Supplementary Material (ESI) for Chemical Communications

Supplementary Information

Title: Side Chain-Directed Assembly of Triangular Molecular Panels into Tetrahedron vs. Open Cone

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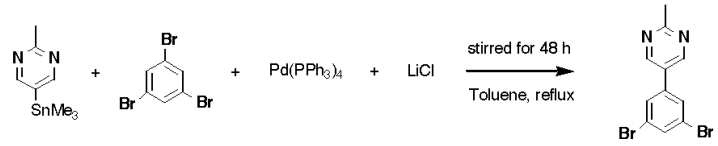
Contents

■ **Preparation of 3,5-Dibromo-1-(4-methyl-3,5-pyrimidyl)benzene.**

Scheme:

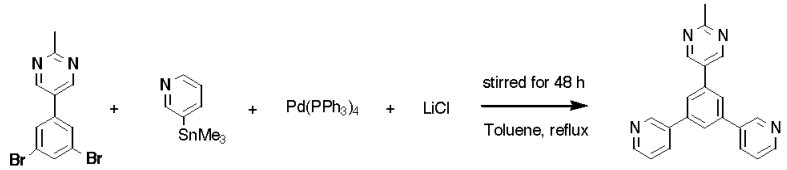


Typical procedure: To a toluene solution (50 mL) of 1,3,5-tribromobenzene (5.51 g; 1.75 mmol) and 2-methyl-5-trimethylstannyl-1,3-pyrimidine (1.50 g; 1.75 mmol), $PdCl_2(PPh_3)_2$ (0.210 g; 0.290 mmol) and LiCl (1.24 g; 29.2 mmol) were added, and the suspension was refluxed for 48 h under an argon atmosphere. The resulting solution was treated with H_2O and the products were extracted with $CHCl_3$. After usual workup, the result was purified by column chromatography on silica gel (eluent: EtOAc-Hexane 7:1) to give the title compound as a colorless solid (0.700 g; 2.12 mmol) in 36% yield.

Physical data: ^{1}H NMR (500.13 MHz, $CDCl_3$, 27 °C): δ 8.80 (s, 2H), 7.75 (s, 1H), 7.63 (s, 2H), 2.81 (s, 3H); ^{13}C NMR (125.77 MHz, $CDCl_3$, 27 °C): δ 168.2 (C_q), 154.9 (*C*H), 138.1 (C_q), 134.1 (*C*H), 128.7 (C_q), 128.6 (*C*H), 123.9 (*C*H), 25.8 (CH_3); IR (KBr, cm^{-1}): 3045, 3026, 2360, 1558, 1563, 854, 752; m.p.: 217-218 °C; MS (EI, m/z) calcd. for $C_{11}H_8N_2Br_2$ (M^+) 328.0, found 328; Elemental Analysis Calcd. for $C_{11}H_8N_2Br_2$: C, 40.28; H, 2.46; N, 8.54. Found: C, 40.47; H, 2.27; N, 8.55.

■ **Preparation of 1-(4-methyl-3,5-pyrimidyl)-3,5-bis(3-pyridyl)benzene (2b).**

Scheme:



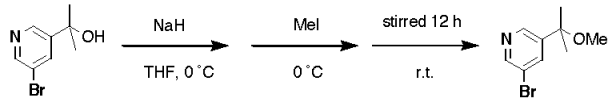
Typical procedure: To a toluene solution (60 mL) of 3,5-dibromo-1-(4-methyl-3,5-pyrimidyl)benzene (0.67 g; 2.64 mmol) and 3-trimethylstannyl-pyridine (2.3 g; 6.1 mmol), $PdCl_2(PPh_3)_2$ (0.14 g; 0.20 mmol) and LiCl (0.87 g; 20.4 mmol) were added, and the mixture was refluxed for 48 h under an argon atmosphere. The gray suspension was filtered and the precipitates were washed with hexane and ethyl acetate. After the evaporation of the solvent, the resulting gray solid was dissolved with 5 M HCl (5.0

mL) and the small amount of insoluble solid was removed by filtration. Acetone (50 mL) was added to the solution, and the resulting white precipitates were filtered and washed with water and a small amount of acetone. Drying under vacuum for 12 h gave the title compound as a gray solid (0.26 g; 0.79 mmol) in 39% yield.

Physical data: ^{1}H NMR (500.13 MHz, DMSO, 27 °C): δ 9.79 (s, 2H), 9.67 (s, 2H), 9.16 (d, J = 8.5 Hz, 2H), 8.87 (d, J = 4.9 Hz, 2H), 8.68 (s, 2H), 8.65 (s, 1H), 8.07 (dd, J = 4.9, 8.5 Hz, 2H), 3.22 (s, 3H); ^{13}C NMR (125.77 MHz, DMSO, 27 °C): δ 166.6 (C_q), 155.4 (*C*H), 149.0 (*C*H), 148.3 (*C*H), 139.1 (*C*H), 135.9 (C_q), 135.1 (C_q), 134.9 (C_q), 129.8 (C_q), 125.6 (*C*H), 125.0 (*C*H), 124.0 (*C*H), 25.5 (*C*H$_3$); IR (KBr, cm^{-1}): 3040, 1654, 1590, 1440, 1025, 708; m.p.: 241-243 °C; MS (FAB, m/z) calcd. for $C_{21}H_{17}N_4$ (M+H$^+$) 325.15, found 325.2; Elemental Analysis Calcd. for $C_{21}H_{16}N_4$: C, 77.76; H, 4.97; N, 17.27. Found: C, 77.64; H,5.10; N, 17.06.

■ **Preparation of 3-bromo-5-(1-methoxyisopropyl)pyridine.**

Scheme:

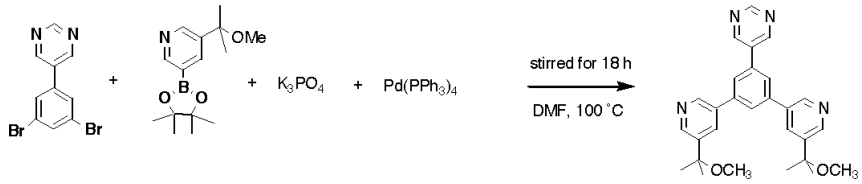


Typical procedure: To a THF solution (20 mL) of NaH (0.500 g; 20.8 mmol) at 0 ºC, a THF solution (20 mL) of 3-bromo-5-(1-hydroxyisopropyl)pyridine (3.00 g; 13.9 mmol) was added dropwise, and the mixture was stirred for 1 h at 0 °C. After MeI (1.30 mL, 20.8 mmol) was added dropwise to the mixture, the solution was stirred for 12 h at ambient temperature. The resulting solution was treated with H_2O (30 mL) and extracted with diethylether. The extract was dried over $MgSO_4$. After purification by column chromatography on silica gel (eluent: Hexane-AcOEt 5:1), the title compound was obtained as orange-color oil (2.35 g; 10.2 mmol) in 73% yield.

Physical data: ^{1}H NMR (500.13 MHz, $CDCl_3$, 27 °C): δ 8.58 (d, J = 2.1 Hz, 1H), 8.56 (d, J = 2.1 Hz, 1H), 7.88 (t, J = 2.1 Hz, 1H), 3.12 (s, 3H), 1.54 (s, 6H); ^{13}C NMR (125.77 MHz, $CDCl_3$, 27 °C): δ 149.1 (*C*H), 145.6 (*C*H), 143.4 (C_q), 136.0 (*C*H), 120.5 (C_q), 75.1 (C_q), 50.5 (*C*H$_3$), 27.4 (*C*H$_3$); IR (KBr, cm^{-1}): 2362, 1414, 1364, 1256, 1175, 1072, 883, 711; MS (EI, m/z) calcd. for $C_9H_{12}ONBr$ (M$^+$) 230.1, found 230; Elemental Analysis Calcd. for $C_9H_{12}NOBr$: C, 46.98; H, 5.26; N, 6.09. Found: C, 46.70; H, 5.19; N, 6.02.

■Preparation of 1-(3,5-Pyrimidyl)-3,5-bis[3-(1-methoxyisopropyl)-5-pyridyl]benzene (2c).

Scheme:

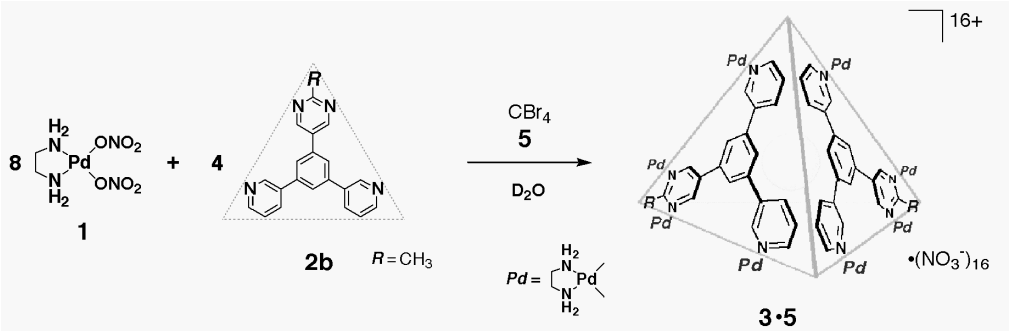


Typical procedure: A DMF solution (15 mL) of 3-(1-methoxyisopropyl)pyridyl-5-boronic acid pinacol ester (2.77 g; 10.0 mmol), 3,5-dibromo-1-(3,5-pyrimidyl)benzene (0.942 g; 3.00 mmol), $Pd(PPh_3)_4$ (0.3467 g; 0.300 mmol), and K_3PO_4 (3.82 g; 18.0 mmol) was heated at 120 °C for 72 h under an argon atmosphere. The resulting brown suspension was treated with an aqueous solution of ethylenediamine and extracted with $CHCl_3$. After usual workup, the result was purified by column chromatography on silica gel (eluent: $CHCl_3$-MeOH 40:1) to give the title compound as a white solid (0.613 g; 1.35 mmol) in 45% yield.

Physical data: ^{1}H NMR (500.13 MHz, $CDCl_3$, 27 °C): δ 9.30 (s, 1H), 9.11 (s, 2H), 8.87 (s, 2H), 8.73 (s, 2H), 8.05 (s, 2H), 7.90 (s, 1H), 7.83 (s, 2H), 3.20 (s, 6H), 1.65 (s, 12H); ^{13}C NMR (125.77 MHz, $CDCl_3$, 27 °C): δ 157.9 (*C*H), 155.0 (*C*H), 147.1 (C_q), 146.8 (*C*H), 141.8 (*C*H), 140.3 (*C*H), 136.1 (C_q), 135.1 (CH), 133.7 (C_q), 132.0 (*C*H), 126.8 (C_q), 125.6 (*C*H), 75.5 (C_q), 50.7 (CH_3), 27.6 (CH_3); IR (KBr, cm^{-1}): 3042, 2988, 1558, 1395, 1072, 874, 728; m.p.: 222-224 °C; MS (FAB, m/z) calcd. for $C_{28}H_{31}O_2N_4$ ($M+H^+$) 455.24, found 455.2; Elemental Analysis Calcd. for $C_{28}H_{30}N_4O_2\cdot(H_2O)_{0.3}$: C, 73.11; H, 6.71; N, 12.18. Found: C, 73.09; H, 6.75; N, 12.02.

□ Self-assembly of Open cone 3•5 (5 = CBr_4).

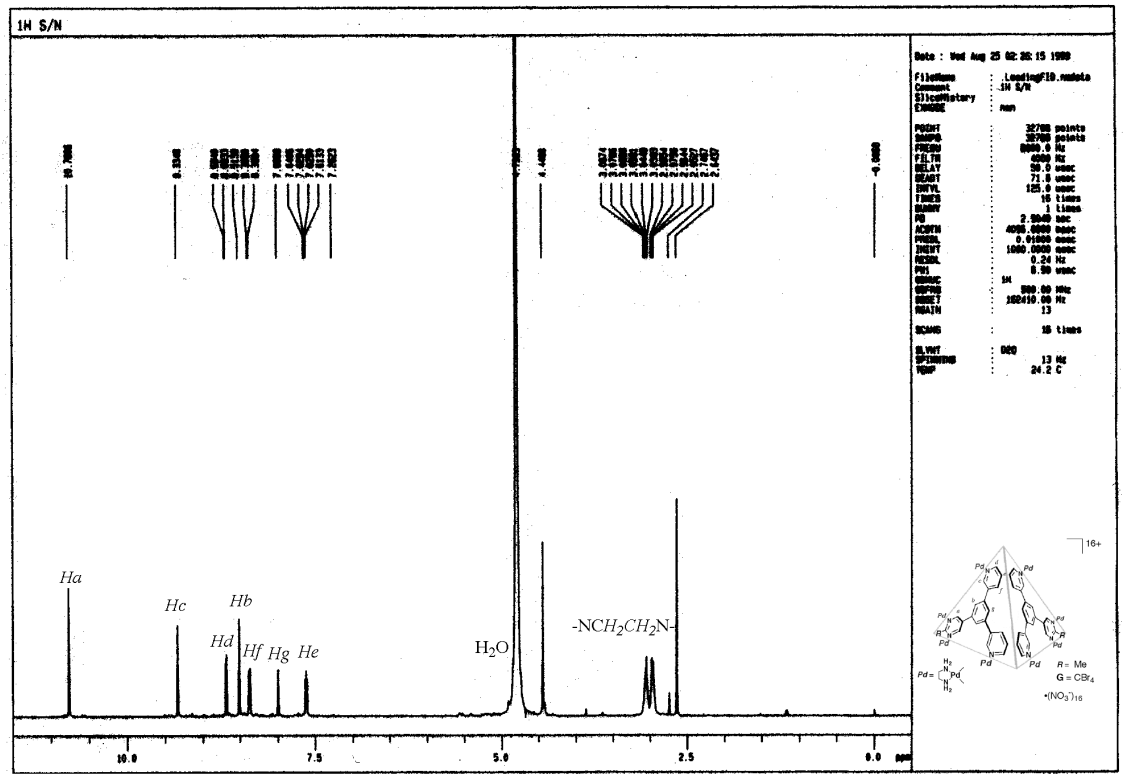
Scheme:



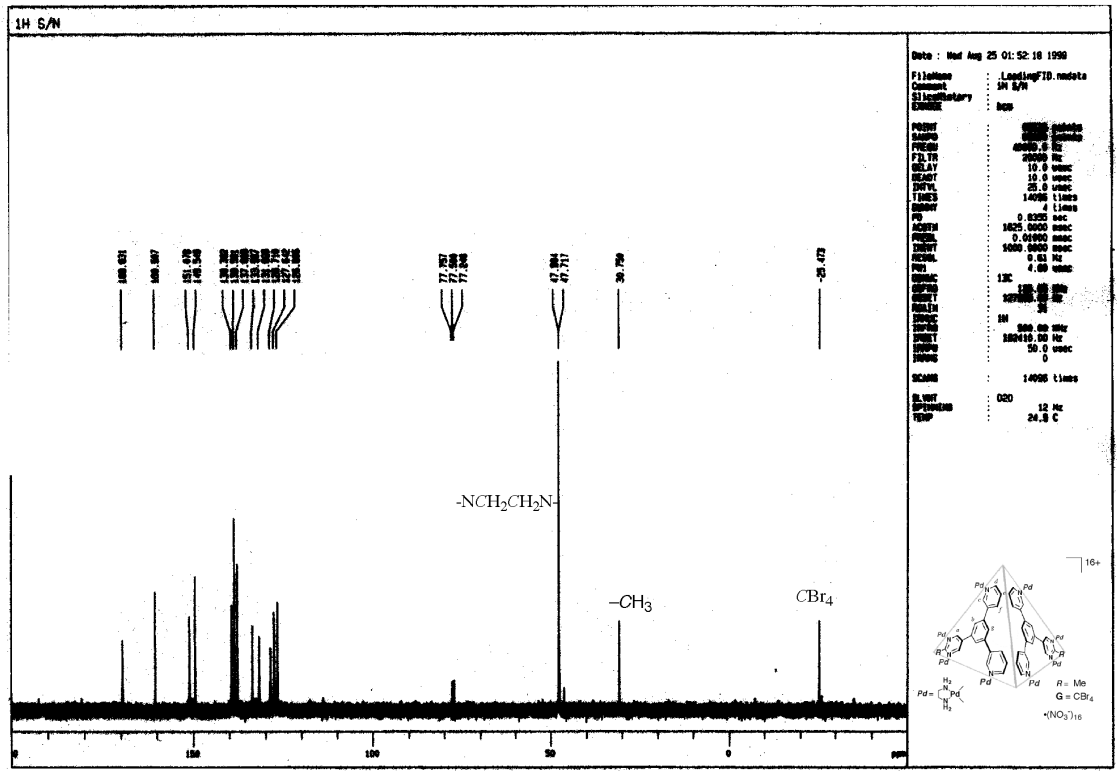
Typical procedure: To an aqueous suspension (D_2O: 1.0 mL) of (en)Pd(NO_3)$_2$ (**1**; 6.2 mg; 21.3 μmol) and **2b** (2.8 mg; 7.9 μmol), excess amount (ca. 27 μmol) of CBr_4 (**5**) was added and the mixture was stirred for 24 h at ambient temperature. After filtration, the resulting clear solution was concentrated to precipitate included complex **3•5** in 77% isolated yield.

Physical data: ^{1}H NMR (500.13 MHz, D_2O, 27 °C, TMS as external standard): δ 10.76 (s, 2H), 9.33 (s, 2H), 8.69 (d, J = 5.4 Hz, 2H), 8.51 (s, 2H), 8.37 (d, J = 8.3 Hz, 2H), 8.00 (s, 1H), 7.63 (d, J = 5.4, 8.3 Hz, 2H), 4.44 (s, 3H), 3.09-3.03 (m, 8H), 2.99-2.95 (m, 8H); ^{13}C NMR (125.77 MHz, D_2O, 27 °C, TMS as external standard): δ 169.6 (C_q), 160.5 (*C*H), 151.1 (*C*H), 149.5 (*C*H), 139.4 (*C*H), 138.6 (C_q), 137.8 (C_q), 133.6 (C_q), 131.8 (C_q), 128.7 (*C*H), 127.6 (*C*H), 126.7 (*C*H), 47.8 (*C*H), 47.7 (*C*H), 30.7 (*C*H$_3$), –25.5 (C_q, **5**); IR (KBr, cm^{-1}): 3404, 3060, 2370, 1558, 1382, 1055, 822; m.p.: ~220 °C (decomposed).

