Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(34)	C(56)	H(36)	90.7	H(34)	C(56)	H(37)	95.4
H(35)	C(56)	H(36)	78.0	H(35)	C(56)	H(37)	75.4
H(36)	C(56)	H(37)	76.6	C(56)	C(57)	H(35)	101.1
C(56)	C(57)	H(36)	104.1	C(56)	C(57)	H(37)	116.0
H(35)	C(57)	H(36)	108.6	H(35)	C(57)	H(37)	109.7
H(36)	C(57)	H(37)	116.0	C(59)	C(58)	H(38)	114.0
C(59)	C(58)	H(39)	101.7	C(59)	C(58)	H(40)	105.5
H(38)	C(58)	H(39)	115.9	H(38)	C(58)	H(40)	114.8
H(39)	C(58)	H(40)	103.3	O(2)	C(59)	H(41)	99.5
O(2)	C(59)	H(42)	99.0	C(58)	C(59)	H(41)	109.8
C(58)	C(59)	H(42)	114.8	H(41)	C(59)	H(42)	112.4
O(2)	C(60)	H(43)	93.6	O(2)	C(60)	H(44)	83.7
C(61)	C(60)	H(43)	113.9	C(61)	C(60)	H(44)	101.5
H(43)	C(60)	H(44)	102.4	C(60)	C(61)	H(45)	107.0
C(60)	C(61)	H(46)	117.9	C(60)	C(61)	H(47)	110.3
H(45)	C(61)	H(46)	113.8	H(45)	C(61)	H(47)	103.3
H(46)	C(61)	H(47)	103.6				

X-ray Structure determination of $[Pd_4(DPOT)_2(py)_2][BAr_f]_2 \cdot 2C_6H_{14}$ (**2'**).

Experimental

Data Collection

An orange prismatic crystal of $C_{114}H_{70}N_2Pd_4F_{48}B_2 \cdot 2C_6H_{14}$ having approximate dimensions of 0.20 x 0.20 x 0.25 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS-CS imaging plate area detector with graphite monochromated Mo-Kα 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 o.1 mm pixel mode.

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

a =	13.417(3) Å	α =	106.00(3)°
b =	19.297(6) Å	β =	94.42(2)°
c =	13.369(3) Å	γ =	100.98(4)°
V =	3235(1) Å^3		

For Z = 1 and $F.W.$ = 2999.32, the calculated density is 1.54 g/cm^3. Based on a statistical analysis of intensity distribution,and the successful solution and refinement of the structure, the space group was determined to be:

$$P\bar{1}\ (\#2)$$

The data were collected at a temperature of -50 ± 1°C to a maximum 2θvalue of 60.4°. A total of 60 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 10501 reflections was collected.

The linear absorption coefficient, μ, for Mo-$K\alpha$ radiation is 6.6 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson 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 refinement[3] was based on 10431 observed reflections ($I > 3.00\sigma(I)$) and 819 variable parameters and converged (largest parameter shift was 11.69 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.064$$

$$Rw = [(\Sigma \, \omega \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, \omega \, Fo^2)]^{1/2} = 0.067$$

The standard deviation of an observation of unit weight[4] was 2.44. The weighting scheme was based on counting statistics and included a factor (p = 0.010) to downweight the intense reflections. Plots of $\Sigma \, \omega \, (|Fo| - |Fc|)^2$ 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 0.64 and -0.92 $e^-/Å^3$, 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) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(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	$C_{114}H_{70}N_2Pd_4F_{48}B_2 \cdot 2C_6H_{14}$
Formula Weight	2999.32
Crystal Color, Habit	orange, prismatic
Crystal Dimensions	0.20 X 0.20 X 0.25 mm
Crystal System	triclinic
Lattice Type	Primitive
Indexing Images	3stills @ 5.0 minutes
Detector Position	143.2mm
Detector Swing Angle	0.00°
Pixel Size	0.1 mm
Lattice Parameters	a = 13.417(3)Å
	b = 19.297(6) Å
	c = 13.369(3) Å
	α = 106.00(3)°
	β = 94.42(2)°
	γ = 100.98(4)°
	V = 3235(1) Å^3
Space Group	$P\bar{1}$ (#2)

Z value	1
D_{calc}	1.539 g/cm^3
F_{000}	1494.00
μ(MoKα)	6.64 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	60 exposures @ 10.0 minutes
Oscillation Range	3.0°
Detector Position	143.2 mm
Detector Swing Angle	0.00°
Pixel Size	0.1 mm
$2\Theta_{max}$	60.4°
No. of Reflections Measured	Total: 10501
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
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))	10431
No. Variables	858
Reflection/Parameter Ratio	12.16
Residuals: R; Rw	0.064 ; 0.067
Residuals: R1	0.064
No. of Reflections to calc R1	10431
Goodness of Fit Indicator	2.40
Max Shift/Error in Final Cycle	0.83
Maximum peak in Final Diff. Map	0.64 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.92 $e^-/Å^3$

