Crystallographic Structural Determination. The single crystal X-ray diffraction experiment was performed on a Siemens P4/CCD diffractometer for **3**. Crystal, data collection, and refinement parameters are given in Table I. Systematic absences and diffraction symmetry are consistent for the space groups, *P*1 and *P* for **3**. The *E*-statistics suggested the centrosymmetric option, which yielded chemically reasonable and computationally stable results of refinement. The structure was solved using direct methods, completed by subsequent difference Fourier syntheses and refined by full-matrix, least-squares procedures. An empirical absorption correction was applied to the data using the program DIFABS. All non-hydrogen atoms were refined with anisotropic displacement coefficients. Hydrogen atoms were treated as idealized contributions. Three molecules of THF co-crystallized with the sample, one of which is disordered over an inversion center. One of the phenyl rings attached to P(1) possesses very large thermal ellipsoids in a pattern consistent with positional disorder. The resolution of the current data did not allow the construction of a multi-site disorder model.

All software and sources of the scattering factors are contained in the SHELXTL (5.03) program library (G. Sheldrick, Siemens XRD, Madison, WI). The program DIFABS is described by Walker, N. and Stuart, D. in *Acta Cryst.* 1983, *A39*, 158.

Table 9S. Crystal data and structure refinement for **3**

Identification code	hart01
Empirical formula	$C_{114}H_{108}Fe_3O_3P_6Pd_2$
Formua weight	2092.17
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal Systems	Triclinic
Space Group	*P* (no. 1)
Unit cell dimensions	a = 11.29580(5) Å α = 68.919(1)°
	b = 13.4092(1) Å β = 83.384(1)°
	c = 17.4577(2) Å γ = 70.923(1)°
Volume, Z	2334.59(3) $Å^3$, 1
Density (calculated)	1.490 g/cm^3
Absorption coefficient	0.992 mm^{-1}
F(000)	1076
Crystal Size	0.40 x 0.25 x 0.08 mm
Cystal Color	yellow blade
θ range for data collection	1.25 to 28.78°
Limiting indices	$-14 \le h \le 14$, $-16 \le k \le 17$, $0 \le l \le 23$
Reflections collected	15174
Independent reflections	10454 (R_{int} = 0.0542)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10443/ 0 / 657
Goodness-of-fit on F^2	1.299
Final R indices [$I>2\sigma(I)$]	R1 = 0.0689, wR2 = 0.1780
R indices (all data)	R1 = 0.1009, wR2 = 0.2137
Largest diff. peak and hole	2.298 and -2.068 $eÅ^{-3}$