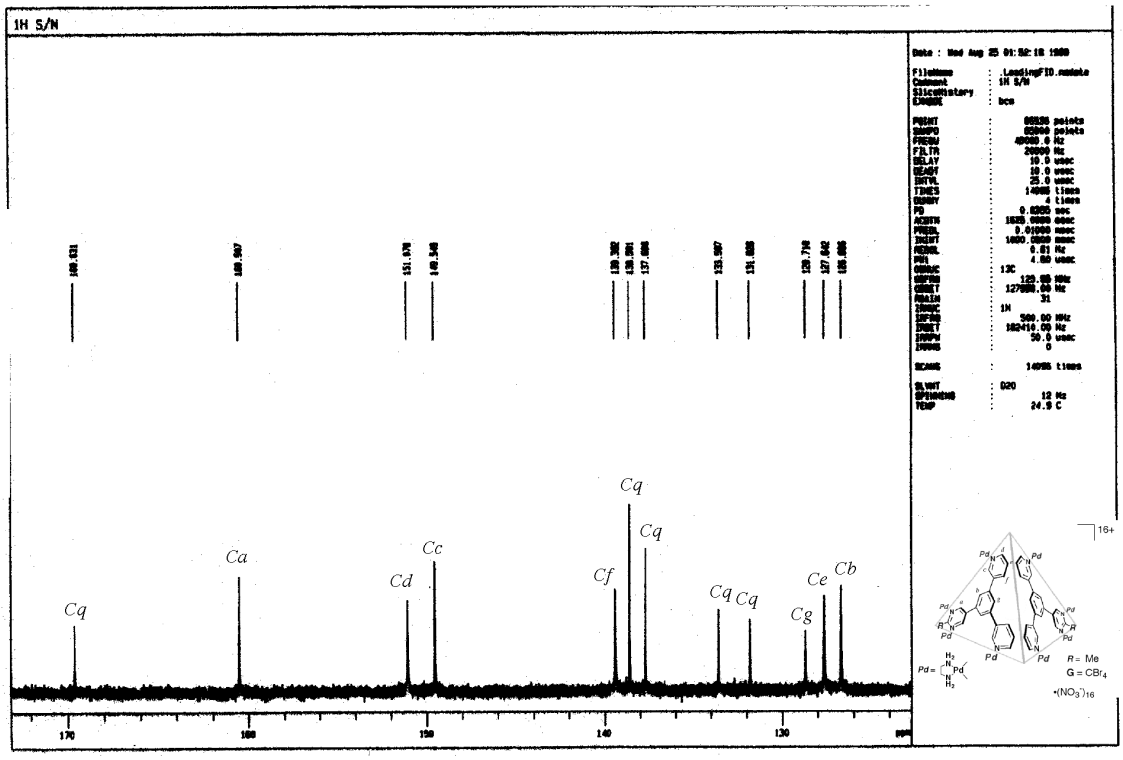
^{1}H NMR of 3•5



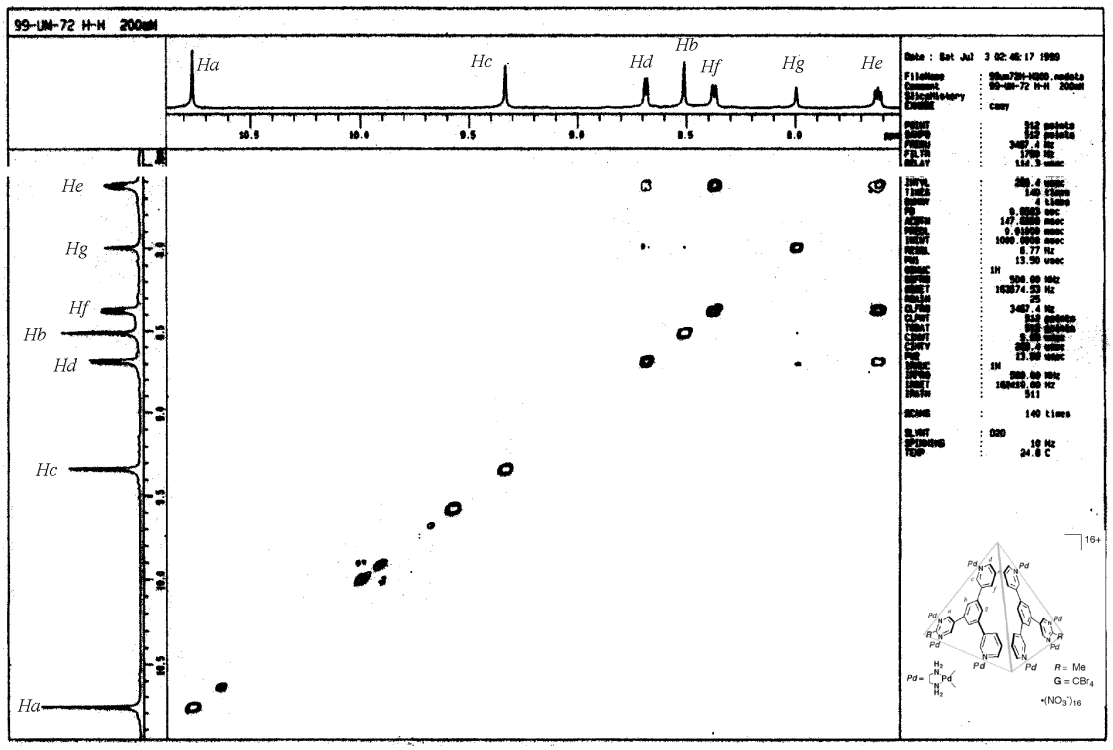
^{13}C NMR of 3•5



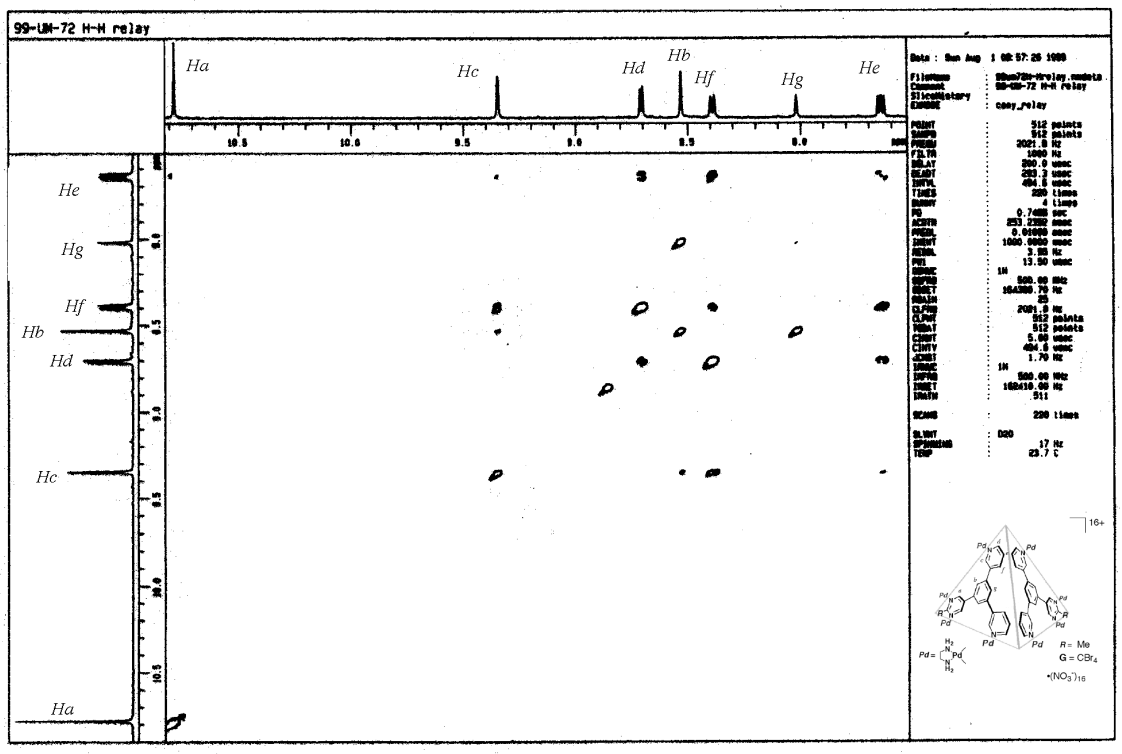
^{13}C NMR of 3•5 (magnification)



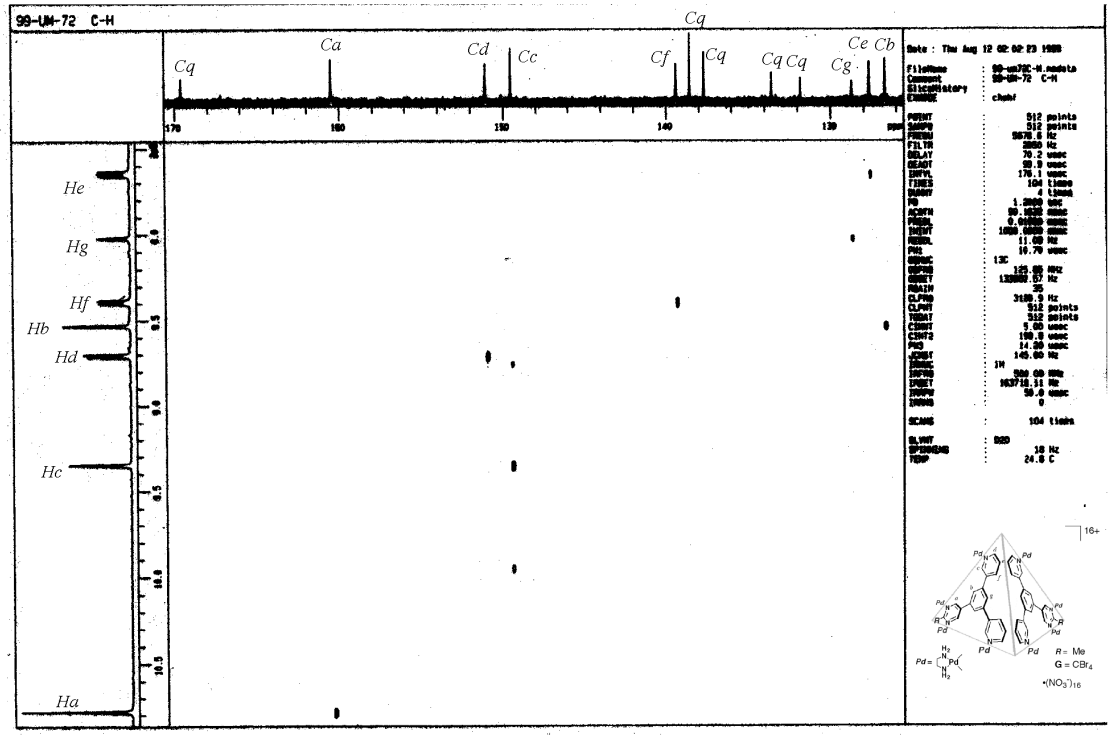
H-H COSY of 3•5



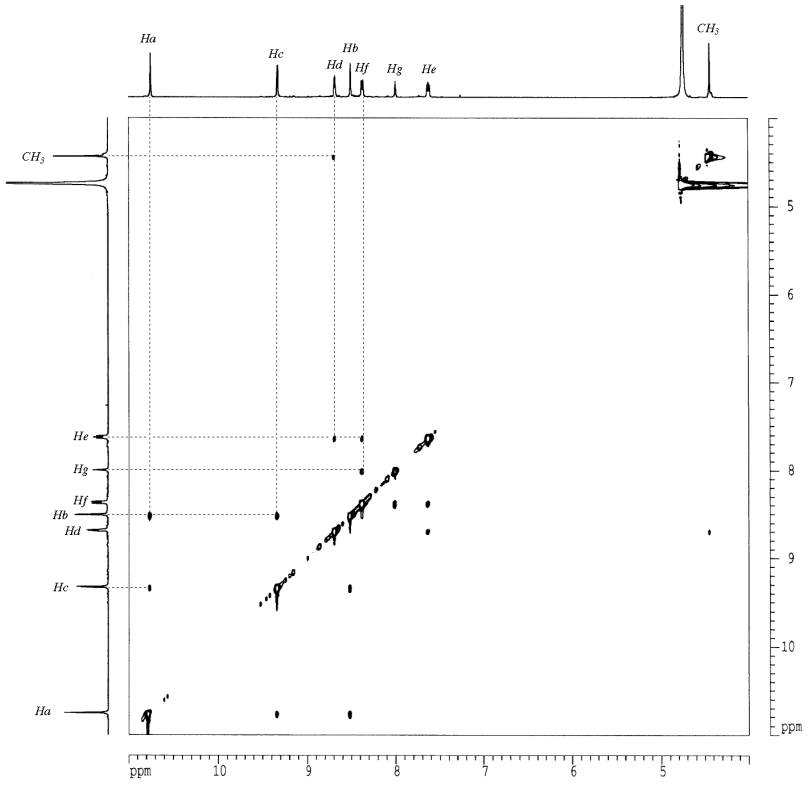
H-H Relay COSY of 3•5

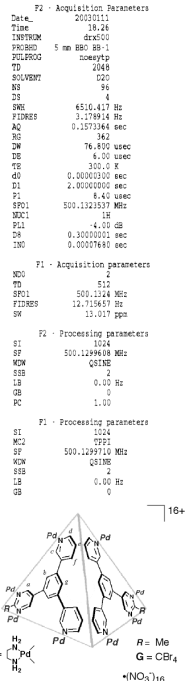


C-H COSY of 3•5



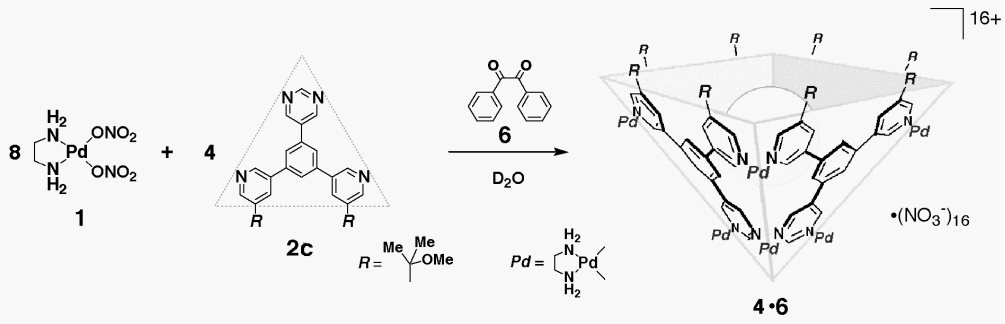
NOESY of 3•5





□ Self-assembly of Open cone 4•6 (6 = benzil).

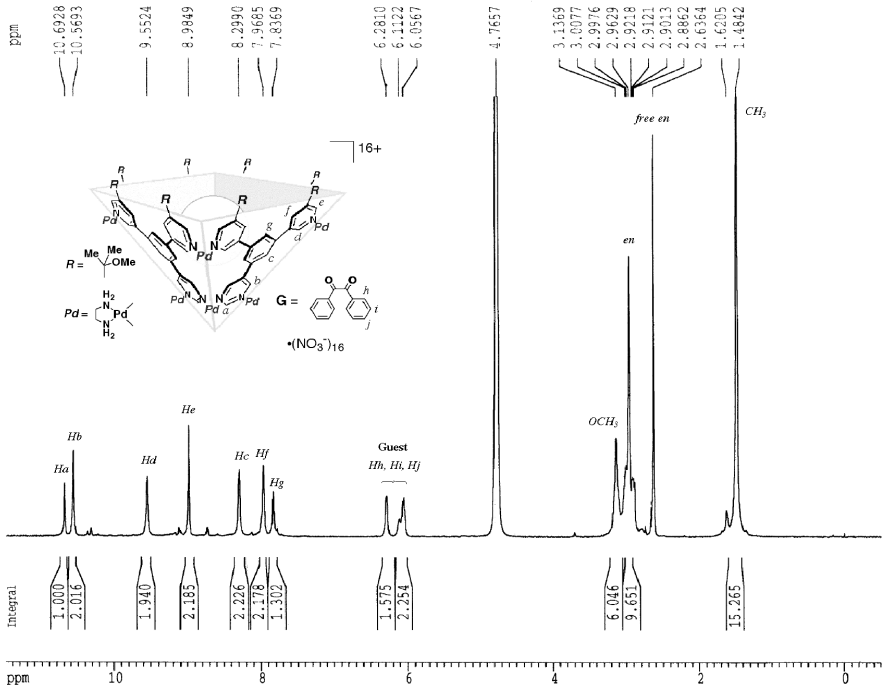
Scheme:



Typical procedure: To an aqueous suspension (D_2O: 1.0 mL) of (en)$Pd(NO_3)_2$ (**1**; 6.9 mg; 23.8 μmol) and **2c** (3.6 mg; 7.9 μmol), excess amount (ca. 10 equivalents based on **4**) of benzil (**6**) was added and the mixture was stirred for 24 h at ambient temperature. After filtration, the resulting solution was concentrated to precipitate included complex **4•6** as a pale yellow solid (8.1 mg; 1.8 μmol) in 94% isolated yield.

Physical data: ^{1}H NMR (500.13 MHz, D_2O, 27 °C, TMS as external standard): δ 10.70(s, 4H), 10.58 (s, 8H), 9.54 (s, 8H), 8.99 (s, 8H), 8.30 (s, 8H), 7.97 (s, 8H), 7.83 (s, 4H), 6.27(s, 4H, **6**), 6.07(m, 6H, **6**), 3.14 (m, 32H), 2.96 (s, 24H), 1.49 (s, 24H); ^{13}C NMR (125.77 MHz, D_2O, 27 °C, TMS as external standard): δ 193.7 (C_q, **6**), 160.6 (*C*H), 159.2 (*C*H), 148.9 (*C*H), 148.3 (*C*H), 145.2 (C_q), 137.2 (C_q), 136.9 (C_q), 135.7 (C_q), 135.5 (*C*H), 133.9 (*C*H, **6**), 131.3 (C_q), 130.9 (C_q, **6**), 128.1 (*C*H), 128.0 (*C*H, **6**), 127.6 (*C*H, **6**), 126.0 (*C*H), 76.4 (C_q), 50.3 (CH_3), 47.8 (CH_2), 46.9 (CH_2), 26.6 (CH_3), 26.1 (CH_3); IR (KBr, cm^{-1}): 3073, 2988, 2290, 1734, 1595, 1356, 1051; m.p.: ~220 °C (decomposed); CSI-MS(H_2O + DMF) 973.1 [**4•6** – **6** – $(NO_3)_4]^{4+}$, 992.2 [**4•6** + DMF – **6** – $(NO_3)_4]^{4+}$, 1010.5 [**4•6** + 2DMF – **6** – $(NO_3)_4]^{4+}$, 1318.4 [**4•6** – **6** – $(NO_3)_3]^{3+}$, 1025.7 [**4•6**− $(NO_3)_4]^{4+}$, 1044.7 [**4•6** + DMF − $(NO_3)_4]^{4+}$, 1063.3[**4•6** + 2DMF – $(NO_3)_4]^{4+}$, 1079.3 [**4•6** + 3DMF − $(NO_3)_4]^{4+}$; Elemental Analysis Calcd for $C_{142}H_{162}N_{32}O_{10}Pd_8P_{16}F_{96}\cdot(H_2O)_{17}$ (counter ions of **4•6** was replaced by PF_6^-): C, 28.56; H, 3.34; N, 7.51. Found: C, 28.75; H, 3.73; N, 7.26.