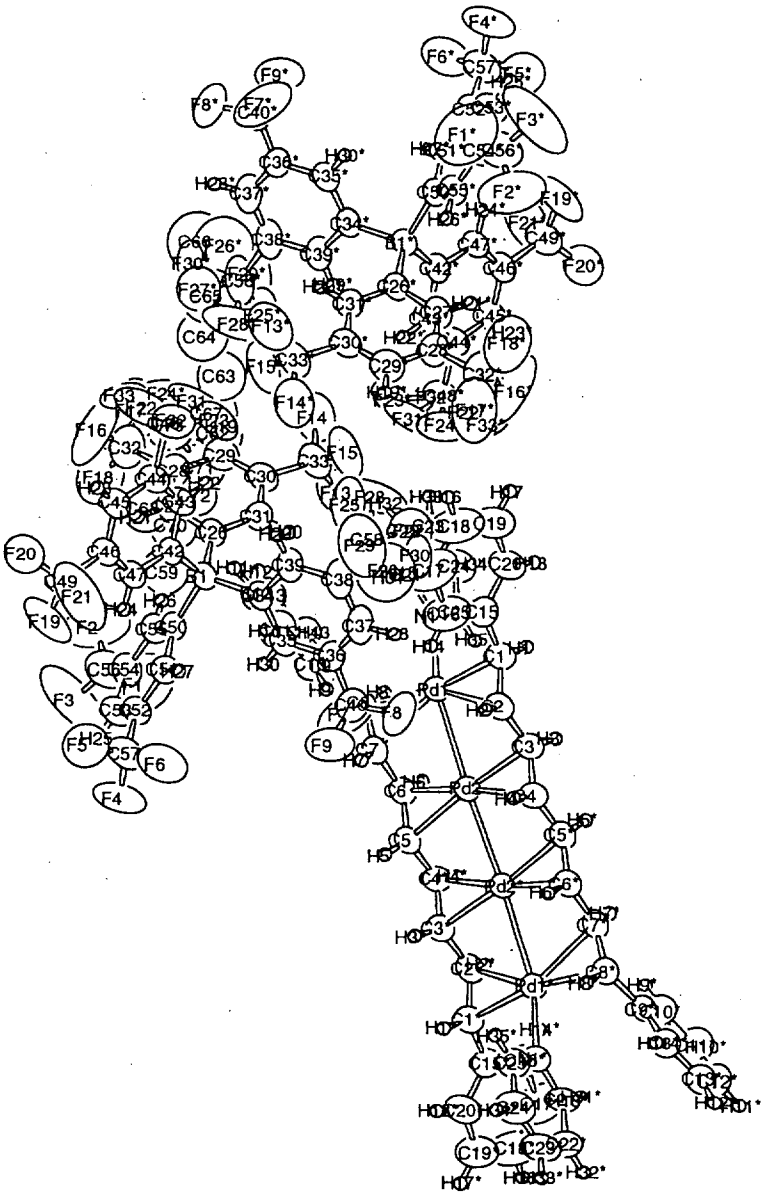

Table 1. Atomic coordinates, B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Pd(1)	0.18211(4)	0.35236(3)	0.40529(4)	3.92(1)	1.0000
Pd(2)	0.06108(4)	0.45073(3)	0.47499(5)	4.17(1)	1.0000
F(1)	0.7072(8)	0.4952(6)	0.7686(9)	16.5(4)	1.0000
F(2)	0.8162(7)	0.4413(4)	0.7877(9)	15.6(3)	1.0000
F(3)	0.8071(9)	0.5355(5)	0.8970(7)	19.4(4)	1.0000
F(4)	0.5656(6)	0.5322(3)	1.1575(5)	10.5(2)	1.0000
F(5)	0.6259(6)	0.4568(4)	1.2189(5)	12.1(3)	1.0000
F(6)	0.4734(6)	0.4331(3)	1.1554(5)	10.8(2)	1.0000
F(7)	0.2356(6)	0.3400(5)	0.7478(8)	14.1(3)	1.0000
F(8)	0.1049(5)	0.2760(4)	0.7655(8)	15.0(3)	1.0000
F(9)	0.2045(7)	0.3437(4)	0.8928(6)	13.2(3)	1.0000
F(13)	0.4449(7)	0.1377(4)	0.4091(6)	14.4(3)	1.0000
F(14)	0.5317(6)	0.0568(6)	0.3694(5)	16.4(3)	1.0000
F(15)	0.4160(6)	0.0449(4)	0.4554(6)	11.9(2)	1.0000
F(16)	0.8934(6)	0.1633(8)	0.697(1)	18.4(5)	1.0000
F(17)	0.8756(6)	0.1581(8)	0.5455(8)	21.4(5)	1.0000
F(18)	0.8922(6)	0.2515(6)	0.655(1)	18.0(4)	1.0000
F(19)	0.7286(7)	0.2869(3)	1.2354(5)	12.5(2)	1.0000
F(20)	0.7915(7)	0.2013(5)	1.2433(6)	16.0(3)	1.0000
F(21)	0.6433(8)	0.1997(6)	1.2722(6)	17.2(4)	1.0000
F(22)	0.665(3)	-0.0416(10)	0.974(2)	17.8(9)	0.7000
F(23)	0.5406(10)	-0.0487(6)	0.863(2)	9.9(4)	0.7000
F(24)	0.316(2)	0.0215(9)	0.175(3)	13.8(7)	0.7000
F(25)	0.260(2)	-0.011(1)	0.771(2)	12.1(7)	0.5000

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

atom	x	y	z	B_{eq}	occ
F(26)	0.134(3)	0.034(2)	0.831(4)	20(1)	0.5000
F(27)	0.155(2)	0.011(1)	0.670(2)	10.8(5)	0.5000
F(28)	0.247(2)	-0.008(1)	0.677(3)	22(1)	0.5000
F(29)	0.188(2)	0.012(1)	0.843(2)	14.1(8)	0.5000
F(30)	0.1096(8)	0.0225(6)	0.720(2)	9.5(4)	0.5000
F(31)	0.614(7)	-0.036(2)	0.812(3)	14(1)	0.3000
F(32)	0.595(3)	-0.048(1)	0.968(4)	8.6(9)	0.3000
F(33)	0.737(2)	-0.017(2)	0.922(4)	9.4(9)	0.3000
N(1)	0.2561(4)	0.2909(3)	0.2848(4)	4.3(1)	1.0000
C(1)	0.0586(6)	0.2529(4)	0.3590(6)	5.2(2)	1.0000
C(2)	0.0182(5)	0.3018(3)	0.4356(6)	5.0(2)	1.0000
C(3)	-0.0455(5)	0.3481(4)	0.4056(7)	5.2(2)	1.0000
C(4)	-0.0960(5)	0.3908(4)	0.4800(7)	5.2(2)	1.0000
C(5)	0.1566(5)	0.5620(4)	0.5530(6)	5.1(2)	1.0000
C(6)	0.2087(5)	0.5190(4)	0.4812(6)	5.0(2)	1.0000
C(7)	0.2673(5)	0.4702(4)	0.5110(5)	4.4(2)	1.0000
C(8)	0.3287(5)	0.4344(3)	0.4432(6)	4.2(2)	1.0000
C(9)	0.4078(5)	0.3991(3)	0.4806(5)	4.2(2)	1.0000
C(10)	0.4043(6)	0.3738(4)	0.5688(7)	5.8(2)	1.0000
C(11)	0.4781(8)	0.3393(6)	0.5983(8)	7.9(3)	1.0000
C(12)	0.5577(7)	0.3291(5)	0.5389(9)	7.1(3)	1.0000
C(13)	0.5635(6)	0.3543(5)	0.4526(8)	6.5(2)	1.0000
C(14)	0.4891(5)	0.3895(4)	0.4220(6)	5.1(2)	1.0000
C(15)	0.0986(5)	0.1911(4)	0.3784(7)	5.4(2)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(16)	0.1426(9)	0.1920(6)	0.4730(9)	8.9(4)	1.0000
C(17)	0.179(1)	0.1319(8)	0.489(1)	11.3(5)	1.0000
C(18)	0.166(1)	0.0697(8)	0.405(2)	12.5(6)	1.0000
C(19)	0.124(1)	0.0680(6)	0.307(1)	10.5(4)	1.0000
C(20)	0.0898(8)	0.1282(5)	0.2938(9)	8.5(3)	1.0000
C(21)	0.3175(6)	0.2453(4)	0.2994(6)	5.0(2)	1.0000
C(22)	0.3654(6)	0.2085(4)	0.2226(7)	5.8(2)	1.0000
C(23)	0.3520(7)	0.2195(5)	0.1255(8)	6.7(3)	1.0000
C(24)	0.2926(8)	0.2652(5)	0.1080(7)	7.0(3)	1.0000
C(25)	0.2442(6)	0.3009(4)	0.1892(6)	5.3(2)	1.0000
C(26)	0.5890(5)	0.1942(3)	0.7313(5)	4.2(2)	1.0000
C(27)	0.6939(5)	0.1990(4)	0.7255(6)	5.0(2)	1.0000
C(28)	0.7329(6)	0.1750(5)	0.6325(7)	5.7(2)	1.0000
C(29)	0.6670(7)	0.1400(4)	0.5400(7)	5.8(2)	1.0000
C(30)	0.5657(6)	0.1324(4)	0.5423(6)	5.1(2)	1.0000
C(31)	0.5257(5)	0.1597(4)	0.6362(6)	4.5(2)	1.0000
C(32)	0.8462(8)	0.1862(9)	0.631(1)	9.5(4)	1.0000
C(33)	0.4917(9)	0.0953(6)	0.4429(8)	7.3(3)	1.0000
C(34)	0.4218(5)	0.2037(3)	0.8298(5)	4.1(1)	1.0000
C(35)	0.3629(5)	0.2554(4)	0.8237(6)	4.9(2)	1.0000
C(36)	0.2557(5)	0.2375(4)	0.8026(6)	5.2(2)	1.0000
C(37)	0.2042(6)	0.1663(5)	0.7826(7)	6.3(2)	1.0000
C(38)	0.2594(6)	0.1136(5)	0.7864(7)	6.0(2)	1.0000
C(39)	0.3667(5)	0.1323(4)	0.8099(6)	5.3(2)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(40)	0.2000(7)	0.2959(6)	0.8019(10)	7.5(3)	1.0000
C(42)	0.5944(5)	0.1825(3)	0.9263(5)	4.0(1)	1.0000
C(43)	0.5989(6)	0.1086(4)	0.8881(6)	4.8(2)	1.0000
C(44)	0.6356(6)	0.0704(4)	0.9532(6)	5.2(2)	1.0000
C(45)	0.6720(6)	0.1046(4)	1.0584(6)	5.7(2)	1.0000
C(46)	0.6696(5)	0.1774(4)	1.0971(6)	4.7(2)	1.0000
C(47)	0.6321(5)	0.2151(3)	1.0319(5)	4.3(2)	1.0000
C(48)	0.637(1)	-0.0107(5)	0.907(1)	7.9(3)	1.0000
C(49)	0.7100(9)	0.2175(5)	1.2116(8)	7.2(3)	1.0000
C(50)	0.5886(5)	0.3135(3)	0.8952(5)	4.1(1)	1.0000
C(51)	0.5583(5)	0.3518(4)	0.9902(5)	4.3(2)	1.0000
C(52)	0.5953(6)	0.4261(4)	1.0367(6)	4.7(2)	1.0000
C(53)	0.6614(6)	0.4678(4)	0.9905(6)	5.5(2)	1.0000
C(54)	0.6882(6)	0.4322(4)	0.8960(6)	5.2(2)	1.0000
C(55)	0.6526(5)	0.3574(4)	0.8480(6)	4.5(2)	1.0000
C(56)	0.758(1)	0.4751(6)	0.840(1)	8.3(3)	1.0000
C(57)	0.5661(8)	0.4614(5)	1.1406(8)	6.6(3)	1.0000
C(58)	0.2102(10)	0.0296(8)	0.757(1)	9.8(4)	1.0000
C(59)	0.923(2)	0.532(2)	0.210(2)	12.2(8)	0.5000
C(62)	0.924(4)	0.345(3)	0.005(5)	17(1)	0.5000
C(63)	0.925(3)	0.253(2)	-0.008(3)	13(1)	0.5000
C(64)	0.968(3)	0.198(2)	0.013(3)	14(1)	0.5000
C(65)	0.975(3)	0.140(3)	-0.014(3)	16(1)	0.5000
C(66)	1.003(4)	0.059(2)	0.000(4)	21(1)	0.5000