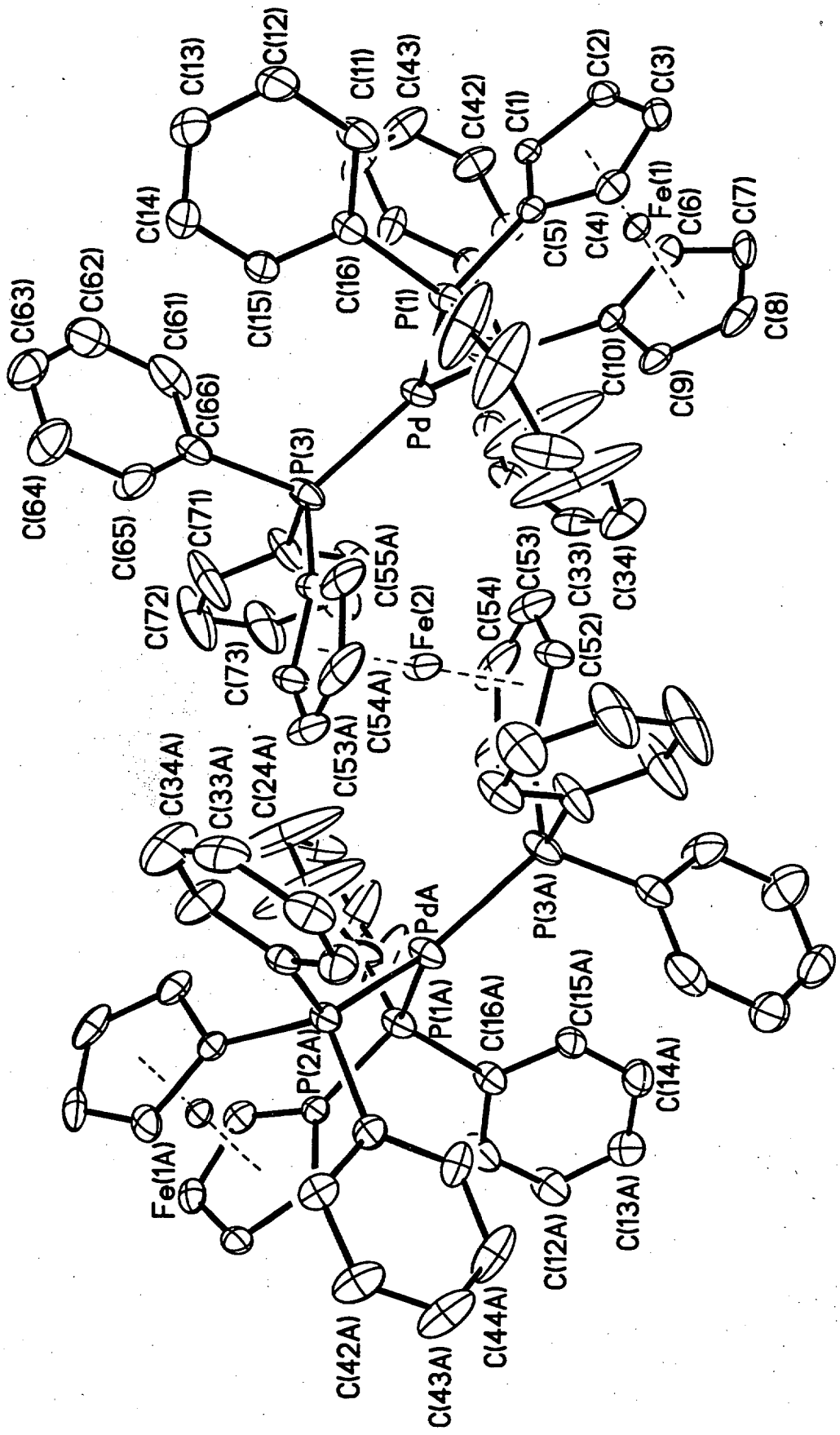

Table 10S. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å2 x 10^3] for **3**. U(eq) is defined as one third of the trace of the orthodonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	2928.0(4)	-74.9(4)	2219.3(2)	37(1)
Fe(1)	4225.1(6)	-2609.8(7)	4408.4(5)	29(1)
Fe(2)	5000	0	0	85(1)
P(1)	2472(2)	-1728(1)	2719(1)	37(1)
P(2)	3786(1)	112(1)	3265(1)	30(1)
P(3)	2405(2)	1200(2)	935(1)	47(1)
C(1)	2352(5)	-2096(5)	4420(3)	33(1)
C(2)	2808(5)	-2937(5)	5173(3)	37(1)
C(3)	3528(5)	-3906(5)	5015(4)	36(1)
C(4)	3516(5)	-3676(5)	4162(4)	37(1)
C(5)	2790(5)	-2550(5)	3788(3)	30(1)
C(6)	4921(5)	-1677(5)	4799(4)	39(1)
C(7)	5743(5)	-2748(5)	4993(4)	47(2)
C(8)	6114(5)	-2983(6)	4274(5)	52(2)
C(9)	5496(5)	-2053(5)	3622(4)	41(1)
C(10)	4739(5)	-1203(5)	3933(3)	31(1)
C(11)	271(7)	-2349(7)	3234(4)	62(2)
C(12)	-947(7)	-2276(7)	3122(4)	65(2)
C(13)	-1582(6)	-1532(6)	2436(4)	49(2)
C(14)	-1037(6)	-830(6)	1875(4)	51(2)
C(15)	167(6)	-879(5)	1981(4)	41(1)
C(16)	851(5)	-1664(5)	2650(3)	37(1)
C(21)	2776(8)	-3426(9)	2102(9)	125(5)
C(22)	3378(8)	-4218(10)	1788(10)	129(6)
C(23)	4479(10)	-4221(7)	1433(5)	81(3)
C(24)	5060(15)	-3621(17)	1607(13)	256(13)
C(25)	4428(13)	-2890(16)	2011(12)	233(12)
C(26)	3278(6)	-2778(6)	2253(4)	46(2)
C(31)	4313(6)	2086(5)	3045(4)	45(2)
C(32)	5063(7)	2755(6)	2904(4)	52(2)
C(33)	6310(7)	2321(7)	2877(4)	57(2)
C(34)	6812(7)	1215(8)	2969(6)	81(3)
C(35)	6056(6)	541(6)	3113(5)	58(2)
C(36)	4800(5)	968(5)	3155(3)	31(1)
C(41)	2868(6)	806(5)	4612(4)	40(1)
C(42)	1920(7)	1224(6)	5085(5)	60(2)
C(43)	713(7)	1430(8)	4911(6)	76(3)
C(44)	436(6)	1252(7)	4250(6)	76(3)
C(45)	1358(5)	858(5)	3753(4)	47(2)
C(46)	2594(5)	627(5)	3932(3)	35(1)
C(51)	3142(6)	707(8)	109(4)	64(2)
C(52)	6392(7)	-1305(12)	657(4)	114(5)
C(53)	5889(8)	-550(17)	1075(5)	158(8)
C(54)	6029(7)	490(14)	603(7)	121(6)
C(55)	6630(6)	389(9)	-126(5)	72(3)
C(61)	-105(9)	2044(6)	1211(4)	69(2)
C(62)	-1373(9)	2348(7)	1075(6)	86(3)

C(63)	-1780(7)	2239(6)	411(6)	66(2)
C(64)	-955(7)	1875(8)	-113(6)	74(2)
C(65)	312(7)	1565(8)	29(5)	69(2)
C(66)	750(6)	1648(5)	683(3)	42(1)
C(71)	1985(11)	3473(9)	47(6)	122(5)
C(72)	2167(11)	4516(8)	-163(7)	125(5)
C(73)	3124(10)	4571(8)	212(6)	102(4)
C(74)	3831(8)	3654(7)	785(5)	72(2)
C(75)	3608(7)	2634(6)	1018(4)	55(2)
C(76)	2660(8)	2566(6)	629(4)	65(2)
O(101)	1425(19)	4600(17)	-2375(11)	269(7)
C(101)	92(24)	4496(21)	-2001(15)	228(10)
C(102)	-891(43)	5588(40)	-2396(30)	421(29)
C(103)	-198(38)	5998(31)	-2288(22)	354(19)
C(104)	1112(22)	5744(19)	-2507(14)	217(9)
O(105)	9223(16)	-4468(15)	5391(11)	104(5)
C(105)	10522(16)	-4674(14)	5354(10)	150(5)
C(106)	8886(22)	-4952(21)	5150(16)	206(9)

Table 11S. Bond lengths [Å] and angles [°] for **3**.

Pd-P(3)	2.278(2)	Pd-P(1)	2.278(2)
Pd-P(2)	2.2872(13)	Fe(1)-C(1)	2.000(5)
Fe(1)-C(9)	2.004(6)	Fe(1)-C(6)	2.007(5)
Fe(1)-C(10)	2.015(5)	Fe(1)-C(5)	2.015(5)
Fe(1)-C(7)	2.019(6)	Fe(1)-C(2)	2.020(5)
Fe(1)-C(3)	2.035(5)	Fe(1)-C(8)	2.031(6)
Fe(1)-C(4)	2.035(5)	Fe(2)-C(52)	2.006(10)
Fe(2)-C(52)#1	2.006(10)	Fe(2)-C(53)	2.007(8)
Fe(2)-C(53)#1	2.007(8)	Fe(2)-C(51)#1	2.019(7)
Fe(2)-C(51)	2.019(7)	Fe(2)-C(55)#1	2.040(7)
Fe(2)-C(55)	2.040(7)	Fe(2)-C(54)#1	2.042(9)
Fe(2)-C(54)	2.042(9)	P(1)-C(26)	1.814(7)
P(1)-C(5)	1.801(5)	P(1)-C(16)	1.821(6)
P(2)-C(10)	1.788(6)	P(2)-C(46)	1.804(6)
P(2)-C(36)	1.821(5)	P(3)-C(76)	1.825(7)
P(3)-C(51)	1.804(8)	P(3)-C(66)	1.819(7)
C(1)-C(2)	1.406(8)	C(1)-C(5)	1.411(7)
C(2)-C(3)	1.392(8)	C(3)-C(4)	1.409(8)
C(4)-C(5)	1.409(8)	C(6)-C(7)	1.375(9)
C(6)-C(10)	1.425(8)	C(7)-C(8)	1.388(10)
C(8)-C(9)	1.390(9)	C(9)-C(10)	1.423(8)
C(11)-C(12)	1.377(9)	C(11)-C(16)	1.371(8)
C(12)-C(13)	1.348(10)	C(13)-C(14)	1.342(9)
C(14)-C(15)	1.372(8)	C(15)-C(16)	1.364(8)
C(21)-C(22)	1.323(12)	C(21)-C(26)	1.291(10)
C(22)-C(23)	1.323(13)	C(23)-C(24)	1.318(13)
C(24)-C(25)	1.375(14)	C(25)-C(26)	1.297(11)
C(31)-C(32)	1.368(9)	C(31)-C(36)	1.365(8)
C(32)-C(33)	1.340(10)	C(33)-C(34)	1.359(11)
C(34)-C(35)	1.378(9)	C(35)-C(36)	1.350(8)
C(41)-C(42)	1.370(8)	C(41)-C(46)	1.380(8)
C(42)-C(43)	1.348(10)	C(43)-C(44)	1.348(12)
C(44)-C(45)	1.372(10)	C(45)-C(46)	1.375(8)
C(51)-C(55)#1	1.396(12)	C(51)-C(52)#1	1.432(9)
C(52)-C(53)	1.39(2)	C(52)-C(51)#1	1.432(9)
C(53)-C(54)	1.39(2)	C(54)-C(55)	1.401(11)
C(55)-C(51)#1	1.396(12)	C(61)-C(62)	1.379(12)
C(61)-C(66)	1.370(10)	C(62)-C(63)	1.366(13)
C(63)-C(64)	1.331(11)	C(64)-C(65)	1.379(10)
C(65)-C(66)	1.350(9)	C(71)-C(72)	1.391(13)
C(71)-C(76)	1.333(11)	C(72)-C(73)	1.361(12)
C(73)-C(74)	1.344(11)	C(74)-C(75)	1.378(10)
C(75)-C(76)	1.375(9)	O(101)-C(104)	1.39(2)
O(101)-C(101)	1.60(2)	C(101)-C(102)	1.50(4)
C(102)-C(103)	1.16(5)	C(103)-C(104)	1.44(3)
O(105)-C(106)	1.07(3)	O(105)-C(105)	1.40(2)
O(105)-C(105)#2	1.97(2)	C(105)-C(106)#2	1.20(2)
C(105)-O(105)#2	1.97(2)	C(106)-C(105)#2	1.20(2)

P(3)-Pd-P(1)	124.02(5)	P(3)-Pd-P(2)	127.90(6)
P(1)-Pd-P(2)	107.80(5)	C(1)-Fe(1)-C(9)	133.2(2)
C(1)-Fe(1)-C(6)	111.4(2)	C(9)-Fe(1)-C(6)	68.8(2)
C(1)-Fe(1)-C(10)	105.9(2)	C(9)-Fe(1)-C(10)	41.5(2)
C(6)-Fe(1)-C(10)	41.5(2)	C(1)-Fe(1)-C(5)	41.1(2)