^{1}H NMR of 4•6



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F2 - Processing parameters

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1D NMR plot parameters

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F2	-250.06 Hz
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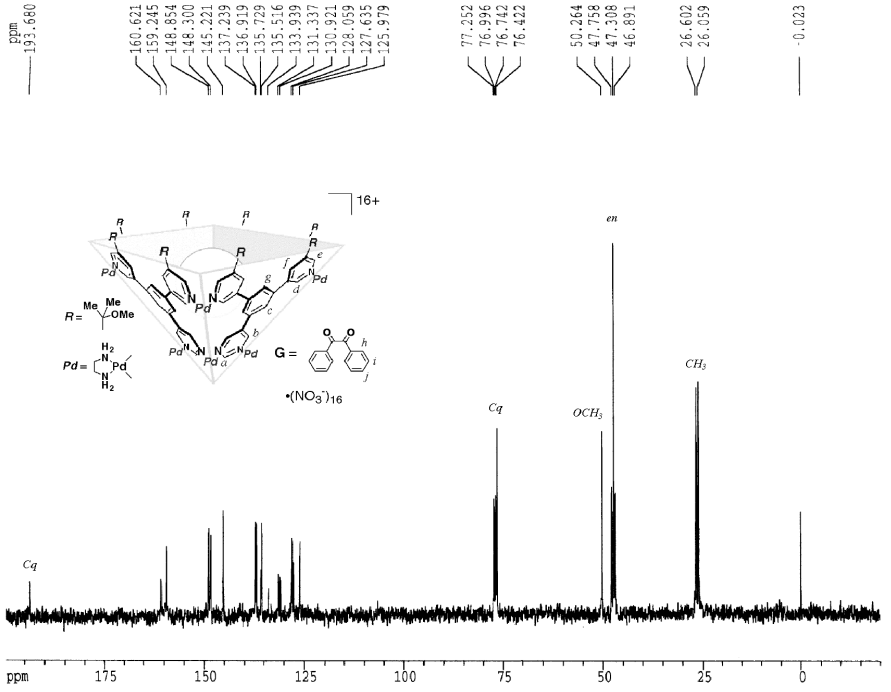
^{13}C NMR of 4•6



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NUC2	1H
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PL12	15.50 dB
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NUC1	13C
PL1	2.00 dB

F2 - Processing parameters

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1D NMR plot parameters

CX	20.00 cm
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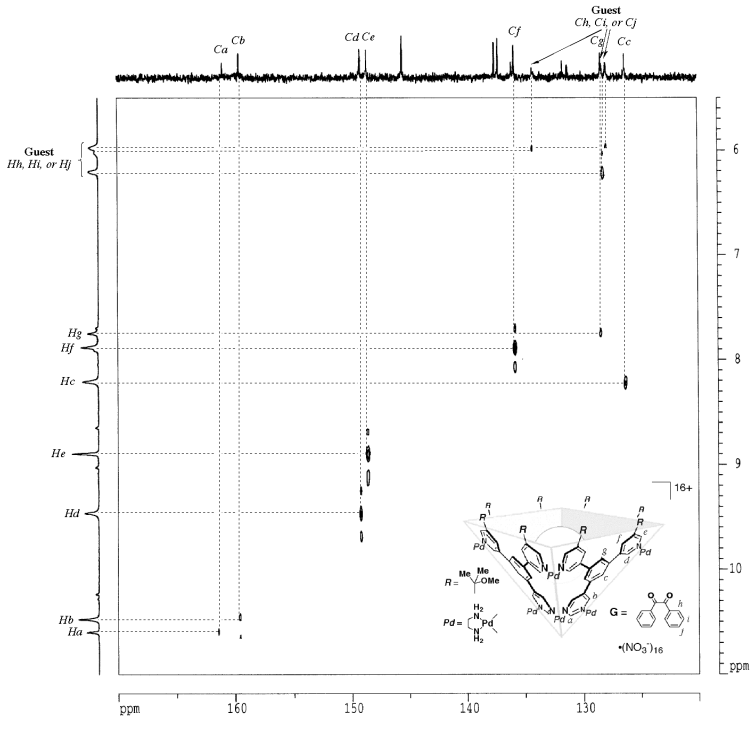
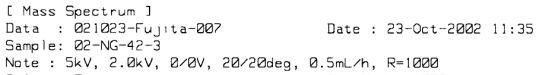
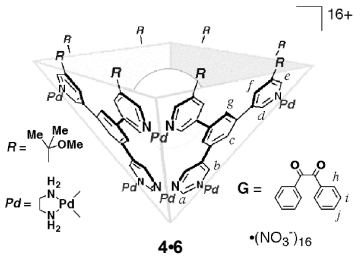
F1	25151.55 Hz
F2P	-20.000 ppm
F2	-2515.16 Hz
PPMCM	11.00000 ppm/cm
HZCM	1383.33557 Hz/cm

C-H COSY of 4•6

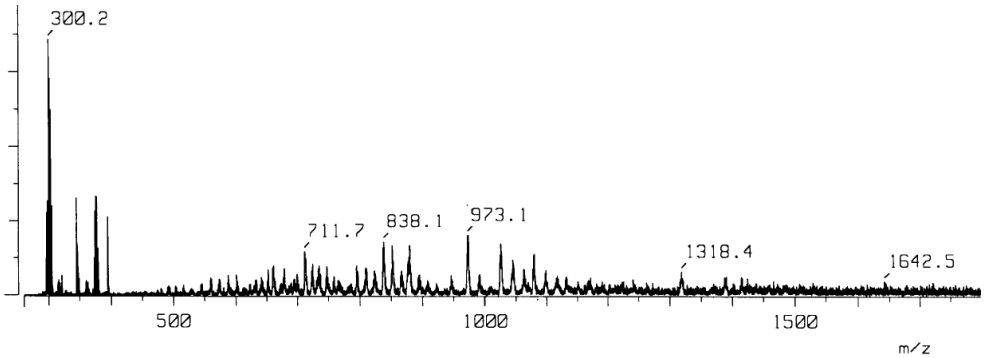


CSI-MS of 4•6

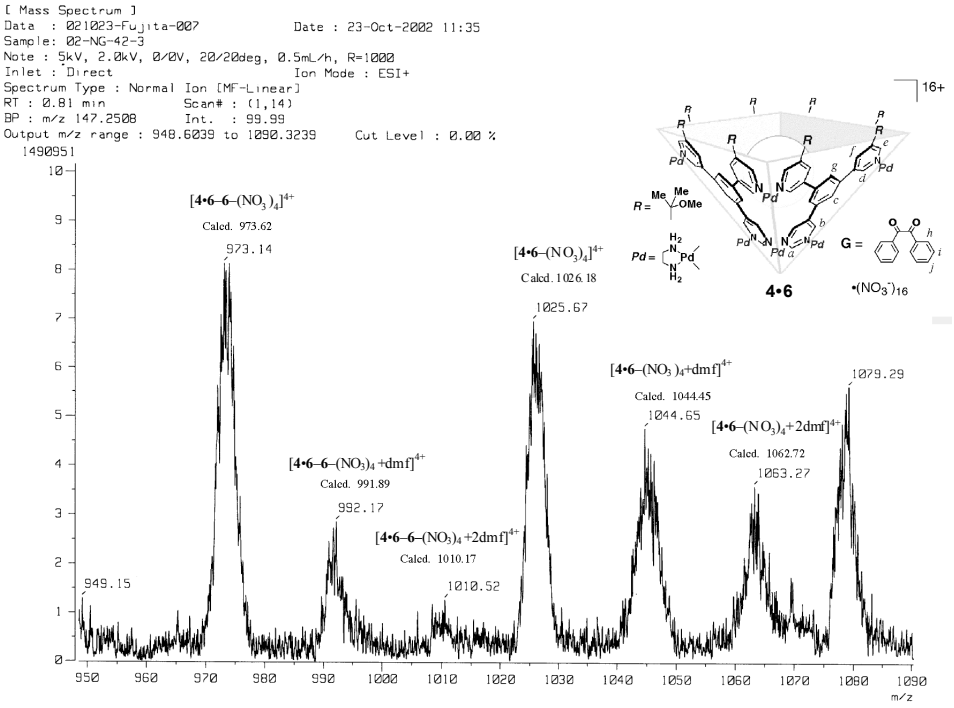




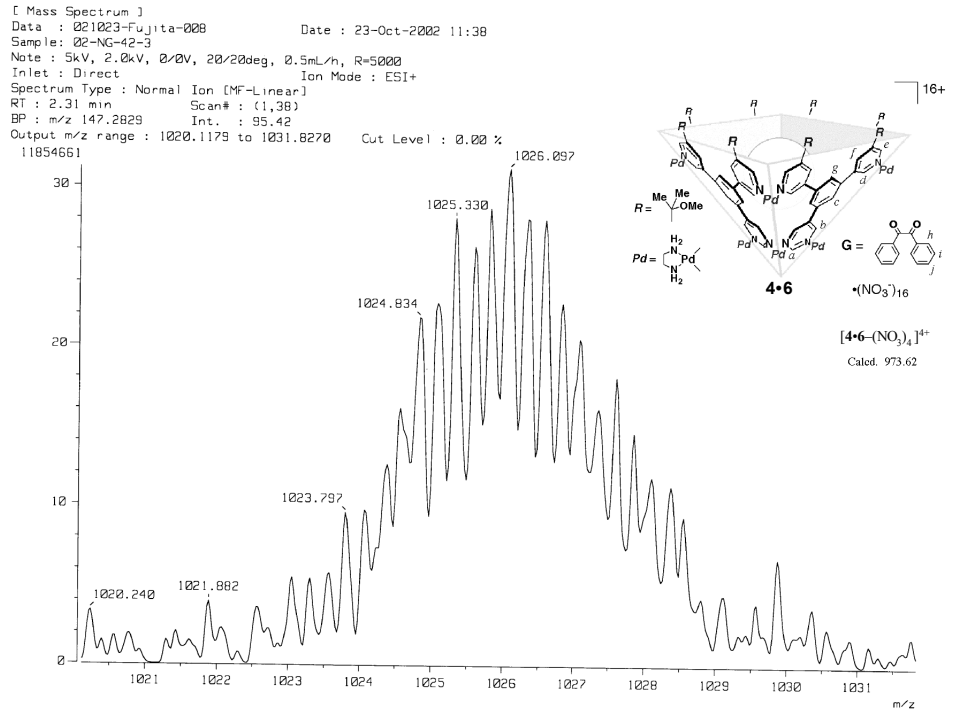
4•6



CSI-MS of 4•6 (magnification)

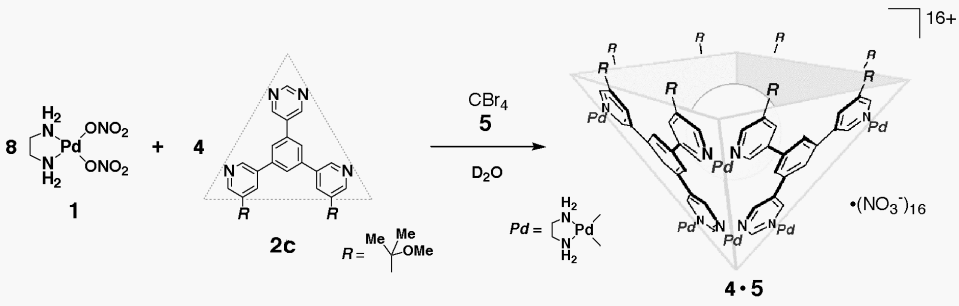


CSI-MS of 4•6 (magnification)



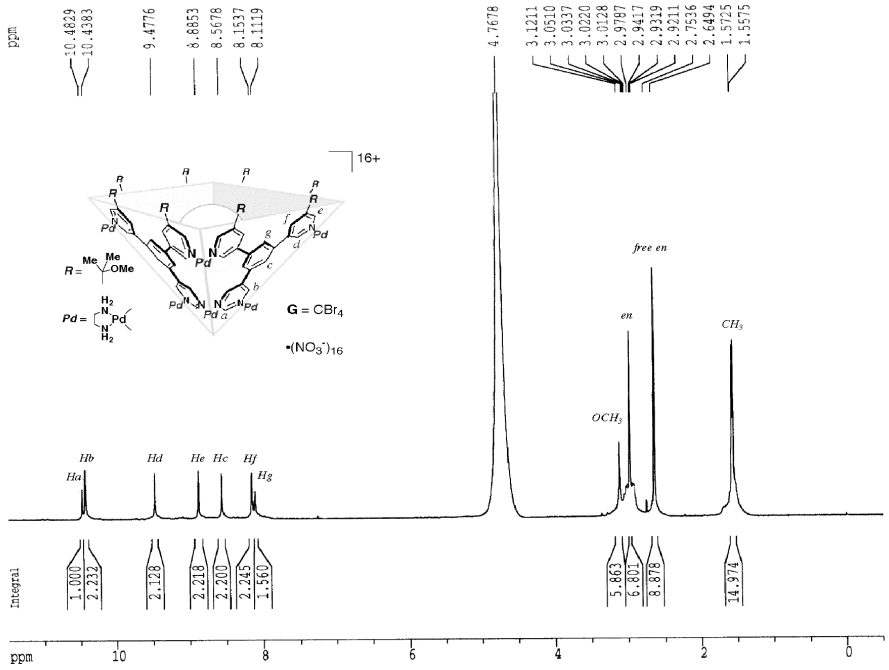
□ Self-assembly of Open cone 4•5 (5 = CBr_4).

Scheme:



Physical data: ^{1}H NMR (500.13 MHz, D_2O, 27 °C, TMS as external standard): δ 10.48(s, 4H), 10.44 (s, 8H), 9.48 (s, 8H), 8.89 (s, 8H), 8.57 (s, 8H), 8.15 (s, 8H), 8.11 (s, 4H), 3.12 (m, 32H), 3.00 (s, 24H), 1.57 (s, 24H), 1.56 (s, 24H); ^{13}C NMR (125.77 MHz, D_2O, 27 °C, TMS as external standard): δ 161.1 (*C*H), 158.8 (*C*H), 149.4 (*C*H), 148.0 (*C*H), 145.3 (C_q), 138.2 (C_q), 137.5 (C_q), 136.2 (*C*H), 135.2 (C_q), 131.8 (C_q), 128.6 (*C*H), 126.2 (*C*H), 76.5 (C_q), 50.4 (CH_3), 47.7 (CH_2), 47.0 (CH_2), 26.6 (CH_3), 26.4 (CH_3), –27.1(C_q, **5**); IR (KBr, cm^{-1}): 3073, 2980, 2296, 1350, 1176, 1053, 707; m.p.: ~220 °C (decomposed); CSI-MS(H_2O + DMF) 766.3 [**4•5** – **5** – $(NO_3)_5]^{5+}$, 780.4 [**4•5** – **5** + DMF – $(NO_3)_5]^{5+}$, 795.4 [**4•5** – **5** + 2DMF – $(NO_3)_5]^{5+}$, 810.6 [**4•5** – **5** + 3DMF – $(NO_3)_5]^{5+}$, 973.1 [**4•5** – **5** – $(NO_3)_4]^{4+}$, 992.2 [**4•5** – **5** + DMF – $(NO_3)_4]^{4+}$, 1010.5 [**4•5** – **5** + 2DMF – $(NO_3)_4]^{4+}$, 1318.8 [**4•5** – **5** – $(NO_3)_3]^{3+}$.

^{1}H NMR of 4•5



F2 - Acquisition Parameters

Date_	20020917
Time	21.36
INSTRUM	drx500
PROBHD	5 mm BBO BB-1
PULPROG	zg30
TD	32768
SOLVENT	D2O
NS	32
DS	2
SWH	10330.578 Hz
FIDRES	0.315264 Hz
AQ	1.5860212 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
P1	9.60 usec
SFO1	500.1330885 MHz
NUC1	1H
PL1	-4.00 dB

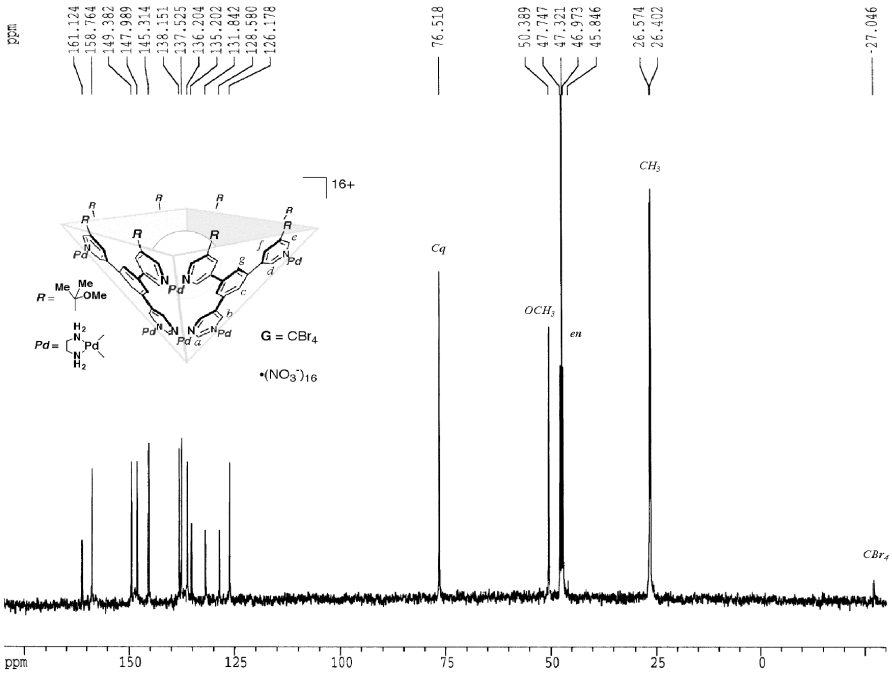
F2 - Processing parameters

SI	16384
SF	500.1299687 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	11.500 ppm
F1	5751.49 Hz
F2P	-0.500 ppm
F2	-250.06 Hz
PPMCM	0.60000 ppm/cm
HZCM	300.07797 Hz/cm

^{13}C NMR of 4•5



F2 - Acquisition Parameters

Date_	20021105
Time	8.32
INSTRUM	drx500
PROBHD	5 mm BBO BB-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	78086
DS	2
SWH	39682.539 Hz
FIDRES	0.605507 Hz
AQ	0.8258036 sec
RG	16384
DW	12.600 usec
DE	6.00 usec
TE	300.0 K
d11	0.03000000 sec
d12	0.00002000 sec
PL13	15.50 dB
D1	2.00000000 sec
CPDPRG2	waltz16
PCPD2	80.00 usec
SFO2	500.1320005 MHz
NUC2	1H
PL2	-4.00 dB
PL12	15.50 dB
P1	7.30 usec
SFO1	125.7736214 MHz
NUC1	13C
PL1	2.00 dB

