4)
S-C(4)	1.748(4)
S-C(32)	1.832(4)
P-C(13)	1.809(4)
P-C(20)	1.810(4)
P-C(26)	1.830(3)
N(1)-C(19)	1.389(4)
N(1)-C(13)	1.406(4)
N(1)-C(1)	1.466(4)
N(2)-C(13)	1.322(4)
N(2)-C(14)	1.415(4)
C(1)-C(3)	1.504(5)
C(1)-C(2)	1.528(5)
C(1)-H(1A)	0.9800
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(2)-H(2D)	0.9600
C(3)-C(7)	1.440(5)
C(3)-C(4)	1.457(5)
C(4)-C(5)	1.407(5)
C(5)-C(6)	1.391(6)
C(5)-H(5A)	0.9800
C(6)-C(7)	1.409(6)

C(6)-H(6A)	0.9800
C(7)-H(7A)	0.9800
C(8)-C(12)	1.403(7)
C(8)-C(9)	1.430(7)
C(8)-H(8A)	0.9800
C(9)-C(10)	1.409(7)
C(9)-H(9A)	0.9800
C(10)-C(11)	1.379(7)
C(10)-H(10A)	0.9800
C(11)-C(12)	1.405(7)
C(11)-H(11A)	0.9800
C(12)-H(12A)	0.9800
C(14)-C(15)	1.383(5)
C(14)-C(19)	1.386(5)
C(15)-C(16)	1.394(5)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.394(6)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.421(5)
C(17)-H(17A)	0.9300
C(18)-C(19)	1.401(5)
C(18)-H(18A)	0.9300
C(20)-C(25)	1.368(5)
C(20)-C(21)	1.381(5)
C(21)-C(22)	1.410(6)
C(21)-H(21A)	0.9300
C(22)-C(23)	1.348(7)
C(22)-H(22A)	0.9300
C(23)-C(24)	1.370(7)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.395(6)
C(24)-H(24A)	0.9300
C(25)-H(25A)	0.9300
C(26)-C(31)	1.378(5)
C(26)-C(27)	1.397(5)
C(27)-C(28)	1.385(5)
C(27)-H(27A)	0.9300
C(28)-C(29)	1.357(6)

C(28)-H(28A)	0.9300
C(29)-C(30)	1.365(6)
C(29)-H(29A)	0.9300
C(30)-C(31)	1.380(6)
C(30)-H(30A)	0.9300
C(31)-H(31A)	0.9300
C(32)-C(33)	1.489(6)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
Pd(2)-P(2)	2.2594(11)
Pd(2)-Cl(4)	2.2999(12)
Pd(2)-S(2)	2.3275(11)
Pd(2)-Cl(3)	2.3540(12)
Fe(2)-C(37)	1.997(4)
Fe(2)-C(38)	2.007(4)
Fe(2)-C(36)	2.015(4)
Fe(2)-C(44)	2.016(5)
Fe(2)-C(42)	2.019(5)
Fe(2)-C(39)	2.031(4)
Fe(2)-C(45)	2.036(5)
Fe(2)-C(40)	2.042(4)
Fe(2)-C(43)	2.047(5)
Fe(2)-C(41)	2.053(5)
S(2)-C(37)	1.768(4)
S(2)-C(65)	1.817(4)
P(2)-C(53)	1.800(4)
P(2)-C(59)	1.808(4)
P(2)-C(46)	1.830(3)
N(3)-C(46)	1.393(4)
N(3)-C(52)	1.396(4)
N(3)-C(34)	1.457(4)
N(4)-C(46)	1.304(5)
N(4)-C(47)	1.405(4)
C(34)-C(36)	1.499(5)
C(34)-C(35)	1.526(5)

C(34)-H(34A)	0.9800
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-C(40)	1.426(5)
C(36)-C(37)	1.428(5)
C(37)-C(38)	1.414(5)
C(38)-C(39)	1.420(6)
C(38)-H(38A)	0.9800
C(39)-C(40)	1.411(5)
C(39)-H(39A)	0.9800
C(40)-H(40A)	0.9800
C(41)-C(45)	1.361(7)
C(41)-C(42)	1.425(7)
C(41)-H(41A)	0.9800
C(42)-C(43)	1.415(8)
C(42)-H(42A)	0.9800
C(43)-C(44)	1.429(8)
C(43)-H(43A)	0.9800
C(44)-C(45)	1.345(7)
C(44)-H(44A)	0.9800
C(45)-H(45A)	0.9800
C(47)-C(52)	1.398(5)
C(47)-C(48)	1.398(5)
C(48)-C(49)	1.375(5)
C(48)-H(48A)	0.9300
C(49)-C(50)	1.409(5)
C(49)-H(49A)	0.9300
C(50)-C(51)	1.378(5)
C(50)-H(50A)	0.9300
C(51)-C(52)	1.389(5)
C(51)-H(51A)	0.9300
C(53)-C(54)	1.357(6)
C(53)-C(58)	1.403(5)
C(54)-C(55)	1.368(6)
C(54)-H(54A)	0.9300
C(55)-C(56)	1.407(7)
C(55)-H(55A)	0.9300

C(56)-C(57)	1.391(8)
C(56)-H(56A)	0.9300
C(57)-C(58)	1.427(8)
C(57)-H(57A)	0.9300
C(58)-H(58A)	0.9300
C(59)-C(60)	1.380(6)
C(59)-C(64)	1.420(5)
C(60)-C(61)	1.361(7)
C(60)-H(60A)	0.9300
C(61)-C(62)	1.368(8)
C(61)-H(61A)	0.9300
C(62)-C(63)	1.389(7)
C(62)-H(62A)	0.9300
C(63)-C(64)	1.379(7)
C(63)-H(63A)	0.9300
C(64)-H(64A)	0.9300
C(65)-C(66)	1.527(6)
C(65)-H(65A)	0.9700
C(65)-H(65B)	0.9700
C(66)-H(66A)	0.9600
C(66)-H(66B)	0.9600
C(66)-H(66C)	0.9600
Cl(5)-C(67)	1.666(6)
Cl(6)-C(67)	1.724(6)
C(67)-H(67A)	0.9700
C(67)-H(67B)	0.9700
P-Pd-Cl(2)	86.21(4)
P-Pd-S	99.75(3)
Cl(2)-Pd-S	172.10(4)
P-Pd-Cl(1)	174.43(4)
Cl(2)-Pd-Cl(1)	89.64(4)
S-Pd-Cl(1)	84.06(4)
C(9)-Fe-C(5)	110.97(19)
C(9)-Fe-C(8)	41.5(2)
C(5)-Fe-C(8)	138.83(18)
C(9)-Fe-C(4)	116.50(16)
C(5)-Fe-C(4)	40.76(15)

C(8)-Fe-C(4)	114.16(16)
C(9)-Fe-C(6)	132.9(2)
C(5)-Fe-C(6)	40.04(16)
C(8)-Fe-C(6)	174.24(18)
C(4)-Fe-C(6)	68.55(15)
C(9)-Fe-C(3)	148.49(17)
C(5)-Fe-C(3)	68.79(15)
C(8)-Fe-C(3)	117.17(17)
C(4)-Fe-C(3)	41.94(14)
C(6)-Fe-C(3)	68.36(15)
C(9)-Fe-C(12)	68.1(2)
C(5)-Fe-C(12)	179.06(18)
C(8)-Fe-C(12)	40.29(19)
C(4)-Fe-C(12)	139.22(17)
C(6)-Fe-C(12)	140.77(18)
C(3)-Fe-C(12)	111.79(16)
C(9)-Fe-C(11)	66.82(18)
C(5)-Fe-C(11)	140.05(18)
C(8)-Fe-C(11)	67.43(19)
C(4)-Fe-C(11)	176.52(17)
C(6)-Fe-C(11)	110.16(18)
C(3)-Fe-C(11)	134.66(16)
C(12)-Fe-C(11)	40.06(19)
C(9)-Fe-C(7)	170.14(19)
C(5)-Fe-C(7)	68.07(16)
C(8)-Fe-C(7)	145.05(18)
C(4)-Fe-C(7)	69.64(14)
C(6)-Fe-C(7)	40.20(16)
C(3)-Fe-C(7)	41.13(14)
C(12)-Fe-C(7)	112.87(17)
C(11)-Fe-C(7)	107.22(17)
C(9)-Fe-C(10)	40.28(19)
C(5)-Fe-C(10)	112.24(18)
C(8)-Fe-C(10)	68.40(19)
C(4)-Fe-C(10)	144.17(17)
C(6)-Fe-C(10)	106.33(18)
C(3)-Fe-C(10)	171.01(16)
C(12)-Fe-C(10)	67.31(19)

C(11)-Fe-C(10)	39.05(18)
C(7)-Fe-C(10)	130.24(17)
C(4)-S-C(32)	102.49(18)
C(4)-S-Pd	114.45(13)
C(32)-S-Pd	111.79(13)
C(13)-P-C(20)	97.83(16)
C(13)-P-C(26)	107.70(15)
C(20)-P-C(26)	105.15(16)
C(13)-P-Pd	116.81(12)
C(20)-P-Pd	119.81(12)
C(26)-P-Pd	108.34(11)
C(19)-N(1)-C(13)	104.8(3)
C(19)-N(1)-C(1)	126.6(3)
C(13)-N(1)-C(1)	128.5(3)
C(13)-N(2)-C(14)	104.6(3)
N(1)-C(1)-C(3)	108.5(3)
N(1)-C(1)-C(2)	112.4(3)
C(3)-C(1)-C(2)	116.4(3)
N(1)-C(1)-H(1A)	106.3
C(3)-C(1)-H(1A)	106.3
C(2)-C(1)-H(1A)	106.3
C(1)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(2)-H(2D)	109.5
H(2B)-C(2)-H(2D)	109.5
H(2C)-C(2)-H(2D)	109.5
C(7)-C(3)-C(4)	107.1(3)
C(7)-C(3)-C(1)	126.9(3)
C(4)-C(3)-C(1)	125.8(3)
C(7)-C(3)-Fe	69.8(2)
C(4)-C(3)-Fe	68.30(18)
C(1)-C(3)-Fe	130.7(2)
C(5)-C(4)-C(3)	106.5(3)
C(5)-C(4)-S	123.2(3)
C(3)-C(4)-S	130.1(3)
C(5)-C(4)-Fe	69.3(2)
C(3)-C(4)-Fe	69.77(18)