C(9)-Fe(1)-C(5)	110.1(2)	C(6)-Fe(1)-C(5)	143.4(2)
C(10)-Fe(1)-C(5)	112.4(2)	C(1)-Fe(1)-C(7)	142.8(3)
C(9)-Fe(1)-C(7)	68.0(3)	C(6)-Fe(1)-C(7)	39.9(3)
C(10)-Fe(1)-C(7)	68.8(2)	C(5)-Fe(1)-C(7)	175.9(3)
C(1)-Fe(1)-C(2)	40.9(2)	C(9)-Fe(1)-C(2)	171.8(3)
C(6)-Fe(1)-C(2)	106.9(2)	C(10)-Fe(1)-C(2)	130.7(2)
C(5)-Fe(1)-C(2)	68.9(2)	C(7)-Fe(1)-C(2)	113.5(3)
C(1)-Fe(1)-C(3)	68.3(2)	C(9)-Fe(1)-C(3)	147.7(2)
C(6)-Fe(1)-C(3)	132.4(2)	C(10)-Fe(1)-C(3)	170.6(2)
C(5)-Fe(1)-C(3)	68.6(2)	C(7)-Fe(1)-C(3)	110.9(2)
C(2)-Fe(1)-C(3)	40.2(2)	C(1)-Fe(1)-C(8)	173.5(3)
C(9)-Fe(1)-C(8)	40.3(3)	C(6)-Fe(1)-C(8)	67.6(3)
C(10)-Fe(1)-C(8)	68.8(2)	C(5)-Fe(1)-C(8)	136.2(3)
C(7)-Fe(1)-C(8)	40.1(3)	C(2)-Fe(1)-C(8)	145.5(3)
C(3)-Fe(1)-C(8)	117.4(2)	C(1)-Fe(1)-C(4)	68.4(2)
C(9)-Fe(1)-C(4)	116.9(2)	C(6)-Fe(1)-C(4)	172.8(2)
C(10)-Fe(1)-C(4)	145.7(2)	C(5)-Fe(1)-C(4)	40.7(2)
C(7)-Fe(1)-C(4)	136.4(3)	C(2)-Fe(1)-C(4)	68.0(2)
C(3)-Fe(1)-C(4)	40.5(2)	C(8)-Fe(1)-C(4)	113.4(3)
C(52)-Fe(2)-C(52)#1	180.0	C(52)-Fe(2)-C(53)	40.6(6)
C(52)#1-Fe(2)-C(53)	139.4(6)	C(52)-Fe(2)-C(53)#1	139.4(6)
C(52)#1-Fe(2)-C(53)#1	40.6(6)	C(53)-Fe(2)-C(53)#1	180.0
C(52)-Fe(2)-C(51)#1	41.7(3)	C(52)#1-Fe(2)-C(51)#1	138.3(3)
C(53)-Fe(2)-C(51)#1	68.7(3)	C(53)#1-Fe(2)-C(51)#1	111.3(3)
C(52)-Fe(2)-C(51)	138.3(3)	C(52)#1-Fe(2)-C(51)	41.7(3)
C(53)-Fe(2)-C(51)	111.3(3)	C(53)#1-Fe(2)-C(51)	68.7(3)
C(51)#1-Fe(2)-C(51)	180.0	C(52)-Fe(2)-C(55)#1	111.5(4)
C(52)#1-Fe(2)-C(55)#1	68.5(4)	C(53)-Fe(2)-C(55)#1	112.4(4)
C(53)#1-Fe(2)-C(55)#1	67.6(4)	C(51)#1-Fe(2)-C(55)#1	139.8(3)
C(51)-Fe(2)-C(55)#1	40.2(3)	C(52)-Fe(2)-C(55)	68.5(4)
C(52)#1-Fe(2)-C(55)	111.5(4)	C(53)-Fe(2)-C(55)	67.6(4)
C(53)#1-Fe(2)-C(55)	112.4(4)	C(51)#1-Fe(2)-C(55)	40.2(3)
C(51)-Fe(2)-C(55)	139.8(3)	C(55)#1-Fe(2)-C(55)	179.998(1)
C(52)-Fe(2)-C(54)#1	111.6(6)	C(52)#1-Fe(2)-C(54)#1	68.4(6)
C(53)-Fe(2)-C(54)#1	139.8(6)	C(53)#1-Fe(2)-C(54)#1	40.2(6)
C(51)#1-Fe(2)-C(54)#1	111.8(4)	C(51)-Fe(2)-C(54)#1	68.2(4)
C(55)#1-Fe(2)-C(54)#1	40.1(3)	C(55)-Fe(2)-C(54)#1	139.9(3)
C(52)-Fe(2)-C(54)	68.4(6)	C(52)#1-Fe(2)-C(54)	111.6(6)
C(53)-Fe(2)-C(54)	40.2(6)	C(53)#1-Fe(2)-C(54)	139.8(6)
C(51)#1-Fe(2)-C(54)	68.2(4)	C(51)-Fe(2)-C(54)	111.8(4)
C(55)#1-Fe(2)-C(54)	139.9(3)	C(55)-Fe(2)-C(54)	40.1(3)
C(54)#1-Fe(2)-C(54)	179.999(1)	C(26)-P(1)-C(5)	100.5(3)
C(26)-P(1)-C(16)	100.9(3)	C(5)-P(1)-C(16)	100.6(2)
C(26)-P(1)-Pd	116.9(2)	C(5)-P(1)-Pd	117.6(2)
C(16)-P(1)-Pd	117.3(2)	C(10)-P(2)-C(46)	103.9(3)
C(10)-P(2)-C(36)	99.5(2)	C(46)-P(2)-C(36)	100.6(2)
C(10)-P(2)-Pd	112.5(2)	C(46)-P(2)-Pd	111.4(2)
C(36)-P(2)-Pd	126.2(2)	C(76)-P(3)-C(51)	102.1(4)
C(76)-P(3)-C(66)	99.9(3)	C(51)-P(3)-C(66)	102.2(3)
C(76)-P(3)-Pd	120.7(2)	C(51)-P(3)-Pd	114.9(3)
C(66)-P(3)-Pd	114.4(2)	C(2)-C(1)-C(5)	108.3(5)
C(2)-C(1)-Fe(1)	70.3(3)	C(5)-C(1)-Fe(1)	70.0(3)
C(3)-C(2)-C(1)	108.1(5)	C(3)-C(2)-Fe(1)	70.5(3)
C(1)-C(2)-Fe(1)	68.8(3)	C(2)-C(3)-C(4)	108.2(5)
C(2)-C(3)-Fe(1)	69.3(3)	C(4)-C(3)-Fe(1)	69.7(3)
C(3)-C(4)-C(5)	108.2(5)	C(3)-C(4)-Fe(1)	69.7(3)
C(5)-C(4)-Fe(1)	68.9(3)	C(1)-C(5)-C(4)	107.2(5)
C(1)-C(5)-P(1)	122.6(4)	C(4)-C(5)-P(1)	130.1(4)
C(1)-C(5)-Fe(1)	68.9(3)	C(4)-C(5)-Fe(1)	70.4(3)

