Characterization data

(1) Synthesis and Characterization data for **1'**.

$[Pd(CH_3CN)_4][BF_4]_2$ (50.0 mg, 0.116 mmol) was dissolved in CH_2Cl_2 and then DPOT (119.6mg, 0.463 mmol) and $Pd_2(dba)_3 \cdot CHCl_3$ (179.6 mg, 0.174 mmol) were added subsequently. The solution was stirred for overnight. The solution turned to orange suspension of **1**. Then $NaBAr_f$ (205.1 mg, 0.231 mmol) was added and the reddish orange solution was filtered off. After recrystallization from CH_3COOEt/n-hexane, orange microcrystals of **1'** (229.2 mg, 0.0859 mmol) were obtained (74% yield). ^1H NMR (acetone-d_6, 23 °C) δ 7.78 (16H, br s, BAr_f) 7.67 (8H, s, BAr_f) 7.58 (8H, t, J = 7.8 Hz, *m*-Ph) 7.25 (4H, t, J = 7.8 Hz, *p*-Ph) 7.15 (8H, d, J = 7.3 Hz, *o*-Ph) 5.33 (4H, d, J = 12.7 Hz, -(CH)-), 4.51 (4H, dd, J = 12.7 Hz, J = 11.3 Hz, -(CH)-) 3.80 (4H, m, -(CH)-) 3.50 (4H, m, -(CH)-). ^1H NMR (CD_2Cl_2, 25 °C) δ 7.67 (16H, br s, BAr_f) 7.53 (8H, t, J = 7.8 Hz, *m*-Ph) 7.50 (8H, t, J = 7.8 Hz, *m*-Ph) 7.26 (4H, t, J = 7.8 Hz, *p*-Ph) 6.86 (8H, d, J = 7.3 Hz, *o*-Ph) 4.89 (4H, d, J = 13.2 Hz, -(CH)-), 3.93 (4H, dd, J = 12.7 Hz, J = 11.3 Hz, -(CH)-) 3.27 (4H, m, -(CH)-) 3.00 (4H, m, -(CH)-). These signals were significantly broadened at -90 °C in acetone-d_6 and -96 °C in CD_2Cl_2. Dissolving crystals of **1'** (*meso* arrangement) for 2h gave a mixture of two isomers (84/16); possibly *meso* and *racemic* arising from chiral mode of Pd_4-(DPOT) association. Anal Calcd (found) for $C_{104}H_{60}Pd_4B_2F_{48}$: C, 46.80 (46.01); H, 2.27 (2.37). A single crystal suited for X-ray crystallographic analysis was grown from CH_2Cl_2/Et_2O/n-hexane.

(2) Synthesis and Characterization data for **2'**.

$[Pd_4(DPOT)_2][BF_4]_2$ (**1**) (150.0 mg, 0.134 mmol) was suspended in CH_2Cl_2, and then pyridine (21.7 ml, 0.268 mmol) was added to afford orange solution. The solution was filtered and the filtrate was concentrated in vacuo. Precipitation by adding n-hexane afforded orange powder of **2** (144.8 mg, 0.114 mmol). **2** was dissolved in CH_2Cl_2, and then $NaBAr_f$ (201.3 mg, 0.227 mmol) was added. The orange solution was filtered and the solvent was removed in vacuo. Recrsytallization from CH_2Cl_2/n-hexane gave orange microcrystals of **2'**

(290.8 mg, 0.103 mmol) in 77% yield. ^{1}H NMR (CD_2Cl_2, 25 °C) δ 7.68 (18H, br s, BAr_f and *p*-py) 7.52 (8H, s, BAr_f) 7.20 (16H, br m, *o*-py, *m*-py, *m*-Ph,) 7.06 (4H, br t, *p*-Ph) 6.75 (8H, m, *o*-Ph) 5.41 (4H, d, J = 12.7 Hz, -(CH)-), 4.09 (4H, dd, J = 12.7 Hz, J = 11.3 Hz, -(CH)-) 3.18 (4H, m, -(CH)-) 3.03 (4H, m, -(CH)-). A single crystal of **2'** suited for X-ray crystallographic analysis was grown from CH_2Cl_2/n-hexane.

Since several resonances for pyridine protons overlapped with BAr_f resonances, ^{1}H NMR data (CD_2Cl_2, -80 °C) for **2** are also included: δ 8.38 (2H, d, J = 5.4 Hz, *o*-py) 7.61 (2H, t, J = 7.3 Hz, *p*-py) 7.30 (2H, t, J = 6.8 Hz, *m*-py) 7.25 (4H, t, J = 7.3 Hz, *m*-Ph) 7.06 (4H, t, J = 7.3 Hz, *m*-Ph) 6.96 (4H, t, J = 6.8 Hz, *p*-Ph), 6.76 (4H, d, J = 7.3 Hz, *o*-Ph) 6.67 (4H, d, J = 7.6 Hz, *o*-Ph) 6.66 (2H, t, *m*-py) 5.82 (2H, d, J = 5.4 Hz, *o*-py) 5.31 (4H, d, J = 12.7 Hz, -(CH)-) 4.09 (4H, t, J = 11.9 Hz, -(CH)-) 3.23 (4H, m, -(CH)-) 3.08 (4H, m, -(CH)-). Raising the temperature resulted in broadening and coalescing (0 °C) of the asymmetric (-80 °C) pyridine and phenyl signals, reflecting the restricted rotation of the pyridine and phenyl rings.

(3) Characterization data for **3'**.

A mixture of two isomers (69/31); major: ^{1}H NMR (CD_2Cl_2, 23 °C) δ 7.74 (16H, br s, BAr_f) 7.62 (8H, s, BAr_f) 7.30 (8H, t, J = 7.8 Hz, *p*-Ph) 7.13 (4H, t, J = 7.8 Hz, *m*-Ph) 6.90 (8H, d, J = 7.8 Hz, *o*-Ph) 6.49 (4H, d, J = 13.8 Hz, -(CH)-), 5.24 (4H, dd, J = 13.8 Hz, J = 11.3 Hz, -(CH)-) 3.47 (4H, m, -(CH)-), 2.94 (4H, m, -(CH)-), minor for $-(CH)_8-$ part: δ 5.72 (m, 8H), 3.07 (br s, 8H). Anal. Calcd. (Found) for $C_{104}H_{60}Pd_3B_2F_{48}$: C, 48.75 (48.67); H, 2.36 (2.39).

(4) Characterization data for **4'**.

^{1}H NMR (CD_2Cl_2, 23 °C) δ 7.65 (16H, br s, BAr_f) 7.47 (8H, s, BAr_f) 7.39 (4H, t, J = 7.3 Hz, *p*-Ph) 7.10 (8H, t, J = 7.8 Hz, *m*-Ph) 6.97 (8H, d, J = 7.8 Hz, *o*-Ph) 6.15 (4H, d, J = 13.2 Hz, -(CH)-), 5.33 (4H, t, J = 10.8 Hz, -(CH)-) 3.15 (4H, t, J = 11.6 Hz, -(CH)-) 3.04 (4H, m, -(CH)-) 2.85 (4H, t, J = 11.3 Hz, -(CH)-) 2.59 (4H, m, -(CH)-), Anal. Calcd. (Found) for $C_{110}H_{68}Pd_5B_2F_{48}$: C, 46.27 (46.51); H, 2.40 (2.36).

X-ray structure determination of $[Pd_4(DPOT)_2][BAr_f]_2 \cdot 3Et_2O \cdot 2H_2O$ (**1'**).

Experimental

Data Collection

An orange prismatic crystal of $C_{104}H_{60}Pd_4F_{48}B_2 \cdot 3Et_2O \cdot 2H_2O$ having approximate dimensions of 0.30 x 0.20 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS-CS imaging plate area detector with graphite monochromated Mo-$K\alpha$ radiation.

Indexing was performed from 3 stills which were exposed for 5.0 minutes. The crystal-to-detector distance was 143.2 mm with the detector at the zero swing position. Readout was performed in the 0.1 mm pixel mode.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 13.094(2) Å
b = 24.229(2) Å $\quad \beta$ = 104.42(1)°
c = 19.497(4) Å
V = 5990(1) Å^3

For Z = 2 and $F.W.$ = 2927.16, the calculated density is 1.62 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_{1/c}$ (#14)

The data were collected at a temperature of -50 ± 1°C to a maximum 2θ value of 60.1°. A total of 38 3.00° oscillation images were collected, each being exposed for 10.0 minutes. The crystal-to-detector distance was 143.2 mm with the detector at the zero swing position. Readout was performed in the 0.1 mm pixel mode.

Data Reduction

A total of 10459 reflections was collected.

The linear absorption coefficient, μ, for Mo-$K\alpha$ radiation is 7.2 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods1 and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement3 was based on 10335 observed reflections ($I > 3.00\sigma(I)$) and 833 variable parameters and converged (largest parameter shift was 6.62 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.072$$

$$Rw = [(\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2)]^{1/2} = 0.068$$

The standard deviation of an observation of unit weight[4] was 2.37. The weighting scheme was based on counting statistics and included a factor (p = 0.010) to downweight the intense reflections. Plots of Σ w $(|Fo| - |Fc|)^2$ versus |Fo|,reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.23 and -0.74 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994), J. Appl. Cryst., 27, 435

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized $\Sigma \, \omega \, (|Fo|-|Fc|)^2$

(4) Standard deviation of an observation of unit weight:

$$[\Sigma \, \omega \, (|Fo|-|Fc|)^2/(No-Nv)]^{1/2}$$

where No = number of observations
Nv = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{104}H_{60}Pd_4F_{48}B_2 \cdot 3Et_2O \cdot 2H_2O$
Formula Weight	2927.16
Crystal Color, Habit	orange, prismatic
Crystal Dimensions	0.30 X 0.20 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 stills @ 5.0 minutes
Detector Position	143.2 mm
Detector Swing Angle	0.00°
Pixel Size	0.1 mm
Lattice Parameters	a = 13.094(2)Å
	b = 24.229(2) Å
	c = 19.497(4) Å
	β = 104.42(1)°
	V = 5990(1) Å°
Space Group	$P2_{1/c}$ (#14)
Z value	2
Dcalc	1.623 g/cm^3
F000	2912.00