S-C(4)-Fe	129.4(2)
C(6)-C(5)-C(4)	110.0(3)
C(6)-C(5)-Fe	71.1(2)
C(4)-C(5)-Fe	69.9(2)
C(6)-C(5)-H(5A)	125.0
C(4)-C(5)-H(5A)	125.0
Fe-C(5)-H(5A)	125.0
C(5)-C(6)-C(7)	109.0(3)
C(5)-C(6)-Fe	68.9(2)
C(7)-C(6)-Fe	70.3(2)
C(5)-C(6)-H(6A)	125.5
C(7)-C(6)-H(6A)	125.5
Fe-C(6)-H(6A)	125.5
C(6)-C(7)-C(3)	107.5(3)
C(6)-C(7)-Fe	69.5(2)
C(3)-C(7)-Fe	69.1(2)
C(6)-C(7)-H(7A)	126.2
C(3)-C(7)-H(7A)	126.2
Fe-C(7)-H(7A)	126.2
C(12)-C(8)-C(9)	107.0(4)
C(12)-C(8)-Fe	70.9(3)
C(9)-C(8)-Fe	69.0(3)
C(12)-C(8)-H(8A)	126.5
C(9)-C(8)-H(8A)	126.5
Fe-C(8)-H(8A)	126.5
C(10)-C(9)-C(8)	108.4(4)
C(10)-C(9)-Fe	72.1(2)
C(8)-C(9)-Fe	69.5(3)
C(10)-C(9)-H(9A)	125.8
C(8)-C(9)-H(9A)	125.8
Fe-C(9)-H(9A)	125.8
C(11)-C(10)-C(9)	106.8(4)
C(11)-C(10)-Fe	69.6(2)
C(9)-C(10)-Fe	67.6(2)
C(11)-C(10)-H(10A)	126.6
C(9)-C(10)-H(10A)	126.6
Fe-C(10)-H(10A)	126.6
C(10)-C(11)-C(12)	110.4(4)

C(10)-C(11)-Fe	71.4(2)
C(12)-C(11)-Fe	69.9(2)
C(10)-C(11)-H(11A)	124.8
C(12)-C(11)-H(11A)	124.8
Fe-C(11)-H(11A)	124.8
C(8)-C(12)-C(11)	107.3(4)
C(8)-C(12)-Fe	68.8(3)
C(11)-C(12)-Fe	70.0(3)
C(8)-C(12)-H(12A)	126.4
C(11)-C(12)-H(12A)	126.4
Fe-C(12)-H(12A)	126.4
N(2)-C(13)-N(1)	113.4(3)
N(2)-C(13)-P	123.8(3)
N(1)-C(13)-P	122.5(2)
C(15)-C(14)-C(19)	121.8(3)
C(15)-C(14)-N(2)	128.5(3)
C(19)-C(14)-N(2)	109.6(3)
C(14)-C(15)-C(16)	118.2(3)
C(14)-C(15)-H(15A)	120.9
C(16)-C(15)-H(15A)	120.9
C(15)-C(16)-C(17)	120.3(3)
C(15)-C(16)-H(16A)	119.8
C(17)-C(16)-H(16A)	119.8
C(16)-C(17)-C(18)	122.0(3)
C(16)-C(17)-H(17A)	119.0
C(18)-C(17)-H(17A)	119.0
C(19)-C(18)-C(17)	115.9(3)
C(19)-C(18)-H(18A)	122.1
C(17)-C(18)-H(18A)	122.1
C(14)-C(19)-N(1)	107.5(3)
C(14)-C(19)-C(18)	121.7(3)
N(1)-C(19)-C(18)	130.8(3)
C(25)-C(20)-C(21)	118.2(3)
C(25)-C(20)-P	120.9(3)
C(21)-C(20)-P	120.6(3)
C(20)-C(21)-C(22)	120.1(4)
C(20)-C(21)-H(21A)	119.9
C(22)-C(21)-H(21A)	119.9

C(23)-C(22)-C(21)	118.5(4)
C(23)-C(22)-H(22A)	120.7
C(21)-C(22)-H(22A)	120.7
C(22)-C(23)-C(24)	123.9(4)
C(22)-C(23)-H(23A)	118.1
C(24)-C(23)-H(23A)	118.1
C(23)-C(24)-C(25)	115.9(4)
C(23)-C(24)-H(24A)	122.0
C(25)-C(24)-H(24A)	122.0
C(20)-C(25)-C(24)	123.3(4)
C(20)-C(25)-H(25A)	118.4
C(24)-C(25)-H(25A)	118.4
C(31)-C(26)-C(27)	118.7(3)
C(31)-C(26)-P	117.2(3)
C(27)-C(26)-P	123.5(3)
C(28)-C(27)-C(26)	119.2(3)
C(28)-C(27)-H(27A)	120.4
C(26)-C(27)-H(27A)	120.4
C(29)-C(28)-C(27)	121.3(4)
C(29)-C(28)-H(28A)	119.3
C(27)-C(28)-H(28A)	119.3
C(28)-C(29)-C(30)	119.5(4)
C(28)-C(29)-H(29A)	120.2
C(30)-C(29)-H(29A)	120.2
C(29)-C(30)-C(31)	120.6(4)
C(29)-C(30)-H(30A)	119.7
C(31)-C(30)-H(30A)	119.7
C(26)-C(31)-C(30)	120.5(4)
C(26)-C(31)-H(31A)	119.8
C(30)-C(31)-H(31A)	119.8
C(33)-C(32)-S	111.9(3)
C(33)-C(32)-H(32A)	109.2
S-C(32)-H(32A)	109.2
C(33)-C(32)-H(32B)	109.2
S-C(32)-H(32B)	109.2
H(32A)-C(32)-H(32B)	107.9
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5

H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
P(2)-Pd(2)-Cl(4)	82.31(4)
P(2)-Pd(2)-S(2)	103.28(3)
Cl(4)-Pd(2)-S(2)	168.48(4)
P(2)-Pd(2)-Cl(3)	170.04(4)
Cl(4)-Pd(2)-Cl(3)	90.31(5)
S(2)-Pd(2)-Cl(3)	85.19(4)
C(37)-Fe(2)-C(38)	41.37(15)
C(37)-Fe(2)-C(36)	41.70(14)
C(38)-Fe(2)-C(36)	70.23(15)
C(37)-Fe(2)-C(44)	152.42(19)
C(38)-Fe(2)-C(44)	115.91(19)
C(36)-Fe(2)-C(44)	162.73(19)
C(37)-Fe(2)-C(42)	112.07(17)
C(38)-Fe(2)-C(42)	130.60(18)
C(36)-Fe(2)-C(42)	121.20(19)
C(44)-Fe(2)-C(42)	68.4(2)
C(37)-Fe(2)-C(39)	69.15(15)
C(38)-Fe(2)-C(39)	41.18(16)
C(36)-Fe(2)-C(39)	69.47(15)
C(44)-Fe(2)-C(39)	103.9(2)
C(42)-Fe(2)-C(39)	166.18(19)
C(37)-Fe(2)-C(45)	168.51(17)
C(38)-Fe(2)-C(45)	148.58(18)
C(36)-Fe(2)-C(45)	128.38(17)
C(44)-Fe(2)-C(45)	38.8(2)
C(42)-Fe(2)-C(45)	66.26(19)
C(39)-Fe(2)-C(45)	115.40(18)
C(37)-Fe(2)-C(40)	69.00(14)
C(38)-Fe(2)-C(40)	69.04(16)
C(36)-Fe(2)-C(40)	41.16(14)
C(44)-Fe(2)-C(40)	123.8(2)
C(42)-Fe(2)-C(40)	153.28(19)
C(39)-Fe(2)-C(40)	40.54(15)
C(45)-Fe(2)-C(40)	107.07(17)

C(37)-Fe(2)-C(43)	120.44(16)
C(38)-Fe(2)-C(43)	107.68(18)
C(36)-Fe(2)-C(43)	155.20(19)
C(44)-Fe(2)-C(43)	41.2(2)
C(42)-Fe(2)-C(43)	40.7(2)
C(39)-Fe(2)-C(43)	126.1(2)
C(45)-Fe(2)-C(43)	66.41(19)
C(40)-Fe(2)-C(43)	162.8(2)
C(37)-Fe(2)-C(41)	132.33(17)
C(38)-Fe(2)-C(41)	170.53(17)
C(36)-Fe(2)-C(41)	109.45(17)
C(44)-Fe(2)-C(41)	67.3(2)
C(42)-Fe(2)-C(41)	40.95(19)
C(39)-Fe(2)-C(41)	148.15(17)
C(45)-Fe(2)-C(41)	38.89(19)
C(40)-Fe(2)-C(41)	117.34(16)
C(43)-Fe(2)-C(41)	68.41(19)
C(37)-S(2)-C(65)	101.93(18)
C(37)-S(2)-Pd(2)	118.51(12)
C(65)-S(2)-Pd(2)	110.28(13)
C(53)-P(2)-C(59)	110.41(17)
C(53)-P(2)-C(46)	101.32(17)
C(59)-P(2)-C(46)	99.73(16)
C(53)-P(2)-Pd(2)	114.20(12)
C(59)-P(2)-Pd(2)	111.98(13)
C(46)-P(2)-Pd(2)	117.89(11)
C(46)-N(3)-C(52)	105.2(3)
C(46)-N(3)-C(34)	127.3(3)
C(52)-N(3)-C(34)	127.5(3)
C(46)-N(4)-C(47)	103.5(3)
N(3)-C(34)-C(36)	110.9(3)
N(3)-C(34)-C(35)	112.2(3)
C(36)-C(34)-C(35)	114.4(3)
N(3)-C(34)-H(34A)	106.2
C(36)-C(34)-H(34A)	106.2
C(35)-C(34)-H(34A)	106.2
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5