P(1)-C(5)-Fe(1)	123.6(3)	C(7)-C(6)-C(10)	109.0(6)
C(7)-C(6)-Fe(1)	70.5(4)	C(10)-C(6)-Fe(1)	69.6(3)
C(6)-C(7)-C(8)	108.8(6)	C(6)-C(7)-Fe(1)	69.6(3)
C(8)-C(7)-Fe(1)	70.4(4)	C(7)-C(8)-C(9)	108.1(6)
C(7)-C(8)-Fe(1)	69.5(3)	C(9)-C(8)-Fe(1)	68.8(3)
C(8)-C(9)-C(10)	108.7(6)	C(8)-C(9)-Fe(1)	70.9(3)
C(10)-C(9)-Fe(1)	69.7(3)	C(6)-C(10)-C(9)	105.3(5)
C(6)-C(10)-P(2)	133.5(4)	C(9)-C(10)-P(2)	121.2(4)
C(6)-C(10)-Fe(1)	68.9(3)	C(9)-C(10)-Fe(1)	68.8(3)
P(2)-C(10)-Fe(1)	124.6(3)	C(12)-C(11)-C(16)	120.5(6)
C(13)-C(12)-C(11)	120.4(6)	C(14)-C(13)-C(12)	119.5(6)
C(13)-C(14)-C(15)	120.9(6)	C(16)-C(15)-C(14)	120.6(6)
C(15)-C(16)-C(11)	117.9(6)	C(15)-C(16)-P(1)	118.1(4)
C(11)-C(16)-P(1)	124.0(5)	C(22)-C(21)-C(26)	124.7(9)
C(21)-C(22)-C(23)	119.7(10)	C(24)-C(23)-C(22)	116.1(8)
C(23)-C(24)-C(25)	119.6(10)	C(24)-C(25)-C(26)	122.9(8)
C(25)-C(26)-C(21)	114.8(8)	C(25)-C(26)-P(1)	120.3(5)
C(21)-C(26)-P(1)	124.9(6)	C(32)-C(31)-C(36)	121.7(6)
C(33)-C(32)-C(31)	120.4(6)	C(32)-C(33)-C(34)	118.8(6)
C(35)-C(34)-C(33)	120.7(7)	C(34)-C(35)-C(36)	120.7(7)
C(35)-C(36)-C(31)	117.6(5)	C(35)-C(36)-P(2)	121.0(5)
C(31)-C(36)-P(2)	121.2(4)	C(42)-C(41)-C(46)	120.2(6)
C(43)-C(42)-C(41)	120.9(7)	C(42)-C(43)-C(44)	119.4(7)
C(45)-C(44)-C(43)	121.4(7)	C(44)-C(45)-C(46)	119.8(7)
C(45)-C(46)-C(41)	118.4(6)	C(45)-C(46)-P(2)	118.7(5)
C(41)-C(46)-P(2)	122.8(4)	C(55)#1-C(51)-C(52)#1	107.2(9)
C(55)#1-C(51)-P(3)	123.9(5)	C(52)#1-C(51)-P(3)	129.0(9)
C(55)#1-C(51)-Fe(2)	70.7(5)	C(52)#1-C(51)-Fe(2)	68.7(5)
P(3)-C(51)-Fe(2)	125.4(3)	C(53)-C(52)-C(51)#1	106.9(12)
C(53)-C(52)-Fe(2)	69.7(7)	C(51)#1-C(52)-Fe(2)	69.6(5)
C(52)-C(53)-C(54)	109.5(8)	C(52)-C(53)-Fe(2)	69.7(5)
C(54)-C(53)-Fe(2)	71.3(5)	C(53)-C(54)-C(55)	107.4(12)
C(53)-C(54)-Fe(2)	68.5(6)	C(55)-C(54)-Fe(2)	69.8(4)
C(51)#1-C(55)-C(54)	109.0(10)	C(51)#1-C(55)-Fe(2)	69.1(4)
C(54)-C(55)-Fe(2)	70.0(5)	C(62)-C(61)-C(66)	120.8(7)
C(61)-C(62)-C(63)	119.5(8)	C(64)-C(63)-C(62)	120.0(8)
C(63)-C(64)-C(65)	120.3(8)	C(64)-C(65)-C(66)	121.5(7)
C(65)-C(66)-C(61)	117.9(7)	C(65)-C(66)-P(3)	124.0(5)
C(61)-C(66)-P(3)	118.1(5)	C(72)-C(71)-C(76)	122.1(8)
C(71)-C(72)-C(73)	117.5(8)	C(74)-C(73)-C(72)	120.7(8)
C(73)-C(74)-C(75)	121.5(7)	C(76)-C(75)-C(74)	118.1(7)
C(75)-C(76)-C(71)	119.9(7)	C(75)-C(76)-P(3)	117.3(5)
C(71)-C(76)-P(3)	122.8(6)	C(104)-O(101)-C(101)	95(2)
C(102)-C(101)-O(101)	109(3)	C(103)-C(102)-C(101)	85(4)
C(102)-C(103)-C(104)	126(4)	O(101)-C(104)-C(103)	101(2)
C(106)-O(105)-C(105)	115(2)	C(106)-O(105)-C(105)#2	32(2)
C(105)-O(105)-C(105)#2	86.3(13)	O(105)-C(105)-C(106)#2	119(2)
O(105)-C(105)-O(105)#2	93.7(13)	C(106)#2-C(105)-O(105)#2	27.9(14)
O(105)-C(106)-C(105)#2	121(3)		

Symmetry transformations used to generate equivalent atoms:

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

Table 12S. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **3**. The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd	49(1)	50(1)	24(1)	-8(1)	-3(1)	-34(1)
Fe(1)	22(1)	35(1)	33(1)	-10(1)	-1(1)	-14(1)
Fe(2)	30(1)	205(2)	25(1)	-31(1)	1(1)	-54(1)
P(1)	45(1)	49(1)	28(1)	-10(1)	-2(1)	-32(1)
P(2)	33(1)	38(1)	25(1)	-9(1)	-2(1)	-21(1)
P(3)	64(1)	62(1)	25(1)	-3(1)	-9(1)	-44(1)
C(1)	21(2)	45(3)	28(3)	-7(2)	0(2)	-13(2)
C(2)	32(3)	51(4)	30(3)	-8(3)	2(2)	-22(3)
C(3)	29(3)	33(3)	44(3)	-3(3)	-6(2)	-15(2)
C(4)	31(3)	41(3)	48(3)	-19(3)	2(2)	-20(2)
C(5)	26(2)	37(3)	31(3)	-10(2)	-1(2)	-16(2)
C(6)	35(3)	49(4)	39(3)	-11(3)	-9(2)	-21(3)
C(7)	28(3)	41(4)	60(4)	2(3)	-21(3)	-11(3)
C(8)	22(3)	37(4)	103(6)	-28(4)	8(3)	-14(3)
C(9)	26(3)	39(3)	59(4)	-16(3)	9(3)	-16(3)
C(10)	21(2)	39(3)	36(3)	-11(2)	1(2)	-15(2)
C(11)	68(5)	86(6)	39(3)	5(4)	-13(3)	-57(4)
C(12)	60(4)	97(6)	47(4)	-6(4)	-7(3)	-56(4)
C(13)	46(4)	67(5)	50(4)	-27(4)	0(3)	-31(3)
C(14)	41(3)	56(4)	53(4)	-13(3)	-8(3)	-14(3)
C(15)	41(3)	35(3)	40(3)	-1(3)	-1(3)	-17(3)
C(16)	46(3)	41(3)	32(3)	-10(3)	-6(2)	-27(3)
C(21)	39(4)	100(8)	287(17)	-139(10)	-25(7)	1(5)
C(22)	42(5)	113(8)	282(17)	-141(11)	-18(7)	0(5)
C(23)	149(9)	71(6)	57(4)	-39(4)	46(5)	-74(6)
C(24)	217(15)	390(25)	435(28)	-382(25)	277(19)	-268(18)
C(25)	174(12)	390(23)	405(24)	-377(23)	225(15)	-238(15)
C(26)	62(4)	65(4)	32(3)	-19(3)	12(3)	-45(3)
C(31)	42(3)	42(4)	52(4)	-12(3)	2(3)	-18(3)
C(32)	82(5)	32(3)	47(4)	-8(3)	5(3)	-32(3)
C(33)	74(5)	73(5)	52(4)	-26(4)	19(4)	-59(4)
C(34)	51(4)	78(6)	131(8)	-37(6)	21(5)	-46(4)
C(35)	41(4)	44(4)	99(6)	-32(4)	21(4)	-25(3)
C(36)	38(3)	38(3)	22(2)	-9(2)	-1(2)	-22(2)
C(41)	39(3)	41(3)	49(3)	-23(3)	6(3)	-17(3)
C(42)	50(4)	65(5)	81(5)	-46(4)	23(4)	-24(4)
C(43)	47(4)	85(6)	126(8)	-73(6)	33(5)	-27(4)
C(44)	27(3)	68(5)	143(9)	-52(6)	4(4)	-11(3)
C(45)	30(3)	42(4)	70(4)	-20(3)	-8(3)	-6(3)
C(46)	31(3)	39(3)	39(3)	-12(3)	0(2)	-18(2)
C(51)	35(3)	133(8)	23(3)	-5(4)	-7(3)	-47(4)
C(52)	37(4)	246(14)	27(4)	14(6)	-10(3)	-69(6)
C(53)	30(4)	397(25)	31(4)	-58(9)	0(4)	-61(9)
C(54)	28(4)	282(18)	92(8)	-131(10)	-4(5)	-23(7)
C(55)	34(3)	153(9)	66(5)	-71(6)	8(3)	-44(5)
C(61)	108(7)	41(4)	37(4)	-11(3)	-9(4)	2(4)
C(62)	75(6)	65(6)	66(5)	-7(5)	17(5)	22(5)