μ(Mo$K\alpha$)	7.17 cm^{-1}

B. Intensity Measurements

Diffractometer	RAXIS-CS
Radiation	Mo$K\alpha$(λ= 0.71070 Å)
	graphite monochromated
Detector Aperture	200 mm x 200 mm
Data Images	38 exposures @ 10.0 minutes
Oscillation Range	3.0°
Detector Position	143.2 mm
Detector Swing Angle	0.00°
Pixel Size	0.1 mm
$2\Theta_{max}$	60.1°
No. of Reflections Measured	Total: 10459
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\ \omega\ (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0100
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00Σ(I))	10335
No. Variables	833

Reflection/Parameter Ratio	12.41
Residuals: R; Rw	0.072 ; 0.068
Residuals: R1	0.072
No. of Reflections to calc R1	10335
Goodness of Fit Indicator	2.37
Max Shift/Error in Final Cycle	6.62
Maximum peak in Final Diff. Map	1.23 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.74 $e^-/Å^3$

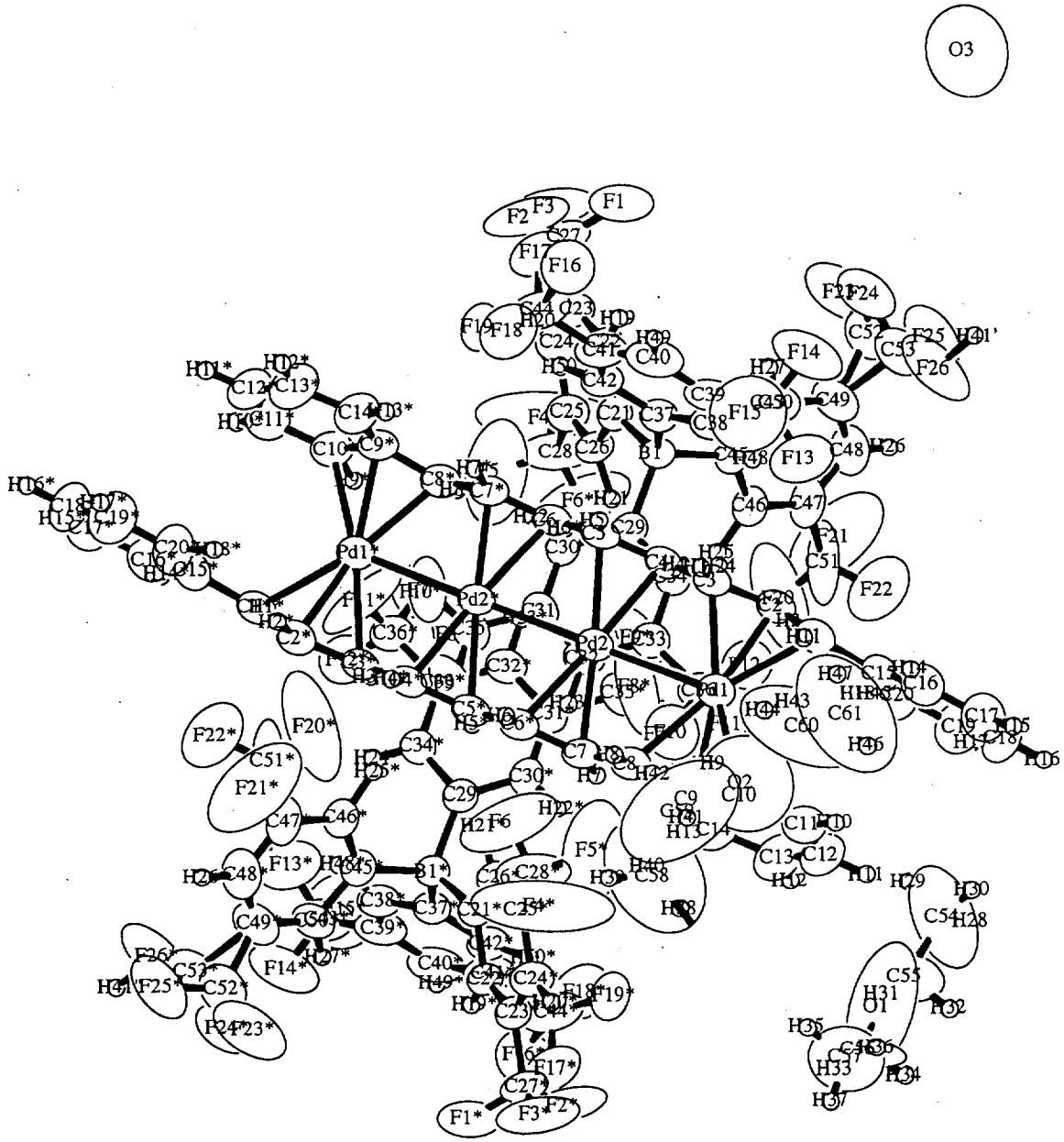

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Pd(1)	0.99943(4)	0.02149(2)	0.29345(3)	4.43(1)	1.0000
Pd(2)	0.99769(4)	0.00719(2)	0.43215(3)	4.06(1)	1.0000
F(1)	0.6183(7)	0.3565(3)	0.6731(4)	12.5(2)	1.0000
F(2)	0.6886(7)	0.3052(3)	0.7505(5)	18.5(3)	1.0000
F(3)	0.5363(6)	0.3303(3)	0.7404(4)	13.0(3)	1.0000
F(4)	0.2812(9)	0.1891(5)	0.646(1)	28.5(7)	1.0000
F(5)	0.354(1)	0.1257(8)	0.6592(7)	28.6(7)	1.0000
F(6)	0.7065(6)	-0.1412(5)	0.4330(5)	17.7(4)	1.0000
F(7)	0.7432(5)	-0.0068(3)	0.6350(3)	11.2(2)	1.0000
F(8)	0.5874(5)	-0.0224(4)	0.5946(4)	14.6(3)	1.0000
F(9)	0.7003(9)	-0.0642(3)	0.5615(4)	16.4(3)	1.0000
F(10)	0.7268(6)	-0.0119(2)	0.3287(3)	11.6(2)	1.0000
F(11)	0.5795(5)	0.0242(4)	0.2900(3)	14.5(3)	1.0000
F(12)	0.7149(6)	0.0676(2)	0.2968(3)	9.8(2)	1.0000
F(13)	0.9099(6)	0.2289(3)	0.3470(4)	11.1(2)	1.0000
F(14)	0.9651(8)	0.3033(3)	0.3954(4)	15.3(3)	1.0000
F(15)	1.0560(6)	0.2330(4)	0.4128(5)	14.9(3)	1.0000
F(16)	1.098(1)	0.2652(5)	0.6586(7)	9.5(3)	0.5000
F(17)	0.9983(7)	0.2679(3)	0.7001(3)	14.0(3)	1.0000
F(18)	1.0834(7)	0.1954(3)	0.6799(4)	13.0(2)	1.0000
F(19)	0.9672(8)	0.1931(4)	0.7160(5)	6.9(3)	0.5000
F(20)	0.2808(9)	0.1505(6)	0.3299(8)	30.1(6)	1.0000
F(21)	0.2075(6)	0.2210(6)	0.3152(5)	20.3(5)	1.0000
F(22)	0.2759(6)	0.1960(4)	0.2431(4)	12.6(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
F(23)	0.442(2)	0.3879(6)	0.430(1)	16.2(8)	0.5000
F(24)	0.5839(8)	0.3894(3)	0.3974(5)	12.9(3)	1.0000
F(25)	0.4400(8)	0.3914(3)	0.3221(5)	15.4(3)	1.0000
F(26)	0.569(2)	0.3640(6)	0.294(1)	15.5(8)	0.5000
O(1)	0.638(2)	-0.124(3)	-0.012(2)	26(1)	0.5000
O(2)	1.272(2)	-0.047(1)	0.198(2)	29(1)	1.0000
O(3)	0.718(1)	0.5979(8)	0.430(1)	25.2(8)	1.0000
C(1)	1.0065(6)	0.1002(3)	0.2305(4)	4.8(2)	1.0000
C(2)	0.9601(6)	0.1086(3)	0.2866(4)	4.8(2)	1.0000
C(3)	1.0195(6)	0.0995(2)	0.3572(4)	4.5(2)	1.0000
C(4)	0.9709(5)	0.0955(2)	0.4148(4)	4.4(2)	1.0000
C(5)	1.0272(5)	0.0884(2)	0.4860(4)	4.5(2)	1.0000
C(6)	0.9771(6)	0.0820(2)	0.5421(4)	4.6(2)	1.0000
C(7)	0.9679(6)	-0.0754(2)	0.3865(4)	4.6(2)	1.0000
C(8)	1.0202(6)	-0.0657(3)	0.3320(4)	4.9(2)	1.0000
C(9)	0.9706(6)	-0.0645(3)	0.2565(4)	5.1(2)	1.0000
C(10)	1.0349(7)	-0.0465(3)	0.2114(4)	6.1(2)	1.0000
C(11)	0.990(1)	-0.0400(4)	0.1387(5)	8.1(3)	1.0000
C(12)	0.886(1)	-0.0497(4)	0.1113(5)	8.6(3)	1.0000
C(13)	0.8211(9)	-0.0657(5)	0.1549(6)	8.4(3)	1.0000
C(14)	0.8615(7)	-0.0734(4)	0.2259(5)	6.5(2)	1.0000
C(15)	0.9494(7)	0.1015(3)	0.1546(4)	5.3(2)	1.0000
C(16)	1.0081(8)	0.1072(3)	0.1049(5)	6.9(3)	1.0000
C(17)	0.958(1)	0.1097(4)	0.0336(6)	8.7(3)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(18)	0.850(1)	0.1076(5)	0.0119(5)	8.8(3)	1.0000
C(19)	0.7925(9)	0.1014(5)	0.0611(6)	9.1(3)	1.0000
C(20)	0.8411(8)	0.0986(4)	0.1318(5)	7.1(3)	1.0000
C(21)	0.5907(5)	0.2032(2)	0.5657(3)	3.7(1)	1.0000
C(22)	0.6198(5)	0.2483(2)	0.6110(3)	3.9(1)	1.0000
C(23)	0.5639(6)	0.2641(3)	0.6593(3)	4.4(2)	1.0000
C(24)	0.4743(6)	0.2368(3)	0.6640(4)	5.3(2)	1.0000
C(25)	0.4417(6)	0.1926(3)	0.6190(4)	4.9(2)	1.0000
C(26)	0.4989(5)	0.1759(3)	0.5717(3)	4.2(1)	1.0000
C(27)	0.6038(8)	0.3117(4)	0.7077(5)	6.3(2)	1.0000
C(28)	0.338(1)	0.1657(5)	0.6149(8)	10.9(4)	1.0000
C(29)	0.6496(4)	0.1230(2)	0.4846(3)	3.5(1)	1.0000
C(30)	0.6573(5)	0.0823(3)	0.5360(3)	4.0(1)	1.0000
C(31)	0.6687(5)	0.0267(3)	0.5219(4)	4.3(1)	1.0000
C(32)	0.6744(5)	0.0100(3)	0.4549(4)	4.7(2)	1.0000
C(33)	0.6663(5)	0.0491(3)	0.4026(4)	4.3(1)	1.0000
C(34)	0.6556(5)	0.1042(3)	0.4179(3)	4.0(1)	1.0000
C(35)	0.6708(7)	-0.0148(3)	0.5778(5)	5.8(2)	1.0000
C(36)	0.6682(7)	0.0321(3)	0.3299(4)	5.6(2)	1.0000
C(37)	0.7664(5)	0.2106(2)	0.5127(3)	3.9(1)	1.0000
C(38)	0.8094(5)	0.2243(3)	0.4567(4)	4.5(2)	1.0000
C(39)	0.9141(6)	0.2382(3)	0.4666(5)	5.6(2)	1.0000
C(40)	0.9801(6)	0.2392(3)	0.5345(6)	6.3(2)	1.0000
C(41)	0.9412(5)	0.2255(3)	0.5914(5)	5.5(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(42)	0.8359(5)	0.2102(3)	0.5806(4)	4.5(2)	1.0000
C(43)	0.9556(9)	0.2533(4)	0.4048(6)	8.1(3)	1.0000
C(44)	1.0073(6)	0.2263(5)	0.6677(6)	8.0(3)	1.0000
C(45)	0.5625(5)	0.2209(3)	0.4346(3)	4.0(1)	1.0000
C(46)	0.4694(5)	0.1958(3)	0.3964(4)	4.5(2)	1.0000
C(47)	0.3898(6)	0.2247(4)	0.3494(4)	5.4(2)	1.0000
C(48)	0.4015(7)	0.2794(4)	0.3386(5)	6.9(2)	1.0000
C(49)	0.4930(9)	0.3052(3)	0.3736(6)	8.1(3)	1.0000
C(50)	0.5715(6)	0.2767(3)	0.4208(4)	5.9(2)	1.0000
C(51)	0.2936(7)	0.1925(7)	0.3078(7)	11.4(4)	1.0000
C(52)	0.486(2)	0.3660(9)	0.380(1)	7.5(6)	0.5000
C(53)	0.528(2)	0.3637(9)	0.339(2)	7.8(7)	0.5000
C(54)	0.540(3)	-0.030(2)	-0.014(3)	20(1)	0.5000
C(55)	0.596(6)	-0.091(2)	-0.014(3)	21(2)	0.5000
C(56)	0.704(4)	-0.167(2)	-0.019(4)	17(2)	0.5000
C(57)	0.743(3)	-0.181(2)	-0.014(4)	14(1)	0.5000
C(58)	1.258(5)	-0.149(2)	0.233(3)	55(3)	1.0000
C(59)	1.317(4)	-0.096(3)	0.242(3)	36(2)	1.0000
C(60)	1.301(4)	0.015(2)	0.175(3)	35(2)	1.0000
C(61)	1.326(3)	0.040(2)	0.140(3)	35(2)	1.0000
B(1)	0.6438(5)	0.1894(3)	0.5004(4)	3.6(1)	1.0000
H(1)	1.0993	0.0899	0.2351	4.5840	1.0000
H(2)	0.8764	0.1087	0.2655	4.5840	1.0000
H(3)	1.1009	0.0999	0.3692	4.5840	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(4)	0.8856	0.1047	0.4028	4.5840	1.0000
H(5)	1.1082	0.0940	0.4896	4.5840	1.0000
H(6)	1.1071	-0.0853	0.4696	4.5840	1.0000
H(7)	0.8788	-0.0808	0.3659	4.5840	1.0000
H(8)	1.1034	-0.0702	0.3469	4.5840	1.0000
H(9)	1.1228	-0.0368	0.2441	4.5840	1.0000
H(10)	1.0321	-0.0282	0.1079	9.8993	1.0000
H(11)	0.8545	-0.0446	0.0620	10.6072	1.0000
H(12)	0.7480	-0.0739	0.1357	10.0188	1.0000
H(13)	0.8166	-0.0835	0.2551	7.7266	1.0000
H(14)	1.0814	0.1102	0.1198	8.2733	1.0000
H(15)	0.9965	0.1133	-0.0012	10.6891	1.0000
H(16)	0.8125	0.1104	-0.0368	10.5062	1.0000