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

atom	x	y	z	B_{eq}	occ
C(67)	0.931(4)	0.309(4)	0.032(6)	18(1)	0.5000
C(68)	0.969(3)	0.439(2)	0.234(3)	13.2(9)	0.5000
C(70)	0.926(2)	0.464(2)	0.176(3)	12.4(9)	0.5000
C(71)	0.915(3)	0.380(2)	0.084(3)	12(1)	0.5000
C(72)	0.916(2)	0.429(2)	0.090(2)	8.8(6)	0.5000
C(73)	0.979(3)	0.328(2)	0.119(3)	14(1)	0.5000
B(1)	0.5485(6)	0.2243(4)	0.8453(6)	4.0(2)	1.0000
H(1)	0.0375	0.2476	0.2760	5.1199	1.0000
H(2)	0.0149	0.2875	0.5153	5.1199	1.0000
H(3)	-0.0635	0.3489	0.3145	5.1199	1.0000
H(4)	-0.0860	0.3807	0.5606	5.1199	1.0000
H(5)	0.1741	0.5766	0.6268	5.1199	1.0000
H(6)	0.2032	0.5198	0.3961	5.1199	1.0000
H(7)	0.2625	0.4666	0.5897	5.1199	1.0000
H(8)	0.3277	0.4363	0.3514	5.1199	1.0000
H(9)	0.3486	0.3797	0.6094	6.9388	1.0000
H(10)	0.4761	0.3238	0.6596	9.6010	1.0000
H(11)	0.6089	0.3051	0.5572	8.4258	1.0000
H(12)	0.6170	0.3479	0.4102	7.8200	1.0000
H(13)	0.4939	0.4073	0.3627	6.0040	1.0000
H(14)	0.1474	0.2351	0.5307	10.8498	1.0000
H(15)	0.2115	0.1349	0.5580	13.8481	1.0000
H(16)	0.1865	0.0275	0.4147	15.2621	1.0000
H(17)	0.1182	0.0257	0.2468	12.9210	1.0000