C(63)	42(4)	43(4)	92(6)	-10(4)	9(4)	-6(3)
C(64)	50(4)	101(7)	95(6)	-51(6)	2(4)	-33(4)
C(65)	41(4)	127(8)	60(4)	-46(5)	8(3)	-41(4)
C(66)	58(4)	39(3)	29(3)	-2(3)	-1(3)	-25(3)
C(71)	164(10)	115(8)	80(6)	55(6)	-86(7)	-102(8)
C(72)	157(10)	68(6)	121(9)	62(6)	-91(8)	-75(7)
C(73)	128(9)	68(6)	90(7)	42(5)	-49(6)	-64(6)
C(74)	91(6)	72(5)	68(5)	-7(4)	-20(5)	-56(5)
C(75)	84(5)	57(4)	36(3)	-4(3)	-13(3)	-46(4)
C(76)	91(5)	57(4)	46(4)	20(3)	-37(4)	-52(4)

Table 13S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å2 x 10^3) for **3**.

	x	y	z	U(eq)
H(1A)	1804(5)	-1312(5)	4345(3)	39
H(2A)	2650(5)	-2853(5)	5725(3)	45
H(3A)	3985(5)	-4635(5)	5434(4)	44
H(4A)	3963(5)	-4214(5)	3871(4)	44
H(6A)	4510(5)	-1295(5)	5202(4)	47
H(7A)	6023(5)	-3275(5)	5560(4)	56
H(8A)	6701(5)	-3705(6)	4234(5)	63
H(9A)	5576(5)	-1990(5)	3031(4)	49
H(11A)	711(7)	-2878(7)	3719(4)	75
H(12A)	-1340(7)	-2754(7)	3532(4)	78
H(13A)	-2410(6)	-1504(6)	2351(4)	58
H(14A)	-1492(6)	-292(6)	1398(4)	61
H(15A)	529(6)	-361(5)	1585(4)	49
H(21A)	1913(8)	-3327(9)	2225(9)	150
H(22A)	3022(8)	-4782(10)	1818(10)	155
H(23A)	4830(10)	-4631(7)	1074(5)	97
H(24A)	5911(15)	-3693(17)	1454(13)	308
H(25A)	4853(13)	-2448(16)	2117(12)	280
H(31A)	3431(6)	2407(5)	3067(4)	54
H(32A)	4696(7)	3531(6)	2825(4)	62
H(33A)	6835(7)	2778(7)	2795(4)	69
H(34A)	7694(7)	902(8)	2933(6)	97
H(35A)	6423(6)	-233(6)	3183(5)	70
H(41A)	3716(6)	639(5)	4754(4)	48
H(42A)	2117(7)	1371(6)	5540(5)	71
H(43A)	63(7)	1699(8)	5252(6)	91
H(44A)	-416(6)	1403(7)	4127(6)	91
H(45A)	1144(5)	744(5)	3287(4)	57
H(52A)	6434(7)	-2115(12)	858(4)	136
H(53A)	5486(8)	-727(17)	1628(5)	190
H(54A)	5744(7)	1184(14)	754(7)	145
H(55A)	6837(6)	1008(9)	-590(5)	86
H(61A)	178(9)	2109(6)	1677(4)	82
H(62A)	-1960(9)	2632(7)	1440(6)	103
H(63A)	-2652(7)	2424(6)	323(6)	79
H(64A)	-1240(7)	1828(8)	-586(6)	89
H(65A)	889(7)	1286(8)	-343(5)	82
H(71A)	1360(11)	3404(9)	-234(6)	147
H(72A)	1642(11)	5166(8)	-553(7)	149
H(73A)	3295(10)	5264(8)	67(6)	123
H(74A)	4500(8)	3710(7)	1034(5)	86
H(75A)	4094(7)	1997(6)	1437(4)	66
H(10A)	-85(24)	3881(21)	-2108(15)	273
H(10B)	93(24)	4321(21)	-1400(15)	273
H(10C)	-1052(43)	5751(40)	-2981(30)	505
H(10D)	-1681(43)	5709(40)	-2082(30)	505
H(10E)	-227(38)	5870(31)	-1692(22)	425
H(10F)	-572(38)	6817(31)	-2565(22)	425

H(10G)	1236(22)	6177(19)	-3087(14)	260
H(10H)	1603(22)	5892(19)	-2147(14)	260
H(10I)	10870(16)	-5199(14)	5900(10)	180
H(10J)	10680(16)	-3957(14)	5269(10)	180
H(10K)	8764(179)	-3723(169)	5643(113)	247
H(10L)	8982(183)	-4455(166)	6067(115)	247

Crystallographic Structural Determination. Crystal, data collection and refinement parameters are given in Table I. The data were collected on a Siemens P4 diffractometer equipped with a SMART/CCD detector.

Systematic absences and diffraction symmetry are consistent for the space groups *P*1 and $P\bar{1}$ for **6**. The *E*-statistics suggested the centrosymmetric option, which yielded chemically reasonable and computationally stable results and refinement. The structure was solved using direct methods, completed by subsequent difference Fourier synthesis and refined by full-matrix least-squares methods. Empirical adsorption corrections were applied using *DIFABS* to the data of **6**. There is one benzene molecule in the asymmetric unit of **6**. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were treated as idealized contributions.

All software and sources of the scattering factors are contained in the SHELXTL (version 5.03) program library (G. Sheldrick, Siemens XRD, Madison, WI). The program *DIFABS* is described by Walker, N and Stuart, D. in *Acta Cryst.* **1983**, 158.

Table 14S. Crystal data and structure refinement for **6**

Identification code	hart05
Empirical formula	$C_{56}H_{43}BrP_2Pd$
Formua weight	964.15
Temperature	198(2) K
Wavelength	0.71073 Å
Crystal Systems	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	a = 12.3757(2) Å α = 83.5768(7)°
	b = 12.9432(2) Å β = 82.1315(4)°
	c = 14.5021(2) Å γ = 77.3821(7)°
Volume, Z	2237.43(6) $Å^3$, 2
Density (calculated)	1.431 g/cm^3
Absorption coefficient	1.417 mm^{-1}
F(000)	980
Crystal Size	0.40 x 0.40 x 0.30 mm
Cystal Color	yellow block
θ range for data collection	1.42 to 28.24°
Limiting indices	$-15 \le h \le 16$, $-16 \le k \le 17$, $-1 \le l \le 19$
Reflections collected	14728
Independent reflections	9662 (R_{int} = 0.0346)
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.810
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9662 / 0 / 541
Goodness-of-fit on F^2	0.985
Final R indices [$I>2\sigma(I)$]	R1 = 0.0335, wR2 = 0.0906
R indices (all data)	R1 = 0.0425, wR2 = 0.0941
Largest diff. peak and hole	0.651 and -8.55 $eÅ^{-3}$