H(17)	0.7191	0.0987	0.0460	11.1881	1.0000
H(18)	0.7949	0.0855	0.1726	4.5840	1.0000
H(19)	0.6800	0.2693	0.6083	4.6543	1.0000
H(20)	0.4363	0.2477	0.6972	6.3378	1.0000
H(21)	0.4713	0.1463	0.5291	4.5840	1.0000
H(22)	0.6545	0.0930	0.5824	4.7632	1.0000
H(23)	0.6776	-0.0303	0.4436	4.5840	1.0000
H(24)	0.6517	0.1305	0.3813	4.7231	1.0000
H(25)	0.4571	0.1500	0.4019	4.5840	1.0000
H(26)	0.3469	0.2998	0.3074	8.2764	1.0000
H(27)	0.6343	0.2957	0.4445	7.1428	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(28)	0.4700	-0.0191	-0.0365	21.3649	0.5000
H(29)	0.5474	-0.0182	0.0381	21.3649	0.5000
H(30)	0.5864	-0.0015	-0.0279	21.3649	0.5000
H(31)	0.5290	-0.1097	0.0019	23.5988	1.0000
H(32)	0.5510	-0.0947	-0.0705	23.5988	1.0000
H(33)	0.6365	-0.1878	-0.0026	16.8733	0.5000
H(34)	0.6577	-0.1654	-0.0723	16.8733	0.5000
H(35)	0.7730	-0.1749	0.0374	14.8270	0.5000
H(36)	0.7844	-0.1630	-0.0385	14.8270	0.5000
H(37)	0.7334	-0.2177	-0.0224	14.8270	0.5000
H(38)	1.2475	-0.1630	0.1922	32.4376	1.0000
H(39)	1.3016	-0.1715	0.2718	32.4376	1.0000
H(40)	1.1933	-0.1420	0.2496	32.4376	1.0000
H(41)	1.3788	-0.1003	0.2280	26.5457	1.0000
H(42)	1.3276	-0.0800	0.2872	26.5457	1.0000
H(43)	1.2624	0.0315	0.1994	30.6911	1.0000
H(44)	1.3760	0.0079	0.2150	30.6911	1.0000
H(45)	1.2753	0.0681	0.1275	29.1139	1.0000
H(46)	1.3440	0.0244	0.1017	29.1139	1.0000
H(47)	1.3937	0.0620	0.1658	29.1139	1.0000
H(48)	0.7510	0.2168	0.4024	4.5840	1.0000
H(49)	1.0515	0.2496	0.5412	7.7225	1.0000
H(50)	0.8090	0.2049	0.6290	4.5840	1.0000
Pd(2*)	1.00231(4)	-0.00719(2)	0.56785(3)	4.06(1)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(6*)	1.0229(6)	-0.0820(2)	0.4579(4)	4.6(2)	1.0000
C(28*)	0.662(1)	-0.1657(5)	0.3851(8)	10.9(4)	1.0000
H(41')	0.6212	0.3997	0.2720	26.5457	1.0000
C(7*)	1.0321(6)	0.0754(2)	0.6135(4)	4.6(2)	1.0000
H(6*)	0.8929	0.0853	0.5304	4.5840	1.0000
F(6*)	0.2935(6)	0.1412(5)	0.5670(5)	17.7(4)	1.0000
Pd(1*)	1.00057(4)	-0.02149(2)	0.70655(3)	4.43(1)	1.0000
C(4*)	1.0291(5)	-0.0955(2)	0.5852(4)	4.4(2)	1.0000
C(5*)	0.9728(5)	-0.0884(2)	0.5140(4)	4.5(2)	1.0000
F(4*)	0.7188(9)	-0.1891(5)	0.354(1)	28.5(7)	1.0000
F(5*)	0.646(1)	-0.1257(8)	0.3408(7)	28.6(7)	1.0000
C(25*)	0.5583(6)	-0.1926(3)	0.3810(4)	4.9(2)	1.0000
C(8*)	0.9798(6)	0.0657(3)	0.6680(4)	4.9(2)	1.0000
H(7*)	1.1212	0.0808	0.6341	4.5840	1.0000
C(1*)	0.9935(6)	-0.1002(3)	0.7695(4)	4.8(2)	1.0000
C(2*)	1.0399(6)	-0.1086(3)	0.7134(4)	4.8(2)	1.0000
C(3*)	0.9805(6)	-0.0995(2)	0.6428(4)	4.5(2)	1.0000
C(9*)	1.0294(6)	0.0645(3)	0.7435(4)	5.1(2)	1.0000
C(10*)	0.9651(7)	0.0465(3)	0.7886(4)	6.1(2)	1.0000
H(4*)	1.1144	-0.1047	0.5972	4.5840	1.0000
H(5*)	0.8918	-0.0940	0.5104	4.5840	1.0000
C(24*)	0.5257(6)	-0.2368(3)	0.3360(4)	5.3(2)	1.0000
C(26*)	0.5011(5)	-0.1759(3)	0.4283(3)	4.2(1)	1.0000
H(8*)	0.8966	0.0702	0.6531	4.5840	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
C(15*)	1.0506(7)	-0.1015(3)	0.8454(4)	5.3(2)	1.0000
H(1*)	0.9007	-0.0899	0.7649	4.5840	1.0000
H(2*)	1.1236	-0.1087	0.7345	4.5840	1.0000
H(3*)	0.8991	-0.0999	0.6308	4.5840	1.0000
C(14*)	1.1385(7)	0.0734(4)	0.7741(5)	6.5(2)	1.0000
C(11*)	1.010(1)	0.0400(4)	0.8613(5)	8.1(3)	1.0000
H(9*)	0.8772	0.0368	0.7559	4.5840	1.0000
C(23*)	0.4361(6)	-0.2641(3)	0.3407(3)	4.4(2)	1.0000
H(20*)	0.5637	-0.2477	0.3028	6.3378	1.0000
C(21*)	0.4093(5)	-0.2032(2)	0.4343(3)	3.7(1)	1.0000
H(21*)	0.5287	-0.1463	0.4709	4.5840	1.0000
C(16*)	0.9919(8)	-0.1072(3)	0.8951(5)	6.9(3)	1.0000
C(20*)	1.1589(8)	-0.0986(4)	0.8682(5)	7.1(3)	1.0000
C(13*)	1.1789(9)	0.0657(5)	0.8451(6)	8.4(3)	1.0000
H(13*)	1.1834	0.0835	0.7449	7.7266	1.0000
C(12*)	1.114(1)	0.0497(4)	0.8887(5)	8.6(3)	1.0000
H(10*)	0.9679	0.0282	0.8921	9.8993	1.0000
C(22*)	0.3802(5)	-0.2483(2)	0.3890(3)	3.9(1)	1.0000
C(27*)	0.3962(8)	-0.3117(4)	0.2923(5)	6.3(2)	1.0000
B(1*)	0.3562(5)	-0.1894(3)	0.4996(4)	3.6(1)	1.0000
C(17*)	1.042(1)	-0.1097(4)	0.9664(6)	8.7(3)	1.0000
H(14*)	0.9186	-0.1102	0.8802	8.2733	1.0000
C(19*)	1.2075(9)	-0.1014(5)	0.9389(6)	9.1(3)	1.0000
H(18*)	1.2051	-0.0855	0.8274	4.5840	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(12*)	1.2520	0.0739	0.8643	10.0188	1.0000
H(11*)	1.1455	0.0446	0.9380	10.6072	1.0000
H(19*)	0.3200	-0.2693	0.3917	4.6543	1.0000
F(1*)	0.3817(7)	-0.3565(3)	0.3269(4)	12.5(2)	1.0000
F(2*)	0.3114(7)	-0.3052(3)	0.2495(5)	18.5(3)	1.0000
F(3*)	0.4637(6)	-0.3303(3)	0.2596(4)	13.0(3)	1.0000
C(29*)	0.3504(4)	-0.1230(2)	0.5154(3)	3.5(1)	1.0000
C(37*)	0.2336(5)	-0.2106(2)	0.4873(3)	3.9(1)	1.0000
C(45*)	0.4375(5)	-0.2208(3)	0.5654(3)	4.0(1)	1.0000
C(18*)	1.150(1)	-0.1076(5)	0.9881(5)	8.8(3)	1.0000
H(15*)	1.0035	-0.1133	1.0012	10.6891	1.0000
H(17*)	1.2809	-0.0987	0.9540	11.1881	1.0000
C(30*)	0.3427(5)	-0.0823(3)	0.4640(3)	4.0(1)	1.0000
C(34*)	0.3444(5)	-0.1042(3)	0.5821(3)	4.0(1)	1.0000
C(38*)	0.1906(5)	-0.2243(3)	0.5433(4)	4.5(2)	1.0000
C(42*)	0.1641(5)	-0.2102(3)	0.4194(4)	4.5(2)	1.0000
C(46*)	0.5306(5)	-0.1958(3)	0.6036(4)	4.5(2)	1.0000
C(50*)	0.4285(6)	-0.2767(3)	0.5792(4)	5.9(2)	1.0000
H(16*)	1.1875	-0.1104	1.0368	10.5062	1.0000
C(31*)	0.3313(5)	-0.0267(3)	0.4781(4)	4.3(1)	1.0000
H(22*)	0.3455	-0.0930	0.4176	4.7632	1.0000
C(33*)	0.3337(5)	-0.0491(3)	0.5974(4)	4.3(1)	1.0000
H(24*)	0.3483	-0.1305	0.6187	4.7231	1.0000
C(39*)	0.0859(6)	-0.2382(3)	0.5334(5)	5.6(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(48*)	0.2490	-0.2168	0.5976	4.5840	1.0000
C(41*)	0.0588(5)	-0.2255(3)	0.4086(5)	5.5(2)	1.0000
H(50*)	0.1910	-0.2049	0.3710	4.5840	1.0000
C(47*)	0.6102(6)	-0.2247(4)	0.6506(4)	5.4(2)	1.0000
H(25*)	0.5429	-0.1500	0.5981	4.5840	1.0000
C(49*)	0.5070(9)	-0.3052(3)	0.6264(6)	8.1(3)	1.0000
H(27*)	0.3657	-0.2957	0.5555	7.1428	1.0000
C(32*)	0.3256(5)	-0.0100(3)	0.5451(4)	4.7(2)	1.0000
C(35*)	0.3292(7)	0.0148(3)	0.4222(5)	5.8(2)	1.0000
C(36*)	0.3318(7)	-0.0321(3)	0.6701(4)	5.6(2)	1.0000
C(40*)	0.0199(6)	-0.2392(3)	0.4655(6)	6.3(2)	1.0000
C(43*)	0.0444(9)	-0.2533(4)	0.5952(6)	8.1(3)	1.0000
C(44*)	-0.0073(6)	-0.2263(5)	0.3323(6)	8.0(3)	1.0000
C(48*)	0.5985(7)	-0.2794(4)	0.6614(5)	6.9(2)	1.0000
C(51*)	0.7064(7)	-0.1925(7)	0.6922(7)	11.4(4)	1.0000
C(52*)	0.514(2)	-0.3660(9)	0.620(1)	7.5(6)	0.5000
C(53*)	0.472(2)	-0.3637(9)	0.661(2)	7.8(7)	0.5000
H(23*)	0.3224	0.0303	0.5564	4.5840	1.0000
F(7*)	0.2568(5)	0.0068(3)	0.3650(3)	11.2(2)	1.0000
F(8*)	0.4126(5)	0.0224(4)	0.4054(4)	14.6(3)	1.0000
F(9*)	0.2997(9)	0.0642(3)	0.4385(4)	16.4(3)	1.0000
F(10*)	0.2732(6)	0.0119(2)	0.6713(3)	11.6(2)	1.0000
F(11*)	0.4205(5)	-0.0242(4)	0.7100(3)	14.5(3)	1.0000
F(12*)	0.2851(6)	-0.0676(2)	0.7032(3)	9.8(2)	1.0000