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

atom	x	y	z	B_{eq}	occ
H(18)	0.0585	0.1271	0.2264	10.1454	1.0000
H(19)	0.6939	0.1221	0.4767	6.9755	1.0000
H(20)	0.4542	0.1555	0.6344	5.2409	1.0000
H(21)	0.7394	0.2205	0.7881	5.7575	1.0000
H(22)	0.5755	0.0832	0.8166	5.7266	1.0000
H(23)	0.6981	0.0790	1.1024	6.9094	1.0000
H(24)	0.6321	0.2659	1.0615	5.0563	1.0000
H(25)	0.6869	0.5193	1.0218	6.5960	1.0000
H(26)	0.6711	0.3351	0.7810	5.3827	1.0000
H(27)	0.5113	0.3253	1.0235	5.2648	1.0000
H(28)	0.1312	0.1534	0.7634	7.4832	1.0000
H(29)	0.4032	0.0948	0.8133	6.1570	1.0000
H(30)	0.3973	0.3057	0.8358	5.7234	1.0000
H(31)	0.3266	0.2383	0.3677	5.9858	1.0000
H(32)	0.4074	0.1767	0.2353	6.9654	1.0000
H(33)	0.3846	0.1955	0.0694	8.1402	1.0000
H(34)	0.2804	0.2715	0.0399	8.4949	1.0000
H(35)	0.2029	0.3337	0.1770	6.0992	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)	0.0498(3)	0.0436(3)	0.0513(3)	0.0096(2)	0.0074(2)	0.0075(2)
Pd(2)	0.0475(3)	0.0451(2)	0.0593(4)	0.0083(2)	0.0066(2)	0.0064(2)
F(1)	0.229(10)	0.26(1)	0.24(1)	0.075(9)	0.106(9)	0.20(1)
F(2)	0.198(8)	0.124(6)	0.34(1)	0.051(6)	0.192(9)	0.120(7)
F(3)	0.33(1)	0.153(7)	0.151(8)	-0.152(8)	0.090(8)	0.001(6)
F(4)	0.202(7)	0.070(3)	0.120(5)	0.034(4)	0.060(5)	0.002(3)
F(5)	0.186(7)	0.221(8)	0.054(4)	0.096(6)	0.006(4)	0.010(4)
F(6)	0.150(6)	0.118(5)	0.123(6)	0.011(4)	0.077(5)	0.000(4)
F(7)	0.171(7)	0.194(8)	0.26(1)	0.113(6)	0.087(7)	0.144(8)
F(8)	0.069(4)	0.129(6)	0.33(1)	0.025(4)	-0.046(6)	0.025(6)
F(9)	0.210(8)	0.160(7)	0.123(6)	0.111(6)	0.001(5)	-0.013(5)
F(13)	0.265(10)	0.133(6)	0.124(6)	0.058(6)	-0.100(6)	0.023(4)
F(14)	0.149(7)	0.32(1)	0.082(5)	0.076(7)	-0.012(4)	-0.076(6)
F(15)	0.156(6)	0.127(5)	0.121(6)	-0.020(5)	-0.064(5)	0.012(4)
F(16)	0.064(5)	0.38(2)	0.33(2)	0.074(7)	0.055(6)	0.22(1)
F(17)	0.096(6)	0.45(2)	0.177(10)	0.023(8)	0.067(6)	-0.04(1)
F(18)	0.083(5)	0.190(9)	0.38(2)	-0.020(6)	0.052(7)	0.07(1)
F(19)	0.270(9)	0.075(4)	0.083(5)	0.013(5)	-0.067(5)	-0.008(3)
F(20)	0.228(9)	0.196(8)	0.131(6)	0.124(7)	-0.109(7)	-0.053(5)
F(21)	0.26(1)	0.25(1)	0.056(6)	-0.073(9)	0.020(6)	-0.007(5)
F(22)	0.41(4)	0.10(1)	0.13(2)	0.12(2)	-0.11(3)	-0.017(9)
F(23)	0.133(9)	0.064(5)	0.14(1)	-0.017(5)	0.012(9)	-0.007(6)
F(24)	0.16(1)	0.097(9)	0.25(3)	0.043(10)	0.10(2)	-0.01(1)
F(25)	0.11(1)	0.09(1)	0.27(3)	-0.035(9)	-0.06(2)	0.12(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(28)	0.19(2)	0.08(1)	0.48(5)	-0.05(1)	0.20(3)	-0.09(2)
F(29)	0.19(2)	0.15(2)	0.21(2)	-0.06(2)	0.00(2)	0.13(2)
F(30)	0.048(6)	0.078(7)	0.20(2)	-0.034(5)	-0.022(8)	0.036(9)
F(31)	0.40(8)	0.07(2)	0.06(2)	0.09(4)	-0.08(4)	-0.02(1)
F(32)	0.12(2)	0.036(9)	0.17(4)	0.01(1)	0.03(3)	0.04(1)
F(33)	0.13(2)	0.09(2)	0.16(3)	0.08(2)	0.04(2)	0.03(2)
N(1)	0.058(3)	0.046(3)	0.055(4)	0.010(2)	0.006(3)	0.009(2)
C(1)	0.060(4)	0.051(4)	0.076(6)	0.008(3)	0.013(4)	0.008(3)
C(2)	0.055(4)	0.040(3)	0.083(6)	-0.003(3)	0.012(4)	0.010(3)
C(3)	0.051(4)	0.041(3)	0.094(6)	0.004(3)	0.010(4)	0.004(3)
C(4)	0.050(4)	0.041(3)	0.097(6)	0.004(3)	0.013(4)	0.006(3)
C(5)	0.045(4)	0.048(4)	0.080(6)	0.000(3)	0.007(3)	-0.006(3)
C(6)	0.048(4)	0.046(4)	0.082(6)	0.000(3)	0.010(3)	0.005(3)
C(7)	0.051(4)	0.052(4)	0.055(5)	0.005(3)	0.002(3)	0.005(3)
C(8)	0.049(4)	0.042(3)	0.065(5)	0.005(3)	0.006(3)	0.012(3)
C(9)	0.050(4)	0.048(3)	0.053(4)	0.006(3)	-0.001(3)	0.003(3)
C(10)	0.078(5)	0.076(5)	0.071(6)	0.027(4)	0.015(4)	0.023(4)
C(11)	0.116(8)	0.120(8)	0.075(7)	0.048(7)	-0.003(6)	0.033(6)
C(12)	0.080(6)	0.092(7)	0.096(8)	0.033(5)	-0.007(5)	0.017(6)
C(13)	0.048(4)	0.066(5)	0.109(8)	0.004(4)	0.013(4)	-0.006(5)
C(14)	0.055(4)	0.062(4)	0.072(5)	0.006(3)	0.015(4)	0.015(4)
C(15)	0.049(4)	0.052(4)	0.099(7)	0.005(3)	0.016(4)	0.018(4)
C(16)	0.15(1)	0.108(8)	0.114(10)	0.067(8)	0.053(8)	0.056(7)
C(17)	0.17(1)	0.15(1)	0.17(1)	0.08(1)	0.07(1)	0.11(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(18)	0.16(1)	0.079(8)	0.26(2)	0.056(9)	0.08(1)	0.07(1)
C(19)	0.12(1)	0.064(6)	0.20(2)	0.028(6)	0.03(1)	0.008(8)
C(20)	0.093(7)	0.057(5)	0.144(10)	0.011(5)	0.010(6)	-0.009(5)
C(21)	0.080(5)	0.053(4)	0.056(5)	0.021(4)	0.021(4)	0.008(3)
C(22)	0.075(5)	0.057(4)	0.087(7)	0.023(4)	0.021(4)	0.009(4)
C(23)	0.108(7)	0.063(5)	0.083(7)	0.024(5)	0.039(5)	0.007(4)
C(24)	0.125(8)	0.093(6)	0.058(6)	0.032(6)	0.032(5)	0.027(5)
C(25)	0.083(5)	0.062(4)	0.061(5)	0.020(4)	0.012(4)	0.021(4)
C(26)	0.051(4)	0.047(3)	0.055(4)	0.003(3)	0.003(3)	0.009(3)
C(27)	0.058(4)	0.066(4)	0.055(5)	0.000(3)	0.006(3)	0.009(3)
C(28)	0.055(4)	0.086(5)	0.073(6)	0.008(4)	0.018(4)	0.018(4)
C(29)	0.081(6)	0.076(5)	0.062(6)	0.015(4)	0.023(4)	0.016(4)
C(30)	0.083(5)	0.062(4)	0.043(5)	0.016(4)	0.003(4)	0.008(3)
C(31)	0.057(4)	0.060(4)	0.054(5)	0.014(3)	0.004(3)	0.017(3)
C(32)	0.061(6)	0.15(1)	0.13(1)	0.007(7)	0.031(7)	0.012(9)
C(33)	0.104(8)	0.094(7)	0.058(6)	0.015(6)	-0.013(5)	-0.005(5)
C(34)	0.048(4)	0.053(4)	0.046(4)	0.001(3)	0.004(3)	0.009(3)
C(35)	0.053(4)	0.064(4)	0.054(5)	0.000(3)	0.008(3)	0.004(3)
C(36)	0.050(4)	0.073(5)	0.066(5)	0.012(4)	0.003(3)	0.010(4)
C(37)	0.047(4)	0.100(6)	0.081(6)	-0.005(4)	0.005(4)	0.027(5)
C(38)	0.057(4)	0.082(5)	0.083(6)	-0.011(4)	-0.005(4)	0.036(5)
C(39)	0.052(4)	0.063(4)	0.080(6)	-0.004(3)	-0.003(4)	0.027(4)
C(40)	0.068(6)	0.093(7)	0.112(9)	0.016(5)	0.008(5)	0.013(6)
C(42)	0.045(3)	0.052(3)	0.048(4)	-0.001(3)	0.003(3)	0.011(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(43)	0.073(5)	0.051(4)	0.052(5)	0.006(3)	0.003(3)	0.010(3)
C(44)	0.079(5)	0.049(4)	0.062(5)	0.012(3)	0.000(4)	0.011(3)
C(45)	0.079(5)	0.056(4)	0.070(6)	0.007(4)	-0.008(4)	0.013(4)
C(46)	0.066(4)	0.056(4)	0.047(4)	0.007(3)	-0.002(3)	0.008(3)
C(47)	0.058(4)	0.045(3)	0.053(4)	0.005(3)	0.000(3)	0.006(3)
C(48)	0.14(1)	0.062(6)	0.092(9)	0.030(7)	-0.015(8)	0.012(6)
C(49)	0.132(9)	0.078(6)	0.059(7)	0.031(6)	-0.012(6)	0.012(5)
C(50)	0.049(4)	0.048(3)	0.052(4)	0.005(3)	-0.004(3)	0.012(3)
C(51)	0.059(4)	0.051(4)	0.055(5)	0.011(3)	0.007(3)	0.017(3)
C(52)	0.068(5)	0.053(4)	0.053(5)	0.008(3)	0.000(3)	0.012(3)
C(53)	0.089(6)	0.046(4)	0.067(6)	0.005(4)	0.005(4)	0.014(3)
C(54)	0.065(5)	0.060(4)	0.071(6)	-0.001(3)	0.005(4)	0.026(4)
C(55)	0.060(4)	0.052(4)	0.057(5)	0.004(3)	0.003(3)	0.018(3)
C(56)	0.131(10)	0.071(6)	0.118(10)	0.002(6)	0.052(8)	0.038(6)
C(57)	0.109(8)	0.062(5)	0.070(7)	0.010(5)	0.015(5)	0.011(4)
C(58)	0.078(8)	0.114(10)	0.15(1)	-0.031(7)	-0.027(8)	0.040(10)
B(1)	0.048(4)	0.047(4)	0.049(5)	0.002(3)	0.004(3)	0.009(3)