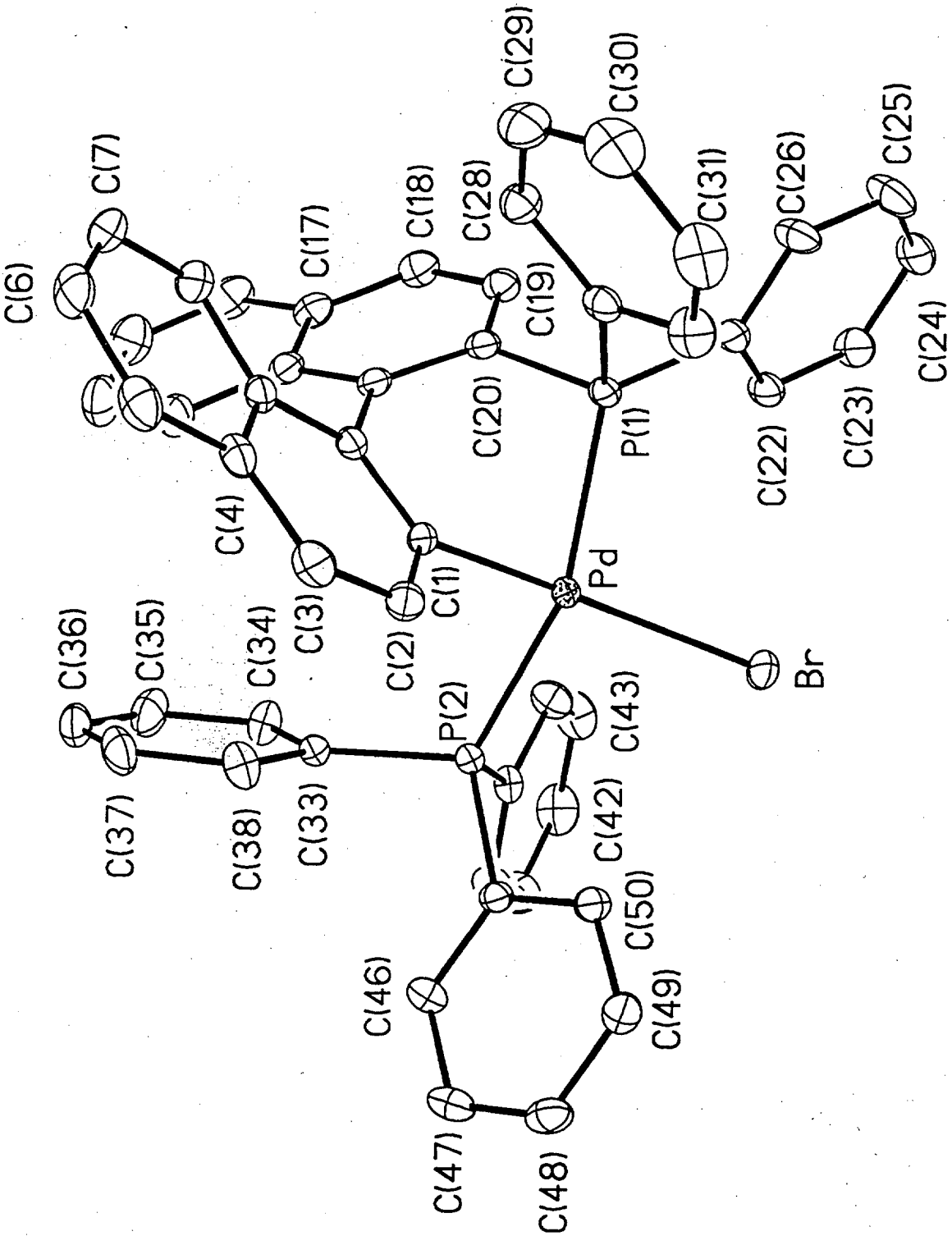

Table 15S. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å2 x 10^3] for 6. U(eq) is defined as one third of the trace of the orthodonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	2612.6(1)	8761.8(1)	-2058.0(1)	22(1)
Br	4278(1)	9609(1)	-2490(1)	37(1)
P(1)	1473(1)	9604(1)	-3168(1)	24(1)
P(2)	3597(1)	7324(1)	-1182(1)	23(1)
C(1)	1157(2)	8402(2)	-1473(2)	24(1)
C(2)	834(2)	8740(2)	-555(2)	32(1)
C(3)	-195(2)	8702(2)	-99(2)	35(1)
C(4)	-1001(2)	8370(2)	-533(2)	30(1)
C(5)	-2107(2)	8405(2)	-94(2)	41(1)
C(6)	-2898(2)	8162(2)	-547(2)	47(1)
C(7)	-2633(2)	7899(3)	-1471(2)	45(1)
C(8)	-1569(2)	7813(2)	-1918(2)	38(1)
C(9)	-707(2)	8038(2)	-1459(2)	28(1)
C(10)	419(2)	8018(2)	-1907(2)	24(1)
C(11)	739(2)	7708(2)	-2891(2)	26(1)
C(12)	676(2)	6682(2)	-3145(2)	31(1)
C(13)	411(3)	5861(2)	-2471(2)	40(1)
C(14)	374(3)	4888(3)	-2737(2)	53(1)
C(15)	590(3)	4683(3)	-3687(3)	56(1)
C(16)	872(3)	5434(3)	-4350(2)	49(1)
C(17)	947(2)	6452(2)	-4105(2)	35(1)
C(18)	1271(2)	7242(2)	-4781(2)	37(1)
C(19)	1377(2)	8196(2)	-4520(2)	32(1)
C(20)	1127(2)	8436(2)	-3566(2)	26(1)
C(21)	2047(2)	10296(2)	-4223(2)	27(1)
C(22)	3132(2)	9887(2)	-4616(2)	33(1)
C(23)	3578(2)	10377(2)	-5446(2)	39(1)
C(24)	2957(3)	11276(3)	-5870(2)	44(1)
C(25)	1895(3)	11703(3)	-5477(2)	50(1)
C(26)	1434(2)	11213(2)	-4655(2)	39(1)
C(27)	159(2)	10510(2)	-2835(2)	29(1)
C(28)	-868(2)	10335(2)	-2998(2)	36(1)
C(29)	-1839(3)	11084(3)	-2760(2)	48(1)
C(30)	-1791(3)	11991(3)	-2378(2)	55(1)
C(31)	-782(3)	12164(3)	-2206(2)	53(1)
C(32)	199(3)	11428(2)	-2431(2)	41(1)
C(33)	2893(2)	6206(2)	-807(2)	26(1)
C(34)	3108(2)	5305(2)	-1299(2)	38(1)
C(35)	2531(3)	4495(2)	-1024(2)	47(1)
C(36)	1723(3)	4574(2)	-273(2)	44(1)
C(37)	1486(3)	5476(2)	209(2)	45(1)
C(38)	2074(2)	6280(2)	-45(2)	39(1)
C(39)	4873(2)	6689(2)	-1886(2)	29(1)
C(40)	5755(2)	6014(2)	-1489(2)	40(1)
C(41)	6683(3)	5520(3)	-2056(2)	53(1)
C(42)	6746(3)	5710(3)	-3012(2)	53(1)
C(43)	5885(3)	6381(3)	-3416(2)	49(1)

C(44)	4947(3)	6866(2)	-2854(2)	39(1)
C(45)	4004(2)	7646(2)	-98(2)	25(1)
C(46)	4382(2)	6861(2)	600(2)	34(1)
C(47)	4711(2)	7142(2)	1401(2)	38(1)
C(48)	4674(2)	8200(2)	1515(2)	38(1)
C(49)	4280(2)	8984(2)	837(2)	34(1)
C(50)	3946(2)	8707(2)	36(2)	28(1)
C(100)	4572(4)	7385(4)	4188(3)	80(1)
C(101)	4541(4)	6357(4)	4135(3)	77(1)
C(102)	5480(4)	5637(3)	3850(3)	72(1)
C(103)	6456(4)	5955(4)	3620(3)	73(1)
C(104)	6506(4)	6997(4)	3668(3)	83(1)
C(105)	5573(5)	7714(3)	3953(3)	86(2)

Table 16S. Bond lengths [Å] and angles [°] for 6.