H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(40)-C(36)-C(37)	106.6(3)
C(40)-C(36)-C(34)	129.0(3)
C(37)-C(36)-C(34)	124.2(3)
C(40)-C(36)-Fe(2)	70.4(2)
C(37)-C(36)-Fe(2)	68.5(2)
C(34)-C(36)-Fe(2)	130.6(3)
C(38)-C(37)-C(36)	109.0(3)
C(38)-C(37)-S(2)	119.5(3)
C(36)-C(37)-S(2)	131.5(3)
C(38)-C(37)-Fe(2)	69.7(2)
C(36)-C(37)-Fe(2)	69.8(2)
S(2)-C(37)-Fe(2)	128.37(19)
C(37)-C(38)-C(39)	107.5(3)
C(37)-C(38)-Fe(2)	68.9(2)
C(39)-C(38)-Fe(2)	70.3(2)
C(37)-C(38)-H(38A)	126.3
C(39)-C(38)-H(38A)	126.3
Fe(2)-C(38)-H(38A)	126.3
C(40)-C(39)-C(38)	108.3(3)
C(40)-C(39)-Fe(2)	70.2(2)
C(38)-C(39)-Fe(2)	68.5(2)
C(40)-C(39)-H(39A)	125.9
C(38)-C(39)-H(39A)	125.9
Fe(2)-C(39)-H(39A)	125.9
C(39)-C(40)-C(36)	108.7(3)
C(39)-C(40)-Fe(2)	69.3(2)
C(36)-C(40)-Fe(2)	68.4(2)
C(39)-C(40)-H(40A)	125.6
C(36)-C(40)-H(40A)	125.6
Fe(2)-C(40)-H(40A)	125.6
C(45)-C(41)-C(42)	105.4(4)
C(45)-C(41)-Fe(2)	69.9(3)
C(42)-C(41)-Fe(2)	68.2(3)
C(45)-C(41)-H(41A)	127.3

C(42)-C(41)-H(41A)	127.3
Fe(2)-C(41)-H(41A)	127.3
C(43)-C(42)-C(41)	108.5(5)
C(43)-C(42)-Fe(2)	70.7(3)
C(41)-C(42)-Fe(2)	70.8(3)
C(43)-C(42)-H(42A)	125.7
C(41)-C(42)-H(42A)	125.7
Fe(2)-C(42)-H(42A)	125.7
C(42)-C(43)-C(44)	105.7(4)
C(42)-C(43)-Fe(2)	68.6(3)
C(44)-C(43)-Fe(2)	68.3(3)
C(42)-C(43)-H(43A)	127.1
C(44)-C(43)-H(43A)	127.1
Fe(2)-C(43)-H(43A)	127.1
C(45)-C(44)-C(43)	107.4(5)
C(45)-C(44)-Fe(2)	71.4(3)
C(43)-C(44)-Fe(2)	70.6(3)
C(45)-C(44)-H(44A)	126.3
C(43)-C(44)-H(44A)	126.3
Fe(2)-C(44)-H(44A)	126.3
C(44)-C(45)-C(41)	112.9(5)
C(44)-C(45)-Fe(2)	69.8(3)
C(41)-C(45)-Fe(2)	71.3(3)
C(44)-C(45)-H(45A)	123.5
C(41)-C(45)-H(45A)	123.5
Fe(2)-C(45)-H(45A)	123.5
N(4)-C(46)-N(3)	114.9(3)
N(4)-C(46)-P(2)	124.1(3)
N(3)-C(46)-P(2)	121.0(3)
C(52)-C(47)-C(48)	120.8(3)
C(52)-C(47)-N(4)	111.2(3)
C(48)-C(47)-N(4)	128.0(3)
C(49)-C(48)-C(47)	116.8(3)
C(49)-C(48)-H(48A)	121.6
C(47)-C(48)-H(48A)	121.6
C(48)-C(49)-C(50)	121.9(3)
C(48)-C(49)-H(49A)	119.0
C(50)-C(49)-H(49A)	119.0

C(51)-C(50)-C(49)	121.7(3)
C(51)-C(50)-H(50A)	119.1
C(49)-C(50)-H(50A)	119.1
C(50)-C(51)-C(52)	116.2(3)
C(50)-C(51)-H(51A)	121.9
C(52)-C(51)-H(51A)	121.9
C(51)-C(52)-N(3)	132.2(3)
C(51)-C(52)-C(47)	122.6(3)
N(3)-C(52)-C(47)	105.2(3)
C(54)-C(53)-C(58)	118.4(4)
C(54)-C(53)-P(2)	121.9(3)
C(58)-C(53)-P(2)	119.7(3)
C(53)-C(54)-C(55)	125.1(4)
C(53)-C(54)-H(54A)	117.5
C(55)-C(54)-H(54A)	117.5
C(54)-C(55)-C(56)	118.3(5)
C(54)-C(55)-H(55A)	120.9
C(56)-C(55)-H(55A)	120.9
C(57)-C(56)-C(55)	118.3(5)
C(57)-C(56)-H(56A)	120.8
C(55)-C(56)-H(56A)	120.8
C(56)-C(57)-C(58)	121.9(4)
C(56)-C(57)-H(57A)	119.1
C(58)-C(57)-H(57A)	119.1
C(53)-C(58)-C(57)	117.9(5)
C(53)-C(58)-H(58A)	121.1
C(57)-C(58)-H(58A)	121.1
C(60)-C(59)-C(64)	117.6(4)
C(60)-C(59)-P(2)	122.3(3)
C(64)-C(59)-P(2)	119.3(3)
C(61)-C(60)-C(59)	121.9(4)
C(61)-C(60)-H(60A)	119.0
C(59)-C(60)-H(60A)	119.0
C(60)-C(61)-C(62)	121.7(5)
C(60)-C(61)-H(61A)	119.2
C(62)-C(61)-H(61A)	119.2
C(61)-C(62)-C(63)	117.3(5)
C(61)-C(62)-H(62A)	121.3

C(63)-C(62)-H(62A)	121.3
C(64)-C(63)-C(62)	122.7(5)
C(64)-C(63)-H(63A)	118.7
C(62)-C(63)-H(63A)	118.7
C(63)-C(64)-C(59)	118.6(4)
C(63)-C(64)-H(64A)	120.7
C(59)-C(64)-H(64A)	120.7
C(66)-C(65)-S(2)	109.2(3)
C(66)-C(65)-H(65A)	109.8
S(2)-C(65)-H(65A)	109.8
C(66)-C(65)-H(65B)	109.8
S(2)-C(65)-H(65B)	109.8
H(65A)-C(65)-H(65B)	108.3
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
Cl(5)-C(67)-Cl(6)	115.7(3)
Cl(5)-C(67)-H(67A)	108.3
Cl(6)-C(67)-H(67A)	108.3
Cl(5)-C(67)-H(67B)	108.3
Cl(6)-C(67)-H(67B)	108.3
H(67A)-C(67)-H(67B)	107.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å^{2}x 10^3) for gama15. The anisotropic displacement factor exponent takes the form: -2 ^{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	44(1)	26(1)	33(1)	-3(1)	4(1)	0(1)
Fe	54(1)	25(1)	48(1)	-2(1)	-1(1)	-8(1)
Cl(1)	77(1)	46(1)	45(1)	-19(1)	4(1)	1(1)
Cl(2)	50(1)	58(1)	62(1)	-14(1)	19(1)	-3(1)
S	45(1)	32(1)	36(1)	-3(1)	-5(1)	-1(1)
P	36(1)	26(1)	35(1)	0(1)	3(1)	-1(1)
N(1)	52(2)	25(1)	38(2)	-4(1)	7(1)	-3(1)
N(2)	38(1)	25(1)	40(1)	-9(1)	2(1)	-3(1)
C(1)	41(2)	19(2)	42(2)	-2(1)	0(2)	-7(1)
C(2)	86(3)	31(2)	48(2)	8(2)	-34(2)	6(2)
C(3)	44(2)	22(1)	31(2)	5(1)	-1(2)	-8(1)
C(4)	39(2)	28(2)	51(2)	2(2)	-3(2)	-6(2)
C(5)	39(2)	54(2)	58(2)	4(2)	-4(2)	-12(2)
C(6)	44(2)	42(2)	81(3)	12(2)	2(2)	-10(2)
C(7)	62(2)	27(2)	62(2)	7(2)	20(2)	6(2)
C(8)	66(3)	43(2)	89(3)	6(2)	13(3)	-10(2)
C(9)	153(5)	51(2)	35(2)	2(2)	-6(3)	19(3)
C(10)	85(3)	37(2)	72(3)	-6(2)	-4(2)	-6(2)
C(11)	102(3)	29(2)	76(3)	-10(2)	-3(3)	10(2)
C(12)	83(3)	53(2)	76(3)	-7(2)	-34(2)	15(2)
C(13)	44(2)	24(2)	46(2)	6(2)	-6(2)	0(2)
C(14)	41(2)	31(2)	36(2)	-6(1)	16(2)	-3(2)
C(15)	62(2)	37(2)	37(2)	-11(2)	0(2)	1(2)
C(16)	62(2)	62(2)	29(2)	2(2)	12(2)	6(2)
C(17)	65(2)	41(2)	42(2)	-6(2)	10(2)	-7(2)
C(18)	56(2)	53(2)	27(2)	-4(2)	9(2)	-7(2)
C(19)	37(2)	40(2)	29(2)	-1(1)	3(2)	-3(2)
C(20)	45(2)	40(2)	29(2)	4(2)	6(2)	-4(2)
C(21)	53(2)	45(2)	56(2)	-11(2)	7(2)	4(2)
C(22)	63(2)	83(3)	53(2)	-13(2)	-11(2)	40(2)
C(23)	49(2)	112(4)	46(2)	2(3)	-14(2)	-7(3)
C(24)	74(3)	71(3)	56(2)	6(2)	-23(2)	-20(2)
C(25)	58(2)	60(2)	47(2)	-5(2)	-5(2)	-13(2)