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(Å)

atom	atom	distance	atom	atom	distance
Pd(1)	Pd(2)	2.7463(8)	Pd(1)	N(1)	2.152(5)
Pd(1)	C(1)	2.188(7)	Pd(1)	C(2)	2.344(7)
Pd(1)	C(7)	2.337(6)	Pd(1)	C(8)	2.202(6)
Pd(2)	Pd(2)	2.721(1)	Pd(2)	C(3)	2.129(6)
Pd(2)	C(4)	2.218(7)	Pd(2)	C(5)	2.203(6)
Pd(2)	C(6)	2.142(6)	F(1)	C(56)	1.31(1)
F(2)	C(56)	1.25(1)	F(3)	C(56)	1.23(1)
F(4)	C(57)	1.322(9)	F(5)	C(57)	1.30(1)
F(6)	C(57)	1.31(1)	F(7)	C(40)	1.31(1)
F(8)	C(40)	1.28(1)	F(9)	C(40)	1.30(1)
F(13)	C(33)	1.27(1)	F(14)	C(33)	1.28(1)
F(15)	C(33)	1.32(1)	F(16)	C(32)	1.27(2)
F(17)	C(32)	1.25(1)	F(18)	C(32)	1.23(1)
F(19)	C(49)	1.26(1)	F(20)	C(49)	1.27(1)
F(21)	C(49)	1.31(1)	F(22)	F(32)	0.92(4)
F(22)	F(33)	1.32(4)	F(22)	C(48)	1.27(2)
F(23)	F(31)	1.27(9)	F(23)	F(32)	1.53(4)
F(23)	C(48)	1.36(2)	F(24)	F(31)	0.91(8)
F(24)	F(33)	1.41(4)	F(24)	C(48)	1.29(2)
F(25)	F(28)	1.28(4)	F(25)	F(29)	1.45(4)
F(25)	C(58)	1.16(2)	F(26)	F(29)	0.95(4)
F(26)	F(30)	1.43(4)	F(26)	C(58)	1.47(4)
F(27)	F(28)	1.36(3)	F(27)	F(30)	0.95(2)
F(27)	C(58)	1.25(2)	F(28)	C(58)	1.31(3)

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

atom	atom	distance	atom	atom	distance
F(29)	C(58)	1.33(2)	F(30)	C(58)	1.37(2)
F(31)	C(48)	1.22(3)	F(32)	C(48)	1.32(3)
F(33)	C(48)	1.38(3)	N(1)	C(21)	1.355(9)
N(1)	C(25)	1.346(9)	C(1)	C(2)	1.407(10)
C(1)	C(15)	1.47(1)	C(2)	C(3)	1.46(1)
C(3)	C(4)	1.412(10)	C(4)	C(5)	1.46(1)
C(5)	C(6)	1.410(9)	C(6)	C(7)	1.451(10)
C(7)	C(8)	1.402(9)	C(8)	C(9)	1.490(9)
C(9)	C(10)	1.40(1)	C(9)	C(14)	1.403(9)
C(10)	C(11)	1.38(1)	C(11)	C(12)	1.39(1)
C(12)	C(13)	1.37(1)	C(13)	C(14)	1.40(1)
C(15)	C(16)	1.35(1)	C(15)	C(20)	1.39(1)
C(16)	C(17)	1.40(1)	C(17)	C(18)	1.37(2)
C(18)	C(19)	1.38(2)	C(19)	C(20)	1.38(2)
C(21)	C(22)	1.359(10)	C(22)	C(23)	1.38(1)
C(23)	C(24)	1.35(1)	C(24)	C(25)	1.39(1)
C(26)	C(27)	1.402(9)	C(26)	C(31)	1.390(9)
C(26)	B(1)	1.647(10)	C(27)	C(28)	1.38(1)
C(28)	C(29)	1.38(1)	C(28)	C(32)	1.50(1)
C(29)	C(30)	1.34(1)	C(30)	C(31)	1.410(10)
C(30)	C(33)	1.50(1)	C(34)	C(35)	1.401(9)
C(34)	C(39)	1.377(9)	C(34)	B(1)	1.653(9)
C(35)	C(36)	1.402(9)	C(36)	C(37)	1.36(1)
C(36)	C(40)	1.47(1)	C(37)	C(38)	1.38(1)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(38)	C(39)	1.404(10)	C(38)	C(58)	1.56(1)
C(42)	C(43)	1.391(9)	C(42)	C(47)	1.387(9)
C(42)	B(1)	1.66(1)	C(43)	C(44)	1.403(10)
C(44)	C(45)	1.38(1)	C(44)	C(48)	1.52(1)
C(45)	C(46)	1.364(9)	C(46)	C(47)	1.402(9)
C(46)	C(49)	1.52(1)	C(50)	C(51)	1.415(9)
C(50)	C(55)	1.398(9)	C(50)	B(1)	1.630(9)
C(51)	C(52)	1.371(9)	C(52)	C(53)	1.38(1)
C(52)	C(57)	1.49(1)	C(53)	C(54)	1.37(1)
C(54)	C(55)	1.380(9)	C(54)	C(56)	1.51(1)
C(59)	C(70)	1.26(4)	C(62)	C(63)	1.76(7)
C(62)	C(67)	0.90(8)	C(62)	C(71)	1.11(6)
C(62)	C(72)	1.73(7)	C(62)	C(73)	1.79(7)
C(63)	C(64)	1.37(4)	C(63)	C(67)	1.05(6)
C(64)	C(65)	1.10(5)	C(65)	C(66)	1.73(5)
C(67)	C(71)	1.43(7)	C(67)	C(73)	1.21(6)
C(68)	C(70)	1.19(4)	C(70)	C(71)	1.72(5)
C(70)	C(72)	1.15(4)	C(71)	C(72)	0.92(4)
C(71)	C(73)	1.58(5)			