Pd-C(1)	2.010(2)	Pd-P(1)	2.3079(6)
Pd-P(2)	2.3382(6)	Pd-Br	2.5141(3)
P(1)-C(21)	1.822(2)	P(1)-C(27)	1.825(3)
P(1)-C(20)	1.829(3)	P(2)-C(45)	1.832(2)
P(2)-C(39)	1.841(3)	P(2)-C(33)	1.842(2)
C(1)-C(10)	1.380(3)	C(1)-C(2)	1.425(3)
C(2)-C(3)	1.360(4)	C(3)-C(4)	1.413(4)
C(4)-C(5)	1.421(4)	C(4)-C(9)	1.431(4)
C(5)-C(6)	1.358(5)	C(6)-C(7)	1.397(5)
C(7)-C(8)	1.373(4)	C(8)-C(9)	1.428(4)
C(9)-C(10)	1.450(3)	C(10)-C(11)	1.503(3)
C(11)-C(20)	1.392(3)	C(11)-C(12)	1.438(4)
C(12)-C(13)	1.423(3)	C(12)-C(17)	1.436(4)
C(13)-C(14)	1.370(4)	C(14)-C(15)	1.410(5)
C(15)-C(16)	1.357(5)	C(16)-C(17)	1.428(4)
C(17)-C(18)	1.419(4)	C(18)-C(19)	1.369(4)
C(19)-C(20)	1.429(3)	C(21)-C(26)	1.395(3)
C(21)-C(22)	1.399(3)	C(22)-C(23)	1.397(3)
C(23)-C(24)	1.379(4)	C(24)-C(25)	1.381(4)
C(25)-C(26)	1.397(4)	C(27)-C(28)	1.395(4)
C(27)-C(32)	1.395(4)	C(28)-C(29)	1.399(4)
C(29)-C(30)	1.368(5)	C(30)-C(31)	1.376(5)
C(31)-C(32)	1.394(4)	C(33)-C(38)	1.391(4)
C(33)-C(34)	1.392(4)	C(34)-C(35)	1.387(4)
C(35)-C(36)	1.371(4)	C(36)-C(37)	1.383(5)
C(37)-C(38)	1.386(4)	C(39)-C(40)	1.390(4)
C(39)-C(44)	1.390(3)	C(40)-C(41)	1.393(4)
C(41)-C(42)	1.376(5)	C(42)-C(43)	1.372(5)
C(43)-C(44)	1.394(4)	C(45)-C(50)	1.394(3)
C(45)-C(46)	1.402(3)	C(46)-C(47)	1.392(4)
C(47)-C(48)	1.387(4)	C(48)-C(49)	1.388(4)
C(49)-C(50)	1.392(4)	C(100)-C(101)	1.351(6)
C(100)-C(105)	1.384(7)	C(101)-C(102)	1.367(6)
C(102)-C(103)	1.348(6)	C(103)-C(104)	1.373(6)
C(104)-C(105)	1.361(7)		

C(1)-Pd-P(1)	80.02(6)	C(1)-Pd-P(2)	90.71(7)
P(1)-Pd-P(2)	156.60(2)	C(1)-Pd-Br	164.27(7)
P(1)-Pd-Br	101.52(2)	P(2)-Pd-Br	93.22(2)
C(21)-P(1)-C(27)	102.94(11)	C(21)-P(1)-C(20)	104.90(11)
C(27)-P(1)-C(20)	107.21(12)	C(21)-P(1)-Pd	120.27(8)
C(27)-P(1)-Pd	120.82(8)	C(20)-P(1)-Pd	98.96(8)
C(45)-P(2)-C(39)	107.65(11)	C(45)-P(2)-C(33)	103.80(11)
C(39)-P(2)-C(33)	102.42(11)	C(45)-P(2)-Pd	115.22(8)
C(39)-P(2)-Pd	110.32(8)	C(33)-P(2)-Pd	116.33(8)
C(10)-C(1)-C(2)	119.6(2)	C(10)-C(1)-Pd	126.9(2)
C(2)-C(1)-Pd	112.8(2)	C(3)-C(2)-C(1)	121.3(2)
C(2)-C(3)-C(4)	121.2(2)	C(3)-C(4)-C(5)	121.9(2)
C(3)-C(4)-C(9)	118.8(2)	C(5)-C(4)-C(9)	119.3(3)
C(6)-C(5)-C(4)	121.4(3)	C(5)-C(6)-C(7)	119.6(3)
C(8)-C(7)-C(6)	121.5(3)	C(7)-C(8)-C(9)	120.5(3)
C(8)-C(9)-C(4)	117.5(2)	C(8)-C(9)-C(10)	123.3(2)
C(4)-C(9)-C(10)	119.0(2)	C(1)-C(10)-C(9)	119.9(2)
C(1)-C(10)-C(11)	119.6(2)	C(9)-C(10)-C(11)	120.1(2)