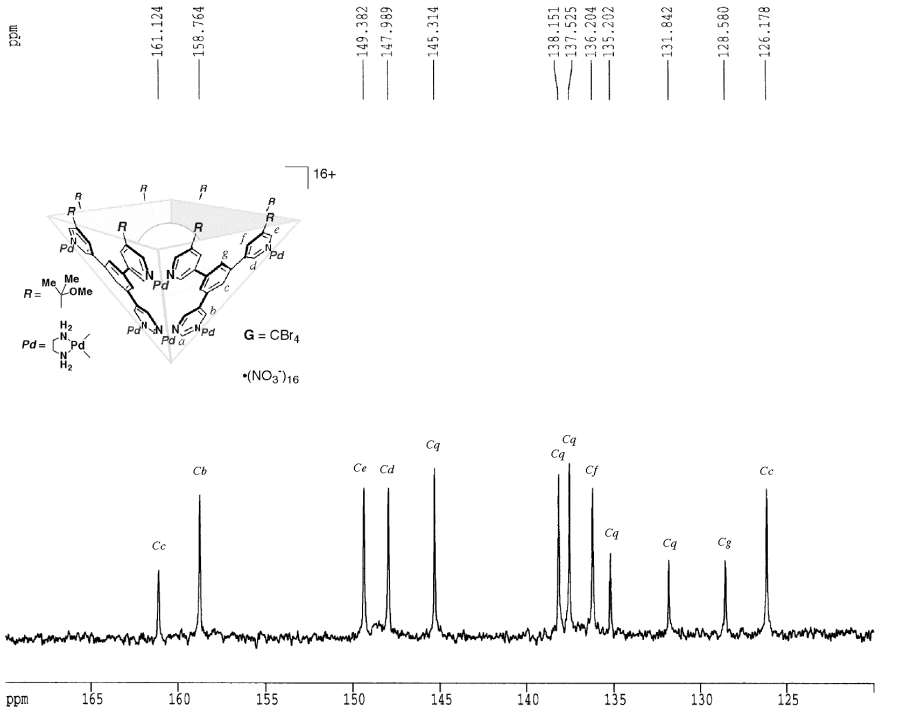
F2 - Processing parameters

SI	32768
SF	125.7577849 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	180.000 ppm
F1	22636.40 Hz
F2P	-30.000 ppm
F2	-3772.74 Hz
PPMCM	10.50000 ppm/cm
HZCM	1320.45667 Hz/cm

^{13}C NMR of 4•5 (magnification)

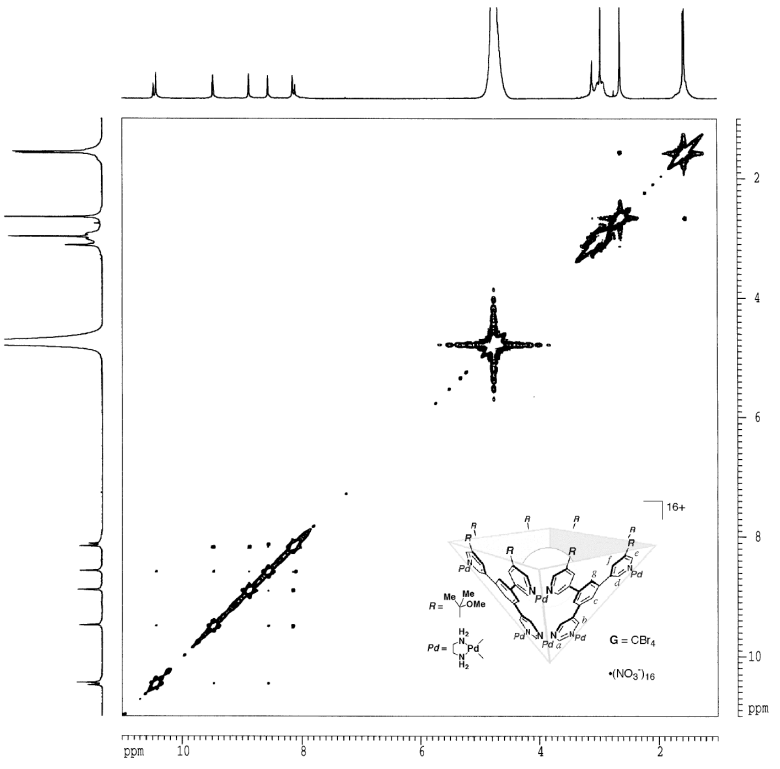



```
F2 - Acquisition Parameters
Date_              20021105
Time                  8.32
INSTRUM             drx500
PROBHD    5 mm BBO BB-1
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                  78086
DS                      2
SWH            39682.539 Hz
FIDRES          0.605507 Hz
AQ              0.8258036 sec
RG                  16384
DW                12.600 usec
DE                 6.00 usec
TE                300.0 K
d11           0.03000000 sec
d12           0.00002000 sec
PL13               15.50 dB
D1            2.00000000 sec
CPDPRG2           waltz16
PCPD2              80.00 usec
SFO2          500.1320005 MHz
NUC2                  1H
PL2                -4.00 dB
PL12               15.50 dB
P1                  7.30 usec
SFO1          125.7736214 MHz
NUC1                 13C
PL1                2.00 dB

F2 - Processing parameters
SI                 32768
SF          125.7577849 MHz
WDW                   EM
SSB                    0
LB                  5.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                20.00 cm
F1P              170.000 ppm
F1              21378.82 Hz
F2P              120.000 ppm
F2              15090.93 Hz
PPMCM            2.50000 ppm/cm
HZCM           314.39447 Hz/cm
```

H-H COSY of 4•5

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F2 - Acquisition Parameters
Date_              20020917
Time                  21.47
INSTRUM             drx500
PROBHD    5 mm BBO BB-1
PULPROG           cosy90
TD                  2048
SOLVENT              D2O
NS                    64
DS                     4
SWH            6009.615 Hz
FIDRES         2.934382 Hz
AQ              0.1704436 sec
RG                   256
DW                83.200 usec
DE                 6.00 usec
TE                300.0 K
d0            0.00000300 sec
D1            2.00000000 sec
P1                 10.00 usec
SFO1          500.1327194 MHz
NUC1                  1H
PL1                4.00 dB
IN0           0.00016640 sec

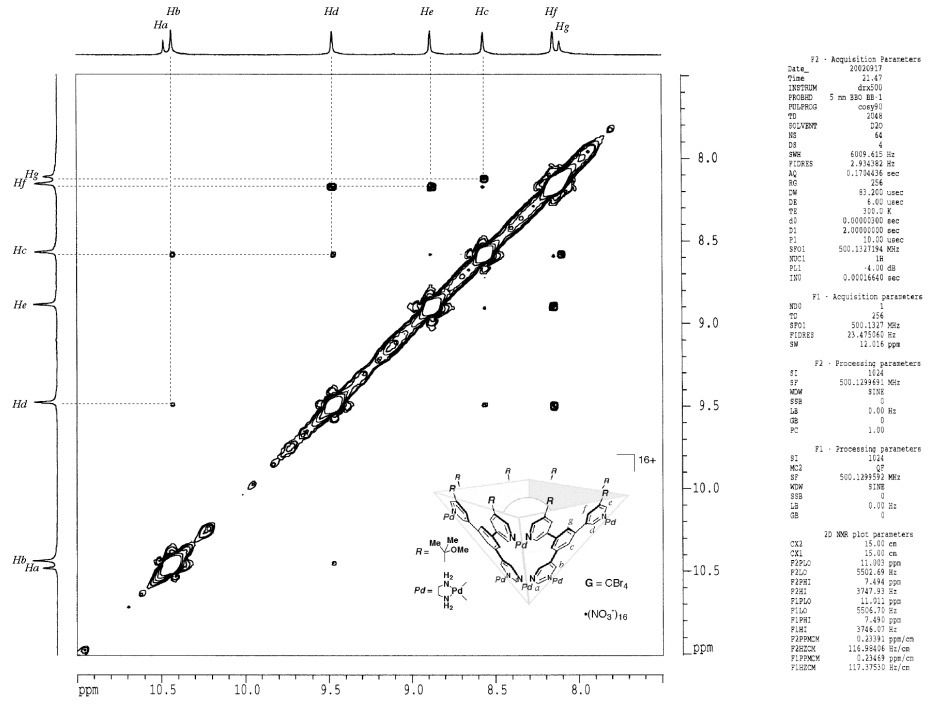
F1 - Acquisition parameters
NDU                    1
TD                   256
SFO1          500.1327 MHz
FIDRES         23.47596 Hz
SW              12.016 ppm

F2 - Processing parameters
SI                  1024
SF          500.1299691 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          500.1299592 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0

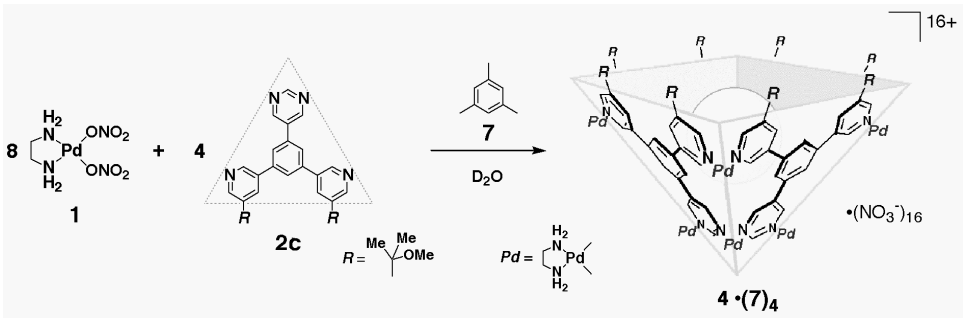
2D NMR plot parameters
CX2                15.00 cm
CX1                15.00 cm
F2PLO           11.000 ppm
F2LO            5501.43 Hz
F2PPI              1.000 ppm
F2HI             500.13 Hz
F1PLO           11.000 ppm
F1LO            5501.43 Hz
F1PPI              1.000 ppm
F1HI             500.13 Hz
F2PPMCM         0.66667 ppm/cm
F2HZCM        333.41998 Hz/cm
F1PPMCM         0.66667 ppm/cm
F1HZCM        333.41998 Hz/cm
```

H-H COSY of 4•5 (magnification)



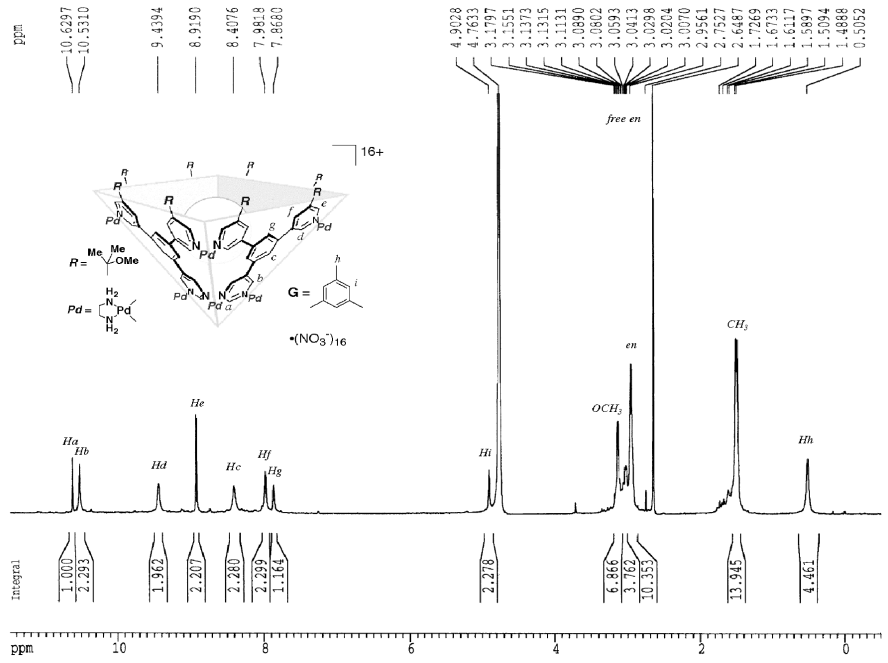
□ Self-assembly of Open cone 4•(7)$_4$ (7 = mesitylene).

Scheme:



Physical data: ^{1}H NMR (500.13 MHz, D_2O, 27 °C, TMS as external standard): δ 10.63 (s, 4H), 10.53 (s, 8H), 9.44 (s, 8H), 8.92 (s, 8H), 8.41 (s, 8H), 7.98 (s, 8H), 7.87 (s, 4H), 4.90 (s, 12H, **7**), 3.14 (m, 32H), 3.06 (s, 24H), 1.51 (s, 24H), 1.49 (s, 24H), 0.50 (s, 36H, **7**); ^{13}C NMR (125.77 MHz, D_2O, 27 °C, TMS as external standard): δ 160.6 (*C*H), 158.9 (*C*H), 148.9 (*C*H), 148.4 (*C*H), 145.2 (C_q), 137.5 (C_q), 137.2 (C_q), 135.7 (*C*H), 135.4 (C_q, **7**), 135.1 (C_q), 131.2 (C_q, **7**), 128.2 (*C*H), 125.8 (*C*H, **7**), 125.1 (*C*H), 76.4 (C_q), 50.3 (CH_3), 47.7 (CH_2), 46.9 (CH_2), 26.5 (CH_3), 26.3 (CH_3), 19.4 (CH_3, **7**); IR (KBr, cm^{-1}): 3073, 2981, 2296, 1369, 1174, 1052, 708; m.p.: ~220 °C (decomposed).

^{1}H NMR of 4•(7)$_4$



F2 - Acquisition Parameters
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Time 17.31
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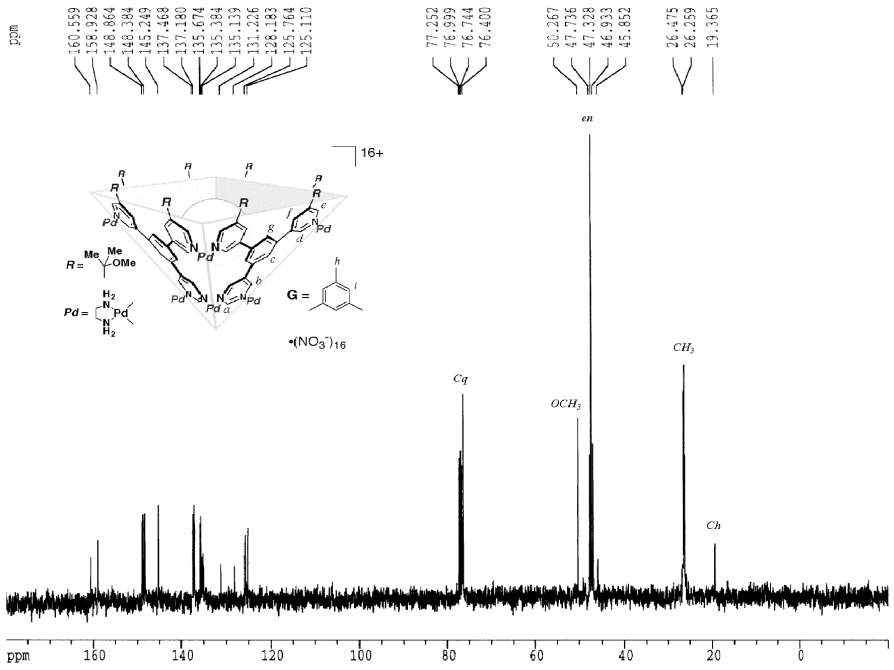
PROBHD 5 mm BBO BB-1
PULPROG zg30
TD 32768
SOLVENT D2O
NS 32
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.00 usec
SFO1 500.1330885 MHz
NUC1 1H
PL1 -4.00 dB

F2 - Processing parameters
SI 16384
SF 500.1299699 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 11.500 ppm
F1 5751.49 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.60000 ppm/cm
HZCM 300.07797 Hz/cm

^{13}C NMR of 4•(7)$_4$

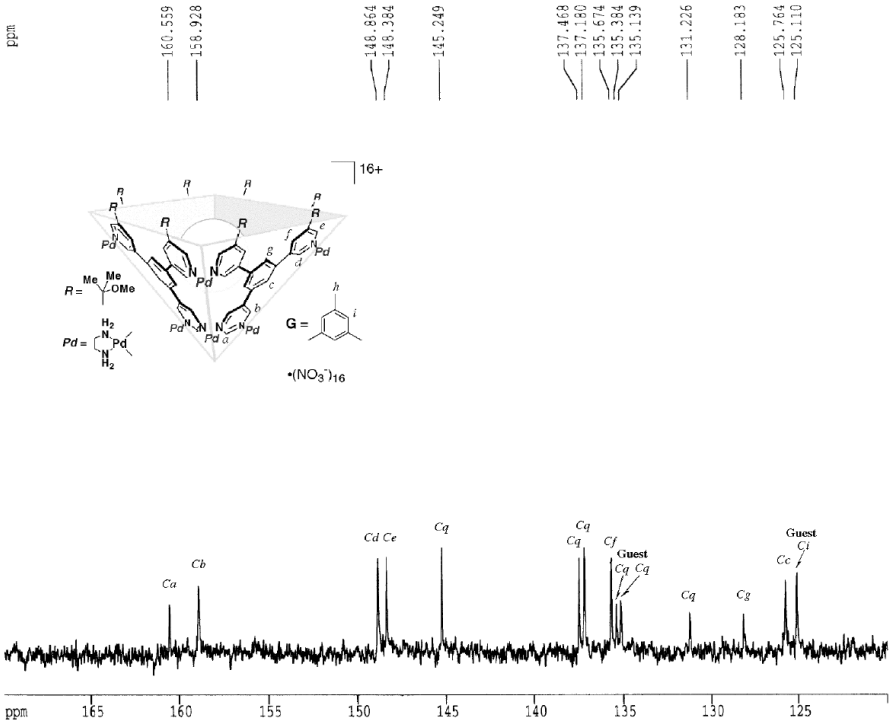


F2 - Acquisition Parameters
Date_ 20021025
Time 23.02
INSTRUM drx500
PROBHD 5 mm BBO BB-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11751
DS 2
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 14596.5
DW 12.600 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
d12 0.00002000 sec
PL13 15.50 dB
D1 2.00000000 sec
CPDPRG2 waltz16
PCPD2 80.00 usec
SFO2 500.1320005 MHz
NUC2 1H
PL2 -4.00 dB
PL12 15.50 dB
P1 7.30 usec
SFO1 125.7736214 MHz
NUC1 13C
PL1 2.00 dB

F2 - Processing parameters
SI 32768
SF 125.7577825 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 180.000 ppm
F1 22636.40 Hz
F2P -20.000 ppm
F2 -2515.16 Hz
PPMCM 10.00000 ppm/cm
HZCM 1257.57788 Hz/cm

^{13}C NMR of 4•$(7)_4$ (magnification)

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F2 - Acquisition Parameters
Date_              20021025
Time                 23.02
INSTRUM              drx500
PROBHD     5 mm BBO BB-1
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                    11751
DS                        2
SWH              39682.539 Hz
FIDRES               0.605507 Hz
AQ                 0.8258036 sec
RG                   14596.5
DW                  12.600 usec
DE                   6.00 usec
TE                  300.0 K
d11              0.03000000 sec
d12              0.00002000 sec
PL13                15.50 dB
D1               2.00000000 sec
CPDPRG2             waltz16
PCPD2               80.00 usec
SFO2            500.1320005 MHz
NUC2                    1H
PL2                 -4.00 dB
PL12                15.50 dB
P1                   7.30 usec
SFO1            125.7736214 MHz
NUC1                   13C
PL1                  2.00 dB

F2 - Processing parameters
SI                    32768
SF              125.7577825 MHz
WDW                      EM
SSB                       0
LB                   3.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                   20.00 cm
F1P                170.000 ppm
F1                 21378.82 Hz
F2P                120.000 ppm
F2                 15090.93 Hz
PPMCM               2.50000 ppm/cm
HZCM              314.39447 Hz/cm
```
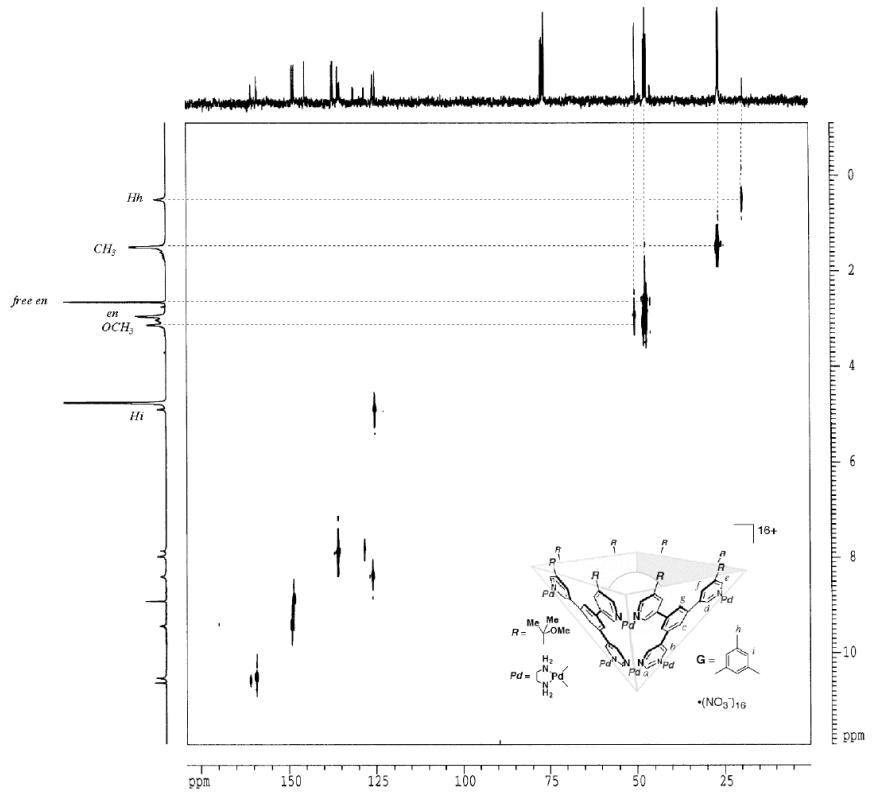
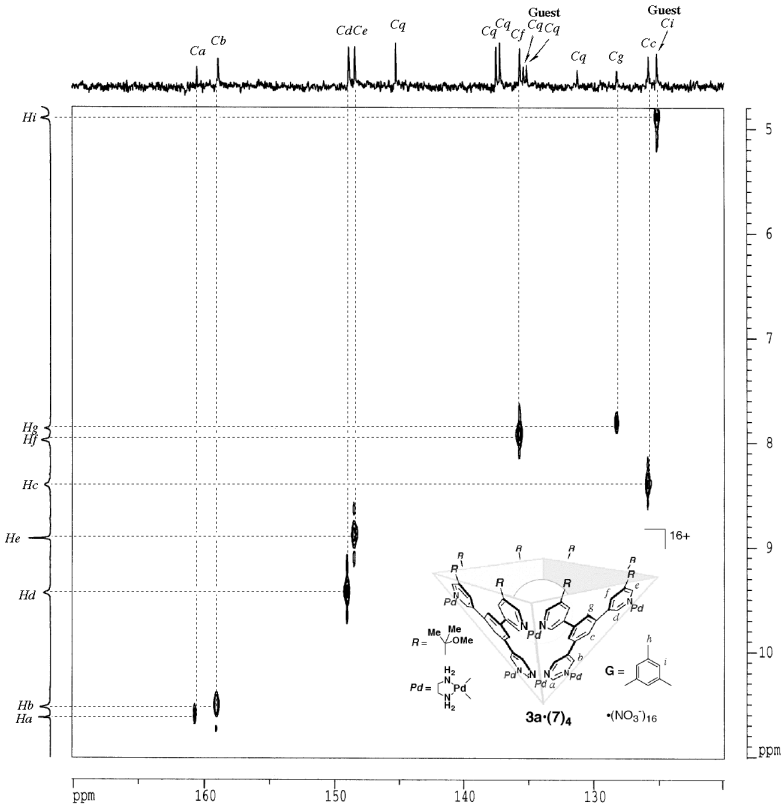