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(49*)	-0.0515	-0.2496	0.4588	7.7225	1.0000
F(13*)	0.0901(6)	-0.2289(3)	0.6530(4)	11.1(2)	1.0000
F(14*)	0.0349(8)	-0.3033(3)	0.6046(4)	15.3(3)	1.0000
F(15*)	-0.0560(6)	-0.2330(4)	0.5872(5)	14.9(3)	1.0000
F(16*)	-0.098(1)	-0.2652(5)	0.3414(7)	9.5(3)	0.5000
F(17*)	0.0017(7)	-0.2679(3)	0.2999(3)	14.0(3)	1.0000
F(18*)	-0.0834(7)	-0.1954(3)	0.3201(4)	13.0(2)	1.0000
F(19*)	0.0328(8)	-0.1931(4)	0.2840(5)	6.9(3)	0.5000
H(26*)	0.6531	-0.2998	0.6926	8.2764	1.0000
F(20*)	0.7192(9)	-0.1505(6)	0.6701(8)	30.1(6)	1.0000
F(21*)	0.7925(6)	-0.2210(6)	0.6848(5)	20.3(5)	1.0000
F(22*)	0.7241(6)	-0.1960(4)	0.7569(4)	12.6(3)	1.0000
F(23*)	0.558(2)	-0.3879(6)	0.570(1)	16.2(8)	0.5000
F(24*)	0.4161(8)	-0.3894(3)	0.6026(5)	12.9(3)	1.0000
F(25*)	0.5600(8)	-0.3914(3)	0.6779(5)	15.4(3)	1.0000
F(26*)	0.431(2)	-0.3640(6)	0.706(1)	15.5(8)	0.5000
H(41")	0.3788	-0.3997	0.7280	26.5457	1.0000