C(26)	43(2)	25(2)	37(2)	4(1)	4(2)	0(2)
C(27)	42(2)	24(2)	59(2)	-5(2)	4(2)	5(2)
C(28)	76(3)	35(2)	55(2)	3(2)	-1(2)	17(2)
C(29)	112(3)	24(2)	45(2)	5(2)	-2(2)	14(2)
C(30)	91(3)	48(2)	43(2)	7(2)	26(2)	-11(2)
C(31)	52(2)	41(2)	57(2)	11(2)	10(2)	-3(2)
C(32)	48(2)	46(2)	75(3)	8(2)	-17(2)	4(2)
C(33)	49(2)	60(3)	100(3)	-18(3)	-28(2)	13(2)
Pd(2)	56(1)	38(1)	35(1)	-9(1)	-8(1)	-2(1)
Fe(2)	37(1)	45(1)	40(1)	2(1)	-2(1)	2(1)
Cl(3)	81(1)	80(1)	48(1)	-20(1)	-24(1)	12(1)
Cl(4)	133(1)	41(1)	69(1)	-18(1)	-33(1)	-6(1)
S(2)	46(1)	41(1)	38(1)	1(1)	-3(1)	-1(1)
P(2)	53(1)	28(1)	40(1)	-5(1)	-8(1)	-2(1)
N(3)	40(2)	31(1)	28(1)	-5(1)	-8(1)	6(1)
N(4)	39(2)	37(1)	34(1)	-2(1)	-1(1)	12(1)
C(34)	34(2)	41(2)	33(2)	-11(2)	-2(2)	-6(2)
C(35)	43(2)	52(2)	47(2)	1(2)	7(2)	6(2)
C(36)	41(2)	43(2)	39(2)	-8(2)	0(2)	-4(2)
C(37)	48(2)	39(2)	29(2)	7(2)	-14(2)	-11(2)
C(38)	63(2)	35(2)	53(2)	4(2)	-13(2)	10(2)
C(39)	59(2)	32(2)	63(2)	8(2)	3(2)	11(2)
C(40)	52(2)	32(2)	50(2)	-7(2)	4(2)	7(2)
C(41)	63(3)	85(3)	53(2)	17(2)	-6(2)	-7(3)
C(42)	45(2)	128(4)	95(3)	-52(3)	-8(2)	-25(3)
C(43)	52(2)	170(5)	70(3)	52(3)	-32(2)	-52(3)
C(44)	41(2)	91(4)	125(4)	24(3)	-8(3)	17(2)
C(45)	70(3)	74(3)	64(3)	21(2)	20(2)	3(2)
C(46)	48(2)	28(2)	30(2)	-2(1)	-2(2)	8(2)
C(47)	32(2)	31(2)	35(2)	-3(1)	-4(2)	2(2)
C(48)	33(2)	47(2)	45(2)	-4(2)	-9(2)	0(2)
C(49)	58(2)	41(2)	38(2)	-9(2)	-3(2)	-21(2)
C(50)	51(2)	24(2)	45(2)	-10(2)	-2(2)	-3(2)
C(51)	46(2)	47(2)	35(2)	-5(2)	-4(2)	1(2)
C(52)	37(2)	34(2)	26(2)	-8(1)	-7(1)	-14(2)
C(53)	61(2)	37(2)	38(2)	-6(2)	-1(2)	5(2)
C(54)	59(2)	60(2)	56(2)	-3(2)	0(2)	17(2)
C(55)	69(3)	75(3)	75(3)	16(3)	12(2)	20(3)

C(56)	90(3)	66(3)	98(3)	-14(3)	22(3)	28(3)
C(57)	148(5)	33(2)	86(3)	-15(2)	-16(4)	33(3)
C(58)	114(4)	21(2)	102(4)	-8(2)	0(3)	10(2)
C(59)	55(2)	35(2)	48(2)	4(2)	-8(2)	-7(2)
C(60)	67(3)	49(2)	57(2)	1(2)	-8(2)	-3(2)
C(61)	127(4)	87(3)	55(3)	26(3)	1(3)	-17(3)
C(62)	102(4)	85(4)	80(3)	6(3)	32(3)	-11(3)
C(63)	82(3)	75(3)	87(3)	-8(3)	12(3)	-34(3)
C(64)	51(2)	57(2)	64(2)	20(2)	-18(2)	-21(2)
C(65)	41(2)	55(2)	48(2)	12(2)	12(2)	5(2)
C(66)	45(2)	90(3)	148(5)	44(3)	-21(3)	-20(3)
Cl(5)	283(3)	78(1)	152(2)	-28(1)	23(2)	-59(1)
Cl(6)	111(1)	175(2)	82(1)	-16(1)	-19(1)	51(1)
C(67)	119(4)	107(4)	90(4)	-25(4)	-8(4)	39(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gama15.

	x	y	z	U(eq)
H(1A)	3053	7216	7660	41
H(2B)	4008	7057	8318	83
H(2C)	3308	6425	8166	83
H(2D)	2597	6858	8504	83
H(5A)	-1449	6788	7123	61
H(6A)	-1803	6249	7826	67
H(7A)	303	6422	8282	61
H(8A)	2950	5935	6980	79
H(9A)	623	5697	6640	95
H(10A)	-815	5080	7178	77
H(11A)	574	4974	7842	83
H(12A)	2898	5474	7730	85
H(15A)	935	9637	8583	55
H(16A)	-86	9155	9166	61
H(17A)	-189	8056	9215	59
H(18A)	806	7394	8696	54
H(21A)	5642	7438	7654	61
H(22A)	7614	7452	8069	79
H(23A)	8482	8400	8278	83
H(24A)	7500	9362	8103	80
H(25A)	5526	9333	7700	66
H(27A)	1844	9439	7188	50
H(28A)	1846	10314	6742	67
H(29A)	3776	10618	6400	73
H(30A)	5685	9996	6446	73
H(31A)	5660	9063	6830	60
H(32A)	370	8417	7333	68
H(32B)	787	8655	6882	68
H(33A)	-1566	8735	7015	104
H(33B)	-1627	7987	7024	104
H(33C)	-1231	8344	6607	104
H(34A)	4692	5196	5092	43
H(35A)	4472	5150	5847	71

H(35B)	3171	5362	5600	71
H(35C)	4070	5874	5828	71
H(38A)	4729	7055	4192	60
H(39A)	3670	7609	4837	62
H(40A)	3683	6820	5452	54
H(41A)	1406	5426	5025	81
H(42A)	2240	5299	4255	107
H(43A)	1878	6376	3876	117
H(44A)	926	7158	4439	103
H(45A)	654	6559	5103	83
H(48A)	10407	5760	5810	50
H(49A)	9939	6691	6177	55
H(50A)	7775	7116	6195	48
H(51A)	5997	6634	5835	51
H(54A)	9212	4654	4520	70
H(55A)	11107	4114	4318	87
H(56A)	11388	3047	4544	101
H(57A)	9635	2560	4910	107
H(58A)	7575	3100	5034	95
H(60A)	6957	3893	5726	69
H(61A)	5580	3440	6213	107
H(62A)	3321	3258	6074	107
H(63A)	2475	3559	5421	97
H(64A)	3853	3976	4905	69
H(65A)	7777	5921	4619	58
H(65B)	8154	5633	4177	58
H(66A)	8805	6691	4154	142
H(66B)	7397	6917	4328	142
H(66C)	7510	6644	3869	142
H(67A)	4704	11201	8288	126
H(67B)	3146	11168	8200	126

Table 6. Torsion angles [°] for gama15.

P-Pd-S-C(4)	-82.21(13)
Cl(2)-Pd-S-C(4)	139.2(3)
Cl(1)-Pd-S-C(4)	101.89(13)
P-Pd-S-C(32)	33.74(16)
Cl(2)-Pd-S-C(32)	-104.9(3)
Cl(1)-Pd-S-C(32)	-142.15(16)
Cl(2)-Pd-P-C(13)	-154.27(13)
S-Pd-P-C(13)	30.95(13)
Cl(1)-Pd-P-C(13)	163.8(4)
Cl(2)-Pd-P-C(20)	-36.53(13)
S-Pd-P-C(20)	148.69(13)
Cl(1)-Pd-P-C(20)	-78.5(4)
Cl(2)-Pd-P-C(26)	83.96(12)
S-Pd-P-C(26)	-90.82(12)
Cl(1)-Pd-P-C(26)	42.0(4)
C(19)-N(1)-C(1)-C(3)	70.2(4)
C(13)-N(1)-C(1)-C(3)	-105.8(4)
C(19)-N(1)-C(1)-C(2)	-60.0(5)
C(13)-N(1)-C(1)-C(2)	124.0(4)
N(1)-C(1)-C(3)-C(7)	-100.1(4)
C(2)-C(1)-C(3)-C(7)	27.9(5)
N(1)-C(1)-C(3)-C(4)	74.5(4)
C(2)-C(1)-C(3)-C(4)	-157.6(3)
N(1)-C(1)-C(3)-Fe	165.6(2)
C(2)-C(1)-C(3)-Fe	-66.5(4)
C(9)-Fe-C(3)-C(7)	176.3(3)
C(5)-Fe-C(3)-C(7)	80.5(2)
C(8)-Fe-C(3)-C(7)	-144.4(2)
C(4)-Fe-C(3)-C(7)	118.9(3)
C(6)-Fe-C(3)-C(7)	37.4(2)
C(12)-Fe-C(3)-C(7)	-100.3(2)
C(11)-Fe-C(3)-C(7)	-60.1(3)
C(10)-Fe-C(3)-C(7)	-17.8(12)
C(9)-Fe-C(3)-C(4)	57.4(4)
C(5)-Fe-C(3)-C(4)	-38.4(2)
C(8)-Fe-C(3)-C(4)	96.7(2)