C-H COSY of 4•$(7)_4$



C-H COSY of 4•$(7)_4$ (magnification)



F2 - Acquisition Parameters
Date_ 20021110
Time 16.18
INSTRUM drx500
PROBHD 5 mm BBO BB-1
PULPROG hsco
TD 4096
SOLVENT H2O
NS 200
DS 4
SWH 12522.523 Hz
FIDRES 5.498663 Hz
AQ 0.0939812 sec
RG 14384
DW 22.200 usec
DE 6.00 usec
TE 300.0 K
P1 7.30 usec
P2 14.40 usec
SD 0.00000200 sec
CNST2 145.0000000
AQ 0.09344828 sec
CNST11 3.0000000
d1 0.00229885 sec
d11 0.03000000 sec
d12 0.00002000 sec
D1 2.00000000 sec
PL2 4.00 dB
P3 10.00 usec
SFO2 500.1327019 MHz
NUC2 1H
SFO1 125.7690053 MHz
NUC1 13C
PL1 2.00 dB
PL12 15.50 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
IN0 0.00007980 sec

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 500.1327 MHz
FIDRES 50.962629 Hz
SW 13.017 ppm

F2 - Processing parameters
SI 2048
SF 125.7577390 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 170.127 ppm
F2LO 21394.84 Hz
F2PHI 119.845 ppm
F2HI 15071.38 Hz
F1PLO 11.013 ppm
F1LO 5507.72 Hz
F1PHI 4.796 ppm
F1HI 2398.75 Hz
F2PPMCM 3.35219 ppm/cm
F2HZCM 421.54418 Hz/cm
F1PPMCM 0.41442 ppm/cm
F1HZCM 207.26521 Hz/cm

□ X-ray crystal data of Tetrahedron 3•5.

Table 1. Crystal data and structure refinement for bk81n.

Identification code	bk81n	
Empirical formula	C101 H174 Br4 N48 O73 Pd8	
Formula weight	4399.72	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 31.439(4) Å	α= 90°.
	b = 44.137(6) Å	β= 107.253(3)°.
	c = 27.987(4) Å	γ = 90°.
Volume	37088(8) $Å^3$	
Z	8	
Density (calculated)	1.576 Mg/m^3	
Absorption coefficient	1.714 mm^{-1}	
F(000)	17664	
Crystal size	0.15 mm x 0.10 mm x 0.10 mm	
Theta range for data collection	1.20 to 25.00°.	
Index ranges	-37<=h<=35, 0<=k<=52, 0<=l<=33	
Reflections collected	44275	
Independent reflections	32651 [R(int) = 0.4402]	
Completeness to theta = 25.00°	99.9 %	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	32651 / 30 / 1863	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2sigma(I)]	R1 = 0.1073, wR2 = 0.2412	
R indices (all data)	R1 = 0.3216, wR2 = 0.2806	
Extinction coefficient	0.000324(12)	
Largest diff. peak and hole	1.312 and -0.845 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for bk81n. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2974(1)	-380(1)	2421(1)	65(1)
Pd(2)	3949(1)	783(1)	890(1)	63(1)
Pd(3)	1931(1)	203(1)	3636(1)	84(1)
Pd(4)	286(1)	1428(1)	-641(1)	48(1)
Pd(5)	-128(1)	2363(1)	676(1)	52(1)
Pd(6)	2648(1)	1403(1)	-798(1)	48(1)
Pd(7)	2486(1)	1796(1)	4462(1)	45(1)
Pd(8)	1726(1)	2742(1)	2941(1)	47(1)
C(1)	8163(8)	1340(4)	3365(9)	91(9)
Br(1)	7870(1)	1580(1)	2779(1)	111(1)
Br(2)	7827(1)	1384(1)	3822(1)	138(1)
Br(3)	8757(1)	1484(1)	3634(1)	108(1)
Br(4)	8177(1)	921(1)	3170(1)	89(1)
N(100)	4267(7)	2605(9)	876(9)	190(20)
O(101)	4558(6)	2635(3)	704(6)	108(6)
O(102)	4088(6)	2851(4)	968(7)	135(8)
O(103)	4105(9)	2358(6)	1022(9)	208(16)
N(200)	2383(6)	1405(4)	6833(6)	69(6)
O(201)	1992(6)	1326(3)	6789(6)	114(6)
O(202)	2688(5)	1273(3)	7159(6)	98(6)
O(203)	2438(5)	1621(3)	6584(5)	87(5)
N(300)	8726(6)	2265(4)	9586(6)	71(6)
O(301)	8488(5)	2294(3)	9143(5)	85(5)
O(302)	8958(5)	2463(3)	9812(5)	76(5)
O(303)	8712(5)	2008(3)	9784(5)	87(5)
N(400)	7158(9)	2074(5)	2070(7)	250(30)
O(401)	6901(7)	2239(4)	1749(7)	157(9)
O(402)	7506(9)	1974(7)	2054(12)	271
O(403)	6991(6)	1998(4)	2431(8)	161(9)
N(500)	1694(5)	2564(4)	4530(6)	50(5)
O(501)	1974(4)	2522(3)	4913(5)	58(4)
O(502)	1594(4)	2834(3)	4369(4)	67(4)
O(503)	1486(4)	2354(3)	4262(4)	53(3)
N(600)	10821(5)	2609(4)	11798(6)	66(5)
O(601)	10820(6)	2715(4)	12189(5)	132(8)
O(602)	10973(4)	2351(3)	11785(4)	62(4)
O(603)	10667(6)	2740(3)	11401(6)	114(6)
N(700)	6421(6)	1645(5)	6505(6)	107(9)
O(701)	6290(6)	1610(3)	6048(6)	120(7)
O(702)	6229(6)	1513(4)	6733(5)	123(7)
O(703)	6718(5)	1823(4)	6678(6)	110(7)

N(800)	6625(7)	4392(5)	3837(9)	134(11)
O(801)	7001(7)	4434(4)	4126(7)	164(9)
O(802)	6617(9)	4205(6)	3556(12)	277(18)
O(803)	6307(7)	4532(6)	3848(13)	278(18)
N(900)	6505(6)	5137(5)	1964(6)	81(7)
O(901)	6831(5)	5311(3)	2079(5)	86(5)
O(902)	6546(6)	4869(3)	2117(6)	118(8)
O(903)	6145(6)	5235(4)	1694(7)	121(7)
N(110)	13204(13)	489(10)	9048(15)	237
O(111)	13238(8)	158(8)	8862(9)	224(13)
O(112)	13273(7)	691(4)	8824(8)	147(9)
O(113)	13078(8)	465(3)	9406(8)	150(9)
N(120)	1446(5)	1413(3)	-735(7)	75(6)
O(121)	1081(6)	1321(7)	-960(6)	241(16)
O(122)	1616(4)	1415(3)	-304(4)	73(5)
O(123)	1614(6)	1481(5)	-1111(6)	164(10)
N(130)	4706(9)	2589(6)	7098(10)	209
O(131)	4368(9)	2742(6)	6921(11)	261(14)
O(132)	4732(9)	2321(6)	7039(10)	246(13)
O(133)	5000	2751(6)	7500	167(11)
N(150)	12251(8)	-1051(6)	9209(8)	149(9)
O(151)	12413(11)	-800(7)	9267(11)	289(16)
O(152)	11955(9)	-1174(6)	9320(9)	238(13)
O(153)	12156(4)	-1048(3)	8687(5)	81(4)
N(140)	13471(9)	160(7)	11635(12)	186
O(141)	13218(5)	335(3)	11626(5)	75
O(142)	13582(8)	-66(4)	11918(10)	195
O(143)	13782(10)	203(6)	11506(10)	224
C(11A)	2284(6)	2123(4)	581(6)	41(5)
C(12A)	2446(6)	2258(4)	1039(6)	47(5)
C(13A)	2141(5)	2342(4)	1308(5)	36(4)
C(14A)	1721(5)	2248(4)	1118(6)	46(5)
C(15A)	1516(6)	2112(4)	628(6)	44(5)
C(16A)	1826(5)	2066(3)	379(6)	35(4)
N(21A)	2776(5)	1756(3)	-332(5)	47(4)
C(21A)	2507(6)	1824(4)	-52(6)	43(5)
C(22A)	2599(6)	2069(4)	289(6)	48(5)
C(23A)	2931(6)	2265(4)	302(6)	43(5)
C(24A)	3217(7)	2195(4)	10(7)	76(7)
C(25A)	3104(6)	1930(4)	-303(6)	53(6)
N(31A)	2184(5)	2674(3)	2567(5)	45(4)
C(31A)	2050(7)	2528(4)	2129(7)	62(6)
C(32A)	2311(6)	2486(4)	1818(7)	45(5)
C(33A)	2716(7)	2600(5)	1995(7)	75(7)
C(34A)	2870(6)	2731(5)	2459(8)	85(8)
C(35A)	2576(6)	2777(5)	2721(6)	65(7)

N(41A)	490(5)	1778(3)	-108(4)	43(4)
N(42A)	304(4)	2142(3)	382(5)	37(4)
C(41A)	1062(6)	2039(4)	426(7)	49(5)
C(42A)	922(6)	1817(4)	91(6)	36(4)
C(43A)	176(5)	1929(4)	12(6)	34(5)
C(44A)	715(6)	2201(4)	578(6)	51(5)
C(45A)	-280(6)	1880(4)	-214(6)	49(5)
C(11B)	1415(6)	609(5)	484(6)	61(6)
C(12B)	1499(6)	327(4)	720(6)	52(5)
C(13B)	1907(6)	205(4)	844(6)	50(5)
C(14B)	2225(5)	343(4)	696(6)	40(5)
C(15B)	2165(7)	611(4)	452(6)	52(6)
C(16B)	1776(6)	753(4)	362(6)	50(5)
N(21B)	456(5)	1118(3)	-73(5)	47(4)
C(21B)	813(7)	988(4)	6(6)	55(6)
C(22B)	992(6)	779(4)	406(6)	51(6)
C(23B)	748(6)	737(4)	745(8)	65(7)
C(24B)	391(7)	879(4)	644(6)	65(6)
C(25B)	194(6)	1081(4)	220(7)	62(6)
N(31B)	2438(5)	-362(3)	1807(5)	51(4)
C(31B)	2363(7)	-126(4)	1529(6)	51(6)
C(32B)	2004(7)	-84(4)	1133(8)	60(7)
C(33B)	1704(8)	-311(5)	996(7)	84(8)
C(34B)	1777(7)	-570(5)	1266(8)	77(7)
C(35B)	2135(7)	-601(4)	1671(7)	54(6)
N(41B)	2773(5)	1098(3)	-210(5)	51(4)
N(42B)	3319(5)	850(3)	436(5)	50(4)
C(41B)	2515(6)	775(4)	301(6)	48(5)
C(42B)	2955(8)	721(4)	542(7)	66(7)
C(43B)	3198(6)	1043(4)	30(6)	43(5)
C(44B)	2438(7)	973(4)	-93(6)	54(6)
C(45B)	3565(5)	1170(4)	-123(6)	46(5)
C(11C)	3354(8)	1183(4)	2404(7)	81(7)
C(12C)	3424(7)	1366(4)	2811(6)	68(7)
C(13C)	3274(6)	1295(4)	3200(7)	54(6)
C(14C)	3062(7)	1037(4)	3219(6)	60(6)
C(15C)	3011(8)	824(4)	2827(7)	81(8)
C(16C)	3158(9)	887(4)	2413(7)	98(9)
N(21C)	3813(5)	1120(2)	1309(4)	77(6)
C(21C)	3667(5)	1044(2)	1716(4)	83(8)
C(22C)	3482(5)	1265(3)	1948(4)	72(6)
C(23C)	3444(5)	1561(3)	1774(6)	126(11)
C(24C)	3591(6)	1638(2)	1368(6)	131(10)
C(25C)	3775(6)	1417(3)	1135(5)	560(30)
N(31C)	2990(5)	1763(3)	4179(5)	50(4)
C(31C)	2967(6)	1568(4)	3821(6)	42(5)