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	1.09	C(2)	H(2)	1.17
C(3)	H(3)	1.23	C(4)	H(4)	1.15
C(5)	H(5)	0.95	C(6)	H(6)	1.14
C(7)	H(7)	1.08	C(8)	H(8)	1.24
C(10)	H(9)	0.96	C(11)	H(10)	0.95
C(12)	H(11)	0.95	C(13)	H(12)	0.95
C(14)	H(13)	0.95	C(16)	H(14)	0.95
C(17)	H(15)	0.97	C(18)	H(16)	0.94
C(19)	H(17)	0.96	C(20)	H(18)	0.96
C(21)	H(31)	0.96	C(22)	H(32)	0.95
C(23)	H(33)	0.95	C(24)	H(34)	0.96
C(25)	H(35)	0.95	C(27)	H(21)	0.94
C(29)	H(19)	0.95	C(31)	H(20)	0.94
C(35)	H(30)	0.96	C(37)	H(28)	0.96
C(39)	H(29)	0.96	C(43)	H(22)	0.94
C(45)	H(23)	0.95	C(47)	H(24)	0.95
C(51)	H(27)	0.95	C(53)	H(25)	0.95
C(55)	H(26)	0.95			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Pd(2)	Pd(1)	N(1)	152.0(2)	Pd(2)	Pd(1)	C(1)	96.3(2)
Pd(2)	Pd(1)	C(2)	63.8(2)	Pd(2)	Pd(1)	C(7)	63.8(2)
Pd(2)	Pd(1)	C(8)	96.5(2)	N(1)	Pd(1)	C(1)	85.1(2)
N(1)	Pd(1)	C(2)	121.0(2)	N(1)	Pd(1)	C(7)	119.9(2)
N(1)	Pd(1)	C(8)	84.2(2)	C(1)	Pd(1)	C(2)	36.0(2)
C(1)	Pd(1)	C(7)	154.8(3)	C(1)	Pd(1)	C(8)	167.0(3)
C(2)	Pd(1)	C(7)	119.1(2)	C(2)	Pd(1)	C(8)	154.4(2)
C(7)	Pd(1)	C(8)	35.8(2)	Pd(1)	Pd(2)	Pd(2)	174.50(4)
Pd(1)	Pd(2)	C(3)	76.0(2)	Pd(1)	Pd(2)	C(4)	110.3(2)
Pd(1)	Pd(2)	C(5)	110.4(2)	Pd(1)	Pd(2)	C(6)	75.6(2)
Pd(2)	Pd(2)	C(3)	103.3(2)	Pd(2)	Pd(2)	C(4)	70.7(2)
Pd(2)	Pd(2)	C(5)	70.4(2)	Pd(2)	Pd(2)	C(6)	103.6(2)
C(3)	Pd(2)	C(4)	37.8(2)	C(3)	Pd(2)	C(5)	173.6(3)
C(3)	Pd(2)	C(6)	148.3(3)	C(4)	Pd(2)	C(5)	136.0(3)
C(4)	Pd(2)	C(6)	173.8(3)	C(5)	Pd(2)	C(6)	37.8(2)
F(32)	F(22)	F(33)	135(3)	F(32)	F(22)	C(48)	72(2)
F(33)	F(22)	C(48)	64(1)	F(31)	F(23)	F(32)	103(2)
F(31)	F(23)	C(48)	55(1)	F(32)	F(23)	C(48)	54(1)
F(31)	F(24)	F(33)	121(5)	F(31)	F(24)	C(48)	64(3)
F(33)	F(24)	C(48)	61(1)	F(28)	F(25)	F(29)	120(2)
F(28)	F(25)	C(58)	64(1)	F(29)	F(25)	C(58)	59(1)
F(29)	F(26)	F(30)	109(4)	F(29)	F(26)	C(58)	62(2)
F(30)	F(26)	C(58)	56(1)	F(28)	F(27)	F(30)	132(2)
F(28)	F(27)	C(58)	60(1)	F(30)	F(27)	C(58)	75(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(25)	F(28)	F(27)	102(2)	F(25)	F(28)	C(58)	53(1)
F(27)	F(28)	C(58)	55(1)	F(25)	F(29)	F(26)	126(3)
F(25)	F(29)	C(58)	49(1)	F(26)	F(29)	C(58)	78(2)
F(26)	F(30)	F(27)	124(2)	F(26)	F(30)	C(58)	63(1)
F(27)	F(30)	C(58)	62(1)	F(23)	F(31)	F(24)	137(4)
F(23)	F(31)	C(48)	66(3)	F(24)	F(31)	C(48)	72(2)
F(22)	F(32)	F(23)	115(4)	F(22)	F(32)	C(48)	66(2)
F(23)	F(32)	C(48)	56(1)	F(22)	F(33)	F(24)	103(3)
F(22)	F(33)	C(48)	56(1)	F(24)	F(33)	C(48)	55(1)
Pd(1)	N(1)	C(21)	124.7(5)	Pd(1)	N(1)	C(25)	117.6(5)
C(21)	N(1)	C(25)	117.6(6)	Pd(1)	C(1)	C(2)	78.0(4)
Pd(1)	C(1)	C(15)	109.0(5)	C(2)	C(1)	C(15)	123.1(8)
Pd(1)	C(2)	C(1)	66.0(4)	Pd(1)	C(2)	C(3)	103.7(4)
C(1)	C(2)	C(3)	120.5(7)	Pd(2)	C(3)	C(2)	96.5(4)
Pd(2)	C(3)	C(4)	74.5(4)	C(2)	C(3)	C(4)	120.9(8)
Pd(2)	C(4)	C(3)	67.7(4)	Pd(2)	C(4)	C(5)	100.5(4)
C(3)	C(4)	C(5)	118.9(8)	Pd(2)	C(5)	C(4)	102.1(4)
Pd(2)	C(5)	C(6)	68.7(4)	C(4)	C(5)	C(6)	120.6(8)
Pd(2)	C(6)	C(5)	73.4(4)	Pd(2)	C(6)	C(7)	95.9(4)
C(5)	C(6)	C(7)	121.8(8)	Pd(1)	C(7)	C(6)	104.0(4)
Pd(1)	C(7)	C(8)	66.8(3)	C(6)	C(7)	C(8)	121.4(7)
Pd(1)	C(8)	C(7)	77.3(4)	Pd(1)	C(8)	C(9)	107.0(4)
C(7)	C(8)	C(9)	121.9(7)	C(8)	C(9)	C(10)	123.9(6)
C(8)	C(9)	C(14)	117.7(7)	C(10)	C(9)	C(14)	118.4(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(9)	C(10)	C(11)	121.5(8)	C(10)	C(11)	C(12)	119.6(9)
C(11)	C(12)	C(13)	119.9(8)	C(12)	C(13)	C(14)	121.0(8)
C(9)	C(14)	C(13)	119.5(8)	C(1)	C(15)	C(16)	123.9(8)
C(1)	C(15)	C(20)	117.7(9)	C(16)	C(15)	C(20)	118.4(9)
C(15)	C(16)	C(17)	122(1)	C(16)	C(17)	C(18)	117(1)
C(17)	C(18)	C(19)	120(1)	C(18)	C(19)	C(20)	119(1)
C(15)	C(20)	C(19)	120(1)	N(1)	C(21)	C(22)	123.6(7)
C(21)	C(22)	C(23)	117.8(8)	C(22)	C(23)	C(24)	120.6(8)
C(23)	C(24)	C(25)	119.3(8)	N(1)	C(25)	C(24)	121.2(7)
C(27)	C(26)	C(31)	114.6(6)	C(27)	C(26)	B(1)	120.4(6)
C(31)	C(26)	B(1)	124.9(6)	C(26)	C(27)	C(28)	123.4(7)
C(27)	C(28)	C(29)	119.9(7)	C(27)	C(28)	C(32)	120.6(9)
C(29)	C(28)	C(32)	119.5(8)	C(28)	C(29)	C(30)	118.7(7)
C(29)	C(30)	C(31)	121.5(7)	C(29)	C(30)	C(33)	120.2(8)
C(31)	C(30)	C(33)	118.3(8)	C(26)	C(31)	C(30)	121.7(6)
F(16)	C(32)	F(17)	104(1)	F(16)	C(32)	F(18)	101(1)
F(16)	C(32)	C(28)	114(1)	F(17)	C(32)	F(18)	103(1)
F(17)	C(32)	C(28)	116(1)	F(18)	C(32)	C(28)	114(1)
F(13)	C(33)	F(14)	110(1)	F(13)	C(33)	F(15)	102.9(10)
F(13)	C(33)	C(30)	115.3(9)	F(14)	C(33)	F(15)	101.7(9)
F(14)	C(33)	C(30)	113.0(9)	F(15)	C(33)	C(30)	112.0(9)
C(35)	C(34)	C(39)	115.0(6)	C(35)	C(34)	B(1)	122.7(6)
C(39)	C(34)	B(1)	121.9(6)	C(34)	C(35)	C(36)	123.4(7)
C(35)	C(36)	C(37)	119.8(7)	C(35)	C(36)	C(40)	119.6(7)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(37)	C(36)	C(40)	120.6(8)	C(36)	C(37)	C(38)	118.6(7)
C(37)	C(38)	C(39)	121.3(7)	C(37)	C(38)	C(58)	123.4(9)
C(39)	C(38)	C(58)	115.2(9)	C(34)	C(39)	C(38)	121.9(7)
F(7)	C(40)	F(8)	102(1)	F(7)	C(40)	F(9)	100.3(10)