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd(1)	0.0596(3)	0.0484(3)	0.0596(3)	-0.0003(2)	0.0133(2)	-0.0041(2)
Pd(2)	0.0534(3)	0.0415(2)	0.0578(3)	-0.0012(2)	0.0108(2)	-0.0057(2)
F(1)	0.264(9)	0.092(4)	0.135(6)	-0.079(5)	0.083(6)	-0.051(4)
F(2)	0.216(9)	0.163(7)	0.222(9)	0.071(6)	-0.139(8)	-0.134(7)
F(3)	0.188(7)	0.159(6)	0.187(7)	-0.085(5)	0.124(6)	-0.125(6)
F(4)	0.23(1)	0.28(1)	0.69(3)	-0.18(1)	0.35(2)	-0.32(2)
F(5)	0.32(2)	0.50(2)	0.21(1)	-0.32(2)	-0.03(1)	0.15(2)
F(6)	0.141(6)	0.35(1)	0.210(9)	-0.170(8)	0.105(7)	-0.169(10)
F(7)	0.128(5)	0.155(6)	0.106(4)	-0.045(4)	-0.037(4)	0.069(4)
F(8)	0.075(4)	0.254(9)	0.228(8)	0.007(5)	0.041(5)	0.178(8)
F(9)	0.42(2)	0.078(4)	0.150(7)	0.060(7)	0.116(8)	0.048(4)
F(10)	0.249(8)	0.101(4)	0.114(5)	0.070(5)	0.085(5)	-0.007(4)
F(11)	0.096(4)	0.36(1)	0.088(4)	-0.045(6)	0.015(4)	-0.116(6)
F(12)	0.194(7)	0.111(4)	0.087(4)	-0.020(4)	0.071(4)	-0.010(3)
F(13)	0.179(7)	0.152(6)	0.116(5)	-0.069(5)	0.086(5)	-0.044(4)
F(14)	0.37(1)	0.074(4)	0.206(8)	-0.051(6)	0.206(9)	-0.023(4)
F(15)	0.132(6)	0.25(1)	0.223(9)	-0.012(6)	0.124(7)	-0.013(7)
F(17)	0.272(10)	0.114(5)	0.099(5)	0.068(6)	-0.044(6)	-0.042(4)
F(18)	0.191(8)	0.136(6)	0.125(6)	0.076(6)	-0.039(5)	-0.019(4)
F(19)	0.072(6)	0.105(7)	0.067(6)	-0.016(5)	-0.020(5)	0.014(5)
F(20)	0.22(1)	0.35(2)	0.41(2)	-0.21(1)	-0.23(1)	0.28(1)
F(21)	0.065(5)	0.51(2)	0.193(9)	-0.012(8)	0.019(5)	-0.10(1)
F(22)	0.121(5)	0.229(9)	0.114(5)	-0.063(6)	0.000(4)	-0.011(6)
F(23)	0.30(3)	0.079(9)	0.27(2)	0.03(1)	0.13(2)	0.01(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(24)	0.206(9)	0.070(4)	0.183(8)	-0.010(5)	-0.010(7)	0.015(5)
F(25)	0.234(10)	0.090(5)	0.212(9)	0.038(6)	-0.034(8)	0.057(5)
F(26)	0.29(3)	0.080(9)	0.27(2)	-0.01(1)	0.17(2)	0.05(1)
O(1)	0.08(1)	0.71(10)	0.21(3)	0.04(3)	0.03(2)	0.14(5)
O(2)	0.36(3)	0.34(3)	0.40(3)	0.16(3)	0.04(2)	0.01(2)
O(3)	0.26(2)	0.33(2)	0.33(2)	-0.11(2)	0.02(2)	0.06(2)
C(1)	0.074(5)	0.043(3)	0.068(5)	-0.004(3)	0.024(4)	-0.001(3)
C(2)	0.071(5)	0.044(3)	0.068(5)	0.000(3)	0.019(4)	-0.002(3)
C(3)	0.068(4)	0.038(3)	0.063(4)	0.001(3)	0.010(4)	-0.004(3)
C(4)	0.068(4)	0.035(3)	0.065(4)	0.002(3)	0.015(3)	-0.002(3)
C(5)	0.064(4)	0.036(3)	0.068(4)	-0.003(3)	0.012(3)	-0.006(3)
C(6)	0.067(4)	0.039(3)	0.066(4)	0.003(3)	0.012(4)	-0.008(3)
C(7)	0.070(4)	0.041(3)	0.059(4)	-0.001(3)	0.010(4)	-0.011(3)
C(8)	0.071(5)	0.047(4)	0.066(5)	0.001(3)	0.013(4)	-0.009(3)
C(9)	0.085(5)	0.048(4)	0.060(4)	-0.003(3)	0.019(4)	-0.014(3)
C(10)	0.107(7)	0.060(4)	0.067(5)	-0.001(4)	0.027(5)	-0.012(4)
C(11)	0.18(1)	0.067(5)	0.070(6)	-0.006(7)	0.050(7)	-0.011(4)
C(12)	0.17(1)	0.088(7)	0.061(6)	0.006(7)	0.012(7)	-0.016(5)
C(13)	0.119(9)	0.113(8)	0.077(7)	0.001(7)	0.006(6)	-0.017(6)
C(14)	0.094(6)	0.083(6)	0.067(5)	-0.003(5)	0.014(5)	-0.016(4)
C(15)	0.089(6)	0.049(4)	0.064(5)	0.006(4)	0.018(4)	0.006(3)
C(16)	0.120(8)	0.068(5)	0.082(6)	-0.003(5)	0.040(6)	0.003(4)
C(17)	0.17(1)	0.089(7)	0.083(8)	-0.001(8)	0.050(8)	0.006(6)
C(18)	0.16(1)	0.108(8)	0.055(6)	0.012(8)	0.012(7)	0.001(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(19)	0.121(9)	0.119(9)	0.092(8)	0.024(7)	0.003(7)	0.000(7)
C(20)	0.097(7)	0.102(7)	0.069(6)	0.015(5)	0.019(5)	0.010(5)
C(21)	0.044(3)	0.048(3)	0.049(3)	0.005(2)	0.007(3)	-0.005(3)
C(22)	0.049(3)	0.051(3)	0.048(4)	-0.005(3)	0.009(3)	-0.008(3)
C(23)	0.067(4)	0.051(4)	0.048(4)	-0.001(3)	0.010(3)	-0.008(3)
C(24)	0.079(5)	0.065(4)	0.068(5)	-0.012(4)	0.036(4)	-0.016(4)
C(25)	0.060(4)	0.063(4)	0.068(5)	-0.012(3)	0.024(4)	-0.011(3)
C(26)	0.053(4)	0.056(4)	0.049(4)	-0.006(3)	0.009(3)	-0.012(3)
C(27)	0.105(7)	0.072(5)	0.064(5)	-0.022(5)	0.027(5)	-0.033(4)
C(28)	0.17(1)	0.126(9)	0.17(1)	-0.093(9)	0.15(1)	-0.088(9)
C(29)	0.033(3)	0.049(3)	0.048(3)	-0.002(2)	0.006(2)	-0.005(3)
C(30)	0.041(3)	0.060(4)	0.046(3)	0.000(3)	0.004(3)	0.001(3)
C(31)	0.045(3)	0.053(4)	0.064(4)	-0.002(3)	0.008(3)	0.009(3)
C(32)	0.054(4)	0.050(4)	0.073(5)	0.001(3)	0.013(3)	-0.007(3)
C(33)	0.055(4)	0.050(4)	0.059(4)	0.003(3)	0.015(3)	-0.005(3)
C(34)	0.050(4)	0.050(3)	0.053(4)	0.000(3)	0.014(3)	0.001(3)
C(35)	0.068(5)	0.060(5)	0.084(6)	-0.005(4)	0.004(4)	0.016(4)
C(36)	0.093(6)	0.059(4)	0.065(5)	0.002(4)	0.026(5)	-0.015(4)
C(37)	0.046(3)	0.045(3)	0.058(4)	0.001(2)	0.011(3)	-0.007(3)
C(38)	0.051(4)	0.052(4)	0.072(5)	-0.006(3)	0.019(3)	-0.015(3)
C(39)	0.064(5)	0.055(4)	0.105(6)	-0.016(3)	0.041(5)	-0.026(4)
C(40)	0.047(4)	0.062(5)	0.132(8)	-0.007(3)	0.026(5)	-0.030(5)
C(41)	0.044(4)	0.064(4)	0.095(6)	0.003(3)	0.003(4)	-0.031(4)
C(42)	0.046(3)	0.054(4)	0.066(4)	0.005(3)	0.007(3)	-0.015(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(43)	0.099(7)	0.098(7)	0.136(10)	-0.039(6)	0.075(7)	-0.039(7)
C(44)	0.041(4)	0.116(8)	0.127(9)	0.011(5)	-0.018(5)	-0.060(7)
C(45)	0.050(4)	0.058(4)	0.045(3)	0.008(3)	0.013(3)	-0.002(3)
C(46)	0.050(4)	0.068(4)	0.051(4)	0.001(3)	0.008(3)	0.005(3)
C(47)	0.048(4)	0.100(6)	0.055(4)	0.008(4)	0.007(3)	0.017(4)
C(48)	0.079(6)	0.089(6)	0.082(6)	0.033(5)	-0.003(5)	0.020(5)
C(49)	0.117(8)	0.052(5)	0.115(8)	0.020(5)	-0.020(6)	0.010(5)
C(50)	0.081(5)	0.043(4)	0.086(6)	0.005(3)	-0.008(4)	-0.002(4)
C(51)	0.048(5)	0.25(2)	0.116(9)	-0.026(7)	-0.021(5)	0.12(1)
C(52)	0.09(2)	0.08(1)	0.11(2)	0.03(1)	0.02(1)	0.02(1)
C(53)	0.13(2)	0.07(1)	0.12(2)	0.00(1)	0.06(2)	0.01(1)
C(54)	0.16(3)	0.28(5)	0.36(6)	0.06(3)	0.09(3)	0.16(5)
C(55)	0.5(1)	0.14(3)	0.22(5)	-0.16(5)	0.21(7)	-0.05(3)
C(56)	0.23(6)	0.07(2)	0.34(7)	-0.04(3)	0.08(6)	-0.10(4)
C(57)	0.12(2)	0.17(4)	0.24(5)	0.08(2)	0.01(2)	-0.02(3)
C(58)	0.79(10)	0.38(6)	0.67(8)	0.14(6)	-0.31(7)	0.16(5)
C(59)	0.45(7)	0.6(1)	0.34(5)	0.09(6)	0.20(5)	-0.18(6)
C(60)	0.60(7)	0.25(4)	0.67(8)	-0.22(4)	0.46(6)	-0.08(4)
C(61)	0.29(4)	0.35(5)	0.66(8)	0.14(4)	0.01(4)	0.18(5)
B(1)	0.039(3)	0.045(3)	0.047(4)	-0.002(3)	0.002(3)	-0.004(3)
Pd(2*)	0.0534(3)	0.0415(2)	0.0578(3)	-0.0012(2)	0.0108(2)	-0.0057(2)
C(6*)	0.067(4)	0.039(3)	0.066(4)	0.003(3)	0.012(4)	-0.008(3)
C(28*)	0.17(1)	0.126(9)	0.17(1)	-0.093(9)	0.15(1)	-0.088(9)
C(7*)	0.070(4)	0.041(3)	0.059(4)	-0.001(3)	0.010(4)	-0.011(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(6*)	0.141(6)	0.35(1)	0.210(9)	-0.170(8)	0.105(7)	-0.169(10)
Pd(1*)	0.0596(3)	0.0484(3)	0.0596(3)	-0.0003(2)	0.0133(2)	-0.0041(2)
C(4*)	0.068(4)	0.035(3)	0.065(4)	0.002(3)	0.015(3)	-0.002(3)
C(5*)	0.064(4)	0.036(3)	0.068(4)	-0.003(3)	0.012(3)	-0.006(3)
F(4*)	0.23(1)	0.28(1)	0.69(3)	-0.18(1)	0.35(2)	-0.32(2)
F(5*)	0.32(2)	0.50(2)	0.21(1)	-0.32(2)	-0.03(1)	0.15(2)
C(25*)	0.060(4)	0.063(4)	0.068(5)	-0.012(3)	0.024(4)	-0.011(3)
C(8*)	0.071(5)	0.047(4)	0.066(5)	0.001(3)	0.013(4)	-0.009(3)
C(1*)	0.074(5)	0.043(3)	0.068(5)	-0.004(3)	0.024(4)	-0.001(3)
C(2*)	0.071(5)	0.044(3)	0.068(5)	0.000(3)	0.019(4)	-0.002(3)
C(3*)	0.068(4)	0.038(3)	0.063(4)	0.001(3)	0.010(4)	-0.004(3)
C(9*)	0.085(5)	0.048(4)	0.060(4)	-0.003(3)	0.019(4)	-0.014(3)
C(10*)	0.107(7)	0.060(4)	0.067(5)	-0.001(4)	0.027(5)	-0.012(4)
C(24*)	0.079(5)	0.065(4)	0.068(5)	-0.012(4)	0.036(4)	-0.016(4)
C(26*)	0.053(4)	0.056(4)	0.049(4)	-0.006(3)	0.009(3)	-0.012(3)
C(15*)	0.089(6)	0.049(4)	0.064(5)	0.006(4)	0.018(4)	0.006(3)
C(14*)	0.094(6)	0.083(6)	0.067(5)	-0.003(5)	0.014(5)	-0.016(4)