C(32C)	3295(7)	1524(4)	3619(6)	59(6)
C(33C)	3708(7)	1689(4)	3817(8)	77(7)
C(34C)	3736(7)	1899(4)	4211(7)	76(7)
C(35C)	3356(7)	1922(4)	4351(7)	60(7)
N(41C)	2744(5)	-10(3)	2713(5)	53(5)
N(42C)	2328(5)	204(3)	3176(5)	56(5)
C(41C)	2794(7)	523(4)	2837(7)	67(7)
C(42C)	2914(7)	246(4)	2649(6)	70(7)
C(43C)	2435(7)	-42(4)	2962(7)	72(7)
C(44C)	2529(7)	489(4)	3127(6)	66(7)
C(45C)	2278(7)	-324(3)	3052(7)	70(7)
C(11D)	435(6)	1508(4)	2091(6)	45(5)
C(12D)	495(6)	1195(5)	2163(6)	59(7)
C(13D)	848(7)	1094(4)	2523(7)	63(7)
C(14D)	1173(6)	1274(4)	2846(6)	48(5)
C(15D)	1113(6)	1600(4)	2740(6)	48(5)
C(16D)	742(6)	1701(4)	2396(6)	46(5)
N(21D)	-219(5)	1976(3)	1050(5)	51(4)
C(21D)	119(6)	1871(4)	1430(6)	54(6)
C(22D)	92(6)	1616(4)	1690(7)	57(6)
C(23D)	-291(8)	1471(4)	1551(7)	81(8)
C(24D)	-681(8)	1575(5)	1141(7)	81(8)
C(25D)	-626(7)	1864(5)	911(7)	79(8)
N(31D)	1395(5)	344(4)	3090(5)	64(5)
C(31D)	1321(7)	634(4)	2973(6)	50(6)
C(32D)	930(7)	753(5)	2672(7)	65(7)
C(33D)	576(7)	548(4)	2473(8)	75(7)
C(34D)	689(9)	227(5)	2615(12)	131(16)
C(35D)	1049(8)	135(5)	2901(10)	101(12)
N(41D)	1762(5)	2307(3)	3183(5)	44(4)
N(42D)	2065(4)	1933(3)	3803(5)	41(4)
C(41D)	1448(6)	1804(4)	3064(6)	43(5)
C(42D)	1489(6)	2114(4)	2926(6)	46(5)
C(43D)	2071(7)	2233(4)	3619(6)	60(7)
C(44D)	1742(6)	1733(4)	3528(6)	50(6)
C(45D)	2424(6)	2436(4)	3941(6)	51(5)
N(1A)	3503(6)	-399(3)	2969(6)	76(6)
N(2A)	3216(6)	-740(3)	2156(6)	69(5)
C(1A)	3777(9)	-636(9)	2923(11)	175(16)
C(2A)	3639(11)	-780(8)	2430(14)	181(17)
N(1B)	4542(7)	712(5)	1344(8)	116(8)
N(2B)	4113(6)	445(4)	510(6)	85(6)
C(1B)	4787(9)	521(8)	1102(14)	153(18)
C(2B)	4524(14)	293(8)	826(12)	190(20)
N(1C)	2444(8)	101(4)	4236(8)	127(9)
N(2C)	1571(7)	206(4)	4133(7)	109(8)

C(1C)	2297(11)	92(10)	4661(9)	210(20)
C(2C)	1872(12)	154(7)	4608(11)	159(17)
N(1D)	152(5)	1709(3)	-1225(5)	55(5)
N(2D)	113(5)	1097(3)	-1159(5)	57(4)
C(1D)	121(8)	1534(4)	-1685(6)	75(7)
C(2D)	-110(10)	1256(5)	-1655(8)	113(10)
N(1E)	-540(5)	2613(4)	947(5)	62(5)
N(2E)	-58(5)	2755(4)	339(5)	76(5)
C(1E)	-608(8)	2903(7)	727(10)	122(12)
C(2E)	-298(9)	2995(5)	546(9)	109(10)
N(1F)	2492(5)	1675(3)	-1394(5)	55(4)
N(2F)	2510(5)	1079(3)	-1294(4)	48(4)
C(1F)	2276(8)	1489(5)	-1847(7)	80(7)
C(2F)	2507(8)	1193(4)	-1798(7)	86(8)
N(1G)	2898(5)	1665(3)	5126(5)	53(4)
N(2G)	2012(5)	1802(3)	4809(5)	53(4)
C(1G)	2618(7)	1592(4)	5443(7)	68(6)
C(2G)	2257(7)	1788(4)	5363(6)	68(6)
N(1H)	1658(5)	3176(3)	2743(5)	64(5)
N(2H)	1272(5)	2833(3)	3281(5)	57(4)
C(1H)	1292(10)	3311(5)	2877(11)	124(11)
C(2H)	1200(8)	3158(5)	3269(8)	84(8)
O(1W)	6041(6)	3686(4)	2932(7)	150(7)
O(2W)	3866(5)	2162(4)	2698(6)	108(5)
O(3W)	9206(5)	1916(3)	8428(5)	91(5)
O(4W)	4022(4)	2498(3)	3564(5)	77(4)
O(5W)	4126(5)	2113(3)	-390(5)	95(5)
O(6W)	3121(5)	2912(4)	1115(6)	109(5)
O(7W)	6301(9)	2477(6)	3339(10)	221(11)
O(8W)	559(5)	720(3)	5956(6)	107(5)
O(9W)	5250(17)	5031(11)	1161(19)	460(30)
O(10W)	13490(10)	-1175(7)	9924(11)	255(13)
O(11W)	12922(10)	-724(7)	10994(11)	268(14)
O(12W)	7783(10)	824(7)	9640(11)	265(13)
O(13W)	11441(10)	-1234(7)	9792(11)	272(14)
O(14W)	5634(8)	4193(5)	3218(9)	199(10)
O(15W)	888(5)	1190(4)	5498(6)	117(6)
O(16W)	10168(10)	3203(6)	11886(10)	244(12)
O(17W)	5924(7)	3123(5)	2575(8)	169(8)
O(18W)	10334(6)	-700(4)	8580(6)	125(6)
O(19W)	1347(6)	1642(4)	6091(6)	129(6)
O(20W)	6430(7)	3970(5)	2303(7)	163(8)
O(21W)	5930(6)	4450(4)	1927(6)	117(6)
O(22W)	4745(5)	2245(3)	4227(6)	32(4)
O(23W)	4210(7)	1854(4)	495(7)	72(6)
O(24W)	11325(15)	-710(11)	9816(17)	410(20)

O(25W)	5552(14)	659(9)	5351(15)	370(20)
C(101)	13656(12)	-1147(8)	11135(13)	192(15)
C(102)	4438(19)	5210(13)	1060(20)	330(30)
C(103)	9958(10)	385(7)	8002(11)	144(11)
C(104)	13530(20)	-142(17)	10300(30)	430(40)
C(105)	9881(14)	3720(10)	11269(16)	241(19)
C(106)	5595(13)	1163(9)	5774(14)	203(16)
C(107)	5000(16)	1639(11)	4132(17)	270(20)
C(108)	4452(11)	1669(8)	2862(13)	176(13)
C(109)	13740(20)	-361(14)	8910(20)	370(30)
C(110)	14180(13)	574(9)	12695(15)	206(16)
C(111)	5042(14)	2511(9)	2146(14)	219

Table 3. Bond lengths [Å] and angles [°] for bk81n.

Pd(1)-N(1A)	1.903(19)	N(300)-O(303)	1.268(18)
Pd(1)-N(2A)	1.996(19)	N(400)-O(402)	1.19(2)
Pd(1)-N(31B)	2.019(16)	N(400)-O(401)	1.25(2)
Pd(1)-N(41C)	2.050(15)	N(400)-O(403)	1.31(2)
Pd(2)-N(1B)	1.95(3)	N(500)-O(501)	1.183(18)
Pd(2)-N(2B)	1.988(18)	N(500)-O(503)	1.247(18)
Pd(2)-N(21C)	2.016(9)	N(500)-O(502)	1.279(19)
Pd(2)-N(42B)	2.034(16)	N(600)-O(601)	1.19(2)
Pd(3)-N(1C)	2.00(2)	N(600)-O(602)	1.24(2)
Pd(3)-N(31D)	2.008(16)	N(600)-O(603)	1.22(2)
Pd(3)-N(2C)	2.037(17)	N(700)-O(702)	1.16(2)
Pd(3)-N(42C)	2.042(15)	N(700)-O(703)	1.21(2)
Pd(4)-N(1D)	1.996(13)	N(700)-O(701)	1.23(2)
Pd(4)-N(2D)	2.014(13)	N(800)-O(802)	1.14(2)
Pd(4)-N(21B)	2.044(15)	N(800)-O(803)	1.18(2)
Pd(4)-N(41A)	2.113(14)	N(800)-O(801)	1.23(2)
Pd(5)-N(2E)	2.015(16)	N(900)-O(903)	1.23(2)
Pd(5)-N(1E)	2.010(16)	N(900)-O(901)	1.24(2)
Pd(5)-N(42A)	2.035(14)	N(900)-O(902)	1.25(3)
Pd(5)-N(21D)	2.066(15)	N(110)-O(112)	1.15(5)
Pd(6)-N(2F)	1.953(13)	N(110)-O(113)	1.18(5)
Pd(6)-N(21A)	1.993(15)	N(110)-O(111)	1.57(5)
Pd(6)-N(1F)	1.995(13)	N(120)-O(122)	1.165(17)
Pd(6)-N(41B)	2.070(16)	N(120)-O(121)	1.21(2)
Pd(7)-N(31C)	1.978(17)	N(120)-O(123)	1.345(18)
Pd(7)-N(2G)	2.005(14)	N(130)-O(132)	1.20(2)
Pd(7)-N(1G)	2.010(15)	N(130)-O(131)	1.23(2)
Pd(7)-N(42D)	2.016(15)	N(130)-O(133)	1.42(2)
Pd(8)-N(1H)	1.988(15)	O(133)-N(130)#1	1.42(2)
Pd(8)-N(2H)	1.978(15)	N(150)-O(151)	1.21(2)
Pd(8)-N(41D)	2.027(14)	N(150)-O(152)	1.20(2)
Pd(8)-N(31A)	2.035(13)	N(150)-O(153)	1.404(19)
C(1)-Br(2)	1.89(2)	N(140)-O(141)	1.10(3)
C(1)-Br(3)	1.90(3)	N(140)-O(143)	1.16(3)
C(1)-Br(1)	1.94(2)	N(140)-O(142)	1.26(3)
C(1)-Br(4)	1.93(2)	C(11A)-C(12A)	1.37(2)
N(100)-O(101)	1.16(3)	C(11A)-C(16A)	1.40(2)
N(100)-O(102)	1.29(4)	C(11A)-C(22A)	1.48(2)
N(100)-O(103)	1.32(5)	C(12A)-C(13A)	1.44(2)
N(200)-O(203)	1.22(2)	C(13A)-C(14A)	1.33(2)
N(200)-O(201)	1.25(2)	C(13A)-C(32A)	1.51(2)
N(200)-O(202)	1.25(2)	C(14A)-C(15A)	1.46(2)
N(300)-O(302)	1.194(19)	C(15A)-C(16A)	1.37(2)
N(300)-O(301)	1.250(18)	C(15A)-C(41A)	1.41(2)

N(21A)-C(25A)	1.27(2)	C(43B)-C(45B)	1.46(2)
N(21A)-C(21A)	1.346(19)	C(11C)-C(12C)	1.36(2)
C(21A)-C(22A)	1.42(2)	C(11C)-C(16C)	1.45(2)
C(22A)-C(23A)	1.35(2)	C(11C)-C(22C)	1.49(2)
C(23A)-C(24A)	1.42(2)	C(12C)-C(13C)	1.35(2)
C(24A)-C(25A)	1.44(2)	C(13C)-C(14C)	1.33(2)
N(31A)-C(35A)	1.26(2)	C(13C)-C(32C)	1.53(2)
N(31A)-C(31A)	1.34(2)	C(14C)-C(15C)	1.42(2)
C(31A)-C(32A)	1.37(2)	C(15C)-C(16C)	1.40(2)
C(32A)-C(33A)	1.32(2)	C(15C)-C(41C)	1.49(3)
C(33A)-C(34A)	1.37(3)	N(21C)-C(21C)	1.3900
C(34A)-C(35A)	1.35(2)	N(21C)-C(25C)	1.3900
N(41A)-C(43A)	1.32(2)	C(21C)-C(22C)	1.3900
N(41A)-C(42A)	1.32(2)	C(22C)-C(23C)	1.3900
N(42A)-C(44A)	1.27(2)	C(23C)-C(24C)	1.3900
N(42A)-C(43A)	1.37(2)	C(24C)-C(25C)	1.3900
C(41A)-C(42A)	1.34(2)	N(31C)-C(35C)	1.31(2)
C(41A)-C(44A)	1.47(2)	N(31C)-C(31C)	1.31(2)
C(43A)-C(45A)	1.40(2)	C(31C)-C(32C)	1.33(2)
C(11B)-C(12B)	1.40(2)	C(32C)-C(33C)	1.45(3)
C(11B)-C(16B)	1.43(2)	C(33C)-C(34C)	1.42(3)
C(11B)-C(22B)	1.49(3)	C(34C)-C(35C)	1.37(3)
C(12B)-C(13B)	1.34(2)	N(41C)-C(42C)	1.29(2)
C(13B)-C(14B)	1.34(2)	N(41C)-C(43C)	1.36(2)
C(13B)-C(32B)	1.49(3)	N(42C)-C(43C)	1.33(2)
C(14B)-C(15B)	1.35(2)	N(42C)-C(44C)	1.43(2)
C(15B)-C(16B)	1.33(2)	C(41C)-C(44C)	1.33(2)
C(15B)-C(41B)	1.48(3)	C(41C)-C(42C)	1.43(2)
N(21B)-C(21B)	1.22(2)	C(43C)-C(45C)	1.39(2)
N(21B)-C(25B)	1.34(2)	C(11D)-C(16D)	1.38(2)
C(21B)-C(22B)	1.43(2)	C(11D)-C(22D)	1.39(3)
C(22B)-C(23B)	1.40(2)	C(11D)-C(12D)	1.40(3)
C(23B)-C(24B)	1.24(2)	C(12D)-C(13D)	1.33(3)
C(24B)-C(25B)	1.47(2)	C(13D)-C(14D)	1.40(3)
N(31B)-C(31B)	1.28(2)	C(13D)-C(32D)	1.56(3)
N(31B)-C(35B)	1.40(2)	C(14D)-C(15D)	1.47(2)
C(31B)-C(32B)	1.34(3)	C(15D)-C(16D)	1.35(2)
C(32B)-C(33B)	1.35(3)	C(15D)-C(41D)	1.48(2)
C(33B)-C(34B)	1.35(3)	N(21D)-C(25D)	1.32(2)
C(34B)-C(35B)	1.35(3)	N(21D)-C(21D)	1.34(2)
N(41B)-C(44B)	1.31(2)	C(21D)-C(22D)	1.36(2)
N(41B)-C(43B)	1.33(2)	C(22D)-C(23D)	1.32(3)
N(42B)-C(43B)	1.38(2)	C(23D)-C(24D)	1.48(3)
N(42B)-C(42B)	1.39(2)	C(24D)-C(25D)	1.46(3)
C(41B)-C(44B)	1.37(2)	N(31D)-C(31D)	1.32(2)
C(41B)-C(42B)	1.37(3)	N(31D)-C(35D)	1.40(3)

C(31D)-C(32D)	1.37(3)	N(2B)-Pd(2)-N(42B)	97.7(6)
C(32D)-C(33D)	1.41(3)	N(21C)-Pd(2)-N(42B)	85.5(6)
C(33D)-C(34D)	1.48(4)	N(1C)-Pd(3)-N(31D)	172.8(7)
C(34D)-C(35D)	1.24(4)	N(1C)-Pd(3)-N(2C)	84.3(9)
N(41D)-C(42D)	1.272(19)	N(31D)-Pd(3)-N(2C)	90.4(8)
N(41D)-C(43D)	1.36(2)	N(1C)-Pd(3)-N(42C)	92.2(7)
N(42D)-C(44D)	1.39(2)	N(31D)-Pd(3)-N(42C)	93.0(6)
N(42D)-C(43D)	1.42(2)	N(2C)-Pd(3)-N(42C)	176.2(8)
C(41D)-C(44D)	1.39(2)	N(1D)-Pd(4)-N(2D)	85.1(6)
C(41D)-C(42D)	1.43(2)	N(1D)-Pd(4)-N(21B)	174.9(6)
C(43D)-C(45D)	1.50(3)	N(2D)-Pd(4)-N(21B)	91.5(6)
N(1A)-C(1A)	1.38(4)	N(1D)-Pd(4)-N(41A)	94.0(5)
N(2A)-C(2A)	1.34(4)	N(2D)-Pd(4)-N(41A)	177.7(6)
C(1A)-C(2A)	1.46(4)	N(21B)-Pd(4)-N(41A)	89.2(5)
N(1B)-C(1B)	1.44(5)	N(2E)-Pd(5)-N(1E)	83.0(7)
N(2B)-C(2B)	1.49(4)	N(2E)-Pd(5)-N(42A)	92.5(6)
C(1B)-C(2B)	1.39(5)	N(1E)-Pd(5)-N(42A)	175.5(6)
N(1C)-C(1C)	1.40(3)	N(2E)-Pd(5)-N(21D)	176.4(6)
N(2C)-C(2C)	1.40(4)	N(1E)-Pd(5)-N(21D)	93.5(6)
C(1C)-C(2C)	1.33(4)	N(42A)-Pd(5)-N(21D)	91.0(5)
N(1D)-C(1D)	1.48(2)	N(2F)-Pd(6)-N(21A)	175.8(5)
N(2D)-C(2D)	1.53(2)	N(2F)-Pd(6)-N(1F)	84.1(6)
C(1D)-C(2D)	1.44(3)	N(21A)-Pd(6)-N(1F)	91.8(6)
N(1E)-C(1E)	1.41(3)	N(2F)-Pd(6)-N(41B)	92.1(5)
N(2E)-C(2E)	1.51(2)	N(21A)-Pd(6)-N(41B)	92.0(6)
C(1E)-C(2E)	1.29(3)	N(1F)-Pd(6)-N(41B)	175.6(6)
N(1F)-C(1F)	1.49(2)	N(31C)-Pd(7)-N(2G)	173.8(6)
N(2F)-C(2F)	1.49(2)	N(31C)-Pd(7)-N(1G)	88.6(6)
C(1F)-C(2F)	1.48(3)	N(2G)-Pd(7)-N(1G)	85.6(6)
N(1G)-C(1G)	1.46(2)	N(31C)-Pd(7)-N(42D)	92.4(6)
N(2G)-C(2G)	1.51(2)	N(2G)-Pd(7)-N(42D)	93.5(5)
C(1G)-C(2G)	1.39(3)	N(1G)-Pd(7)-N(42D)	178.9(6)
N(1H)-C(1H)	1.44(3)	N(1H)-Pd(8)-N(2H)	84.5(6)
N(2H)-C(2H)	1.45(2)	N(1H)-Pd(8)-N(41D)	174.9(5)
C(1H)-C(2H)	1.39(3)	N(2H)-Pd(8)-N(41D)	90.5(6)
		N(1H)-Pd(8)-N(31A)	91.8(6)
N(1A)-Pd(1)-N(2A)	85.7(7)	N(2H)-Pd(8)-N(31A)	176.2(6)
N(1A)-Pd(1)-N(31B)	176.1(6)	N(41D)-Pd(8)-N(31A)	93.2(5)
N(2A)-Pd(1)-N(31B)	91.7(6)	Br(2)-C(1)-Br(3)	112.2(14)
N(1A)-Pd(1)-N(41C)	92.3(6)	Br(2)-C(1)-Br(1)	107.1(10)
N(2A)-Pd(1)-N(41C)	178.0(7)	Br(3)-C(1)-Br(1)	108.4(11)
N(31B)-Pd(1)-N(41C)	90.3(6)	Br(2)-C(1)-Br(4)	110.6(11)
N(1B)-Pd(2)-N(2B)	82.9(10)	Br(3)-C(1)-Br(4)	109.3(10)
N(1B)-Pd(2)-N(21C)	93.9(8)	Br(1)-C(1)-Br(4)	109.2(13)
N(2B)-Pd(2)-N(21C)	176.7(7)	O(101)-N(100)-O(102)	115(5)
N(1B)-Pd(2)-N(42B)	177.8(7)	O(101)-N(100)-O(103)	131(5)