C(6)-Fe-C(3)-C(4)	-81.5(2)
C(12)-Fe-C(3)-C(4)	140.8(2)
C(11)-Fe-C(3)-C(4)	-179.0(2)
C(7)-Fe-C(3)-C(4)	-118.9(3)
C(10)-Fe-C(3)-C(4)	-136.7(11)
C(9)-Fe-C(3)-C(1)	-61.8(5)
C(5)-Fe-C(3)-C(1)	-157.6(3)
C(8)-Fe-C(3)-C(1)	-22.5(4)
C(4)-Fe-C(3)-C(1)	-119.2(4)
C(6)-Fe-C(3)-C(1)	159.2(3)
C(12)-Fe-C(3)-C(1)	21.6(3)
C(11)-Fe-C(3)-C(1)	61.8(4)
C(7)-Fe-C(3)-C(1)	121.9(4)
C(10)-Fe-C(3)-C(1)	104.1(11)
C(7)-C(3)-C(4)-C(5)	0.6(4)
C(1)-C(3)-C(4)-C(5)	-174.8(3)
Fe-C(3)-C(4)-C(5)	59.9(2)
C(7)-C(3)-C(4)-S	175.7(3)
C(1)-C(3)-C(4)-S	0.2(5)
Fe-C(3)-C(4)-S	-125.1(3)
C(7)-C(3)-C(4)-Fe	-59.2(2)
C(1)-C(3)-C(4)-Fe	125.3(3)
C(32)-S-C(4)-C(5)	82.9(3)
Pd-S-C(4)-C(5)	-155.9(3)
C(32)-S-C(4)-C(3)	-91.4(3)
Pd-S-C(4)-C(3)	29.8(4)
C(32)-S-C(4)-Fe	172.4(2)
Pd-S-C(4)-Fe	-66.4(3)
C(9)-Fe-C(4)-C(5)	91.9(3)
C(8)-Fe-C(4)-C(5)	138.0(3)
C(6)-Fe-C(4)-C(5)	-36.5(2)
C(3)-Fe-C(4)-C(5)	-117.5(3)
C(12)-Fe-C(4)-C(5)	178.6(3)
C(11)-Fe-C(4)-C(5)	-105(3)
C(7)-Fe-C(4)-C(5)	-79.6(2)
C(10)-Fe-C(4)-C(5)	51.9(4)
C(9)-Fe-C(4)-C(3)	-150.5(2)
C(5)-Fe-C(4)-C(3)	117.5(3)

C(8)-Fe-C(4)-C(3)	-104.5(2)
C(6)-Fe-C(4)-C(3)	81.1(2)
C(12)-Fe-C(4)-C(3)	-63.9(3)
C(11)-Fe-C(4)-C(3)	12(3)
C(7)-Fe-C(4)-C(3)	37.9(2)
C(10)-Fe-C(4)-C(3)	169.4(3)
C(9)-Fe-C(4)-S	-24.6(3)
C(5)-Fe-C(4)-S	-116.6(4)
C(8)-Fe-C(4)-S	21.5(3)
C(6)-Fe-C(4)-S	-153.0(3)
C(3)-Fe-C(4)-S	125.9(4)
C(12)-Fe-C(4)-S	62.0(4)
C(11)-Fe-C(4)-S	138(3)
C(7)-Fe-C(4)-S	163.8(3)
C(10)-Fe-C(4)-S	-64.6(4)
C(3)-C(4)-C(5)-C(6)	-0.2(4)
S-C(4)-C(5)-C(6)	-175.7(3)
Fe-C(4)-C(5)-C(6)	60.0(3)
C(3)-C(4)-C(5)-Fe	-60.2(2)
S-C(4)-C(5)-Fe	124.4(3)
C(9)-Fe-C(5)-C(6)	132.6(3)
C(8)-Fe-C(5)-C(6)	171.3(3)
C(4)-Fe-C(5)-C(6)	-120.7(3)
C(3)-Fe-C(5)-C(6)	-81.2(2)
C(12)-Fe-C(5)-C(6)	150(11)
C(11)-Fe-C(5)-C(6)	54.1(4)
C(7)-Fe-C(5)-C(6)	-36.8(2)
C(10)-Fe-C(5)-C(6)	89.2(3)
C(9)-Fe-C(5)-C(4)	-106.7(3)
C(8)-Fe-C(5)-C(4)	-68.0(3)
C(6)-Fe-C(5)-C(4)	120.7(3)
C(3)-Fe-C(5)-C(4)	39.5(2)
C(12)-Fe-C(5)-C(4)	-89(11)
C(11)-Fe-C(5)-C(4)	174.8(3)
C(7)-Fe-C(5)-C(4)	83.8(2)
C(10)-Fe-C(5)-C(4)	-150.2(2)
C(4)-C(5)-C(6)-C(7)	-0.3(5)
Fe-C(5)-C(6)-C(7)	59.0(3)

C(4)-C(5)-C(6)-Fe	-59.3(3)
C(9)-Fe-C(6)-C(5)	-69.7(3)
C(8)-Fe-C(6)-C(5)	-82.0(18)
C(4)-Fe-C(6)-C(5)	37.1(2)
C(3)-Fe-C(6)-C(5)	82.4(2)
C(12)-Fe-C(6)-C(5)	-179.3(3)
C(11)-Fe-C(6)-C(5)	-146.3(2)
C(7)-Fe-C(6)-C(5)	120.6(3)
C(10)-Fe-C(6)-C(5)	-105.3(3)
C(9)-Fe-C(6)-C(7)	169.7(2)
C(5)-Fe-C(6)-C(7)	-120.6(3)
C(8)-Fe-C(6)-C(7)	157.4(17)
C(4)-Fe-C(6)-C(7)	-83.4(2)
C(3)-Fe-C(6)-C(7)	-38.2(2)
C(12)-Fe-C(6)-C(7)	60.2(3)
C(11)-Fe-C(6)-C(7)	93.1(3)
C(10)-Fe-C(6)-C(7)	134.1(2)
C(5)-C(6)-C(7)-C(3)	0.7(4)
Fe-C(6)-C(7)-C(3)	58.9(2)
C(5)-C(6)-C(7)-Fe	-58.2(3)
C(4)-C(3)-C(7)-C(6)	-0.8(4)
C(1)-C(3)-C(7)-C(6)	174.6(3)
Fe-C(3)-C(7)-C(6)	-59.1(3)
C(4)-C(3)-C(7)-Fe	58.3(2)
C(1)-C(3)-C(7)-Fe	-126.3(3)
C(9)-Fe-C(7)-C(6)	-49.6(11)
C(5)-Fe-C(7)-C(6)	36.7(2)
C(8)-Fe-C(7)-C(6)	-176.1(3)
C(4)-Fe-C(7)-C(6)	80.5(2)
C(3)-Fe-C(7)-C(6)	119.1(3)
C(12)-Fe-C(7)-C(6)	-143.5(2)
C(11)-Fe-C(7)-C(6)	-101.1(3)
C(10)-Fe-C(7)-C(6)	-64.5(3)
C(9)-Fe-C(7)-C(3)	-168.7(10)
C(5)-Fe-C(7)-C(3)	-82.4(2)
C(8)-Fe-C(7)-C(3)	64.8(3)
C(4)-Fe-C(7)-C(3)	-38.6(2)
C(6)-Fe-C(7)-C(3)	-119.1(3)

C(12)-Fe-C(7)-C(3)	97.4(2)
C(11)-Fe-C(7)-C(3)	139.8(2)
C(10)-Fe-C(7)-C(3)	176.4(2)
C(9)-Fe-C(8)-C(12)	-117.7(4)
C(5)-Fe-C(8)-C(12)	-179.5(3)
C(4)-Fe-C(8)-C(12)	139.0(3)
C(6)-Fe-C(8)-C(12)	-104.0(18)
C(3)-Fe-C(8)-C(12)	92.3(3)
C(11)-Fe-C(8)-C(12)	-37.7(3)
C(7)-Fe-C(8)-C(12)	50.3(4)
C(10)-Fe-C(8)-C(12)	-80.0(3)
C(5)-Fe-C(8)-C(9)	-61.8(4)
C(4)-Fe-C(8)-C(9)	-103.4(3)
C(6)-Fe-C(8)-C(9)	13.7(19)
C(3)-Fe-C(8)-C(9)	-150.0(2)
C(12)-Fe-C(8)-C(9)	117.7(4)
C(11)-Fe-C(8)-C(9)	80.0(3)
C(7)-Fe-C(8)-C(9)	168.0(3)
C(10)-Fe-C(8)-C(9)	37.7(3)
C(12)-C(8)-C(9)-C(10)	-0.9(5)
Fe-C(8)-C(9)-C(10)	-62.0(3)
C(12)-C(8)-C(9)-Fe	61.1(3)
C(5)-Fe-C(9)-C(10)	-100.1(3)
C(8)-Fe-C(9)-C(10)	118.3(4)
C(4)-Fe-C(9)-C(10)	-144.4(3)
C(6)-Fe-C(9)-C(10)	-59.8(4)
C(3)-Fe-C(9)-C(10)	176.6(3)
C(12)-Fe-C(9)-C(10)	80.3(3)
C(11)-Fe-C(9)-C(10)	36.7(3)
C(7)-Fe-C(9)-C(10)	-17.6(12)
C(5)-Fe-C(9)-C(8)	141.6(3)
C(4)-Fe-C(9)-C(8)	97.3(3)
C(6)-Fe-C(9)-C(8)	-178.1(3)
C(3)-Fe-C(9)-C(8)	58.3(4)
C(12)-Fe-C(9)-C(8)	-38.1(3)
C(11)-Fe-C(9)-C(8)	-81.6(3)
C(7)-Fe-C(9)-C(8)	-136.0(10)
C(10)-Fe-C(9)-C(8)	-118.3(4)