F(7)	C(40)	C(36)	115.0(9)	F(8)	C(40)	F(9)	104.8(9)
F(8)	C(40)	C(36)	117.5(9)	F(9)	C(40)	C(36)	114.7(10)
C(43)	C(42)	C(47)	114.5(6)	C(43)	C(42)	B(1)	119.5(6)
C(47)	C(42)	B(1)	125.9(6)	C(42)	C(43)	C(44)	121.9(7)
C(43)	C(44)	C(45)	121.9(7)	C(43)	C(44)	C(48)	119.5(8)
C(45)	C(44)	C(48)	118.6(8)	C(44)	C(45)	C(46)	117.1(7)
C(45)	C(46)	C(47)	120.8(7)	C(45)	C(46)	C(49)	119.0(7)
C(47)	C(46)	C(49)	120.3(7)	C(42)	C(47)	C(46)	123.7(6)
F(22)	C(48)	F(23)	106(1)	F(22)	C(48)	F(24)	114(1)
F(22)	C(48)	F(31)	129(1)	F(22)	C(48)	F(32)	41(1)
F(22)	C(48)	F(33)	59(1)	F(22)	C(48)	C(44)	114(1)
F(23)	C(48)	F(24)	100(1)	F(23)	C(48)	F(31)	58(4)
F(23)	C(48)	F(32)	69(1)	F(23)	C(48)	F(33)	143(1)
F(23)	C(48)	C(44)	108(1)	F(24)	C(48)	F(31)	42(3)
F(24)	C(48)	F(32)	139(1)	F(24)	C(48)	F(33)	63(1)
F(24)	C(48)	C(44)	111(1)	F(31)	C(48)	F(32)	119(3)
F(31)	C(48)	F(33)	103(3)	F(31)	C(48)	C(44)	115(1)
F(32)	C(48)	F(33)	100(1)	F(32)	C(48)	C(44)	108(1)
F(33)	C(48)	C(44)	107(1)	F(19)	C(49)	F(20)	106(1)
F(19)	C(49)	F(21)	105(1)	F(19)	C(49)	C(46)	115.0(8)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(20)	C(49)	F(21)	105(1)	F(20)	C(49)	C(46)	113.5(9)
F(21)	C(49)	C(46)	110.6(9)	C(51)	C(50)	C(55)	115.5(6)
C(51)	C(50)	B(1)	121.0(6)	C(55)	C(50)	B(1)	123.5(6)
C(50)	C(51)	C(52)	122.1(6)	C(51)	C(52)	C(53)	121.2(7)
C(51)	C(52)	C(57)	119.0(7)	C(53)	C(52)	C(57)	119.8(7)
C(52)	C(53)	C(54)	117.5(7)	C(53)	C(54)	C(55)	122.4(7)
C(53)	C(54)	C(56)	120.1(8)	C(55)	C(54)	C(56)	117.5(8)
C(50)	C(55)	C(54)	121.1(7)	F(1)	C(56)	F(2)	101(1)
F(1)	C(56)	F(3)	101(1)	F(1)	C(56)	C(54)	112(1)
F(2)	C(56)	F(3)	109(1)	F(2)	C(56)	C(54)	116.1(9)
F(3)	C(56)	C(54)	113(1)	F(4)	C(57)	F(5)	106.9(8)
F(4)	C(57)	F(6)	103.0(8)	F(4)	C(57)	C(52)	113.7(8)
F(5)	C(57)	F(6)	104.5(9)	F(5)	C(57)	C(52)	112.8(8)
F(6)	C(57)	C(52)	115.0(8)	F(25)	C(58)	F(26)	109(2)
F(25)	C(58)	F(27)	116(2)	F(25)	C(58)	F(28)	62(2)
F(25)	C(58)	F(29)	71(2)	F(25)	C(58)	F(30)	135(1)
F(25)	C(58)	C(38)	119(1)	F(26)	C(58)	F(27)	101(1)
F(26)	C(58)	F(28)	150(1)	F(26)	C(58)	F(29)	39(1)
F(26)	C(58)	F(30)	60(1)	F(26)	C(58)	C(38)	97(1)
F(27)	C(58)	F(28)	63(1)	F(27)	C(58)	F(29)	127(1)
F(27)	C(58)	F(30)	42(1)	F(27)	C(58)	C(38)	108(1)
F(28)	C(58)	F(29)	128(2)	F(28)	C(58)	F(30)	104(2)
F(28)	C(58)	C(38)	110(1)	F(29)	C(58)	F(30)	93(1)
F(29)	C(58)	C(38)	109(1)	F(30)	C(58)	C(38)	105(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(63)	C(62)	C(67)	27(6)	C(63)	C(62)	C(71)	116(5)
C(63)	C(62)	C(72)	145(3)	C(63)	C(62)	C(73)	64(2)
C(67)	C(62)	C(71)	90(7)	C(67)	C(62)	C(72)	118(8)
C(67)	C(62)	C(73)	37(6)	C(71)	C(62)	C(72)	28(3)
C(71)	C(62)	C(73)	60(3)	C(72)	C(62)	C(73)	85(3)
C(62)	C(63)	C(64)	153(3)	C(62)	C(63)	C(67)	23(5)
C(64)	C(63)	C(67)	134(6)	C(63)	C(64)	C(65)	147(5)
C(64)	C(65)	C(66)	155(5)	C(62)	C(67)	C(63)	128(11)
C(62)	C(67)	C(71)	50(5)	C(62)	C(67)	C(73)	115(9)
C(63)	C(67)	C(71)	167(6)	C(63)	C(67)	C(73)	113(7)
C(71)	C(67)	C(73)	72(4)	C(59)	C(70)	C(68)	117(4)
C(59)	C(70)	C(71)	156(4)	C(59)	C(70)	C(72)	127(4)
C(68)	C(70)	C(71)	85(3)	C(68)	C(70)	C(72)	112(3)
C(71)	C(70)	C(72)	29(2)	C(62)	C(71)	C(67)	38(3)
C(62)	C(71)	C(70)	152(5)	C(62)	C(71)	C(72)	115(6)
C(62)	C(71)	C(73)	81(4)	C(67)	C(71)	C(70)	161(4)
C(67)	C(71)	C(72)	153(6)	C(67)	C(71)	C(73)	47(2)
C(70)	C(71)	C(72)	38(2)	C(70)	C(71)	C(73)	114(3)
C(72)	C(71)	C(73)	142(4)	C(62)	C(72)	C(70)	145(3)
C(62)	C(72)	C(71)	35(3)	C(70)	C(72)	C(71)	111(4)
C(62)	C(73)	C(67)	27(3)	C(62)	C(73)	C(71)	37(2)
C(67)	C(73)	C(71)	60(3)	C(26)	B(1)	C(34)	109.6(5)
C(26)	B(1)	C(42)	107.8(5)	C(26)	B(1)	C(50)	111.3(5)
C(34)	B(1)	C(42)	110.0(5)	C(34)	B(1)	C(50)	108.8(5)
C(42)	B(1)	C(50)	109.3(5)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Pd(1)	C(1)	H(1)	101.0	C(2)	C(1)	H(1)	119.0
C(15)	C(1)	H(1)	114.8	Pd(1)	C(2)	H(2)	115.3
C(1)	C(2)	H(2)	114.5	C(3)	C(2)	H(2)	121.6
Pd(2)	C(3)	H(3)	102.0	C(2)	C(3)	H(3)	122.6
C(4)	C(3)	H(3)	116.3	Pd(2)	C(4)	H(4)	101.1
C(3)	C(4)	H(4)	112.8	C(5)	C(4)	H(4)	128.2
Pd(2)	C(5)	H(5)	118.3	C(4)	C(5)	H(5)	111.8
C(6)	C(5)	H(5)	124.3	Pd(2)	C(6)	H(6)	98.9
C(5)	C(6)	H(6)	120.4	C(7)	C(6)	H(6)	117.7
Pd(1)	C(7)	H(7)	103.4	C(6)	C(7)	H(7)	114.5
C(8)	C(7)	H(7)	124.0	Pd(1)	C(8)	H(8)	92.5
C(7)	C(8)	H(8)	122.1	C(9)	C(8)	H(8)	115.6
C(9)	C(10)	H(9)	119.3	C(11)	C(10)	H(9)	119.2
C(10)	C(11)	H(10)	120.7	C(12)	C(11)	H(10)	119.6
C(11)	C(12)	H(11)	121.1	C(13)	C(12)	H(11)	118.9
C(12)	C(13)	H(12)	121.8	C(14)	C(13)	H(12)	117.3
C(9)	C(14)	H(13)	119.9	C(13)	C(14)	H(13)	120.5
C(15)	C(16)	H(14)	117.8	C(17)	C(16)	H(14)	119.7
C(16)	C(17)	H(15)	120.2	C(18)	C(17)	H(15)	122.0
C(17)	C(18)	H(16)	119.4	C(19)	C(18)	H(16)	119.8
C(18)	C(19)	H(17)	121.3	C(20)	C(19)	H(17)	118.9
C(15)	C(20)	H(18)	119.0	C(19)	C(20)	H(18)	120.3
N(1)	C(21)	H(31)	117.9	C(22)	C(21)	H(31)	118.6
C(21)	C(22)	H(32)	121.4	C(23)	C(22)	H(32)	120.8