O(102)-N(100)-O(103)	114(3)	C(14A)-C(13A)-C(32A)	122.7(16)
O(203)-N(200)-O(201)	117(2)	C(12A)-C(13A)-C(32A)	120.1(17)
O(203)-N(200)-O(202)	125(2)	C(13A)-C(14A)-C(15A)	127.8(16)
O(201)-N(200)-O(202)	118(2)	C(16A)-C(15A)-C(41A)	123.5(17)
O(302)-N(300)-O(301)	123(2)	C(16A)-C(15A)-C(14A)	110.8(17)
O(302)-N(300)-O(303)	121(2)	C(41A)-C(15A)-C(14A)	125.7(16)
O(301)-N(300)-O(303)	116(2)	C(15A)-C(16A)-C(11A)	124.6(16)
O(402)-N(400)-O(401)	126(3)	C(25A)-N(21A)-C(21A)	117.8(16)
O(402)-N(400)-O(403)	121(3)	C(25A)-N(21A)-Pd(6)	121.2(13)
O(401)-N(400)-O(403)	112(2)	C(21A)-N(21A)-Pd(6)	121.0(12)
O(501)-N(500)-O(503)	123(2)	N(21A)-C(21A)-C(22A)	121.7(17)
O(501)-N(500)-O(502)	120.3(19)	C(23A)-C(22A)-C(21A)	120.8(17)
O(503)-N(500)-O(502)	116.6(18)	C(23A)-C(22A)-C(11A)	121.5(17)
O(601)-N(600)-O(602)	120(2)	C(21A)-C(22A)-C(11A)	117.2(17)
O(601)-N(600)-O(603)	123(2)	C(22A)-C(23A)-C(24A)	117.6(17)
O(602)-N(600)-O(603)	117(2)	C(23A)-C(24A)-C(25A)	116.2(18)
O(702)-N(700)-O(703)	125(2)	N(21A)-C(25A)-C(24A)	125.5(17)
O(702)-N(700)-O(701)	116(3)	C(35A)-N(31A)-C(31A)	119.7(16)
O(703)-N(700)-O(701)	119(2)	C(35A)-N(31A)-Pd(8)	122.6(15)
O(802)-N(800)-O(803)	123(3)	C(31A)-N(31A)-Pd(8)	117.6(14)
O(802)-N(800)-O(801)	113(3)	N(31A)-C(31A)-C(32A)	124.1(19)
O(803)-N(800)-O(801)	124(3)	C(33A)-C(32A)-C(31A)	114(2)
O(903)-N(900)-O(901)	119(3)	C(33A)-C(32A)-C(13A)	123.3(18)
O(903)-N(900)-O(902)	122(3)	C(31A)-C(32A)-C(13A)	123.0(18)
O(901)-N(900)-O(902)	120(2)	C(32A)-C(33A)-C(34A)	123(2)
O(112)-N(110)-O(113)	134(6)	C(35A)-C(34A)-C(33A)	118.1(19)
O(112)-N(110)-O(111)	120(5)	N(31A)-C(35A)-C(34A)	120.9(19)
O(113)-N(110)-O(111)	106(4)	C(43A)-N(41A)-C(42A)	125.7(17)
O(122)-N(120)-O(121)	128(2)	C(43A)-N(41A)-Pd(4)	117.3(13)
O(122)-N(120)-O(123)	129.9(19)	C(42A)-N(41A)-Pd(4)	116.9(14)
O(121)-N(120)-O(123)	101.6(19)	C(44A)-N(42A)-C(43A)	120.0(16)
O(132)-N(130)-O(131)	125(3)	C(44A)-N(42A)-Pd(5)	116.2(14)
O(132)-N(130)-O(133)	123(3)	C(43A)-N(42A)-Pd(5)	123.7(13)
O(131)-N(130)-O(133)	109(2)	C(42A)-C(41A)-C(15A)	122.1(19)
N(130)-O(133)-N(130)#1	119(3)	C(42A)-C(41A)-C(44A)	116.3(18)
O(151)-N(150)-O(152)	135(3)	C(15A)-C(41A)-C(44A)	121.7(17)
O(151)-N(150)-O(153)	95(2)	N(41A)-C(42A)-C(41A)	118.3(19)
O(152)-N(150)-O(153)	109(2)	N(41A)-C(43A)-N(42A)	117.9(17)
O(141)-N(140)-O(143)	123(3)	N(41A)-C(43A)-C(45A)	123.3(17)
O(141)-N(140)-O(142)	129(3)	N(42A)-C(43A)-C(45A)	118.8(17)
O(143)-N(140)-O(142)	103(3)	N(42A)-C(44A)-C(41A)	121.5(17)
C(12A)-C(11A)-C(16A)	120.6(15)	C(12B)-C(11B)-C(16B)	117(2)
C(12A)-C(11A)-C(22A)	117.5(18)	C(12B)-C(11B)-C(22B)	123.6(19)
C(16A)-C(11A)-C(22A)	121.6(16)	C(16B)-C(11B)-C(22B)	119(2)
C(11A)-C(12A)-C(13A)	118.9(17)	C(13B)-C(12B)-C(11B)	120.8(19)
C(14A)-C(13A)-C(12A)	116.4(17)	C(12B)-C(13B)-C(14B)	119(2)

C(12B)-C(13B)-C(32B)	121(2)	C(14C)-C(13C)-C(32C)	116(2)
C(14B)-C(13B)-C(32B)	120(2)	C(12C)-C(13C)-C(32C)	121.3(17)
C(15B)-C(14B)-C(13B)	123.4(19)	C(13C)-C(14C)-C(15C)	118.7(18)
C(14B)-C(15B)-C(16B)	119(2)	C(16C)-C(15C)-C(14C)	121.3(18)
C(14B)-C(15B)-C(41B)	125(2)	C(16C)-C(15C)-C(41C)	117.2(18)
C(16B)-C(15B)-C(41B)	115.9(19)	C(14C)-C(15C)-C(41C)	121.5(18)
C(15B)-C(16B)-C(11B)	120(2)	C(11C)-C(16C)-C(15C)	116.3(18)
C(21B)-N(21B)-C(25B)	122.2(19)	C(21C)-N(21C)-C(25C)	120.0
C(21B)-N(21B)-Pd(4)	118.1(14)	C(21C)-N(21C)-Pd(2)	118.4(8)
C(25B)-N(21B)-Pd(4)	119.5(15)	C(25C)-N(21C)-Pd(2)	120.2(8)
N(21B)-C(21B)-C(22B)	125(2)	C(22C)-C(21C)-N(21C)	120.0
C(23B)-C(22B)-C(21B)	116.6(19)	C(21C)-C(22C)-C(23C)	120.0
C(23B)-C(22B)-C(11B)	118.7(19)	C(21C)-C(22C)-C(11C)	119.1(13)
C(21B)-C(22B)-C(11B)	124.7(17)	C(23C)-C(22C)-C(11C)	120.8(13)
C(24B)-C(23B)-C(22B)	115(2)	C(22C)-C(23C)-C(24C)	120.0
C(23B)-C(24B)-C(25B)	129(2)	C(23C)-C(24C)-C(25C)	120.0
N(21B)-C(25B)-C(24B)	112.5(18)	C(24C)-C(25C)-N(21C)	120.0
C(31B)-N(31B)-C(35B)	117.5(17)	C(35C)-N(31C)-C(31C)	118.6(18)
C(31B)-N(31B)-Pd(1)	120.4(15)	C(35C)-N(31C)-Pd(7)	122.2(14)
C(35B)-N(31B)-Pd(1)	122.1(14)	C(31C)-N(31C)-Pd(7)	119.2(14)
N(31B)-C(31B)-C(32B)	125(2)	N(31C)-C(31C)-C(32C)	123.3(19)
C(31B)-C(32B)-C(33B)	118(2)	C(31C)-C(32C)-C(33C)	118.8(19)
C(31B)-C(32B)-C(13B)	124(2)	C(31C)-C(32C)-C(13C)	124(2)
C(33B)-C(32B)-C(13B)	118(2)	C(33C)-C(32C)-C(13C)	117(2)
C(32B)-C(33B)-C(34B)	119(2)	C(34C)-C(33C)-C(32C)	118(2)
C(35B)-C(34B)-C(33B)	121(2)	C(35C)-C(34C)-C(33C)	114(2)
C(34B)-C(35B)-N(31B)	119.2(18)	N(31C)-C(35C)-C(34C)	126.9(19)
C(44B)-N(41B)-C(43B)	123.9(18)	C(42C)-N(41C)-C(43C)	123.3(18)
C(44B)-N(41B)-Pd(6)	119.5(14)	C(42C)-N(41C)-Pd(1)	115.8(14)
C(43B)-N(41B)-Pd(6)	116.6(15)	C(43C)-N(41C)-Pd(1)	120.9(13)
C(43B)-N(42B)-C(42B)	112.8(18)	C(43C)-N(42C)-C(44C)	119.7(17)
C(43B)-N(42B)-Pd(2)	125.8(14)	C(43C)-N(42C)-Pd(3)	124.4(14)
C(42B)-N(42B)-Pd(2)	121.2(15)	C(44C)-N(42C)-Pd(3)	115.7(12)
C(44B)-C(41B)-C(42B)	115(2)	C(44C)-C(41C)-C(42C)	114.0(19)
C(44B)-C(41B)-C(15B)	125(2)	C(44C)-C(41C)-C(15C)	119(2)
C(42B)-C(41B)-C(15B)	120.2(19)	C(42C)-C(41C)-C(15C)	126(2)
N(42B)-C(42B)-C(41B)	127(2)	N(41C)-C(42C)-C(41C)	122.6(19)
N(41B)-C(43B)-N(42B)	121.4(17)	N(42C)-C(43C)-N(41C)	117.6(19)
N(41B)-C(43B)-C(45B)	123(2)	N(42C)-C(43C)-C(45C)	120.0(18)
N(42B)-C(43B)-C(45B)	115.5(18)	N(41C)-C(43C)-C(45C)	122(2)
N(41B)-C(44B)-C(41B)	120(2)	C(41C)-C(44C)-N(42C)	122.2(17)
C(12C)-C(11C)-C(16C)	119.0(18)	C(16D)-C(11D)-C(22D)	121(2)
C(12C)-C(11C)-C(22C)	123.6(18)	C(16D)-C(11D)-C(12D)	119(2)
C(16C)-C(11C)-C(22C)	117.4(18)	C(22D)-C(11D)-C(12D)	120(2)
C(13C)-C(12C)-C(11C)	122.0(19)	C(13D)-C(12D)-C(11D)	119(2)
C(14C)-C(13C)-C(12C)	122.1(18)	C(12D)-C(13D)-C(14D)	126(2)

C(12D)-C(13D)-C(32D)	124(2)	N(41D)-C(43D)-N(42D)	117.9(19)
C(14D)-C(13D)-C(32D)	110(2)	N(41D)-C(43D)-C(45D)	126.9(17)
C(13D)-C(14D)-C(15D)	114(2)	N(42D)-C(43D)-C(45D)	115.2(18)
C(16D)-C(15D)-C(14D)	120.0(19)	C(41D)-C(44D)-N(42D)	123.2(17)
C(16D)-C(15D)-C(41D)	123.1(17)	C(1A)-N(1A)-Pd(1)	112.2(18)
C(14D)-C(15D)-C(41D)	116.6(19)	C(2A)-N(2A)-Pd(1)	108.5(19)
C(15D)-C(16D)-C(11D)	122(2)	C(2A)-C(1A)-N(1A)	113(3)
C(25D)-N(21D)-C(21D)	125.1(18)	N(2A)-C(2A)-C(1A)	117(3)
C(25D)-N(21D)-Pd(5)	115.4(15)	C(1B)-N(1B)-Pd(2)	109(2)
C(21D)-N(21D)-Pd(5)	119.4(14)	C(2B)-N(2B)-Pd(2)	109.8(19)
N(21D)-C(21D)-C(22D)	123.4(19)	C(2B)-C(1B)-N(1B)	112(4)
C(23D)-C(22D)-C(21D)	116(2)	C(1B)-C(2B)-N(2B)	106(3)
C(23D)-C(22D)-C(11D)	120(2)	C(1C)-N(1C)-Pd(3)	109(2)
C(21D)-C(22D)-C(11D)	124(2)	C(2C)-N(2C)-Pd(3)	107.0(19)
C(22D)-C(23D)-C(24D)	124(2)	C(2C)-C(1C)-N(1C)	118(3)
C(25D)-C(24D)-C(23D)	116(2)	C(1C)-C(2C)-N(2C)	121(3)
N(21D)-C(25D)-C(24D)	115(2)	C(1D)-N(1D)-Pd(4)	109.4(10)
C(31D)-N(31D)-C(35D)	119(2)	C(2D)-N(2D)-Pd(4)	105.9(12)
C(31D)-N(31D)-Pd(3)	122.3(17)	C(2D)-C(1D)-N(1D)	107.3(16)
C(35D)-N(31D)-Pd(3)	118(2)	C(1D)-C(2D)-N(2D)	110(2)
N(31D)-C(31D)-C(32D)	125(2)	C(1E)-N(1E)-Pd(5)	111.4(14)
C(31D)-C(32D)-C(33D)	117(2)	C(2E)-N(2E)-Pd(5)	106.7(14)
C(31D)-C(32D)-C(13D)	125(2)	C(2E)-C(1E)-N(1E)	115(2)
C(33D)-C(32D)-C(13D)	118(2)	C(1E)-C(2E)-N(2E)	117(2)
C(32D)-C(33D)-C(34D)	114(2)	C(1F)-N(1F)-Pd(6)	108.6(11)
C(35D)-C(34D)-C(33D)	126(4)	C(2F)-N(2F)-Pd(6)	111.2(11)
C(34D)-C(35D)-N(31D)	119(4)	N(1F)-C(1F)-C(2F)	108.5(18)
C(42D)-N(41D)-C(43D)	122.1(17)	N(2F)-C(2F)-C(1F)	104.6(16)
C(42D)-N(41D)-Pd(8)	118.9(14)	C(1G)-N(1G)-Pd(7)	106.7(12)
C(43D)-N(41D)-Pd(8)	118.9(12)	C(2G)-N(2G)-Pd(7)	105.8(12)
C(44D)-N(42D)-C(43D)	118.4(17)	C(2G)-C(1G)-N(1G)	111.9(16)
C(44D)-N(42D)-Pd(7)	119.3(13)	C(1G)-C(2G)-N(2G)	109.4(16)
C(43D)-N(42D)-Pd(7)	122.2(14)	C(1H)-N(1H)-Pd(8)	110.7(13)
C(44D)-C(41D)-C(42D)	112.4(17)	C(2H)-N(2H)-Pd(8)	108.8(12)
C(44D)-C(41D)-C(15D)	126.3(18)	C(2H)-C(1H)-N(1H)	112(2)
C(42D)-C(41D)-C(15D)	121.3(17)	C(1H)-C(2H)-N(2H)	115.4(18)
N(41D)-C(42D)-C(41D)	125.7(18)		

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for bk81n. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	114(2)	28(1)	54(1)	-3(1)	29(1)	0(1)
Pd(2)	74(1)	75(1)	43(1)	3(1)	21(1)	5(1)
Pd(3)	162(2)	39(1)	76(1)	10(1)	73(1)	-1(1)
Pd(4)	59(1)	48(1)	34(1)	-1(1)	11(1)	-7(1)
Pd(5)	59(1)	62(1)	41(1)	-11(1)	23(1)	-4(1)
Pd(6)	69(1)	44(1)	37(1)	1(1)	23(1)	1(1)
Pd(7)	73(1)	32(1)	33(1)	-5(1)	19(1)	-1(1)
Pd(8)	71(1)	36(1)	39(1)	-2(1)	24(1)	-4(1)
C(1)	130(20)	48(14)	130(20)	47(14)	89(18)	69(14)
Br(1)	131(3)	64(2)	144(3)	20(2)	52(2)	12(2)
Br(2)	208(4)	79(2)	177(3)	-17(2)	132(3)	10(2)
Br(3)	143(3)	72(2)	113(2)	-17(2)	48(2)	11(2)
Br(4)	130(2)	56(2)	91(2)	-2(1)	50(2)	16(2)
N(100)	40(20)	390(70)	130(30)	-130(40)	7(17)	20(30)
O(101)	142(19)	77(12)	106(14)	-5(10)	37(13)	33(12)
O(102)	99(17)	141(18)	190(20)	6(16)	74(15)	-30(13)
O(103)	210(30)	210(30)	210(30)	-10(20)	70(20)	-120(20)
N(200)	80(18)	50(14)	83(16)	-20(12)	33(14)	-36(14)
O(201)	147(19)	72(13)	130(16)	19(11)	53(15)	5(12)
O(202)	129(16)	55(11)	88(13)	16(9)	0(11)	22(10)
O(203)	126(14)	70(11)	71(11)	15(9)	38(10)	-15(10)
N(300)	78(17)	91(19)	40(14)	2(14)	13(12)	21(14)
O(301)	115(14)	83(12)	66(11)	-3(10)	41(10)	-6(10)
O(302)	77(12)	81(12)	65(11)	-11(9)	10(9)	-4(9)
O(303)	91(13)	77(11)	96(13)	31(10)	35(10)	12(10)
N(400)	550(70)	170(30)	53(18)	-32(19)	130(30)	-240(40)
O(401)	230(20)	170(20)	109(18)	37(15)	96(18)	-5(17)
O(403)	135(18)	77(14)	250(30)	-47(16)	28(18)	-8(12)
N(500)	37(12)	59(14)	43(12)	-11(11)	-6(10)	-15(11)
O(501)	54(10)	63(10)	61(10)	0(8)	24(8)	-10(8)
O(502)	94(12)	56(10)	45(9)	5(8)	11(8)	3(9)
O(503)	63(10)	64(9)	42(8)	3(7)	29(7)	-8(8)
N(600)	59(13)	68(15)	63(15)	6(13)	4(11)	14(11)
O(601)	210(20)	143(17)	36(9)	-42(10)	25(11)	68(14)
O(602)	51(10)	73(11)	60(9)	5(9)	15(8)	-17(8)
O(603)	159(18)	85(13)	82(13)	27(11)	12(12)	12(12)
N(700)	100(20)	190(30)	29(14)	-3(17)	24(15)	5(18)
O(701)	200(20)	87(12)	93(14)	-21(11)	76(14)	-31(12)
O(702)	154(19)	165(18)	67(12)	-16(12)	57(12)	-56(14)
O(703)	91(16)	123(16)	131(17)	-47(13)	54(13)	-21(12)
O(801)	240(30)	132(18)	128(17)	41(15)	60(19)	109(18)