C(11*)	0.18(1)	0.067(5)	0.070(6)	-0.006(7)	0.050(7)	-0.011(4)
C(23*)	0.067(4)	0.051(4)	0.048(4)	-0.001(3)	0.010(3)	-0.008(3)
C(21*)	0.044(3)	0.048(3)	0.049(3)	0.005(2)	0.007(3)	-0.005(3)
C(16*)	0.120(8)	0.068(5)	0.082(6)	-0.003(5)	0.040(6)	0.003(4)
C(20*)	0.097(7)	0.102(7)	0.069(6)	0.015(5)	0.019(5)	0.010(5)
C(13*)	0.119(9)	0.113(8)	0.077(7)	0.001(7)	0.006(6)	-0.017(6)
C(12*)	0.17(1)	0.088(7)	0.061(6)	0.006(7)	0.012(7)	-0.016(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(22*)	0.049(3)	0.051(3)	0.048(4)	-0.005(3)	0.009(3)	-0.008(3)
C(27*)	0.105(7)	0.072(5)	0.064(5)	-0.022(5)	0.027(5)	-0.033(4)
B(1*)	0.039(3)	0.045(3)	0.047(4)	-0.002(3)	0.002(3)	-0.004(3)
C(17*)	0.17(1)	0.089(7)	0.083(8)	-0.001(8)	0.050(8)	0.006(6)
C(19*)	0.121(9)	0.119(9)	0.092(8)	0.024(7)	0.003(7)	0.000(7)
F(1*)	0.264(9)	0.092(4)	0.135(6)	-0.079(5)	0.083(6)	-0.051(4)
F(2*)	0.216(9)	0.163(7)	0.222(9)	0.071(6)	-0.139(8)	-0.134(7)
F(3*)	0.188(7)	0.159(6)	0.187(7)	-0.085(5)	0.124(6)	-0.125(6)
C(29*)	0.033(3)	0.049(3)	0.048(3)	-0.002(2)	0.006(2)	-0.005(3)
C(37*)	0.046(3)	0.045(3)	0.058(4)	0.001(2)	0.011(3)	-0.007(3)
C(45*)	0.050(4)	0.058(4)	0.045(3)	0.008(3)	0.013(3)	-0.002(3)
C(18*)	0.16(1)	0.108(8)	0.055(6)	0.012(8)	0.012(7)	0.001(5)
C(30*)	0.041(3)	0.060(4)	0.046(3)	0.000(3)	0.004(3)	0.001(3)
C(34*)	0.050(4)	0.050(3)	0.053(4)	0.000(3)	0.014(3)	0.001(3)
C(38*)	0.051(4)	0.052(4)	0.072(5)	-0.006(3)	0.019(3)	-0.015(3)
C(42*)	0.046(3)	0.054(4)	0.066(4)	0.005(3)	0.007(3)	-0.015(3)
C(46*)	0.050(4)	0.068(4)	0.051(4)	0.001(3)	0.008(3)	0.005(3)
C(50*)	0.081(5)	0.043(4)	0.086(6)	0.005(3)	-0.008(4)	-0.002(4)
C(31*)	0.045(3)	0.053(4)	0.064(4)	-0.002(3)	0.008(3)	0.009(3)
C(33*)	0.055(4)	0.050(4)	0.059(4)	0.003(3)	0.015(3)	-0.005(3)
C(39*)	0.064(5)	0.055(4)	0.105(6)	-0.016(3)	0.041(5)	-0.026(4)
C(41*)	0.044(4)	0.064(4)	0.095(6)	0.003(3)	0.003(4)	-0.031(4)
C(47*)	0.048(4)	0.100(6)	0.055(4)	0.008(4)	0.007(3)	0.017(4)
C(49*)	0.117(8)	0.052(5)	0.115(8)	0.020(5)	-0.020(6)	0.010(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(32*)	0.054(4)	0.050(4)	0.073(5)	0.001(3)	0.013(3)	-0.007(3)
C(35*)	0.068(5)	0.060(5)	0.084(6)	-0.005(4)	0.004(4)	0.016(4)
C(36*)	0.093(6)	0.059(4)	0.065(5)	0.002(4)	0.026(5)	-0.015(4)
C(40*)	0.047(4)	0.062(5)	0.132(8)	-0.007(3)	0.026(5)	-0.030(5)
C(43*)	0.099(7)	0.098(7)	0.136(10)	-0.039(6)	0.075(7)	-0.039(7)
C(44*)	0.041(4)	0.116(8)	0.127(9)	0.011(5)	-0.018(5)	-0.060(7)
C(48*)	0.079(6)	0.089(6)	0.082(6)	0.033(5)	-0.003(5)	0.020(5)
C(51*)	0.048(5)	0.25(2)	0.116(9)	-0.026(7)	-0.021(5)	0.12(1)
C(52*)	0.09(2)	0.08(1)	0.11(2)	0.03(1)	0.02(1)	0.02(1)
C(53*)	0.13(2)	0.07(1)	0.12(2)	0.00(1)	0.06(2)	0.01(1)
F(7*)	0.128(5)	0.155(6)	0.106(4)	-0.045(4)	-0.037(4)	0.069(4)
F(8*)	0.075(4)	0.254(9)	0.228(8)	0.007(5)	0.041(5)	0.178(8)
F(9*)	0.42(2)	0.078(4)	0.150(7)	0.060(7)	0.116(8)	0.048(4)
F(10*)	0.249(8)	0.101(4)	0.114(5)	0.070(5)	0.085(5)	-0.007(4)
F(11*)	0.096(4)	0.36(1)	0.088(4)	-0.045(6)	0.015(4)	-0.116(6)
F(12*)	0.194(7)	0.111(4)	0.087(4)	-0.020(4)	0.071(4)	-0.010(3)
F(13*)	0.179(7)	0.152(6)	0.116(5)	-0.069(5)	0.086(5)	-0.044(4)
F(14*)	0.37(1)	0.074(4)	0.206(8)	-0.051(6)	0.206(9)	-0.023(4)
F(15*)	0.132(6)	0.25(1)	0.223(9)	-0.012(6)	0.124(7)	-0.013(7)
F(17*)	0.272(10)	0.114(5)	0.099(5)	0.068(6)	-0.044(6)	-0.042(4)
F(18*)	0.191(8)	0.136(6)	0.125(6)	0.076(6)	-0.039(5)	-0.019(4)
F(19*)	0.072(6)	0.105(7)	0.067(6)	-0.016(5)	-0.020(5)	0.014(5)
F(20*)	0.22(1)	0.35(2)	0.41(2)	-0.21(1)	-0.23(1)	0.28(1)
F(21*)	0.065(5)	0.51(2)	0.193(9)	-0.012(8)	0.019(5)	-0.10(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(22*)	0.121(5)	0.229(9)	0.114(5)	-0.063(6)	0.000(4)	-0.011(6)
F(23*)	0.30(3)	0.079(9)	0.27(2)	0.03(1)	0.13(2)	0.01(1)
F(24*)	0.206(9)	0.070(4)	0.183(8)	-0.010(5)	-0.010(7)	0.015(5)
F(25*)	0.234(10)	0.090(5)	0.212(9)	0.038(6)	-0.034(8)	0.057(5)
F(26*)	0.29(3)	0.080(9)	0.27(2)	-0.01(1)	0.17(2)	0.05(1)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Pd(1)	Pd(2)	2.7322(8)	Pd(1)	C(1)	2.282(7)
Pd(1)	C(2)	2.168(7)	Pd(1)	C(3)	2.242(6)
Pd(1)	C(8)	2.236(7)	Pd(1)	C(9)	2.206(7)
Pd(1)	C(10)	2.421(8)	Pd(2)	Pd(2)	2.654(1)
Pd(2)	C(4)	2.182(6)	Pd(2)	C(5)	2.219(6)
Pd(2)	C(6)	2.223(6)	Pd(2)	C(7)	2.185(6)
F(1)	C(27)	1.32(1)	F(2)	C(27)	1.22(1)
F(3)	C(27)	1.293(10)	F(4)	C(28)	1.21(1)
F(5)	C(28)	1.28(2)	F(6)	C(28)	1.14(1)
F(7)	C(35)	1.286(9)	F(8)	C(35)	1.231(10)
F(9)	C(35)	1.32(1)	F(10)	C(36)	1.317(9)
F(11)	C(36)	1.242(10)	F(12)	C(36)	1.314(9)
F(13)	C(43)	1.28(1)	F(14)	C(43)	1.24(1)
F(15)	C(43)	1.38(1)	F(16)	F(17)	1.70(1)
F(16)	C(44)	1.56(2)	F(17)	C(44)	1.211(10)
F(18)	C(44)	1.221(10)	F(19)	C(44)	1.43(1)
F(20)	C(51)	1.13(1)	F(21)	C(51)	1.36(2)
F(22)	C(51)	1.23(1)	F(23)	C(52)	1.36(3)
F(24)	C(52)	1.37(2)	F(24)	C(53)	1.35(3)
F(25)	C(52)	1.29(2)	F(25)	C(53)	1.30(3)
F(26)	C(53)	1.14(3)	O(1)	C(55)	0.96(8)
O(1)	C(56)	1.39(6)	O(2)	C(59)	1.49(6)
O(2)	C(60)	1.65(4)	C(1)	C(2)	1.393(10)
C(1)	C(15)	1.48(1)	C(2)	C(3)	1.420(10)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(3)	C(4)	1.425(10)	C(4)	C(5)	1.410(9)
C(5)	C(6)	1.419(10)	C(6)	C(7)	1.408(10)
C(7)	C(8)	1.42(1)	C(8)	C(9)	1.454(10)
C(9)	C(10)	1.43(1)	C(9)	C(14)	1.42(1)
C(10)	C(11)	1.40(1)	C(11)	C(12)	1.35(2)
C(12)	C(13)	1.40(2)	C(13)	C(14)	1.37(1)
C(15)	C(16)	1.39(1)	C(15)	C(20)	1.38(1)
C(16)	C(17)	1.38(1)	C(17)	C(18)	1.37(2)
C(18)	C(19)	1.37(2)	C(19)	C(20)	1.37(1)
C(21)	C(22)	1.396(8)	C(21)	C(26)	1.403(9)
C(21)	B(1)	1.631(9)	C(22)	C(23)	1.384(9)
C(23)	C(24)	1.369(10)	C(23)	C(27)	1.498(9)
C(24)	C(25)	1.381(9)	C(25)	C(26)	1.385(9)
C(25)	C(28)	1.49(1)	C(29)	C(30)	1.392(8)
C(29)	C(34)	1.399(8)	C(29)	B(1)	1.643(9)
C(30)	C(31)	1.391(9)	C(31)	C(32)	1.385(10)
C(31)	C(35)	1.479(10)	C(32)	C(33)	1.378(9)
C(33)	C(34)	1.381(8)	C(33)	C(36)	1.483(10)
C(37)	C(38)	1.388(9)	C(37)	C(42)	1.407(9)
C(37)	B(1)	1.645(9)	C(38)	C(39)	1.377(9)
C(39)	C(40)	1.39(1)	C(39)	C(43)	1.49(1)
C(40)	C(41)	1.37(1)	C(41)	C(42)	1.392(9)
C(41)	C(44)	1.52(1)	C(45)	C(46)	1.398(9)
C(45)	C(50)	1.390(9)	C(45)	B(1)	1.637(9)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(46)	C(47)	1.393(9)	C(47)	C(48)	1.36(1)
C(47)	C(51)	1.53(1)	C(48)	C(49)	1.37(1)
C(49)	C(50)	1.38(1)	C(49)	C(52)	1.48(2)
C(49)	C(53)	1.68(3)	C(52)	C(53)	1.08(3)
C(54)	C(55)	1.66(7)	C(56)	C(57)	0.60(7)
C(58)	C(59)	1.49(7)	C(60)	C(61)	1.03(5)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
F(26)	H(41)	1.24	C(1)	H(1)	1.22
C(2)	H(2)	1.07	C(3)	H(3)	1.03
C(4)	H(4)	1.10	C(5)	H(5)	1.05
C(6)	H(6)	1.07	C(7)	H(7)	1.14
C(8)	H(8)	1.06	C(10)	H(9)	1.19
C(11)	H(10)	0.96	C(12)	H(11)	0.95
C(13)	H(12)	0.96	C(14)	H(13)	0.95
C(16)	H(14)	0.93	C(17)	H(15)	0.95
C(18)	H(16)	0.96	C(19)	H(17)	0.93
C(20)	H(18)	1.16	C(22)	H(19)	0.95
C(24)	H(20)	0.95	C(26)	H(21)	1.09
C(30)	H(22)	0.95	C(32)	H(23)	1.00
C(34)	H(24)	0.95	C(38)	H(48)	1.16
C(40)	H(49)	0.95	C(42)	H(50)	1.09
C(46)	H(25)	1.13	C(48)	H(26)	0.95
C(50)	H(27)	0.95	C(54)	H(28)	0.95
C(54)	H(29)	1.03	C(54)	H(30)	1.00
C(55)	H(31)	1.10	C(55)	H(32)	1.11
C(56)	H(33)	1.12	C(56)	H(34)	1.07
C(56)	H(35)	1.25	C(56)	H(36)	1.21
C(56)	H(37)	1.29	C(57)	H(35)	0.99
C(57)	H(36)	0.92	C(57)	H(37)	0.91
C(58)	H(38)	0.84	C(58)	H(39)	0.98
C(58)	H(40)	0.99	C(59)	H(41)	0.92