C(20)-C(11)-C(12)	119.7(2)	C(20)-C(11)-C(10)	118.4(2)
C(12)-C(11)-C(10)	121.9(2)	C(13)-C(12)-C(17)	118.4(2)
C(13)-C(12)-C(11)	122.4(2)	C(17)-C(12)-C(11)	119.2(2)
C(14)-C(13)-C(12)	120.8(3)	C(13)-C(14)-C(15)	120.5(3)
C(16)-C(15)-C(14)	120.7(3)	C(15)-C(16)-C(17)	120.8(3)
C(18)-C(17)-C(16)	122.1(3)	C(18)-C(17)-C(12)	119.2(2)
C(16)-C(17)-C(12)	118.7(3)	C(19)-C(18)-C(17)	120.8(2)
C(18)-C(19)-C(20)	120.9(2)	C(11)-C(20)-C(19)	120.0(2)
C(11)-C(20)-P(1)	117.8(2)	C(19)-C(20)-P(1)	121.7(2)
C(26)-C(21)-C(22)	119.0(2)	C(26)-C(21)-P(1)	122.1(2)
C(22)-C(21)-P(1)	118.9(2)	C(23)-C(22)-C(21)	120.1(2)
C(24)-C(23)-C(22)	120.1(3)	C(23)-C(24)-C(25)	120.4(2)
C(24)-C(25)-C(26)	120.0(3)	C(21)-C(26)-C(25)	120.3(3)
C(28)-C(27)-C(32)	119.3(3)	C(28)-C(27)-P(1)	122.5(2)
C(32)-C(27)-P(1)	118.2(2)	C(27)-C(28)-C(29)	119.5(3)
C(30)-C(29)-C(28)	120.8(3)	C(29)-C(30)-C(31)	120.0(3)
C(30)-C(31)-C(32)	120.5(3)	C(31)-C(32)-C(27)	119.9(3)
C(38)-C(33)-C(34)	118.3(2)	C(38)-C(33)-P(2)	119.7(2)
C(34)-C(33)-P(2)	121.9(2)	C(35)-C(34)-C(33)	120.7(3)
C(36)-C(35)-C(34)	120.7(3)	C(35)-C(36)-C(37)	119.1(3)
C(36)-C(37)-C(38)	120.8(3)	C(37)-C(38)-C(33)	120.4(3)
C(40)-C(39)-C(44)	118.5(2)	C(40)-C(39)-P(2)	122.5(2)
C(44)-C(39)-P(2)	119.0(2)	C(39)-C(40)-C(41)	120.2(3)
C(42)-C(41)-C(40)	120.5(3)	C(43)-C(42)-C(41)	120.0(3)
C(42)-C(43)-C(44)	119.8(3)	C(39)-C(44)-C(43)	121.0(3)
C(50)-C(45)-C(46)	118.8(2)	C(50)-C(45)-P(2)	118.9(2)
C(46)-C(45)-P(2)	122.3(2)	C(47)-C(46)-C(45)	120.2(2)
C(48)-C(47)-C(46)	120.4(2)	C(47)-C(48)-C(49)	119.9(3)
C(48)-C(49)-C(50)	120.0(2)	C(49)-C(50)-C(45)	120.8(2)
C(101)-C(100)-C(105)	119.3(4)	C(100)-C(101)-C(102)	121.2(5)
C(103)-C(102)-C(101)	119.6(4)	C(102)-C(103)-C(104)	120.1(4)
C(105)-C(104)-C(103)	120.4(5)	C(104)-C(105)-C(100)	119.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 17S. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **6**. The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2U_{11} + ... + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd	22(1)	25(1)	21(1)	4(1)	-4(1)	-9(1)
Br	37(1)	46(1)	33(1)	7(1)	-5(1)	-25(1)
P(1)	23(1)	29(1)	20(1)	4(1)	-3(1)	-7(1)
P(2)	23(1)	23(1)	22(1)	2(1)	-3(1)	-7(1)
C(1)	21(1)	30(1)	21(1)	3(1)	-2(1)	-9(1)
C(2)	37(1)	36(1)	25(1)	-3(1)	-5(1)	-11(1)
C(3)	40(2)	38(1)	24(1)	-4(1)	5(1)	-7(1)
C(4)	30(1)	26(1)	31(1)	4(1)	4(1)	-4(1)
C(5)	37(2)	38(2)	40(1)	3(1)	11(1)	-3(1)
C(6)	27(1)	48(2)	57(2)	9(1)	10(1)	-7(1)
C(7)	28(1)	55(2)	54(2)	9(1)	-6(1)	-18(1)
C(8)	31(1)	47(2)	36(1)	4(1)	-2(1)	-14(1)
C(9)	25(1)	28(1)	29(1)	6(1)	-1(1)	-8(1)
C(10)	25(1)	25(1)	23(1)	3(1)	-2(1)	-6(1)
C(11)	21(1)	36(1)	22(1)	-1(1)	-5(1)	-7(1)
C(12)	26(1)	36(1)	31(1)	-3(1)	-5(1)	-9(1)
C(13)	46(2)	40(2)	37(1)	-5(1)	-4(1)	-17(1)
C(14)	65(2)	44(2)	56(2)	-5(1)	-3(2)	-27(2)
C(15)	66(2)	44(2)	66(2)	-18(2)	-7(2)	-22(2)
C(16)	52(2)	52(2)	49(2)	-21(1)	-10(2)	-15(2)
C(17)	32(1)	42(2)	33(1)	-9(1)	-6(1)	-9(1)
C(18)	34(1)	53(2)	25(1)	-9(1)	-2(1)	-9(1)
C(19)	30(1)	43(1)	22(1)	-1(1)	-3(1)	-9(1)
C(20)	20(1)	36(1)	22(1)	0(1)	-5(1)	-6(1)
C(21)	27(1)	33(1)	22(1)	5(1)	-3(1)	-11(1)
C(22)	29(1)	39(1)	28(1)	6(1)	-2(1)	-8(1)
C(23)	32(1)	54(2)	30(1)	3(1)	4(1)	-13(1)
C(24)	46(2)	55(2)	30(1)	15(1)	1(1)	-20(1)
C(25)	54(2)	50(2)	37(2)	20(1)	-7(1)	-2(2)
C(26)	34(2)	49(2)	29(1)	11(1)	-5(1)	-1(1)
C(27)	28(1)	35(1)	21(1)	5(1)	1(1)	-5(1)
C(28)	30(1)	40(1)	36(1)	0(1)	-3(1)	-7(1)
C(29)	30(2)	56(2)	52(2)	-1(1)	-2(1)	-2(1)
C(30)	41(2)	52(2)	59(2)	-6(2)	12(2)	7(2)
C(31)	60(2)	42(2)	50(2)	-13(1)	14(2)	-8(2)
C(32)	43(2)	44(2)	34(1)	-7(1)	5(1)	-10(1)
C(33)	25(1)	25(1)	29(1)	4(1)	-6(1)	-7(1)
C(34)	36(2)	35(1)	46(2)	-7(1)	1(1)	-15(1)
C(35)	45(2)	34(2)	68(2)	-7(1)	-7(2)	-16(1)
C(36)	39(2)	35(2)	58(2)	13(1)	-9(1)	-16(1)
C(37)	43(2)	47(2)	42(2)	10(1)	7(1)	-16(1)
C(38)	44(2)	34(1)	36(1)	1(1)	5(1)	-10(1)
C(39)	30(1)	26(1)	30(1)	0(1)	0(1)	-9(1)
C(40)	33(2)	42(2)	39(1)	3(1)	-2(1)	-3(1)
C(41)	35(2)	57(2)	59(2)	-2(2)	-3(2)	7(1)
C(42)	43(2)	52(2)	58(2)	-13(2)	17(2)	-5(2)
C(43)	58(2)	49(2)	36(2)	-8(1)	12(1)	-10(2)

C(44)	42(2)	40(2)	31(1)	-3(1)	-2(1)	-2(1)
C(45)	23(1)	29(1)	24(1)	-1(1)	-4(1)	-6(1)
C(46)	38(2)	32(1)	29(1)	2(1)	-7(1)	-2(1)
C(47)	40(2)	46(2)	26(1)	3(1)	-11(1)	0(1)
C(48)	38(2)	52(2)	26(1)	-7(1)	-7(1)	-11(1)
C(49)	36(2)	36(1)	32(1)	-6(1)	0(1)	-12(1)
C(50)	27(1)	32(1)	26(1)	0(1)	-4(1)	-8(1)
C(100)	88(3)	75(3)	70(3)	-16(2)	-21(2)	11(3)
C(101)	75(3)	86(3)	71(3)	-13(2)	3(2)	-28(3)
C(102)	89(3)	56(2)	73(3)	-9(2)	-16(2)	-18(2)
C(103)	65(3)	80(3)	72(3)	-18(2)	-11(2)	-1(2)
C(104)	81(3)	94(4)	80(3)	9(3)	-13(3)	-36(3)
C(105)	145(5)	44(2)	74(3)	4(2)	-43(3)	-19(3)

Table 18S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å2 x 10^3) for **6**.

	x	y	z	U(eq)
H(2A)	1348(2)	8996(2)	-256(2)	38
H(3A)	-375(2)	8903(2)	523(2)	42
H(5A)	-2296(2)	8602(2)	528(2)	49
H(6A)	-3627(2)	8171(2)	-236(2)	56
H(7A)	-3202(2)	7778(3)	-1798(2)	54
H(8A)	-1405(2)	7602(2)	-2537(2)	45
H(13A)	256(3)	5990(2)	-1829(2)	47
H(14A)	202(3)	4346(3)	-2278(2)	63
H(15A)	537(3)	4012(3)	-3864(3)	67
H(16A)	1022(3)	5281(3)	-4986(2)	58
H(18A)	1417(2)	7107(2)	-5421(2)	44
H(19A)	1621(2)	8705(2)	-4979(2)	38
H(22A)	3568(2)	9276(2)	-4319(2)	39
H(23A)	4309(2)	10089(2)	-5718(2)	47
H(24A)	3262(3)	11603(3)	-6436(2)	53
H(25A)	1477(3)	12330(3)	-5766(2)	60
H(26A)	701(2)	11505(2)	-4388(2)	47
H(28A)	-908(2)	9711(2)	-3269(2)	43
H(29A)	-2541(3)	10963(3)	-2865(2)	57
H(30A)	-2455(3)	12501(3)	-2232(2)	66
H(31A)	-753(3)	12788(3)	-1931(2)	63
H(32A)	894(3)	11552(2)	-2310(2)	49
H(34A)	3656(2)	5244(2)	-1828(2)	46
H(35A)	2697(3)	3880(2)	-1360(2)	57
H(36A)	1331(3)	4017(2)	-85(2)	52
H(37A)	913(3)	5545(2)	720(2)	54
H(38A)	1918(2)	6885(2)	305(2)	47
H(40A)	5727(2)	5890(2)	-829(2)	47
H(41A)	7276(3)	5048(3)	-1780(2)	64
H(42A)	7386(3)	5378(3)	-3393(2)	64
H(43A)	5929(3)	6514(3)	-4076(2)	59
H(44A)	4350(3)	7324(2)	-3136(2)	47
H(46A)	4413(2)	6134(2)	526(2)	41
H(47A)	4963(2)	6607(2)	1873(2)	46
H(48A)	4917(2)	8387(2)	2055(2)	45
H(49A)	4239(2)	9710(2)	919(2)	41
H(50A)	3675(2)	9248(2)	-424(2)	34
H(10A)	3913(4)	7878(4)	4385(3)	96
H(10B)	3855(4)	6130(4)	4299(3)	92
H(10C)	5443(4)	4917(3)	3815(3)	86
H(10D)	7111(4)	5457(4)	3424(3)	88
H(10E)	7195(4)	7218(4)	3501(3)	100
H(10F)	5609(5)	8434(3)	3990(3)	103