C(8)-C(9)-C(10)-C(11)	1.6(5)
Fe-C(9)-C(10)-C(11)	-58.7(3)
C(8)-C(9)-C(10)-Fe	60.3(3)
C(9)-Fe-C(10)-C(11)	119.2(4)
C(5)-Fe-C(10)-C(11)	-144.2(3)
C(8)-Fe-C(10)-C(11)	80.4(3)
C(4)-Fe-C(10)-C(11)	-177.9(3)
C(6)-Fe-C(10)-C(11)	-102.1(3)
C(3)-Fe-C(10)-C(11)	-49.4(12)
C(12)-Fe-C(10)-C(11)	36.7(3)
C(7)-Fe-C(10)-C(11)	-64.7(4)
C(5)-Fe-C(10)-C(9)	96.6(3)
C(8)-Fe-C(10)-C(9)	-38.8(3)
C(4)-Fe-C(10)-C(9)	62.9(4)
C(6)-Fe-C(10)-C(9)	138.7(3)
C(3)-Fe-C(10)-C(9)	-168.6(10)
C(12)-Fe-C(10)-C(9)	-82.5(3)
C(11)-Fe-C(10)-C(9)	-119.2(4)
C(7)-Fe-C(10)-C(9)	176.1(3)
C(9)-C(10)-C(11)-C(12)	-1.8(5)
Fe-C(10)-C(11)-C(12)	-59.2(3)
C(9)-C(10)-C(11)-Fe	57.5(3)
C(9)-Fe-C(11)-C(10)	-37.9(3)
C(5)-Fe-C(11)-C(10)	57.6(4)
C(8)-Fe-C(11)-C(10)	-83.1(3)
C(4)-Fe-C(11)-C(10)	159(3)
C(6)-Fe-C(11)-C(10)	91.3(3)
C(3)-Fe-C(11)-C(10)	170.4(3)
C(12)-Fe-C(11)-C(10)	-121.0(4)
C(7)-Fe-C(11)-C(10)	133.8(3)
C(9)-Fe-C(11)-C(12)	83.1(3)
C(5)-Fe-C(11)-C(12)	178.5(3)
C(8)-Fe-C(11)-C(12)	37.9(3)
C(4)-Fe-C(11)-C(12)	-80(3)
C(6)-Fe-C(11)-C(12)	-147.7(3)
C(3)-Fe-C(11)-C(12)	-68.6(3)
C(7)-Fe-C(11)-C(12)	-105.3(3)
C(10)-Fe-C(11)-C(12)	121.0(4)

C(9)-C(8)-C(12)-C(11)	-0.2(5)
Fe-C(8)-C(12)-C(11)	59.7(3)
C(9)-C(8)-C(12)-Fe	-59.9(3)
C(10)-C(11)-C(12)-C(8)	1.2(5)
Fe-C(11)-C(12)-C(8)	-58.9(3)
C(10)-C(11)-C(12)-Fe	60.1(3)
C(9)-Fe-C(12)-C(8)	39.2(3)
C(5)-Fe-C(12)-C(8)	21(11)
C(4)-Fe-C(12)-C(8)	-66.5(4)
C(6)-Fe-C(12)-C(8)	171.1(3)
C(3)-Fe-C(12)-C(8)	-106.8(3)
C(11)-Fe-C(12)-C(8)	118.7(4)
C(7)-Fe-C(12)-C(8)	-151.4(3)
C(10)-Fe-C(12)-C(8)	82.9(3)
C(9)-Fe-C(12)-C(11)	-79.5(3)
C(5)-Fe-C(12)-C(11)	-97(11)
C(8)-Fe-C(12)-C(11)	-118.7(4)
C(4)-Fe-C(12)-C(11)	174.8(3)
C(6)-Fe-C(12)-C(11)	52.4(4)
C(3)-Fe-C(12)-C(11)	134.5(3)
C(7)-Fe-C(12)-C(11)	89.9(3)
C(10)-Fe-C(12)-C(11)	-35.8(3)
C(14)-N(2)-C(13)-N(1)	0.8(4)
C(14)-N(2)-C(13)-P	-173.3(3)
C(19)-N(1)-C(13)-N(2)	-0.6(4)
C(1)-N(1)-C(13)-N(2)	176.1(3)
C(19)-N(1)-C(13)-P	173.5(3)
C(1)-N(1)-C(13)-P	-9.8(5)
C(20)-P-C(13)-N(2)	88.5(3)
C(26)-P-C(13)-N(2)	-20.2(4)
Pd-P-C(13)-N(2)	-142.3(3)
C(20)-P-C(13)-N(1)	-85.0(3)
C(26)-P-C(13)-N(1)	166.3(3)
Pd-P-C(13)-N(1)	44.2(3)
C(13)-N(2)-C(14)-C(15)	178.3(4)
C(13)-N(2)-C(14)-C(19)	-0.6(4)
C(19)-C(14)-C(15)-C(16)	1.0(6)
N(2)-C(14)-C(15)-C(16)	-177.8(3)

C(14)-C(15)-C(16)-C(17)	-2.7(6)
C(15)-C(16)-C(17)-C(18)	1.5(6)
C(16)-C(17)-C(18)-C(19)	1.4(6)
C(15)-C(14)-C(19)-N(1)	-178.8(3)
N(2)-C(14)-C(19)-N(1)	0.2(4)
C(15)-C(14)-C(19)-C(18)	2.0(6)
N(2)-C(14)-C(19)-C(18)	-179.0(3)
C(13)-N(1)-C(19)-C(14)	0.2(4)
C(1)-N(1)-C(19)-C(14)	-176.6(3)
C(13)-N(1)-C(19)-C(18)	179.4(4)
C(1)-N(1)-C(19)-C(18)	2.6(6)
C(17)-C(18)-C(19)-C(14)	-3.1(5)
C(17)-C(18)-C(19)-N(1)	177.8(4)
C(13)-P-C(20)-C(25)	-81.0(3)
C(26)-P-C(20)-C(25)	29.8(3)
Pd-P-C(20)-C(25)	151.9(3)
C(13)-P-C(20)-C(21)	93.2(3)
C(26)-P-C(20)-C(21)	-156.0(3)
Pd-P-C(20)-C(21)	-33.9(3)
C(25)-C(20)-C(21)-C(22)	-1.5(6)
P-C(20)-C(21)-C(22)	-175.8(3)
C(20)-C(21)-C(22)-C(23)	0.3(6)
C(21)-C(22)-C(23)-C(24)	0.4(7)
C(22)-C(23)-C(24)-C(25)	0.1(7)
C(21)-C(20)-C(25)-C(24)	2.1(6)
P-C(20)-C(25)-C(24)	176.4(3)
C(23)-C(24)-C(25)-C(20)	-1.4(6)
C(13)-P-C(26)-C(31)	154.7(3)
C(20)-P-C(26)-C(31)	51.1(3)
Pd-P-C(26)-C(31)	-78.1(3)
C(13)-P-C(26)-C(27)	-33.8(3)
C(20)-P-C(26)-C(27)	-137.4(3)
Pd-P-C(26)-C(27)	93.4(3)
C(31)-C(26)-C(27)-C(28)	-0.2(5)
P-C(26)-C(27)-C(28)	-171.6(3)
C(26)-C(27)-C(28)-C(29)	-3.4(6)
C(27)-C(28)-C(29)-C(30)	3.4(6)
C(28)-C(29)-C(30)-C(31)	0.2(6)

C(27)-C(26)-C(31)-C(30)	3.7(6)
P-C(26)-C(31)-C(30)	175.6(3)
C(29)-C(30)-C(31)-C(26)	-3.8(6)
C(4)-S-C(32)-C(33)	-79.4(3)
Pd-S-C(32)-C(33)	157.5(3)
P(2)-Pd(2)-S(2)-C(37)	-71.30(14)
Cl(4)-Pd(2)-S(2)-C(37)	170.7(2)
Cl(3)-Pd(2)-S(2)-C(37)	103.39(14)
P(2)-Pd(2)-S(2)-C(65)	45.53(14)
Cl(4)-Pd(2)-S(2)-C(65)	-72.5(3)
Cl(3)-Pd(2)-S(2)-C(65)	-139.78(14)
Cl(4)-Pd(2)-P(2)-C(53)	61.62(14)
S(2)-Pd(2)-P(2)-C(53)	-108.13(14)
Cl(3)-Pd(2)-P(2)-C(53)	104.1(3)
Cl(4)-Pd(2)-P(2)-C(59)	-64.80(13)
S(2)-Pd(2)-P(2)-C(59)	125.45(13)
Cl(3)-Pd(2)-P(2)-C(59)	-22.3(3)
Cl(4)-Pd(2)-P(2)-C(46)	-179.62(14)
S(2)-Pd(2)-P(2)-C(46)	10.63(14)
Cl(3)-Pd(2)-P(2)-C(46)	-137.2(2)
C(46)-N(3)-C(34)-C(36)	-115.9(3)
C(52)-N(3)-C(34)-C(36)	65.1(4)
C(46)-N(3)-C(34)-C(35)	114.8(3)
C(52)-N(3)-C(34)-C(35)	-64.2(4)
N(3)-C(34)-C(36)-C(40)	-103.0(4)
C(35)-C(34)-C(36)-C(40)	25.1(5)
N(3)-C(34)-C(36)-C(37)	70.0(4)
C(35)-C(34)-C(36)-C(37)	-162.0(3)
N(3)-C(34)-C(36)-Fe(2)	159.8(2)
C(35)-C(34)-C(36)-Fe(2)	-72.1(4)
C(37)-Fe(2)-C(36)-C(40)	117.7(3)
C(38)-Fe(2)-C(36)-C(40)	80.4(2)
C(44)-Fe(2)-C(36)-C(40)	-33.7(7)
C(42)-Fe(2)-C(36)-C(40)	-153.4(2)
C(39)-Fe(2)-C(36)-C(40)	36.4(2)
C(45)-Fe(2)-C(36)-C(40)	-70.3(3)
C(43)-Fe(2)-C(36)-C(40)	169.9(4)
C(41)-Fe(2)-C(36)-C(40)	-109.6(2)