Table 4. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(59)	H(42)	0.94	C(60)	H(43)	0.88
C(60)	H(44)	1.10	C(61)	H(45)	0.93
C(61)	H(46)	0.92	C(61)	H(47)	1.05

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Pd(2)	Pd(1)	C(1)	130.6(2)	Pd(2)	Pd(1)	C(2)	97.1(2)
Pd(2)	Pd(1)	C(3)	65.6(2)	Pd(2)	Pd(1)	C(8)	65.0(2)
Pd(2)	Pd(1)	C(9)	99.2(2)	Pd(2)	Pd(1)	C(10)	128.2(2)
C(1)	Pd(1)	C(2)	36.4(2)	C(1)	Pd(1)	C(3)	65.1(3)
C(1)	Pd(1)	C(8)	162.2(3)	C(1)	Pd(1)	C(9)	129.8(3)
C(1)	Pd(1)	C(10)	99.9(3)	C(2)	Pd(1)	C(3)	37.5(2)
C(2)	Pd(1)	C(8)	161.3(3)	C(2)	Pd(1)	C(9)	151.7(3)
C(2)	Pd(1)	C(10)	134.7(3)	C(3)	Pd(1)	C(8)	128.5(3)
C(3)	Pd(1)	C(9)	164.7(3)	C(3)	Pd(1)	C(10)	157.7(3)
C(8)	Pd(1)	C(9)	38.2(3)	C(8)	Pd(1)	C(10)	63.4(3)
C(9)	Pd(1)	C(10)	35.6(3)	Pd(1)	Pd(2)	Pd(2)	178.25(4)
Pd(1)	Pd(2)	C(4)	76.3(2)	Pd(1)	Pd(2)	C(5)	108.2(2)
Pd(1)	Pd(2)	C(6)	108.0(2)	Pd(1)	Pd(2)	C(7)	76.0(2)
Pd(2)	Pd(2)	C(4)	104.2(2)	Pd(2)	Pd(2)	C(5)	71.8(2)
Pd(2)	Pd(2)	C(6)	71.5(2)	Pd(2)	Pd(2)	C(7)	104.1(2)
C(4)	Pd(2)	C(5)	37.4(2)	C(4)	Pd(2)	C(6)	175.7(3)
C(4)	Pd(2)	C(7)	146.1(3)	C(5)	Pd(2)	C(6)	139.2(3)
C(5)	Pd(2)	C(7)	175.9(3)	C(6)	Pd(2)	C(7)	37.2(2)
F(17)	F(16)	C(44)	43.4(5)	F(16)	F(17)	C(44)	62.2(8)
C(52)	F(24)	C(53)	46(1)	C(52)	F(25)	C(53)	49(1)
C(55)	O(1)	C(56)	169(7)	C(59)	O(2)	C(60)	142(4)
Pd(1)	C(1)	C(2)	67.4(4)	Pd(1)	C(1)	C(15)	118.5(5)
C(2)	C(1)	C(15)	124.8(7)	Pd(1)	C(2)	C(1)	76.3(4)
Pd(1)	C(2)	C(3)	74.1(4)	C(1)	C(2)	C(3)	119.9(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Pd(1)	C(3)	C(2)	68.4(4)	Pd(1)	C(3)	C(4)	111.5(4)
C(2)	C(3)	C(4)	122.0(7)	Pd(2)	C(4)	C(3)	95.9(4)
Pd(2)	C(4)	C(5)	72.7(4)	C(3)	C(4)	C(5)	123.8(7)
Pd(2)	C(5)	C(4)	69.9(3)	Pd(2)	C(5)	C(6)	102.0(4)
C(4)	C(5)	C(6)	122.9(6)	Pd(2)	C(6)	C(5)	102.1(4)
Pd(2)	C(6)	C(7)	69.9(4)	C(5)	C(6)	C(7)	123.7(7)
Pd(2)	C(7)	C(6)	72.9(4)	Pd(2)	C(7)	C(8)	94.8(4)
C(6)	C(7)	C(8)	122.3(7)	Pd(1)	C(8)	C(7)	111.5(5)
Pd(1)	C(8)	C(9)	69.8(4)	C(7)	C(8)	C(9)	125.7(7)
Pd(1)	C(9)	C(8)	72.0(4)	Pd(1)	C(9)	C(10)	80.4(4)
Pd(1)	C(9)	C(14)	110.6(5)	C(8)	C(9)	C(10)	116.5(7)
C(8)	C(9)	C(14)	124.8(7)	C(10)	C(9)	C(14)	118.2(8)
Pd(1)	C(10)	C(9)	64.0(4)	Pd(1)	C(10)	C(11)	119.3(6)
C(9)	C(10)	C(11)	119.5(9)	C(10)	C(11)	C(12)	120(1)
C(11)	C(12)	C(13)	120.7(10)	C(12)	C(13)	C(14)	121(1)
C(9)	C(14)	C(13)	120.0(9)	C(1)	C(15)	C(16)	118.1(8)
C(1)	C(15)	C(20)	123.0(8)	C(16)	C(15)	C(20)	119.0(8)
C(15)	C(16)	C(17)	120.0(10)	C(16)	C(17)	C(18)	120(1)
C(17)	C(18)	C(19)	119(1)	C(18)	C(19)	C(20)	120(1)
C(15)	C(20)	C(19)	120.4(10)	C(22)	C(21)	C(26)	114.9(6)
C(22)	C(21)	B(1)	123.5(6)	C(26)	C(21)	B(1)	120.6(5)
C(21)	C(22)	C(23)	122.6(6)	C(22)	C(23)	C(24)	121.2(6)
C(22)	C(23)	C(27)	118.7(7)	C(24)	C(23)	C(27)	120.1(7)
C(23)	C(24)	C(25)	117.8(6)	C(24)	C(25)	C(26)	121.1(6)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(24)	C(25)	C(28)	120.3(7)	C(26)	C(25)	C(28)	118.3(7)
C(21)	C(26)	C(25)	122.3(6)	F(1)	C(27)	F(2)	103.5(9)
F(1)	C(27)	F(3)	99.6(8)	F(1)	C(27)	C(23)	112.6(7)
F(2)	C(27)	F(3)	108.9(9)	F(2)	C(27)	C(23)	116.6(8)
F(3)	C(27)	C(23)	113.8(8)	F(4)	C(28)	F(5)	92(1)
F(4)	C(28)	F(6)	113(1)	F(4)	C(28)	C(25)	115.8(9)
F(5)	C(28)	F(6)	96(1)	F(5)	C(28)	C(25)	107(1)
F(6)	C(28)	C(25)	123.0(9)	C(30)	C(29)	C(34)	115.3(5)
C(30)	C(29)	B(1)	123.9(6)	C(34)	C(29)	B(1)	120.7(5)
C(29)	C(30)	C(31)	122.4(6)	C(30)	C(31)	C(32)	120.2(6)
C(30)	C(31)	C(35)	119.7(7)	C(32)	C(31)	C(35)	120.0(7)
C(31)	C(32)	C(33)	118.9(6)	C(32)	C(33)	C(34)	119.9(6)
C(32)	C(33)	C(36)	119.9(6)	C(34)	C(33)	C(36)	120.1(6)
C(29)	C(34)	C(33)	123.2(6)	F(7)	C(35)	F(8)	107.6(9)
F(7)	C(35)	F(9)	98.5(8)	F(7)	C(35)	C(31)	114.3(7)
F(8)	C(35)	F(9)	105.2(9)	F(8)	C(35)	C(31)	116.3(7)
F(9)	C(35)	C(31)	113.1(8)	F(10)	C(36)	F(11)	108.9(8)
F(10)	C(36)	F(12)	100.2(7)	F(10)	C(36)	C(33)	113.1(7)
F(11)	C(36)	F(12)	105.6(8)	F(11)	C(36)	C(33)	113.9(7)
F(12)	C(36)	C(33)	114.1(7)	C(38)	C(37)	C(42)	116.6(6)
C(38)	C(37)	B(1)	122.1(6)	C(42)	C(37)	B(1)	121.0(6)
C(37)	C(38)	C(39)	122.2(7)	C(38)	C(39)	C(40)	120.0(8)
C(38)	C(39)	C(43)	119.9(9)	C(40)	C(39)	C(43)	120.1(8)
C(39)	C(40)	C(41)	119.9(7)	C(40)	C(41)	C(42)	119.7(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(40)	C(41)	C(44)	123.5(8)	C(42)	C(41)	C(44)	116.9(9)
C(37)	C(42)	C(41)	121.7(7)	F(13)	C(43)	F(14)	111(1)
F(13)	C(43)	F(15)	99.2(9)	F(13)	C(43)	C(39)	114.6(8)
F(14)	C(43)	F(15)	103.7(9)	F(14)	C(43)	C(39)	115.6(8)
F(15)	C(43)	C(39)	110(1)	F(16)	C(44)	F(17)	74.4(9)
F(16)	C(44)	F(18)	77.6(8)	F(16)	C(44)	F(19)	145.8(9)
F(16)	C(44)	C(41)	99(1)	F(17)	C(44)	F(18)	126.2(9)
F(17)	C(44)	F(19)	91(1)	F(17)	C(44)	C(41)	114.4(9)
F(18)	C(44)	F(19)	86(1)	F(18)	C(44)	C(41)	114.8(8)
F(19)	C(44)	C(41)	115.0(8)	C(46)	C(45)	C(50)	115.1(6)
C(46)	C(45)	B(1)	121.8(6)	C(50)	C(45)	B(1)	122.3(6)
C(45)	C(46)	C(47)	122.9(7)	C(46)	C(47)	C(48)	119.9(7)
C(46)	C(47)	C(51)	118.4(8)	C(48)	C(47)	C(51)	121.7(8)
C(47)	C(48)	C(49)	119.1(7)	C(48)	C(49)	C(50)	121.0(8)
C(48)	C(49)	C(52)	115(1)	C(48)	C(49)	C(53)	118(1)
C(50)	C(49)	C(52)	119(1)	C(50)	C(49)	C(53)	117(1)
C(52)	C(49)	C(53)	39(1)	C(45)	C(50)	C(49)	122.0(7)
F(20)	C(51)	F(21)	102(1)	F(20)	C(51)	F(22)	116(1)
F(20)	C(51)	C(47)	115.8(8)	F(21)	C(51)	F(22)	97.2(9)
F(21)	C(51)	C(47)	106(1)	F(22)	C(51)	C(47)	115.5(9)
F(23)	C(52)	F(24)	101(2)	F(23)	C(52)	F(25)	104(1)
F(23)	C(52)	C(49)	119(1)	F(23)	C(52)	C(53)	159(2)
F(24)	C(52)	F(25)	103(1)	F(24)	C(52)	C(49)	110(1)
F(24)	C(52)	C(53)	65(2)	F(25)	C(52)	C(49)	115(2)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(25)	C(52)	C(53)	66(2)	C(49)	C(52)	C(53)	80(2)
F(24)	C(53)	F(25)	103(1)	F(24)	C(53)	F(26)	113(2)
F(24)	C(53)	C(49)	101(1)	F(24)	C(53)	C(52)	67(2)
F(25)	C(53)	F(26)	111(2)	F(25)	C(53)	C(49)	102(1)
F(25)	C(53)	C(52)	64(1)	F(26)	C(53)	C(49)	123(1)
F(26)	C(53)	C(52)	175(3)	C(49)	C(53)	C(52)	60(1)
O(1)	C(55)	C(54)	171(7)	O(1)	C(56)	C(57)	158(10)
O(2)	C(59)	C(58)	120(5)	O(2)	C(60)	C(61)	149(6)
C(21)	B(1)	C(29)	113.3(5)	C(21)	B(1)	C(37)	114.3(5)
C(21)	B(1)	C(45)	101.3(5)	C(29)	B(1)	C(37)	104.1(5)
C(29)	B(1)	C(45)	111.1(5)	C(37)	B(1)	C(45)	113.0(5)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(53)	F(26)	H(41)	132.2	Pd(1)	C(1)	H(1)	87.9
C(2)	C(1)	H(1)	126.3	C(15)	C(1)	H(1)	108.9
Pd(1)	C(2)	H(2)	103.4	C(1)	C(2)	H(2)	107.7
C(3)	C(2)	H(2)	129.4	Pd(1)	C(3)	H(3)	96.1
C(2)	C(3)	H(3)	120.2	C(4)	C(3)	H(3)	117.4
Pd(2)	C(4)	H(4)	110.2	C(3)	C(4)	H(4)	116.4
C(5)	C(4)	H(4)	119.1	Pd(2)	C(5)	H(5)	101.5
C(4)	C(5)	H(5)	108.8	C(6)	C(5)	H(5)	127.9
Pd(2)	C(6)	H(6)	102.0	C(5)	C(6)	H(6)	118.5
C(7)	C(6)	H(6)	117.7	Pd(2)	C(7)	H(7)	108.1
C(6)	C(7)	H(7)	124.1	C(8)	C(7)	H(7)	113.4
Pd(1)	C(8)	H(8)	102.7	C(7)	C(8)	H(8)	115.6
C(9)	C(8)	H(8)	116.7	Pd(1)	C(10)	H(9)	80.2
C(9)	C(10)	H(9)	111.7	C(11)	C(10)	H(9)	128.7
C(10)	C(11)	H(10)	120.3	C(12)	C(11)	H(10)	119.2
C(11)	C(12)	H(11)	120.7	C(13)	C(12)	H(11)	118.6
C(12)	C(13)	H(12)	121.1	C(14)	C(13)	H(12)	117.8
C(9)	C(14)	H(13)	119.8	C(13)	C(14)	H(13)	120.2
C(15)	C(16)	H(14)	119.7	C(17)	C(16)	H(14)	120.3
C(16)	C(17)	H(15)	121.3	C(18)	C(17)	H(15)	118.4
C(17)	C(18)	H(16)	122.4	C(19)	C(18)	H(16)	118.1
C(18)	C(19)	H(17)	119.2	C(20)	C(19)	H(17)	119.8
C(15)	C(20)	H(18)	117.6	C(19)	C(20)	H(18)	121.0
C(21)	C(22)	H(19)	118.8	C(23)	C(22)	H(19)	118.5