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(22)	C(23)	H(33)	121.0	C(24)	C(23)	H(33)	118.4
C(23)	C(24)	H(34)	121.1	C(25)	C(24)	H(34)	119.5
N(1)	C(25)	H(35)	119.6	C(24)	C(25)	H(35)	119.2
C(26)	C(27)	H(21)	117.7	C(28)	C(27)	H(21)	118.9
C(28)	C(29)	H(19)	119.8	C(30)	C(29)	H(19)	121.5
C(26)	C(31)	H(20)	118.9	C(30)	C(31)	H(20)	119.3
C(34)	C(35)	H(30)	118.5	C(36)	C(35)	H(30)	118.1
C(36)	C(37)	H(28)	119.9	C(38)	C(37)	H(28)	121.5
C(34)	C(39)	H(29)	118.4	C(38)	C(39)	H(29)	119.7
C(42)	C(43)	H(22)	119.1	C(44)	C(43)	H(22)	119.0
C(44)	C(45)	H(23)	122.0	C(46)	C(45)	H(23)	120.9
C(42)	C(47)	H(24)	117.8	C(46)	C(47)	H(24)	118.4
C(50)	C(51)	H(27)	119.2	C(52)	C(51)	H(27)	118.7
C(52)	C(53)	H(25)	121.8	C(54)	C(53)	H(25)	120.8
C(50)	C(55)	H(26)	119.1	C(54)	C(55)	H(26)	119.8