C(38)-Fe(2)-C(36)-C(37)	-37.3(2)
C(44)-Fe(2)-C(36)-C(37)	-151.4(6)
C(42)-Fe(2)-C(36)-C(37)	88.9(3)
C(39)-Fe(2)-C(36)-C(37)	-81.3(2)
C(45)-Fe(2)-C(36)-C(37)	172.0(2)
C(40)-Fe(2)-C(36)-C(37)	-117.7(3)
C(43)-Fe(2)-C(36)-C(37)	52.2(5)
C(41)-Fe(2)-C(36)-C(37)	132.6(2)
C(37)-Fe(2)-C(36)-C(34)	-117.2(4)
C(38)-Fe(2)-C(36)-C(34)	-154.5(4)
C(44)-Fe(2)-C(36)-C(34)	91.4(7)
C(42)-Fe(2)-C(36)-C(34)	-28.3(4)
C(39)-Fe(2)-C(36)-C(34)	161.5(4)
C(45)-Fe(2)-C(36)-C(34)	54.7(4)
C(40)-Fe(2)-C(36)-C(34)	125.0(4)
C(43)-Fe(2)-C(36)-C(34)	-65.0(6)
C(41)-Fe(2)-C(36)-C(34)	15.4(4)
C(40)-C(36)-C(37)-C(38)	-1.6(4)
C(34)-C(36)-C(37)-C(38)	-175.8(3)
Fe(2)-C(36)-C(37)-C(38)	58.9(3)
C(40)-C(36)-C(37)-S(2)	175.6(3)
C(34)-C(36)-C(37)-S(2)	1.4(6)
Fe(2)-C(36)-C(37)-S(2)	-123.9(3)
C(40)-C(36)-C(37)-Fe(2)	-60.5(3)
C(34)-C(36)-C(37)-Fe(2)	125.3(3)
C(65)-S(2)-C(37)-C(38)	88.0(3)
Pd(2)-S(2)-C(37)-C(38)	-150.8(3)
C(65)-S(2)-C(37)-C(36)	-89.0(4)
Pd(2)-S(2)-C(37)-C(36)	32.2(4)
C(65)-S(2)-C(37)-Fe(2)	174.5(2)
Pd(2)-S(2)-C(37)-Fe(2)	-64.3(2)
C(36)-Fe(2)-C(37)-C(38)	-120.3(3)
C(44)-Fe(2)-C(37)-C(38)	41.8(5)
C(42)-Fe(2)-C(37)-C(38)	127.0(3)
C(39)-Fe(2)-C(37)-C(38)	-38.2(2)
C(45)-Fe(2)-C(37)-C(38)	-153.7(8)
C(40)-Fe(2)-C(37)-C(38)	-81.7(2)
C(43)-Fe(2)-C(37)-C(38)	82.3(3)

C(41)-Fe(2)-C(37)-C(38)	169.9(2)
C(38)-Fe(2)-C(37)-C(36)	120.3(3)
C(44)-Fe(2)-C(37)-C(36)	162.1(4)
C(42)-Fe(2)-C(37)-C(36)	-112.7(3)
C(39)-Fe(2)-C(37)-C(36)	82.1(2)
C(45)-Fe(2)-C(37)-C(36)	-33.4(9)
C(40)-Fe(2)-C(37)-C(36)	38.6(2)
C(43)-Fe(2)-C(37)-C(36)	-157.4(3)
C(41)-Fe(2)-C(37)-C(36)	-69.8(3)
C(38)-Fe(2)-C(37)-S(2)	-112.2(3)
C(36)-Fe(2)-C(37)-S(2)	127.5(3)
C(44)-Fe(2)-C(37)-S(2)	-70.4(5)
C(42)-Fe(2)-C(37)-S(2)	14.9(3)
C(39)-Fe(2)-C(37)-S(2)	-150.3(3)
C(45)-Fe(2)-C(37)-S(2)	94.2(9)
C(40)-Fe(2)-C(37)-S(2)	166.1(3)
C(43)-Fe(2)-C(37)-S(2)	-29.9(3)
C(41)-Fe(2)-C(37)-S(2)	57.7(3)
C(36)-C(37)-C(38)-C(39)	1.0(4)
S(2)-C(37)-C(38)-C(39)	-176.6(3)
Fe(2)-C(37)-C(38)-C(39)	60.0(3)
C(36)-C(37)-C(38)-Fe(2)	-59.0(3)
S(2)-C(37)-C(38)-Fe(2)	123.4(3)
C(36)-Fe(2)-C(38)-C(37)	37.6(2)
C(44)-Fe(2)-C(38)-C(37)	-159.9(2)
C(42)-Fe(2)-C(38)-C(37)	-77.0(3)
C(39)-Fe(2)-C(38)-C(37)	118.7(3)
C(45)-Fe(2)-C(38)-C(37)	170.2(3)
C(40)-Fe(2)-C(38)-C(37)	81.6(2)
C(43)-Fe(2)-C(38)-C(37)	-116.3(3)
C(41)-Fe(2)-C(38)-C(37)	-52.1(11)
C(37)-Fe(2)-C(38)-C(39)	-118.7(3)
C(36)-Fe(2)-C(38)-C(39)	-81.1(2)
C(44)-Fe(2)-C(38)-C(39)	81.4(3)
C(42)-Fe(2)-C(38)-C(39)	164.3(3)
C(45)-Fe(2)-C(38)-C(39)	51.6(4)
C(40)-Fe(2)-C(38)-C(39)	-37.1(2)
C(43)-Fe(2)-C(38)-C(39)	125.0(3)

C(41)-Fe(2)-C(38)-C(39)	-170.8(10)
C(37)-C(38)-C(39)-C(40)	-0.1(5)
Fe(2)-C(38)-C(39)-C(40)	59.0(3)
C(37)-C(38)-C(39)-Fe(2)	-59.1(3)
C(37)-Fe(2)-C(39)-C(40)	-81.7(2)
C(38)-Fe(2)-C(39)-C(40)	-120.0(3)
C(36)-Fe(2)-C(39)-C(40)	-37.0(2)
C(44)-Fe(2)-C(39)-C(40)	126.3(3)
C(42)-Fe(2)-C(39)-C(40)	-179.5(7)
C(45)-Fe(2)-C(39)-C(40)	86.8(3)
C(43)-Fe(2)-C(39)-C(40)	165.2(2)
C(41)-Fe(2)-C(39)-C(40)	57.1(4)
C(37)-Fe(2)-C(39)-C(38)	38.3(2)
C(36)-Fe(2)-C(39)-C(38)	83.1(2)
C(44)-Fe(2)-C(39)-C(38)	-113.6(3)
C(42)-Fe(2)-C(39)-C(38)	-59.4(8)
C(45)-Fe(2)-C(39)-C(38)	-153.1(2)
C(40)-Fe(2)-C(39)-C(38)	120.0(3)
C(43)-Fe(2)-C(39)-C(38)	-74.8(3)
C(41)-Fe(2)-C(39)-C(38)	177.2(3)
C(38)-C(39)-C(40)-C(36)	-0.9(5)
Fe(2)-C(39)-C(40)-C(36)	57.1(3)
C(38)-C(39)-C(40)-Fe(2)	-58.0(3)
C(37)-C(36)-C(40)-C(39)	1.5(4)
C(34)-C(36)-C(40)-C(39)	175.4(4)
Fe(2)-C(36)-C(40)-C(39)	-57.7(3)
C(37)-C(36)-C(40)-Fe(2)	59.2(2)
C(34)-C(36)-C(40)-Fe(2)	-126.9(4)
C(37)-Fe(2)-C(40)-C(39)	82.1(2)
C(38)-Fe(2)-C(40)-C(39)	37.6(2)
C(36)-Fe(2)-C(40)-C(39)	121.2(3)
C(44)-Fe(2)-C(40)-C(39)	-70.2(3)
C(42)-Fe(2)-C(40)-C(39)	179.7(4)
C(45)-Fe(2)-C(40)-C(39)	-109.4(3)
C(43)-Fe(2)-C(40)-C(39)	-44.4(7)
C(41)-Fe(2)-C(40)-C(39)	-150.1(2)
C(37)-Fe(2)-C(40)-C(36)	-39.1(2)
C(38)-Fe(2)-C(40)-C(36)	-83.6(2)

C(44)-Fe(2)-C(40)-C(36)	168.6(3)
C(42)-Fe(2)-C(40)-C(36)	58.5(5)
C(39)-Fe(2)-C(40)-C(36)	-121.2(3)
C(45)-Fe(2)-C(40)-C(36)	129.5(2)
C(43)-Fe(2)-C(40)-C(36)	-165.6(5)
C(41)-Fe(2)-C(40)-C(36)	88.7(3)
C(37)-Fe(2)-C(41)-C(45)	169.1(3)
C(38)-Fe(2)-C(41)-C(45)	-146.0(10)
C(36)-Fe(2)-C(41)-C(45)	127.7(3)
C(44)-Fe(2)-C(41)-C(45)	-34.1(3)
C(42)-Fe(2)-C(41)-C(45)	-116.8(4)
C(39)-Fe(2)-C(41)-C(45)	45.5(4)
C(40)-Fe(2)-C(41)-C(45)	83.4(3)
C(43)-Fe(2)-C(41)-C(45)	-78.8(3)
C(37)-Fe(2)-C(41)-C(42)	-74.1(3)
C(38)-Fe(2)-C(41)-C(42)	-29.2(12)
C(36)-Fe(2)-C(41)-C(42)	-115.6(3)
C(44)-Fe(2)-C(41)-C(42)	82.6(3)
C(39)-Fe(2)-C(41)-C(42)	162.3(3)
C(45)-Fe(2)-C(41)-C(42)	116.8(4)
C(40)-Fe(2)-C(41)-C(42)	-159.8(3)
C(43)-Fe(2)-C(41)-C(42)	38.0(3)
C(45)-C(41)-C(42)-C(43)	-0.6(5)
Fe(2)-C(41)-C(42)-C(43)	-60.9(3)
C(45)-C(41)-C(42)-Fe(2)	60.4(3)
C(37)-Fe(2)-C(42)-C(43)	-111.5(3)
C(38)-Fe(2)-C(42)-C(43)	-67.5(3)
C(36)-Fe(2)-C(42)-C(43)	-157.4(3)
C(44)-Fe(2)-C(42)-C(43)	38.7(3)
C(39)-Fe(2)-C(42)-C(43)	-19.2(9)
C(45)-Fe(2)-C(42)-C(43)	80.8(3)
C(40)-Fe(2)-C(42)-C(43)	161.6(3)
C(41)-Fe(2)-C(42)-C(43)	118.6(4)
C(37)-Fe(2)-C(42)-C(41)	129.9(3)
C(38)-Fe(2)-C(42)-C(41)	173.9(3)
C(36)-Fe(2)-C(42)-C(41)	84.0(3)
C(44)-Fe(2)-C(42)-C(41)	-79.9(3)
C(39)-Fe(2)-C(42)-C(41)	-137.8(7)