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(23)	C(24)	H(20)	121.0	C(25)	C(24)	H(20)	121.2
C(21)	C(26)	H(21)	112.1	C(25)	C(26)	H(21)	124.6
C(29)	C(30)	H(22)	118.7	C(31)	C(30)	H(22)	118.9
C(31)	C(32)	H(23)	120.5	C(33)	C(32)	H(23)	120.4
C(29)	C(34)	H(24)	118.3	C(33)	C(34)	H(24)	118.5
C(37)	C(38)	H(48)	112.2	C(39)	C(38)	H(48)	125.2
C(39)	C(40)	H(49)	119.7	C(41)	C(40)	H(49)	120.4
C(37)	C(42)	H(50)	122.7	C(41)	C(42)	H(50)	114.9
C(45)	C(46)	H(25)	120.1	C(47)	C(46)	H(25)	117.0
C(47)	C(48)	H(26)	120.7	C(49)	C(48)	H(26)	120.2
C(45)	C(50)	H(27)	118.7	C(49)	C(50)	H(27)	119.3
C(55)	C(54)	H(28)	127.6	C(55)	C(54)	H(29)	108.5
C(55)	C(54)	H(30)	108.2	H(28)	C(54)	H(29)	103.3
H(28)	C(54)	H(30)	105.7	H(29)	C(54)	H(30)	100.2
O(1)	C(55)	H(31)	97.9	O(1)	C(55)	H(32)	98.3
C(54)	C(55)	H(31)	88.9	C(54)	C(55)	H(32)	87.3
H(31)	C(55)	H(32)	89.3	O(1)	C(56)	H(33)	76.0
O(1)	C(56)	H(34)	81.3	O(1)	C(56)	H(35)	110.8
O(1)	C(56)	H(36)	124.9	O(1)	C(56)	H(37)	158.0
C(57)	C(56)	H(33)	114.3	C(57)	C(56)	H(34)	116.1
C(57)	C(56)	H(35)	50.9	C(57)	C(56)	H(36)	47.4
C(57)	C(56)	H(37)	39.3	H(33)	C(56)	H(34)	90.1
H(33)	C(56)	H(35)	97.9	H(33)	C(56)	H(36)	158.9
H(33)	C(56)	H(37)	82.3	H(34)	C(56)	H(35)	166.7