O(802)	230(30)	230(30)	410(50)	-170(30)	140(30)	-100(20)
O(803)	90(18)	210(30)	540(60)	-70(30)	110(30)	40(17)
N(900)	43(15)	140(30)	50(14)	-33(15)	-5(12)	5(16)
O(901)	116(15)	71(12)	78(12)	-18(9)	40(11)	-7(10)
O(902)	210(20)	42(10)	100(14)	31(10)	34(13)	6(12)
O(903)	107(16)	131(16)	148(17)	78(14)	75(14)	57(13)
O(111)	160(20)	360(40)	140(20)	80(20)	30(17)	-30(30)
O(112)	148(19)	105(16)	180(20)	-59(15)	39(16)	22(14)
O(113)	260(30)	17(9)	190(20)	-27(11)	81(19)	-24(11)
N(120)	28(13)	55(12)	120(20)	-22(15)	-3(14)	-4(10)
O(121)	130(20)	540(50)	46(12)	-30(20)	3(13)	50(30)
O(122)	54(11)	93(12)	51(9)	-31(10)	-17(8)	5(9)
O(123)	170(20)	240(20)	127(16)	-64(16)	111(16)	-120(17)
N(140)	123	195	299	108	154	35
O(141)	122	62	51	-11	39	-17
O(142)	205	114	296	128	122	35
C(11A)	49(14)	54(13)	25(11)	-12(10)	21(10)	22(10)
C(12A)	35(12)	75(14)	34(12)	19(11)	16(10)	15(10)
C(13A)	33(13)	51(12)	19(10)	7(9)	3(9)	-13(10)
C(14A)	34(13)	84(15)	25(11)	10(11)	15(10)	11(11)
C(15A)	59(15)	57(13)	25(11)	-4(10)	26(11)	23(11)
C(16A)	29(12)	37(11)	29(11)	-4(9)	-9(9)	-9(9)
N(21A)	52(11)	48(10)	55(11)	10(8)	37(9)	-13(9)
C(21A)	70(15)	35(11)	32(11)	9(10)	26(11)	-10(10)
C(22A)	62(15)	36(12)	48(13)	-14(10)	18(11)	-8(11)
C(23A)	69(15)	32(11)	29(11)	-8(9)	12(10)	-10(11)
C(24A)	98(19)	60(15)	82(17)	-21(14)	45(15)	-30(13)
C(25A)	85(18)	52(14)	35(12)	19(11)	39(12)	21(13)
N(31A)	67(13)	43(10)	39(10)	-6(8)	35(9)	-1(9)
C(31A)	108(19)	43(13)	56(14)	-3(11)	58(14)	-30(12)
C(32A)	26(12)	54(13)	61(14)	-6(11)	23(11)	-6(10)
C(33A)	74(19)	94(18)	70(17)	-33(14)	41(15)	-28(14)
C(34A)	34(14)	150(20)	75(17)	-37(17)	27(13)	-40(14)
C(35A)	47(16)	109(19)	28(12)	-29(12)	-9(11)	-25(14)
N(41A)	63(13)	44(10)	22(8)	5(7)	14(8)	-6(9)
N(42A)	31(10)	37(9)	44(10)	12(8)	10(8)	-13(8)
C(41A)	18(12)	47(13)	81(15)	-4(12)	12(11)	-8(10)
C(43A)	31(13)	49(13)	22(10)	-6(9)	7(10)	-14(10)
C(44A)	67(17)	49(13)	29(11)	-12(10)	4(11)	-11(12)
C(45A)	75(17)	38(12)	39(12)	-7(9)	28(12)	3(11)
C(11B)	54(16)	103(19)	13(10)	19(12)	-9(10)	-17(14)
C(12B)	51(15)	58(14)	51(13)	18(11)	23(12)	-15(12)
C(13B)	56(16)	57(15)	41(13)	-19(11)	17(12)	-7(13)
C(14B)	22(12)	58(14)	31(11)	-19(10)	-8(9)	18(10)
C(15B)	89(19)	34(13)	38(13)	3(10)	26(13)	5(13)
C(16B)	67(16)	51(14)	26(11)	2(10)	5(11)	-10(13)

N(21B)	61(13)	32(10)	48(11)	2(8)	17(10)	-2(9)
C(21B)	90(20)	33(13)	47(14)	21(11)	31(14)	7(12)
C(22B)	68(16)	58(14)	45(13)	-11(11)	43(12)	-13(12)
C(23B)	42(15)	49(14)	100(19)	32(13)	14(14)	22(12)
C(24B)	100(20)	60(15)	38(13)	23(12)	22(13)	-25(14)
C(25B)	61(16)	69(15)	67(15)	-4(13)	36(13)	-3(12)
N(31B)	87(13)	29(9)	38(10)	1(8)	18(9)	-4(10)
C(31B)	93(19)	49(15)	9(10)	-1(10)	11(12)	-7(13)
C(32B)	86(19)	9(11)	90(20)	-19(13)	31(16)	-19(12)
C(33B)	150(30)	71(18)	23(12)	23(13)	11(14)	33(18)
C(34B)	57(17)	100(20)	77(18)	15(16)	16(15)	10(15)
C(35B)	92(19)	19(11)	51(14)	26(10)	20(13)	3(12)
N(41B)	49(13)	66(12)	21(9)	-13(8)	-13(9)	4(10)
N(42B)	94(14)	42(10)	14(8)	-14(8)	18(9)	-5(9)
C(41B)	61(16)	39(13)	46(13)	6(11)	21(12)	22(12)
C(42B)	150(20)	18(11)	62(15)	-10(11)	80(18)	-6(14)
C(43B)	46(15)	56(13)	37(12)	-4(11)	27(12)	9(11)
C(44B)	87(18)	36(12)	51(14)	14(11)	40(13)	17(12)
C(45B)	61(14)	52(13)	21(10)	3(9)	8(10)	3(10)
C(11C)	150(20)	53(15)	60(15)	13(13)	67(16)	-12(15)
C(12C)	140(20)	32(12)	39(13)	-11(11)	44(14)	9(13)
C(13C)	82(17)	16(11)	57(14)	-15(10)	8(12)	-17(10)
C(14C)	130(20)	29(12)	39(12)	-3(10)	49(13)	10(12)
C(15C)	180(30)	29(13)	44(14)	19(11)	46(15)	0(14)
C(16C)	230(30)	25(12)	70(16)	-10(11)	98(19)	-27(15)
N(21C)	157(18)	42(10)	38(10)	-10(8)	37(11)	-52(11)
C(21C)	150(20)	30(12)	107(18)	34(12)	94(18)	25(13)
C(23C)	220(30)	90(20)	110(20)	-57(17)	100(20)	-19(19)
C(25C)	1160(90)	270(30)	620(70)	-380(30)	820(70)	-522
N(31C)	45(12)	26(9)	67(12)	-20(9)	-1(9)	-13(8)
C(31C)	34(13)	45(13)	47(13)	-4(11)	11(11)	-10(10)
C(32C)	100(20)	38(13)	35(13)	-7(10)	21(13)	-13(13)
C(33C)	100(20)	58(16)	89(19)	32(14)	60(17)	24(15)
C(34C)	110(20)	52(15)	63(15)	-29(12)	23(15)	-25(14)
C(35C)	110(20)	33(12)	64(15)	-1(11)	69(16)	20(13)
N(41C)	86(14)	17(9)	51(11)	12(8)	13(10)	-10(9)
N(42C)	101(14)	35(10)	37(10)	13(8)	28(10)	6(10)
C(41C)	110(20)	59(16)	37(13)	4(11)	31(13)	-28(13)
C(42C)	150(20)	36(13)	36(12)	-5(11)	49(14)	36(14)
C(43C)	120(20)	52(15)	72(16)	-9(13)	71(16)	-9(14)
C(44C)	140(20)	29(12)	37(13)	-6(10)	38(14)	4(13)
C(45C)	140(20)	14(11)	73(15)	-4(10)	61(15)	-12(12)
C(11D)	61(16)	45(14)	33(13)	0(11)	19(12)	-16(12)
C(12D)	38(15)	100(20)	36(14)	-6(14)	5(11)	-19(14)
C(13D)	120(20)	33(13)	58(15)	-35(13)	63(16)	-31(15)
C(14D)	49(13)	66(14)	44(12)	-24(11)	39(11)	-25(11)

C(15D)	78(17)	22(11)	45(13)	-6(10)	22(12)	-12(11)
C(16D)	38(13)	58(14)	27(11)	-8(10)	-14(10)	-17(11)
N(21D)	54(13)	59(11)	42(11)	-4(9)	17(10)	-8(10)
C(21D)	55(16)	72(16)	27(12)	13(11)	-2(11)	-36(12)
C(22D)	48(16)	67(17)	39(14)	-17(13)	-15(12)	-30(13)
C(23D)	160(30)	51(16)	40(15)	18(13)	43(17)	18(18)
C(24D)	110(20)	89(19)	66(17)	-28(15)	58(17)	-36(16)
C(25D)	80(20)	110(20)	68(16)	-6(15)	48(15)	-42(16)
N(31D)	59(13)	79(14)	55(11)	17(11)	17(10)	-1(12)
C(31D)	91(19)	17(11)	47(13)	-2(10)	26(13)	-5(12)
C(32D)	68(17)	87(19)	44(14)	10(14)	22(13)	-40(16)
C(33D)	90(20)	63(17)	78(17)	-4(14)	30(15)	6(15)
C(34D)	140(30)	70(20)	230(50)	-70(30)	130(30)	-80(20)
C(35D)	90(30)	90(20)	150(30)	-20(20)	90(30)	-20(20)
N(41D)	63(12)	33(10)	41(10)	-29(9)	22(9)	-35(9)
N(42D)	51(11)	47(10)	31(9)	-29(8)	20(8)	-17(8)
C(41D)	64(15)	30(11)	26(11)	1(10)	1(10)	-4(11)
C(42D)	51(14)	61(14)	26(11)	12(11)	14(10)	0(11)
C(43D)	130(20)	29(12)	37(13)	17(11)	52(14)	23(13)
C(44D)	82(17)	36(12)	49(14)	-10(11)	45(13)	-4(12)
C(45D)	64(14)	41(12)	42(12)	-22(10)	7(11)	-40(11)
N(1A)	101(16)	20(9)	103(15)	-23(9)	22(12)	8(10)
N(2A)	75(14)	51(11)	73(13)	-3(10)	10(11)	-8(11)
C(1A)	90(30)	280(50)	110(30)	50(30)	-40(20)	70(30)
C(2A)	140(30)	200(40)	200(40)	-140(30)	40(30)	0(30)
N(1B)	100(20)	130(20)	127(19)	36(16)	40(16)	-15(15)
N(2B)	114(17)	55(12)	89(14)	11(11)	36(13)	9(11)
C(1B)	60(20)	170(40)	210(50)	50(40)	20(30)	0(20)
C(2B)	270(60)	160(40)	150(40)	60(30)	90(40)	180(40)
N(1C)	230(30)	65(13)	132(18)	23(13)	124(19)	53(15)
N(2C)	180(20)	95(15)	73(14)	26(13)	75(15)	-29(15)
C(1C)	150(30)	430(60)	54(19)	0(30)	60(20)	-100(40)
C(2C)	210(40)	180(30)	120(30)	110(20)	120(30)	130(30)
N(1D)	104(14)	23(8)	53(10)	10(8)	46(10)	-2(8)
N(2D)	65(12)	53(10)	37(10)	-15(8)	-7(8)	-3(9)
C(1D)	150(20)	53(14)	22(12)	8(11)	23(13)	-29(14)
C(2D)	210(30)	68(17)	45(15)	28(14)	4(17)	30(19)
N(1E)	69(13)	71(12)	38(10)	8(9)	4(9)	26(10)
N(2E)	83(14)	102(15)	36(10)	7(10)	6(9)	-6(11)
C(1E)	80(20)	170(30)	150(30)	-30(20)	80(20)	30(20)
C(2E)	140(30)	65(17)	130(20)	-21(16)	50(20)	58(18)
N(1F)	60(12)	60(11)	53(11)	29(9)	31(9)	24(9)
N(2F)	80(12)	30(9)	22(8)	6(7)	-4(8)	8(8)
C(1F)	130(20)	77(18)	31(13)	17(13)	19(13)	-11(15)
C(2F)	180(30)	33(13)	47(14)	15(11)	39(15)	27(15)
N(1G)	68(12)	55(10)	41(10)	-8(8)	22(9)	-12(9)

N(2G)	75(12)	44(10)	40(10)	-7(8)	19(9)	10(9)
C(1G)	95(19)	57(14)	51(14)	38(12)	18(13)	21(13)
C(2G)	100(20)	68(15)	23(12)	-12(11)	4(12)	-7(14)
N(1H)	97(14)	44(10)	59(11)	1(9)	35(10)	4(10)
N(2H)	55(11)	57(11)	54(11)	-8(9)	9(9)	-5(9)
C(1H)	200(30)	43(15)	180(30)	26(17)	140(30)	36(17)
C(2H)	130(20)	66(17)	80(17)	-14(14)	68(16)	-10(15)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for bk81n.

	x	y	z	U(eq)
H(12A)	2750	2294	1174	56
H(14A)	1538	2271	1322	55
H(16A)	1726	1991	54	42
H(21A)	2255	1706	-83	52
H(23A)	2970	2440	496	52
H(24A)	3464	2314	19	91
H(25A)	3287	1882	-499	63
H(31A)	1762	2450	2028	74
H(33A)	2905	2592	1796	90
H(34A)	3167	2786	2590	102
H(35A)	2665	2886	3019	79
H(42A)	1125	1694	0	43
H(44A)	797	2350	823	61
H(45A)	-449	2015	-73	73
H(45B)	-352	1674	-158	73
H(45C)	-350	1916	-567	73
H(12B)	1268	223	793	62
H(14B)	2502	250	765	48
H(16B)	1740	945	221	60
H(21B)	981	1027	-210	67
H(23B)	845	612	1023	78
H(24B)	226	854	868	78
H(25B)	-83	1173	163	75
H(31B)	2575	27	1607	61
H(33B)	1453	-290	720	100
H(34B)	1576	-730	1172	93
H(35B)	2180	-779	1858	65
H(42B)	3017	584	806	79
H(44B)	2147	1019	-278	65
H(45D)	3449	1298	-409	69
H(45E)	3735	1008	-207	69
H(45F)	3754	1286	147	69
H(12C)	3581	1546	2820	82
H(14C)	2949	997	3485	71
H(16C)	3132	747	2158	118
H(21C)	3692	846	1832	100
H(23C)	3321	1709	1930	152
H(24C)	3565	1836	1251	157
H(25C)	3873	1468	863	673
H(31C)	2707	1455	3701	50

H(33C)	3947	1659	3691	92
H(34C)	3991	2011	4361	91
H(35C)	3357	2066	4594	72
H(42C)	3122	251	2473	84
H(44C)	2472	655	3302	80
H(45G)	2066	-299	3234	105
H(45H)	2523	-445	3244	105
H(45I)	2139	-422	2739	105
H(12D)	292	1059	1963	70
H(14D)	1407	1196	3103	57
H(16D)	691	1909	2364	55
H(21D)	385	1979	1520	65
H(23D)	-319	1294	1719	98
H(24D)	-944	1464	1037	98
H(25D)	-862	1962	681	95
H(31D)	1554	768	3105	60
H(33D)	297	608	2271	90
H(34D)	472	82	2479	157
H(35D)	1089	-68	2988	121
H(42D)	1298	2179	2621	55
H(44D)	1723	1542	3661	60
H(45J)	2595	2326	4231	76
H(45K)	2286	2608	4044	76
H(45L)	2617	2504	3754	76
H(1A1)	3652	-223	2990	91
H(1A2)	3430	-422	3255	91
H(2A1)	3054	-906	2175	82
H(2A2)	3201	-710	1834	82
H(1A3)	4078	-560	2986	210
H(1A4)	3781	-787	3176	210
H(2A3)	3829	-706	2239	217
H(2A4)	3692	-996	2476	217
H(1B1)	4685	890	1428	139
H(1B2)	4522	622	1625	139
H(2B1)	3889	311	420	102
H(2B2)	4161	518	230	102
H(1B3)	4905	644	883	183
H(1B4)	5037	432	1354	183
H(2B3)	4451	145	1045	226
H(2B4)	4678	191	618	226
H(1C1)	2557	-81	4192	152
H(1C2)	2659	241	4276	152
H(2C1)	1436	386	4126	130
H(2C2)	1362	60	4057	130
H(1C3)	2359	-109	4806	246
H(1C4)	2477	234	4902	246

H(2C3)	1865	331	4810	190
H(2C4)	1754	-13	4756	190
H(1D1)	-107	1805	-1256	66
H(1D2)	369	1849	-1178	66
H(2D1)	356	994	-1176	68
H(2D2)	-77	966	-1083	68
H(1D3)	-41	1648	-1978	90
H(1D4)	417	1490	-1709	90
H(2D3)	-106	1124	-1930	136
H(2D4)	-418	1300	-1679	136
H(1E1)	-803	2517	886	74
H(1E2)	-423	2631	1280	74
H(2E1)	232	2803	406	92
H(2E2)	-178	2740	6	92
H(1E3)	-887	2903	460	147
H(1E4)	-636	3048	977	147
H(2E3)	-78	3104	807	130
H(2E4)	-428	3139	281	130
H(1F1)	2305	1821	-1358	65
H(1F2)	2740	1763	-1427	65
H(2F1)	2714	930	-1198	57
H(2F2)	2241	1000	-1313	57
H(1F3)	2297	1593	-2145	96
H(1F4)	1964	1459	-1877	96
H(2F3)	2348	1054	-2059	103
H(2F4)	2808	1217	-1816	103
H(1G1)	3056	1502	5088	64
H(1G2)	3089	1815	5264	64
H(2G1)	1849	1973	4735	63
H(2G2)	1830	1642	4716	63
H(1G3)	2510	1386	5375	82
H(1G4)	2796	1603	5791	82
H(2G3)	2360	1989	5485	82
H(2G4)	2057	1717	5545	82
H(1H1)	1911	3276	2896	77
H(1H2)	1610	3191	2410	77
H(2H1)	1016	2737	3125	68
H(2H2)	1366	2768	3600	68
H(1H3)	1364	3520	2973	149
H(1H4)	1030	3309	2588	149
H(2H3)	891	3195	3251	101
H(2H4)	1383	3243	3582	101