C(45)-Fe(2)-C(42)-C(41)	-37.8(3)
C(40)-Fe(2)-C(42)-C(41)	43.0(5)
C(43)-Fe(2)-C(42)-C(41)	-118.6(4)
C(41)-C(42)-C(43)-C(44)	2.6(5)
Fe(2)-C(42)-C(43)-C(44)	-58.4(3)
C(41)-C(42)-C(43)-Fe(2)	61.0(3)
C(37)-Fe(2)-C(43)-C(42)	89.2(3)
C(38)-Fe(2)-C(43)-C(42)	132.6(3)
C(36)-Fe(2)-C(43)-C(42)	51.6(5)
C(44)-Fe(2)-C(43)-C(42)	-118.0(4)
C(39)-Fe(2)-C(43)-C(42)	174.4(3)
C(45)-Fe(2)-C(43)-C(42)	-80.4(3)
C(40)-Fe(2)-C(43)-C(42)	-151.3(5)
C(41)-Fe(2)-C(43)-C(42)	-38.2(3)
C(37)-Fe(2)-C(43)-C(44)	-152.8(3)
C(38)-Fe(2)-C(43)-C(44)	-109.4(3)
C(36)-Fe(2)-C(43)-C(44)	169.6(4)
C(42)-Fe(2)-C(43)-C(44)	118.0(4)
C(39)-Fe(2)-C(43)-C(44)	-67.6(4)
C(45)-Fe(2)-C(43)-C(44)	37.5(3)
C(40)-Fe(2)-C(43)-C(44)	-33.3(7)
C(41)-Fe(2)-C(43)-C(44)	79.8(3)
C(42)-C(43)-C(44)-C(45)	-3.7(5)
Fe(2)-C(43)-C(44)-C(45)	-62.3(3)
C(42)-C(43)-C(44)-Fe(2)	58.6(3)
C(37)-Fe(2)-C(44)-C(45)	175.1(3)
C(38)-Fe(2)-C(44)-C(45)	-155.5(3)
C(36)-Fe(2)-C(44)-C(45)	-48.3(8)
C(42)-Fe(2)-C(44)-C(45)	78.6(3)
C(39)-Fe(2)-C(44)-C(45)	-113.4(3)
C(40)-Fe(2)-C(44)-C(45)	-74.4(4)
C(43)-Fe(2)-C(44)-C(45)	116.9(5)
C(41)-Fe(2)-C(44)-C(45)	34.2(3)
C(37)-Fe(2)-C(44)-C(43)	58.2(5)
C(38)-Fe(2)-C(44)-C(43)	87.6(3)
C(36)-Fe(2)-C(44)-C(43)	-165.2(5)
C(42)-Fe(2)-C(44)-C(43)	-38.3(3)
C(39)-Fe(2)-C(44)-C(43)	129.7(3)

C(45)-Fe(2)-C(44)-C(43)	-116.9(5)
C(40)-Fe(2)-C(44)-C(43)	168.7(3)
C(41)-Fe(2)-C(44)-C(43)	-82.7(3)
C(43)-C(44)-C(45)-C(41)	3.6(6)
Fe(2)-C(44)-C(45)-C(41)	-58.2(4)
C(43)-C(44)-C(45)-Fe(2)	61.8(3)
C(42)-C(41)-C(45)-C(44)	-1.9(6)
Fe(2)-C(41)-C(45)-C(44)	57.4(4)
C(42)-C(41)-C(45)-Fe(2)	-59.3(3)
C(37)-Fe(2)-C(45)-C(44)	-168.6(8)
C(38)-Fe(2)-C(45)-C(44)	45.6(5)
C(36)-Fe(2)-C(45)-C(44)	163.6(3)
C(42)-Fe(2)-C(45)-C(44)	-84.5(4)
C(39)-Fe(2)-C(45)-C(44)	80.4(4)
C(40)-Fe(2)-C(45)-C(44)	123.2(3)
C(43)-Fe(2)-C(45)-C(44)	-39.8(3)
C(41)-Fe(2)-C(45)-C(44)	-124.2(4)
C(37)-Fe(2)-C(45)-C(41)	-44.4(10)
C(38)-Fe(2)-C(45)-C(41)	169.8(3)
C(36)-Fe(2)-C(45)-C(41)	-72.2(3)
C(44)-Fe(2)-C(45)-C(41)	124.2(4)
C(42)-Fe(2)-C(45)-C(41)	39.7(3)
C(39)-Fe(2)-C(45)-C(41)	-155.4(3)
C(40)-Fe(2)-C(45)-C(41)	-112.6(3)
C(43)-Fe(2)-C(45)-C(41)	84.4(3)
C(47)-N(4)-C(46)-N(3)	0.7(4)
C(47)-N(4)-C(46)-P(2)	-178.3(2)
C(52)-N(3)-C(46)-N(4)	0.1(4)
C(34)-N(3)-C(46)-N(4)	-179.1(3)
C(52)-N(3)-C(46)-P(2)	179.2(2)
C(34)-N(3)-C(46)-P(2)	0.0(4)
C(53)-P(2)-C(46)-N(4)	-2.2(3)
C(59)-P(2)-C(46)-N(4)	111.0(3)
Pd(2)-P(2)-C(46)-N(4)	-127.6(3)
C(53)-P(2)-C(46)-N(3)	178.8(3)
C(59)-P(2)-C(46)-N(3)	-67.9(3)
Pd(2)-P(2)-C(46)-N(3)	53.4(3)
C(46)-N(4)-C(47)-C(52)	-1.3(4)

C(46)-N(4)-C(47)-C(48)	179.1(3)
C(52)-C(47)-C(48)-C(49)	-1.0(5)
N(4)-C(47)-C(48)-C(49)	178.5(3)
C(47)-C(48)-C(49)-C(50)	1.2(5)
C(48)-C(49)-C(50)-C(51)	-0.5(6)
C(49)-C(50)-C(51)-C(52)	-0.4(5)
C(50)-C(51)-C(52)-N(3)	179.4(3)
C(50)-C(51)-C(52)-C(47)	0.6(5)
C(46)-N(3)-C(52)-C(51)	-179.9(3)
C(34)-N(3)-C(52)-C(51)	-0.7(6)
C(46)-N(3)-C(52)-C(47)	-0.9(3)
C(34)-N(3)-C(52)-C(47)	178.3(3)
C(48)-C(47)-C(52)-C(51)	0.1(5)
N(4)-C(47)-C(52)-C(51)	-179.5(3)
C(48)-C(47)-C(52)-N(3)	-179.0(3)
N(4)-C(47)-C(52)-N(3)	1.4(4)
C(59)-P(2)-C(53)-C(54)	-166.0(3)
C(46)-P(2)-C(53)-C(54)	-61.1(3)
Pd(2)-P(2)-C(53)-C(54)	66.7(3)
C(59)-P(2)-C(53)-C(58)	16.4(4)
C(46)-P(2)-C(53)-C(58)	121.4(3)
Pd(2)-P(2)-C(53)-C(58)	-110.8(3)
C(58)-C(53)-C(54)-C(55)	2.9(7)
P(2)-C(53)-C(54)-C(55)	-174.7(4)
C(53)-C(54)-C(55)-C(56)	-5.2(7)
C(54)-C(55)-C(56)-C(57)	2.9(7)
C(55)-C(56)-C(57)-C(58)	1.4(8)
C(54)-C(53)-C(58)-C(57)	1.6(6)
P(2)-C(53)-C(58)-C(57)	179.2(4)
C(56)-C(57)-C(58)-C(53)	-3.7(8)
C(53)-P(2)-C(59)-C(60)	57.9(4)
C(46)-P(2)-C(59)-C(60)	-48.1(4)
Pd(2)-P(2)-C(59)-C(60)	-173.6(3)
C(53)-P(2)-C(59)-C(64)	-132.3(3)
C(46)-P(2)-C(59)-C(64)	121.6(3)
Pd(2)-P(2)-C(59)-C(64)	-3.9(3)
C(64)-C(59)-C(60)-C(61)	3.8(6)
P(2)-C(59)-C(60)-C(61)	173.7(4)

C(59)-C(60)-C(61)-C(62)	-2.5(8)
C(60)-C(61)-C(62)-C(63)	-0.5(8)
C(61)-C(62)-C(63)-C(64)	2.1(8)
C(62)-C(63)-C(64)-C(59)	-0.8(7)
C(60)-C(59)-C(64)-C(63)	-2.1(6)
P(2)-C(59)-C(64)-C(63)	-172.4(3)
C(37)-S(2)-C(65)-C(66)	-70.5(3)
Pd(2)-S(2)-C(65)-C(66)	162.8(3)

Symmetry transformations used to generate equivalent atoms: