Studies on the palladium catalysed methoxycarbonylation of ethene

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X-ray Data

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Order Of Presentation

Crystal Data For [*o*-$C_6H_4(CH_2PCy_2)Pd(H_2O)]^{2+}$ $2[CH_3SO_3]^-$ (45)

Crystal Data For [*o*-$C_6H_4(CH_2PPe^t_2)_2Pd$ (O_2)] (46)

Crystal Data For [$C_{10}H_6(2,3,CH_2PBu^t_2)_2Pd(O_2)$] (47)

Crystal Data For [*o*-$C_6H_4(CH_2PBu^t_2)_2Pd(O_2)$] (48)

Crystal Data For [$(Bu^t_2P(CH_2)_3PBu^t_2)Pd(Cl)_2$] (50)

Crystal Data For [$\{(Bu^t_2P(CH_2)_3PBu^t_2)Pd(OAc)_2\}_4$].10.5 CH_2Cl_2 (52)

Crystal Data For [*o*-$C_6H_4(CH_2PBu^t_2)_2Pd(Cl)_2$] (53)

Crystal Data For [*o*-$C_6H_4(CH_2PBu^t_2)_2Pd(COC_2H_5)(Cl)$].dba (54)

Crystal Data For [*o*-$C_6H_4(CH_2PBu^t_2)_2Pd(Cl)_2$]. CH_2Cl_2 (55)

Table 1A. Crystal data, structure solution and refinement for (7).

Identification code	exti32
Chemical formula	$C_{24}H_{43}NO_2P_2$
Formula weight	439.53
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 8.8024(8) Å α = 108.079(3)°
	b = 11.1937(11) Å β = 95.683(2)°
	c = 14.4535(14) Å γ = 101.607(2)°
Volume	1306.0(2) Å^3
Z	2
Density (calculated)	1.118 g/cm^3
Absorption coefficient μ	0.185 mm^{-1}
F(000)	480
Reflections for cell refinement	7368 (θ range 1.97 to 28.19°)
Crystal colour	pale yellow
Crystal size	0.32 × 0.24 × 0.22 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.50 to 28.36°
Index ranges	$-11 \le h \le 11$, $-14 \le k \le 14$, $-18 \le \ell \le 19$
Standard reflections	0 every 0 minutes
Intensity decay	0%
Reflections collected	9923
Independent reflections	5684 (R_{int} = 0.0184)
Reflections with I>2σ(I)	4954
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.976 and 0.848
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0499, 1.0898
Data / restraints / parameters	5684 / 0 / 274
Final R indices [I>2σ(I)]	R1 = 0.0521, wR2 = 0.1215
R indices (all data)	R1 = 0.0613, wR2 = 0.1275
Goodness-of-fit on F^2	1.053
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	0.424 and -0.487 eÅ^{-3}

The Crystal Structure of [4-nitro-*o*-$C_6H_4(CH_2P(Bu^t)_2$]

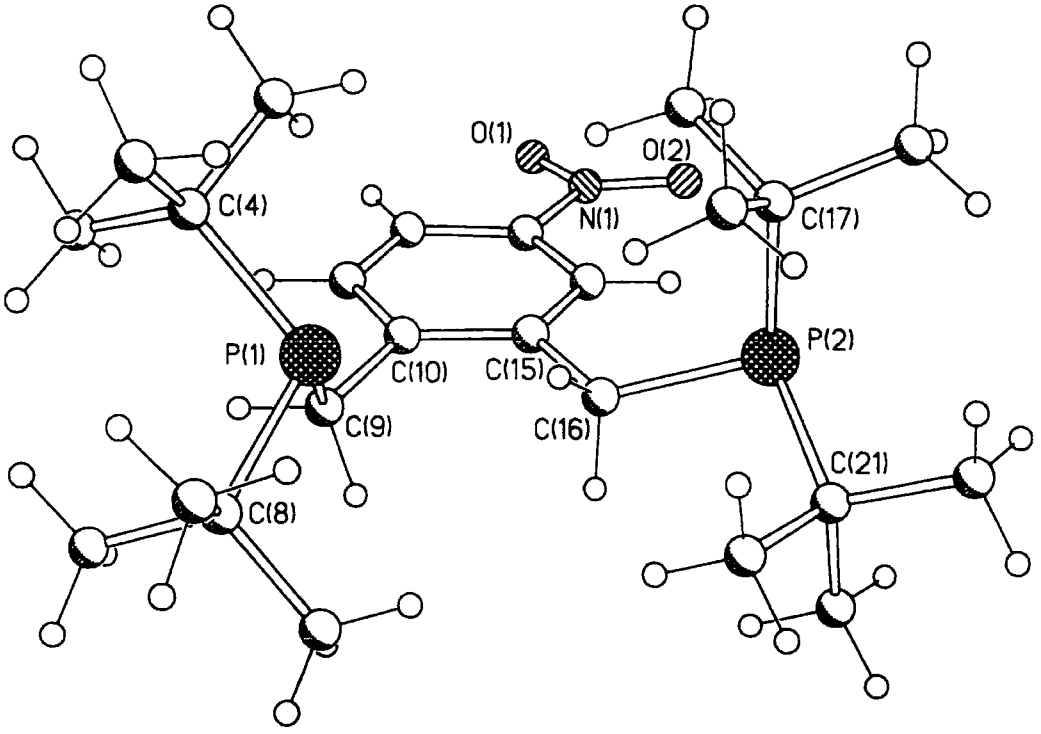


Table 1B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (7). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	2701.9(6)	-50.7(5)	2679.9(4)	25.69(13)
P(2)	2174.5(6)	3953.2(5)	1977.9(4)	22.85(13)
N(1)	7718(2)	6144.6(17)	4384.0(13)	29.6(4)
O(1)	8955.0(17)	6457.8(16)	4980.7(12)	39.3(4)
O(2)	7341.3(19)	6835.3(15)	3937.5(13)	41.8(4)
C(1)	5615(4)	50(3)	2208(3)	65.0(9)
C(2)	5199(4)	-1011(4)	3454(3)	82.2(12)
C(3)	3877(4)	-2147(3)	1700(3)	82.4(12)
C(4)	4401(3)	-844(2)	2534.2(17)	34.0(5)
C(5)	1508(3)	-1490(4)	3933(2)	74.4(11)
C(6)	-135(3)	-244(3)	3330(4)	92.6(15)
C(7)	228(4)	-2235(3)	2186(2)	66.9(9)
C(8)	1056(2)	-1047(2)	3074.6(16)	32.0(5)
C(9)	3416(2)	1324.3(19)	3874.1(14)	28.0(4)
C(10)	4561(2)	2543.5(18)	3911.4(14)	24.2(4)
C(11)	6055(2)	2891(2)	4488.5(15)	30.3(4)
C(12)	7115(2)	4051(2)	4642.1(15)	29.8(4)
C(13)	6640(2)	4883.4(19)	4211.2(14)	25.6(4)
C(14)	5182(2)	4581.7(18)	3627.2(14)	24.3(4)
C(15)	4124(2)	3396.3(18)	3452.7(14)	22.8(4)
C(16)	2503(2)	3041.4(19)	2825.2(15)	25.6(4)
C(17)	2887(2)	3055(2)	833.1(15)	32.4(5)
C(18)	1975(3)	1648(2)	275.4(18)	45.6(6)
C(19)	2900(3)	3851(3)	135.2(17)	42.0(6)
C(20)	4595(3)	3063(3)	1166.3(19)	51.9(7)
C(21)	-51(2)	3546(2)	1757.5(15)	27.6(4)
C(22)	-917(3)	2154(2)	1617(2)	42.4(6)
C(23)	-644(3)	3916(2)	875.6(17)	36.0(5)
C(24)	-463(3)	4444(3)	2689.1(18)	41.2(5)

Table 1C. Bond lengths (Å) and angles (°) for (7).

P(1)-C(9)	1.868(2)	P(1)-C(4)	1.885(2)
P(1)-C(8)	1.892(2)	P(2)-C(16)	1.8572(19)
P(2)-C(17)	1.889(2)	P(2)-C(21)	1.891(2)
N(1)-O(2)	1.222(2)	N(1)-O(1)	1.235(2)
N(1)-C(13)	1.466(2)	C(1)-C(4)	1.526(3)
C(2)-C(4)	1.522(4)	C(3)-C(4)	1.523(4)
C(5)-C(8)	1.518(3)	C(6)-C(8)	1.515(4)
C(7)-C(8)	1.521(3)	C(9)-C(10)	1.507(3)
C(10)-C(11)	1.397(3)	C(10)-C(15)	1.410(3)
C(11)-C(12)	1.378(3)	C(12)-C(13)	1.377(3)
C(13)-C(14)	1.381(3)	C(14)-C(15)	1.393(3)
C(15)-C(16)	1.519(3)	C(17)-C(20)	1.530(3)
C(17)-C(18)	1.533(3)	C(17)-C(19)	1.538(3)
C(21)-C(22)	1.531(3)	C(21)-C(23)	1.534(3)
C(21)-C(24)	1.536(3)		
C(9)-P(1)-C(4)	103.25(10)	C(9)-P(1)-C(8)	98.40(9)
C(4)-P(1)-C(8)	110.54(10)	C(16)-P(2)-C(17)	103.23(9)
C(16)-P(2)-C(21)	98.98(9)	C(17)-P(2)-C(21)	109.91(9)
O(2)-N(1)-O(1)	123.40(17)	O(2)-N(1)-C(13)	118.46(17)
O(1)-N(1)-C(13)	118.13(17)	C(2)-C(4)-C(3)	109.9(3)
C(2)-C(4)-C(1)	107.9(3)	C(3)-C(4)-C(1)	107.8(2)
C(2)-C(4)-P(1)	116.73(18)	C(3)-C(4)-P(1)	109.47(18)
C(1)-C(4)-P(1)	104.61(17)	C(6)-C(8)-C(5)	109.2(3)
C(6)-C(8)-C(7)	106.4(3)	C(5)-C(8)-C(7)	108.6(2)
C(6)-C(8)-P(1)	106.92(17)	C(5)-C(8)-P(1)	116.92(15)
C(7)-C(8)-P(1)	108.28(17)	C(10)-C(9)-P(1)	120.06(14)
C(11)-C(10)-C(15)	119.09(17)	C(11)-C(10)-C(9)	118.70(17)
C(15)-C(10)-C(9)	121.98(17)	C(12)-C(11)-C(10)	122.44(19)
C(13)-C(12)-C(11)	117.25(18)	C(12)-C(13)-C(14)	122.60(18)
C(12)-C(13)-N(1)	118.82(17)	C(14)-C(13)-N(1)	118.58(18)
C(13)-C(14)-C(15)	120.15(18)	C(14)-C(15)-C(10)	118.42(17)
C(14)-C(15)-C(16)	121.49(17)	C(10)-C(15)-C(16)	120.03(16)
C(15)-C(16)-P(2)	118.01(13)	C(20)-C(17)-C(18)	108.3(2)
C(20)-C(17)-C(19)	107.58(19)	C(18)-C(17)-C(19)	109.85(19)
C(20)-C(17)-P(2)	106.30(15)	C(18)-C(17)-P(2)	116.85(16)
C(19)-C(17)-P(2)	107.60(15)	C(22)-C(21)-C(23)	109.54(18)
C(22)-C(21)-C(24)	107.70(19)	C(23)-C(21)-C(24)	107.94(18)
C(22)-C(21)-P(2)	117.55(15)	C(23)-C(21)-P(2)	109.17(14)
C(24)-C(21)-P(2)	104.46(14)		

Table 1D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (7).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
P(1)	27.8(3)	23.1(3)	24.6(3)	8.7(2)	0.87(19)	3.34(19)
P(2)	20.9(2)	23.7(2)	25.2(3)	10.08(19)	4.83(18)	5.06(18)
N(1)	27.7(9)	29.3(9)	27.1(9)	5.7(7)	7.6(7)	1.6(7)
O(1)	27.5(8)	42.2(9)	35.4(9)	7.7(7)	-3.3(6)	-6.7(6)
O(2)	38.7(9)	34.7(9)	50.6(10)	20.7(8)	2.3(7)	-1.0(7)
C(1)	59.8(17)	51.0(16)	94(2)	24.5(16)	52.4(18)	15.2(14)
C(2)	62(2)	149(4)	86(2)	74(3)	34.7(18)	73(2)
C(3)	62(2)	45.7(17)	110(3)	-19.1(18)	20.6(19)	18.4(15)
C(4)	31.8(11)	33.5(11)	39.4(12)	13.0(9)	12.5(9)	9.7(9)
C(5)	40.8(15)	123(3)	61.9(19)	64(2)	-3.4(13)	-20.5(16)
C(6)	27.8(13)	51.5(18)	197(5)	36(2)	38(2)	9.2(13)
C(7)	72(2)	46.9(16)	56.2(18)	12.0(14)	-0.2(15)	-28.0(14)
C(8)	23.1(9)	32.9(11)	37.6(12)	13.7(9)	0.4(8)	1.2(8)
C(9)	32.1(10)	24.8(9)	24.8(10)	9.5(8)	1.3(8)	1.9(8)
C(10)	26.1(9)	22.8(9)	21.3(9)	5.3(7)	4.8(7)	4.2(7)
C(11)	32.1(10)	29.6(10)	27.4(10)	10.1(8)	-2.7(8)	6.5(8)
C(12)	25.1(10)	32.6(11)	25.7(10)	6.1(8)	-2.5(8)	3.4(8)
C(13)	23.8(9)	25.9(9)	22.6(9)	4.0(7)	6.9(7)	1.4(7)
C(14)	23.8(9)	25.0(9)	25.0(9)	8.9(8)	7.3(7)	6.0(7)
C(15)	21.5(9)	24.4(9)	21.2(9)	6.1(7)	5.5(7)	4.7(7)
C(16)	21.2(9)	27.6(10)	29.9(10)	13.8(8)	3.9(8)	3.8(7)
C(17)	29.0(10)	43.2(12)	27.4(10)	11.0(9)	9.1(8)	13.4(9)
C(18)	59.2(16)	40.5(13)	34.0(12)	2.6(10)	9.4(11)	20.4(12)
C(19)	38.3(12)	59.9(15)	32.0(12)	21.2(11)	11.7(10)	9.1(11)
C(20)	35.9(13)	90(2)	36.2(13)	17.4(13)	15.2(11)	31.5(13)
C(21)	22.7(9)	32.1(10)	31.0(10)	13.4(9)	5.9(8)	8.2(8)
C(22)	25.3(10)	42.9(13)	57.9(15)	23.6(12)	2.4(10)	-2.4(9)
C(23)	28.2(10)	48.5(13)	37.0(12)	20.4(10)	3.3(9)	13.8(9)
C(24)	34.7(12)	57.4(15)	39.3(13)	17.7(11)	14.8(10)	22.1(11)

Table 1E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (7).

	x	y	z	U
H(1A)	6004	886	2743	98
H(1B)	5125	184	1621	98
H(1C)	6496	-345	2050	98
H(2A)	6106	-1374	3302	123
H(2B)	4449	-1601	3669	123
H(2C)	5555	-167	3982	123
H(3A)	4805	-2453	1507	124
H(3B)	3277	-2048	1132	124
H(3C)	3213	-2777	1926	124
H(5A)	2220	-2062	3752	112
H(5B)	558	-1961	4088	112
H(5C)	2039	-733	4512	112
H(6A)	291	470	3955	139
H(6B)	-1110	-790	3395	139
H(6C)	-358	109	2804	139
H(7A)	-12	-1969	1614	100
H(7B)	-753	-2669	2335	100
H(7C)	915	-2834	2036	100
H(9A)	2478	1578	4121	34
H(9B)	3909	985	4352	34
H(11)	6350	2306	4786	36
H(12)	8132	4268	5029	36
H(14)	4900	5184	3344	29
H(16A)	1727	3145	3277	31
H(16B)	2264	2110	2423	31
H(18A)	1908	1161	734	68
H(18B)	2522	1253	-253	68
H(18C)	911	1632	-12	68
H(19A)	3501	4745	492	63
H(19B)	1817	3846	-104	63
H(19C)	3391	3468	-428	63
H(20A)	5176	3946	1573	78
H(20B)	5085	2762	585	78
H(20C)	4617	2486	1554	78
H(22A)	-572	1932	2195	64
H(22B)	-679	1558	1024	64
H(22C)	-2054	2081	1542	64
H(23A)	-1757	3924	864	54
H(23B)	-527	3281	261	54
H(23C)	-28	4779	938	54
H(24A)	-137	4201	3259	62
H(24B)	-1602	4363	2600	62
H(24C)	88	5343	2802	62

Table 2A. Crystal data, structure solution and refinement for (11).

Identification code	exti29
Chemical formula	$C_{24}H_{44}OP_2$
Formula weight	410.53
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 12.3600(10) Å $\alpha = 90^\circ$
	b = 10.6211(9) Å $\beta = 99.818(2)^\circ$
	c = 19.3962(17) Å $\gamma = 90^\circ$
Volume	2509.0(4) $Å^3$
Z	4
Density (calculated)	1.087 g/cm^3
Absorption coefficient μ	0.184 mm^{-1}
F(000)	904
Reflections for cell refinement	13275 (θ range 1.67 to 28.21°)
Crystal colour	pale yellow
Crystal size	0.56 × 0.55 × 0.44 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.67 to 28.29°
Index ranges	$-15 \le h \le 16$, $-13 \le k \le 13$, $-24 \le \ell \le 25$
Intensity decay	0%
Reflections collected	17543
Independent reflections	5794 (R_{int} = 0.0194)
Reflections with I>2σ(I)	5201
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.928 and 0.813
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0416, 0.9743
Data / restraints / parameters	5794 / 0 / 257
Final R indices [I>2σ(I)]	R1 = 0.0358, wR2 = 0.0888
R indices (all data)	R1 = 0.0418, wR2 = 0.0922
Goodness-of-fit on F^2	1.080
Extinction coefficient	0.0013(5)
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.486 and -0.302 $eÅ^{-3}$

Crystal Structure of C_6H_3-1-($CH_2P(O)Bu^t_2$)-2-($CH_2PBu^t_2$) (11)

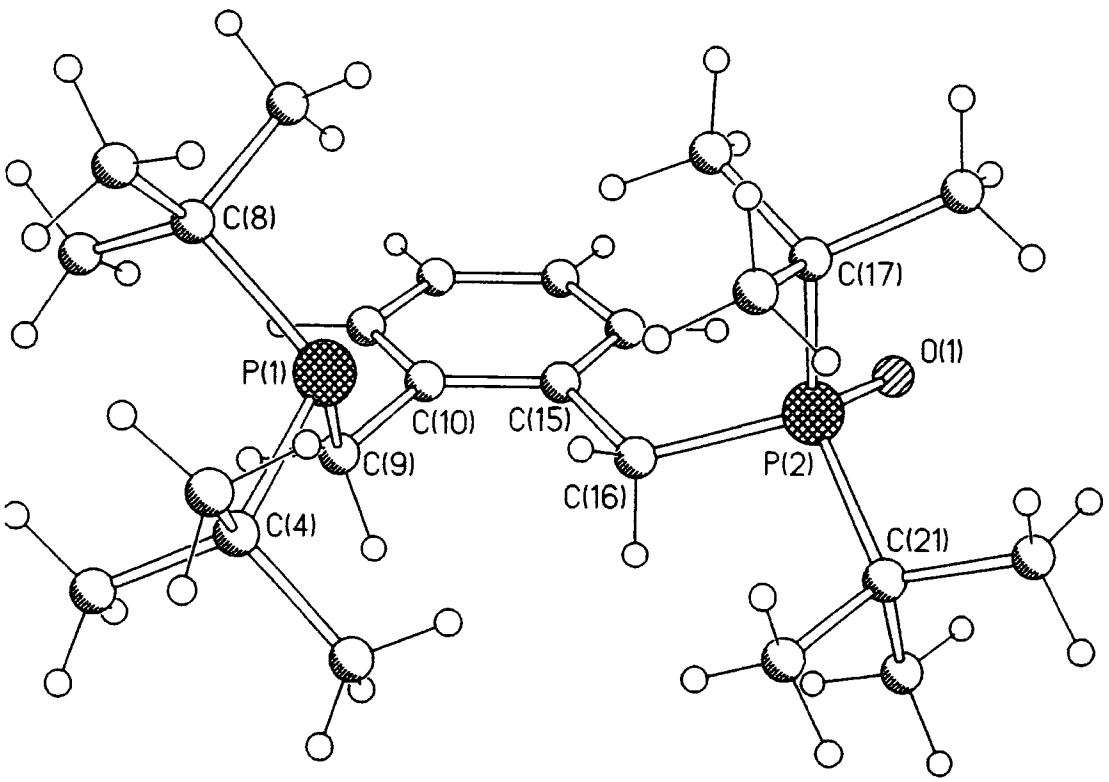


Table 2B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (11). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	6334.9(3)	6188.7(3)	1396.17(17)	20.94(9)
P(2)	9572.4(3)	3530.6(3)	1870.70(16)	18.43(9)
O(1)	10134.3(8)	2683.3(9)	2435.6(5)	27.6(2)
C(1)	5928.6(17)	7504.9(18)	123.3(9)	49.3(5)
C(2)	7698.4(13)	7862.0(16)	891.1(9)	40.1(4)
C(3)	6021.2(15)	8892.2(14)	1180.7(10)	44.3(4)
C(4)	6462.8(12)	7697.9(13)	893.7(7)	29.0(3)
C(5)	4871.2(12)	4577.5(14)	1811.2(9)	34.6(3)
C(6)	4079.9(12)	6015.6(16)	846.0(8)	34.8(3)
C(7)	4466.8(12)	6818.6(16)	2067.7(8)	35.4(3)
C(8)	4874.6(10)	5940.6(13)	1542.6(7)	25.0(3)
C(9)	7068.4(10)	6655.1(12)	2285.2(7)	22.3(3)
C(10)	7380.4(10)	5615.0(12)	2818.2(6)	21.1(2)
C(11)	6880.5(11)	5566.2(14)	3413.4(7)	27.6(3)
C(12)	7199.2(12)	4701.8(15)	3942.3(7)	32.3(3)
C(13)	8036.3(13)	3865.2(15)	3889.3(7)	33.7(3)
C(14)	8550.0(12)	3897.8(13)	3308.4(7)	27.9(3)
C(15)	8232.0(10)	4760.5(12)	2768.3(6)	20.3(2)
C(16)	8853.9(10)	4877.0(11)	2160.9(6)	19.6(2)
C(17)	8527.6(11)	2633.2(12)	1262.7(7)	24.4(3)
C(18)	9003.6(13)	1342.6(13)	1112.8(8)	34.0(3)
C(19)	8094.3(13)	3309.6(15)	572.1(7)	33.1(3)
C(20)	7554.4(12)	2419.6(14)	1648.6(8)	31.2(3)
C(21)	10601.4(10)	4306.8(13)	1419.1(7)	24.2(3)
C(22)	11116.3(13)	3352.7(15)	977.5(8)	35.5(3)
C(23)	11501.7(12)	4779.2(15)	2012.8(8)	33.8(3)
C(24)	10166.6(12)	5453.7(13)	972.6(7)	29.8(3)

Table 2C. Bond lengths (Å) and angles (°) for (11).

P(1)-C(9)	1.8728(13)	P(1)-C(8)	1.8928(13)
P(1)-C(4)	1.8965(14)	P(2)-O(1)	1.4944(10)
P(2)-C(16)	1.8224(12)	P(2)-C(21)	1.8560(13)
P(2)-C(17)	1.8567(13)	C(1)-C(4)	1.541(2)
C(2)-C(4)	1.538(2)	C(3)-C(4)	1.523(2)
C(5)-C(8)	1.5389(19)	C(6)-C(8)	1.5311(19)
C(7)-C(8)	1.528(2)	C(9)-C(10)	1.5172(18)
C(10)-C(11)	1.4003(18)	C(10)-C(15)	1.4056(18)
C(11)-C(12)	1.383(2)	C(12)-C(13)	1.381(2)
C(13)-C(14)	1.3848(19)	C(14)-C(15)	1.3968(18)
C(15)-C(16)	1.5176(16)	C(17)-C(19)	1.5339(19)
C(17)-C(20)	1.5381(19)	C(17)-C(18)	1.5388(19)
C(21)-C(22)	1.5334(19)	C(21)-C(24)	1.5374(19)
C(21)-C(23)	1.5425(19)		

C(9)-P(1)-C(8)	102.88(6)	C(9)-P(1)-C(4)	100.36(6)
C(8)-P(1)-C(4)	111.10(6)	O(1)-P(2)-C(16)	115.86(6)
O(1)-P(2)-C(21)	110.08(6)	C(16)-P(2)-C(21)	101.91(6)
O(1)-P(2)-C(17)	110.03(6)	C(16)-P(2)-C(17)	106.03(6)
C(21)-P(2)-C(17)	112.75(6)	C(3)-C(4)-C(2)	108.95(13)
C(3)-C(4)-C(1)	110.13(14)	C(2)-C(4)-C(1)	105.86(13)
C(3)-C(4)-P(1)	116.71(11)	C(2)-C(4)-P(1)	105.50(10)
C(1)-C(4)-P(1)	109.05(10)	C(7)-C(8)-C(6)	108.75(12)
C(7)-C(8)-C(5)	109.15(12)	C(6)-C(8)-C(5)	108.02(12)
C(7)-C(8)-P(1)	116.51(10)	C(6)-C(8)-P(1)	110.19(10)
C(5)-C(8)-P(1)	103.86(9)	C(10)-C(9)-P(1)	117.49(9)
C(11)-C(10)-C(15)	118.28(12)	C(11)-C(10)-C(9)	119.48(12)
C(15)-C(10)-C(9)	121.98(11)	C(12)-C(11)-C(10)	121.75(13)
C(13)-C(12)-C(11)	119.61(13)	C(12)-C(13)-C(14)	119.86(13)
C(13)-C(14)-C(15)	121.14(13)	C(14)-C(15)-C(10)	119.35(11)
C(14)-C(15)-C(16)	121.38(11)	C(10)-C(15)-C(16)	119.02(11)
C(15)-C(16)-P(2)	120.92(9)	C(19)-C(17)-C(20)	107.97(12)
C(19)-C(17)-C(18)	109.87(11)	C(20)-C(17)-C(18)	108.45(11)
C(19)-C(17)-P(2)	114.56(9)	C(20)-C(17)-P(2)	106.47(9)
C(18)-C(17)-P(2)	109.29(10)	C(22)-C(21)-C(24)	110.34(11)
C(22)-C(21)-C(23)	108.46(12)	C(24)-C(21)-C(23)	107.53(12)
C(22)-C(21)-P(2)	110.68(10)	C(24)-C(21)-P(2)	114.58(9)
C(23)-C(21)-P(2)	104.90(9)		

Table 2D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (11).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
P(1)	21.76(16)	18.88(16)	21.82(17)	-0.08(12)	2.67(12)	0.12(12)
P(2)	19.52(16)	19.12(16)	16.71(15)	1.01(11)	3.25(11)	1.42(11)
O(1)	30.8(5)	27.1(5)	24.4(5)	4.6(4)	3.1(4)	6.1(4)
C(1)	63.1(12)	48.6(10)	31.8(9)	14.2(7)	-4.4(8)	-16.9(9)
C(2)	40.3(9)	39.7(9)	42.4(9)	11.0(7)	12.6(7)	-7.0(7)
C(3)	51.9(10)	22.9(7)	59.3(11)	8.4(7)	12.9(8)	4.5(7)
C(4)	33.3(7)	23.1(6)	29.4(7)	5.0(5)	2.3(6)	-3.3(5)
C(5)	28.3(7)	31.1(7)	44.3(9)	6.2(6)	5.6(6)	-6.1(6)
C(6)	25.1(7)	40.7(8)	35.8(8)	-0.9(6)	-3.0(6)	-2.1(6)
C(7)	25.9(7)	43.1(9)	38.3(8)	-7.7(7)	8.7(6)	2.0(6)
C(8)	20.1(6)	25.2(6)	29.1(7)	-0.5(5)	2.6(5)	-0.5(5)
C(9)	21.5(6)	21.3(6)	23.9(6)	-3.3(5)	3.2(5)	1.4(5)
C(10)	20.0(6)	22.9(6)	20.0(6)	-3.2(5)	2.4(5)	-2.7(5)
C(11)	24.6(6)	34.0(7)	25.3(7)	-5.7(6)	7.3(5)	-0.7(5)
C(12)	35.5(8)	41.8(8)	22.6(7)	-2.2(6)	12.9(6)	-5.2(6)
C(13)	43.5(8)	36.3(8)	22.5(7)	6.1(6)	9.3(6)	1.1(6)
C(14)	32.3(7)	29.2(7)	23.1(7)	4.5(5)	7.3(5)	5.0(6)
C(15)	22.4(6)	20.9(6)	17.9(6)	-1.2(5)	3.9(5)	-3.0(5)
C(16)	20.7(6)	19.7(6)	18.6(6)	1.0(5)	4.2(5)	1.1(5)
C(17)	26.8(6)	22.6(6)	23.0(6)	-2.2(5)	2.0(5)	-1.8(5)
C(18)	42.0(8)	24.3(7)	36.0(8)	-7.1(6)	7.4(6)	-0.2(6)
C(19)	37.9(8)	35.7(8)	22.3(7)	-2.1(6)	-4.0(6)	-0.8(6)
C(20)	27.4(7)	29.7(7)	36.5(8)	-2.8(6)	5.0(6)	-6.7(6)
C(21)	23.3(6)	26.5(6)	24.5(6)	1.4(5)	9.0(5)	0.8(5)
C(22)	35.4(8)	37.3(8)	37.8(8)	-1.4(6)	18.0(6)	6.2(6)
C(23)	22.4(7)	40.6(8)	38.3(8)	0.3(7)	4.8(6)	-5.0(6)
C(24)	34.8(7)	29.0(7)	28.1(7)	6.0(6)	12.6(6)	-0.8(6)

Table 2E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (11).

	x	y	z	U
H(1A)	5128	7492	86	74
H(1B)	6177	6704	-46	74
H(1C)	6141	8196	-160	74
H(2A)	7811	8552	575	60
H(2B)	7997	7081	731	60
H(2C)	8075	8057	1366	60
H(3A)	6360	9001	1672	66
H(3B)	5223	8825	1146	66
H(3C)	6197	9619	909	66
H(5A)	5395	4500	2250	52
H(5B)	5083	4004	1461	52
H(5C)	4133	4360	1894	52
H(6A)	3373	5644	900	52
H(6B)	4386	5552	487	52
H(6C)	3971	6899	705	52
H(7A)	4911	6695	2532	53
H(7B)	3696	6630	2087	53
H(7C)	4532	7694	1921	53
H(9A)	7748	7104	2226	27
H(9B)	6599	7264	2484	27
H(11)	6307	6142	3455	33
H(12)	6844	4684	4340	39
H(13)	8259	3269	4250	40
H(14)	9129	3324	3277	33
H(16A)	9402	5556	2281	23
H(16B)	8324	5175	1752	23
H(18A)	9606	1461	849	51
H(18B)	8427	829	838	51
H(18C)	9281	916	1556	51
H(19A)	7815	4142	671	50
H(19B)	7500	2813	302	50
H(19C)	8691	3406	302	50
H(20A)	7824	2075	2115	47
H(20B)	7037	1826	1383	47
H(20C)	7182	3223	1694	47
H(22A)	11759	3731	825	53
H(22B)	10577	3117	567	53
H(22C)	11342	2601	1259	53
H(23A)	12081	5199	1811	51
H(23B)	11814	4063	2298	51
H(23C)	11181	5375	2307	51
H(24A)	9900	6088	1270	45
H(24B)	9564	5191	605	45
H(24C)	10760	5814	758	45

Table 3A. Crystal data, structure solution and refinement for (12).

Identification code	extil
Chemical formula	$C_{41}H_{58}OP_2Pd$
Formula weight	735.21
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 9.264(2) Å α = 97.72(2)°
	b = 11.482(3) Å β = 93.63(2)°
	c = 19.466(4) Å γ = 112.725(12)°
Volume	1877.5(7) $Å^3$
Z	2
Density (calculated)	1.301 g/cm^3
Absorption coefficient μ	0.609 mm^{-1}
F(000)	776
Reflections for cell refinement	362 (θ range 2.0 to 25.0°)
Crystal colour	orange-yellow
Crystal size	0.38 x 0.21 x 0.10 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.06 to 25.49°
Index ranges	$-10 \le h \le 11$, $-12 \le k \le 13$, $-15 \le \ell \le 22$
Reflections collected	8043
Independent reflections	5889 (R_{int} = 0.0343)
Reflections with I>2σ(I)	5072
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.936 and 0.777
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0409, 4.5793
Data / restraints / parameters	5889 / 89 / 447
Final R indices [I>2σ(I)]	R1 = 0.0432, wR2 = 0.1016
R indices (all data)	R1 = 0.0526, wR2 = 0.1092
Goodness-of-fit on F^2	1.035
Extinction coefficient	0.0016(5)
Largest and mean shift/esd	0.003 and 0.000
Largest diff. peak and hole	0.896 and -0.976 $eÅ^{-3}$

The Crystal Structure of [*o*-$C_6H_4(CH_2PBu'_2)_2$ Pd (dba)] (12)

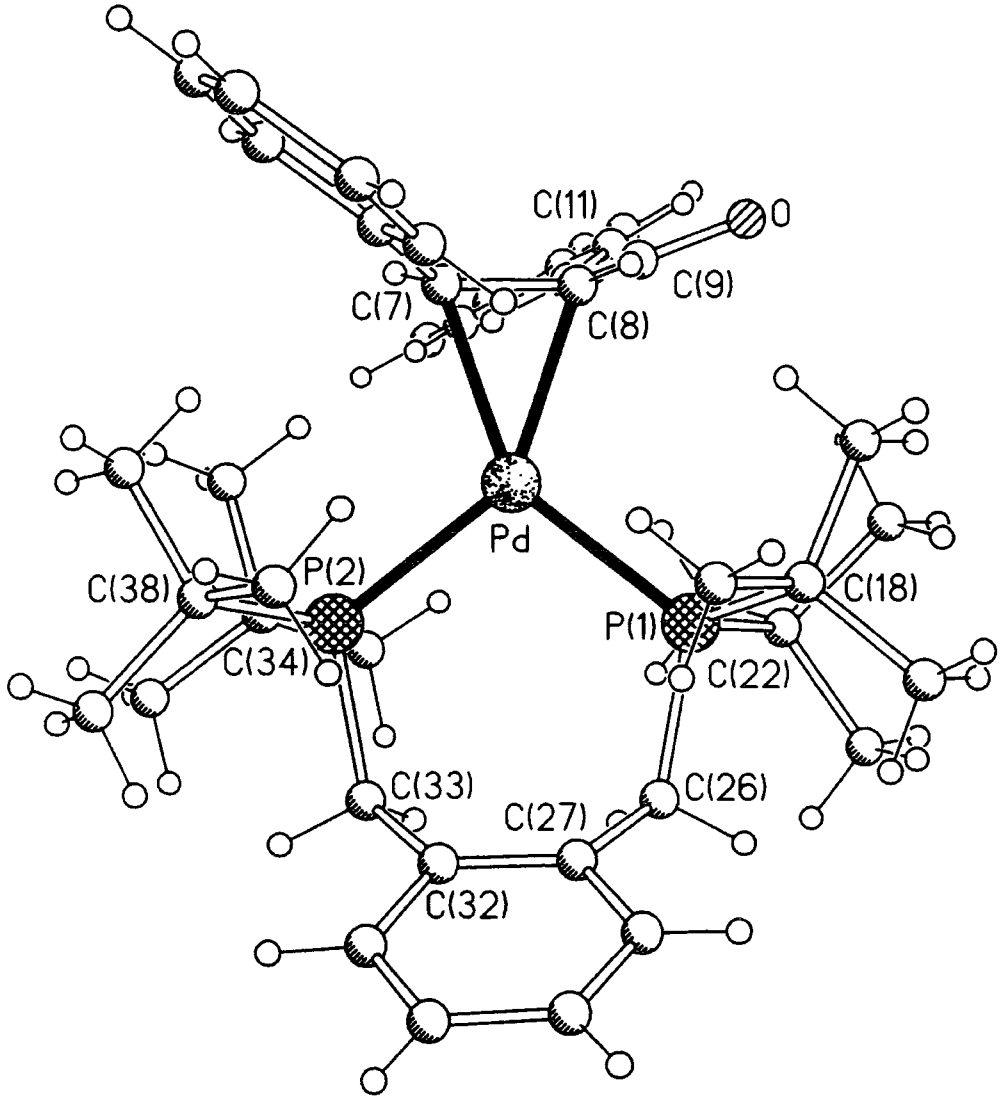


Table 3B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (12). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	3903.0(4)	-8696.4(4)	2636.9(2)	28.3(2)
P(1)	2416(2)	-10604.4(14)	1836.4(7)	37.8(3)
P(2)	1980.3(15)	-8078.7(12)	3112.6(7)	29.9(3)
O	7563(5)	-8499(4)	1596(2)	49.2(10)
C(1)	6331(6)	-8545(5)	4159(3)	38.9(13)
C(2)	6817(7)	-8521(7)	4855(3)	51(2)
C(3)	7655(7)	-7373(7)	5294(3)	56(2)
C(4)	8007(7)	-6253(7)	5041(3)	54(2)
C(5)	7516(6)	-6258(6)	4353(3)	44.3(14)
C(6)	6663(6)	-7413(5)	3895(3)	36.3(12)
C(7)	6199(6)	-7386(5)	3155(3)	35.1(12)
C(8)	6371(6)	-8259(5)	2607(3)	37.0(12)
C(9)	6918(6)	-7912(6)	1953(3)	42.8(14)
C(10)	6721(7)	-6790(6)	1711(3)	49(2)
C(11)	7376(7)	-6328(6)	1166(3)	49(2)
C(12)	7225(8)	-5306(6)	832(3)	53(2)
C(13)	6349(9)	-4624(8)	1068(4)	71(2)
C(14)	6210(11)	-3704(8)	722(5)	87(3)
C(15)	6928(11)	-3443(8)	128(5)	83(3)
C(16)	7807(10)	-4103(7)	-111(4)	71(2)
C(17)	7955(8)	-5021(6)	234(3)	55(2)
C(18)	2990(10)	-11923(7)	2067(4)	79(3)
C(19)	4730(11)	-11602(9)	1963(8)	187(8)
C(20)	2832(17)	-11916(9)	2847(4)	150(6)
C(21)	1994(9)	-13267(6)	1661(4)	65(2)
C(22)	2511(6)	-10533(5)	871(3)	59(2)
C(23A)	1111(11)	-11674(8)	408(5)	39(3)
C(24A)	3968(10)	-10899(9)	695(5)	40(3)
C(25A)	2737(13)	-9307(8)	701(6)	50(3)
C(23B)	2118(15)	-11643(9)	313(5)	53(3)
C(24B)	4088(10)	-9409(9)	752(5)	47(3)
C(25B)	1292(11)	-9873(10)	647(5)	51(3)
C(26)	244(6)	-11258(5)	1817(3)	41.6(13)
C(27)	-530(7)	-11494(6)	2479(3)	47.4(15)
C(28)	-1225(10)	-12747(6)	2598(4)	79(3)
C(29)	-2106(12)	-13061(7)	3144(4)	102(4)
C(30)	-2359(10)	-12141(7)	3565(4)	85(3)
C(31)	-1697(7)	-10893(7)	3458(3)	60(2)
C(32)	-740(6)	-10529(6)	2930(3)	42.7(14)
C(33)	-127(6)	-9150(5)	2829(3)	40.1(13)
C(34)	2035(6)	-6586(5)	2777(3)	36.3(12)
C(35)	1717(8)	-6938(6)	1976(3)	47.4(15)
C(36)	831(7)	-6068(6)	3039(3)	47.0(15)
C(37)	3692(7)	-5516(6)	2950(4)	53(2)
C(38)	2109(6)	-7836(5)	4102(3)	35.0(12)
C(39)	2306(7)	-9020(6)	4301(3)	41.7(13)
C(40)	668(7)	-7726(6)	4413(3)	46.1(14)
C(41)	3566(6)	-6637(6)	4430(3)	44.1(14)

Table 3C. Bond lengths (Å) and angles (°) for (12).

Pd-C(8)	2.150(5)	Pd-C(7)	2.157(5)
Pd-P(2)	2.3540(14)	Pd-P(1)	2.367(2)
P(1)-C(26)	1.852(6)	P(1)-C(18)	1.884(7)
P(1)-C(22)	1.897(6)	P(2)-C(33)	1.858(5)
P(2)-C(38)	1.897(5)	P(2)-C(34)	1.898(5)
O-C(9)	1.237(7)	C(1)-C(6)	1.393(8)
C(1)-C(2)	1.395(8)	C(2)-C(3)	1.377(10)
C(3)-C(4)	1.367(9)	C(4)-C(5)	1.385(9)
C(5)-C(6)	1.401(8)	C(6)-C(7)	1.484(7)
C(7)-C(8)	1.423(8)	C(8)-C(9)	1.450(8)
C(9)-C(10)	1.499(8)	C(10)-C(11)	1.326(8)
C(11)-C(12)	1.462(8)	C(12)-C(13)	1.387(9)
C(12)-C(17)	1.397(8)	C(13)-C(14)	1.367(10)
C(14)-C(15)	1.381(11)	C(15)-C(16)	1.372(11)
C(16)-C(17)	1.368(9)	C(18)-C(21)	1.529(9)
C(18)-C(20)	1.534(13)	C(18)-C(19)	1.542(13)
C(22)-C(25A)	1.429(8)	C(22)-C(23B)	1.469(8)
C(22)-C(23A)	1.560(8)	C(22)-C(24B)	1.588(8)
C(22)-C(24A)	1.604(8)	C(22)-C(25B)	1.652(8)
C(26)-C(27)	1.520(8)	C(27)-C(28)	1.390(9)
C(27)-C(32)	1.400(8)	C(28)-C(29)	1.382(10)
C(29)-C(30)	1.351(12)	C(30)-C(31)	1.374(10)
C(31)-C(32)	1.402(8)	C(32)-C(33)	1.507(8)
C(34)-C(37)	1.531(8)	C(34)-C(36)	1.536(7)
C(34)-C(35)	1.537(8)	C(38)-C(41)	1.531(8)
C(38)-C(39)	1.535(7)	C(38)-C(40)	1.541(7)
C(8)-Pd-C(7)	38.6(2)	C(8)-Pd-P(2)	147.1(2)
C(7)-Pd-P(2)	108.7(2)	C(8)-Pd-P(1)	108.9(2)
C(7)-Pd-P(1)	147.09(15)	P(2)-Pd-P(1)	103.99(5)
C(26)-P(1)-C(18)	104.6(3)	C(26)-P(1)-C(22)	98.3(2)
C(18)-P(1)-C(22)	109.8(3)	C(26)-P(1)-Pd	117.2(2)
C(18)-P(1)-Pd	108.8(2)	C(22)-P(1)-Pd	117.2(2)
C(33)-P(2)-C(38)	103.0(3)	C(33)-P(2)-C(34)	99.6(2)
C(38)-P(2)-C(34)	110.8(2)	C(33)-P(2)-Pd	117.8(2)
C(38)-P(2)-Pd	115.5(2)	C(34)-P(2)-Pd	109.1(2)
C(6)-C(1)-C(2)	121.0(6)	C(3)-C(2)-C(1)	120.4(6)
C(4)-C(3)-C(2)	119.3(6)	C(3)-C(4)-C(5)	121.0(6)
C(4)-C(5)-C(6)	120.9(6)	C(1)-C(6)-C(5)	117.4(5)
C(1)-C(6)-C(7)	123.1(5)	C(5)-C(6)-C(7)	119.6(5)
C(8)-C(7)-C(6)	120.2(5)	C(8)-C(7)-Pd	70.4(3)
C(6)-C(7)-Pd	119.7(4)	C(7)-C(8)-C(9)	123.7(5)
C(7)-C(8)-Pd	71.0(3)	C(9)-C(8)-Pd	113.8(4)
O-C(9)-C(8)	122.0(5)	O-C(9)-C(10)	119.3(5)
C(8)-C(9)-C(10)	118.7(5)	C(11)-C(10)-C(9)	121.2(5)
C(10)-C(11)-C(12)	128.6(6)	C(13)-C(12)-C(17)	117.9(6)
C(13)-C(12)-C(11)	123.3(6)	C(17)-C(12)-C(11)	118.8(6)
C(14)-C(13)-C(12)	120.7(7)	C(13)-C(14)-C(15)	120.7(7)
C(16)-C(15)-C(14)	119.5(7)	C(17)-C(16)-C(15)	120.1(7)
C(16)-C(17)-C(12)	121.2(7)	C(21)-C(18)-C(20)	109.0(8)
C(21)-C(18)-C(19)	108.3(6)	C(20)-C(18)-C(19)	108.7(9)
C(21)-C(18)-P(1)	115.8(5)	C(20)-C(18)-P(1)	105.4(5)
C(19)-C(18)-P(1)	109.6(7)	C(25A)-C(22)-C(23A)	114.1(6)
C(23B)-C(22)-C(24B)	109.5(6)	C(25A)-C(22)-C(24A)	110.8(6)
C(23A)-C(22)-C(24A)	101.1(5)	C(23B)-C(22)-C(25B)	103.9(5)
C(24B)-C(22)-C(25B)	96.8(5)	C(25A)-C(22)-P(1)	113.6(6)
C(23B)-C(22)-P(1)	125.4(6)	C(23A)-C(22)-P(1)	111.6(5)
C(24B)-C(22)-P(1)	111.1(5)	C(24A)-C(22)-P(1)	104.4(5)

C(25B)-C(22)-P(1)	105.9(5)	C(27)-C(26)-P(1)	121.5(4)
C(28)-C(27)-C(32)	118.4(6)	C(28)-C(27)-C(26)	118.4(6)
C(32)-C(27)-C(26)	122.8(5)	C(29)-C(28)-C(27)	122.0(7)
C(30)-C(29)-C(28)	119.8(7)	C(29)-C(30)-C(31)	119.6(6)
C(30)-C(31)-C(32)	122.3(7)	C(27)-C(32)-C(31)	117.9(6)
C(27)-C(32)-C(33)	123.2(5)	C(31)-C(32)-C(33)	118.6(6)
C(32)-C(33)-P(2)	120.1(4)	C(37)-C(34)-C(36)	109.1(5)
C(37)-C(34)-C(35)	106.3(5)	C(36)-C(34)-C(35)	108.8(5)
C(37)-C(34)-P(2)	110.5(4)	C(36)-C(34)-P(2)	115.3(4)
C(35)-C(34)-P(2)	106.5(4)	C(41)-C(38)-C(39)	108.9(4)
C(41)-C(38)-C(40)	107.7(4)	C(39)-C(38)-C(40)	108.7(4)
C(41)-C(38)-P(2)	110.5(4)	C(39)-C(38)-P(2)	104.8(4)
C(40)-C(38)-P(2)	116.0(4)		

Table 3D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (12).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	24.4(2)	30.8(2)	31.1(2)	8.3(2)	3.86(15)	11.6(2)
P(1)	35.8(8)	41.2(8)	33.1(8)	-2.1(6)	-1.2(6)	15.4(6)
P(2)	23.7(7)	29.4(7)	38.3(7)	8.2(6)	4.2(5)	11.7(5)
O	41(2)	66(3)	57(3)	25(2)	22(2)	31(2)
C(1)	26(3)	43(3)	49(3)	15(3)	4(2)	13(2)
C(2)	39(3)	70(4)	57(4)	29(4)	15(3)	28(3)
C(3)	44(4)	89(5)	40(4)	15(4)	9(3)	30(4)
C(4)	45(4)	72(5)	47(4)	-3(3)	5(3)	28(3)
C(5)	34(3)	43(3)	53(4)	3(3)	2(3)	16(3)
C(6)	24(3)	46(3)	44(3)	11(3)	6(2)	18(2)
C(7)	27(3)	33(3)	47(3)	14(2)	1(2)	12(2)
C(8)	31(3)	40(3)	47(3)	17(3)	9(2)	18(2)
C(9)	29(3)	55(4)	53(4)	24(3)	11(3)	20(3)
C(10)	41(3)	63(4)	63(4)	34(3)	27(3)	31(3)
C(11)	43(3)	60(4)	57(4)	24(3)	18(3)	27(3)
C(12)	57(4)	61(4)	56(4)	30(3)	24(3)	31(3)
C(13)	85(5)	90(6)	74(5)	45(4)	40(4)	58(5)
C(14)	112(7)	92(6)	103(7)	50(5)	41(6)	74(6)
C(15)	107(7)	71(5)	90(6)	45(5)	18(5)	43(5)
C(16)	83(5)	71(5)	64(5)	36(4)	22(4)	25(4)
C(17)	56(4)	57(4)	57(4)	22(3)	21(3)	22(3)
C(18)	93(6)	52(4)	88(6)	-33(4)	-48(5)	48(4)
C(19)	84(7)	94(7)	347(20)	-126(10)	-97(10)	69(6)
C(20)	309(17)	90(7)	70(6)	-39(5)	-101(8)	136(9)
C(21)	97(6)	42(4)	54(4)	-4(3)	-17(4)	35(4)
C(22)	33(3)	90(5)	32(3)	-7(3)	1(2)	7(3)
C(23A)	58(7)	38(6)	28(6)	5(5)	-2(6)	27(6)
C(24A)	45(6)	39(6)	33(6)	7(5)	9(5)	12(5)
C(25A)	42(8)	56(7)	44(7)	-6(6)	-2(6)	18(6)
C(23B)	76(10)	47(6)	34(6)	4(5)	-2(6)	25(6)
C(24B)	54(7)	46(6)	35(6)	7(5)	2(5)	13(5)
C(25B)	67(8)	52(7)	35(6)	13(5)	9(6)	22(6)
C(26)	40(3)	38(3)	35(3)	4(2)	0(2)	5(3)
C(27)	47(3)	40(3)	35(3)	5(3)	6(3)	-4(3)
C(28)	109(6)	35(4)	54(4)	0(3)	23(4)	-13(4)
C(29)	139(8)	43(4)	67(5)	6(4)	39(5)	-27(5)
C(30)	86(6)	65(5)	49(4)	2(4)	27(4)	-28(4)
C(31)	48(4)	59(4)	50(4)	0(3)	17(3)	-4(3)
C(32)	31(3)	47(3)	38(3)	7(3)	5(2)	3(3)
C(33)	27(3)	43(3)	51(3)	11(3)	6(2)	14(2)
C(34)	32(3)	32(3)	48(3)	10(2)	2(2)	15(2)
C(35)	59(4)	39(3)	49(4)	13(3)	10(3)	22(3)
C(36)	56(4)	46(3)	50(4)	7(3)	3(3)	34(3)
C(37)	46(4)	36(3)	76(5)	19(3)	2(3)	13(3)
C(38)	33(3)	40(3)	37(3)	7(2)	7(2)	19(2)
C(39)	42(3)	51(3)	38(3)	13(3)	10(3)	23(3)
C(40)	39(3)	61(4)	45(3)	10(3)	15(3)	26(3)
C(41)	36(3)	51(4)	47(3)	1(3)	3(3)	21(3)

Table 3E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (12).

	x	y	z	U
H(1)	5765(6)	-9345(5)	3860(3)	47
H(2)	6567(7)	-9303(7)	5028(3)	61
H(3)	7986(7)	-7358(7)	5768(3)	67
H(4)	8598(7)	-5459(7)	5341(3)	65
H(5)	7762(6)	-5468(6)	4190(3)	53
H(7)	6375(63)	-6558(30)	3062(28)	42
H(8)	6590(64)	-8945(38)	2727(28)	44
H(10)	6117(7)	-6403(6)	1952(3)	59
H(11)	8029(7)	-6712(6)	965(3)	59
H(13)	5840(9)	-4797(8)	1474(4)	86
H(14)	5613(11)	-3241(8)	892(5)	105
H(15)	6815(11)	-2811(8)	-114(5)	100
H(16)	8314(10)	-3922(7)	-516(4)	86
H(17)	8565(8)	-5473(6)	64(3)	66
H(19A)	5389(11)	-10742(9)	2219(8)	281
H(19B)	4842(11)	-11630(9)	1464(8)	281
H(19C)	5065(11)	-12230(9)	2139(8)	281
H(20A)	3468(17)	-11057(9)	3110(4)	225
H(20B)	3203(17)	-12535(9)	3010(4)	225
H(20C)	1723(17)	-12152(9)	2918(4)	225
H(21A)	2089(9)	-13279(6)	1162(4)	97
H(21B)	887(9)	-13501(6)	1734(4)	97
H(21C)	2367(9)	-13883(6)	1827(4)	97
H(23A)	1028(11)	-12480(8)	554(5)	59
H(23B)	1299(11)	-11702(8)	-83(5)	59
H(23C)	128(11)	-11558(8)	461(5)	59
H(24A)	3789(10)	-11741(9)	816(5)	60
H(24B)	4942(10)	-10254(9)	967(5)	60
H(24C)	4063(10)	-10925(9)	196(5)	60
H(25A)	3631(13)	-8640(8)	1012(6)	75
H(25B)	1782(13)	-9148(8)	759(6)	75
H(25C)	2954(13)	-9291(8)	216(6)	75
H(23D)	1145(15)	-12337(9)	387(5)	79
H(23E)	2980(15)	-11937(9)	320(5)	79
H(23F)	1967(15)	-11396(9)	-140(5)	79
H(24D)	4349(10)	-8669(9)	1124(5)	71
H(24E)	3938(10)	-9162(9)	299(5)	71
H(24F)	4951(10)	-9703(9)	758(5)	71
H(25D)	1473(11)	-9114(10)	995(5)	77
H(25E)	200(11)	-10492(10)	623(5)	77
H(25F)	1479(11)	-9620(10)	188(5)	77
H(26A)	-127(6)	-10669(5)	1605(3)	50
H(26B)	-187(6)	-12084(5)	1489(3)	50
H(28)	-1090(10)	-13409(6)	2295(4)	95
H(29)	-2534(12)	-13921(7)	3223(4)	122
H(30)	-2989(10)	-12355(7)	3933(4)	102
H(31)	-1894(7)	-10256(7)	3753(3)	73
H(33A)	-768(6)	-8751(5)	3075(3)	48
H(33B)	-343(6)	-9149(5)	2325(3)	48
H(35A)	2427(34)	-7329(36)	1806(3)	71
H(35B)	1901(47)	-6161(8)	1776(3)	71
H(35C)	620(15)	-7547(30)	1836(3)	71

H(36A)	-223(10)	-6763(10)	2958(20)	71
H(36B)	833(35)	-5385(27)	2786(15)	71
H(36C)	1115(28)	-5725(36)	3540(5)	71
H(37A)	4469(9)	-5849(12)	2799(21)	79
H(37B)	3917(21)	-5206(29)	3455(5)	79
H(37C)	3749(17)	-4809(19)	2706(19)	79
H(39A)	3267(25)	-9061(21)	4138(18)	63
H(39B)	1392(22)	-9794(6)	4082(16)	63
H(39C)	2383(45)	-8960(18)	4810(3)	63
H(40A)	-254(13)	-8537(14)	4268(18)	69
H(40B)	456(30)	-7034(26)	4244(17)	69
H(40C)	887(19)	-7538(39)	4924(3)	69
H(41A)	4467(13)	-6605(21)	4183(13)	66
H(41B)	3805(28)	-6666(19)	4923(6)	66
H(41C)	3358(18)	-5871(6)	4393(19)	66

Table 4A. Crystal data, structure solution and refinement for (13).

Identification code	exti13
Chemical formula	$C_{37}H_{51}OP_2Pd$
Formula weight	680.12
Temperature	205(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 9.1626(11) Å α = 81.331(3)°
	b = 13.858(2) Å β = 78.5110(10)°
	c = 14.353(2) Å γ = 77.523(3)°
Volume	1732.7(4) $Å^3$
Z	2
Density (calculated)	1.304 g/cm^3
Absorption coefficient μ	0.654 mm^{-1}
F(000)	714
Reflections for cell refinement	5655 (θ range 2.21 to 26.33°)
Crystal colour	yellow
Crystal size	0.30 × 0.28 × 0.24 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.46 to 26.39°
Index ranges	$-11 \le h \le 6$, $-17 \le k \le 17$, $-17 \le \ell \le 16$
Intensity decay	0%
Reflections collected	10165
Independent reflections	6930 (R_{int} = 0.0630)
Reflections with I>2σ(I)	5718
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.944 and 0.558
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0856, 4.4583
Data / restraints / parameters	6926 / 2 / 384
Final R indices [I>2σ(I)]	R1 = 0.0652, wR2 = 0.1568
R indices (all data)	R1 = 0.0834, wR2 = 0.1799
Goodness-of-fit on F^2	1.151
Largest and mean shift/esd	-0.001 and 0.000
Largest diff. peak and hole	2.092 and -1.946 $eÅ^{-3}$

The Crystal Structure of [*o*-$C_6H_4(CH_2PPr^i_2)_2$ Pd (dba)] (13)

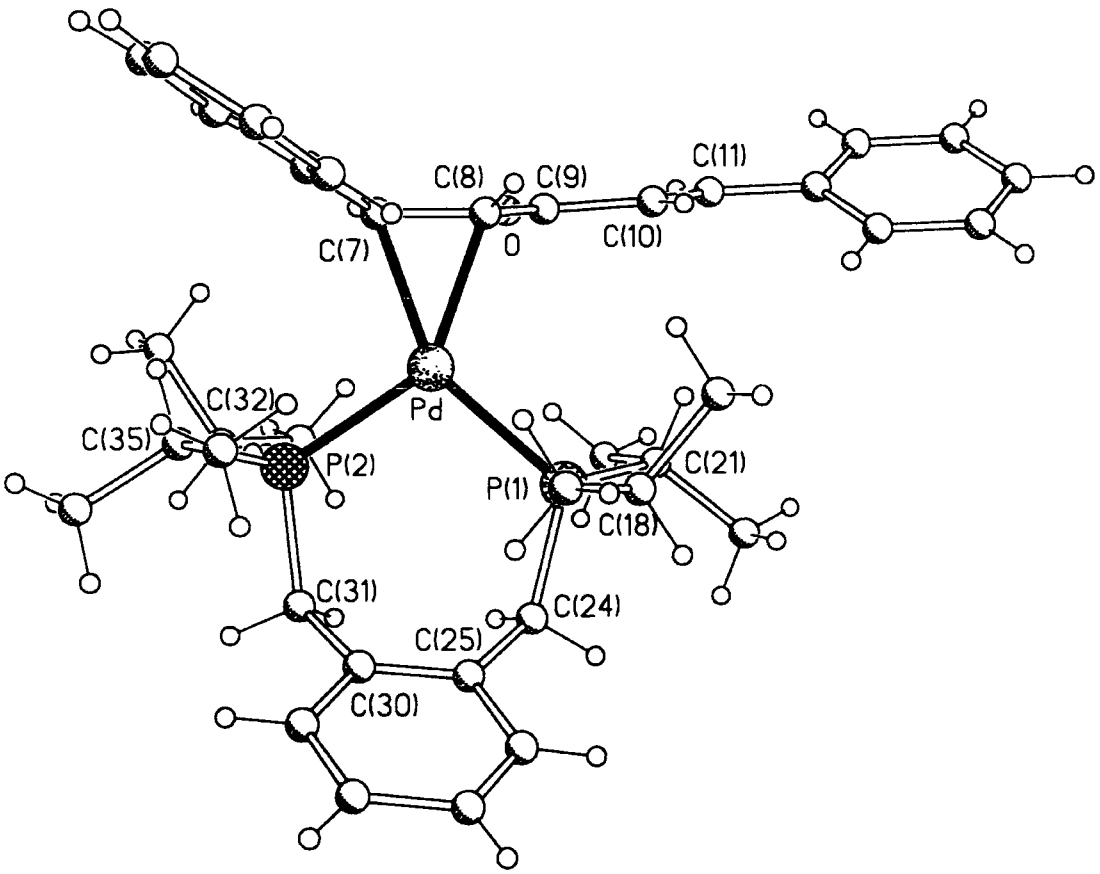


Table 4B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (13). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	5182.7(4)	7420.9(3)	7264.3(3)	25.80(15)
P(1)	5340(2)	8809.5(10)	7930.6(10)	29.2(3)
P(2)	7633.0(15)	6552.9(11)	7004.4(10)	30.1(3)
O	3008(6)	8403(4)	5567(3)	52.8(12)
C(1)	3469(6)	5339(4)	8204(4)	33.5(12)
C(2)	3342(7)	4399(5)	8618(4)	40.6(14)
C(3)	3524(8)	3628(5)	8061(5)	49(2)
C(4)	3884(7)	3817(4)	7079(5)	45(2)
C(5)	4011(7)	4775(4)	6658(4)	36.1(13)
C(6)	3796(6)	5568(4)	7208(4)	29.9(11)
C(7)	3901(6)	6574(4)	6731(4)	29.6(11)
C(8)	2910(6)	7430(4)	7093(4)	28.8(11)
C(9)	2492(7)	8320(4)	6432(4)	36.6(13)
C(10)	1362(6)	9147(5)	6870(5)	38.0(13)
C(11)	814(8)	9979(5)	6346(5)	43.2(14)
C(12)	-277(7)	10862(4)	6700(5)	38.9(13)
C(13)	-1160(8)	11488(5)	6093(5)	48(2)
C(14)	-2192(8)	12320(5)	6416(6)	55(2)
C(15)	-2315(8)	12544(5)	7332(6)	52(2)
C(16)	-1419(8)	11927(5)	7939(5)	49(2)
C(17)	-409(7)	11089(5)	7630(5)	43.2(14)
C(18)	4394(7)	8809(4)	9207(4)	34.4(12)
C(19)	2663(7)	9116(5)	9284(5)	41.6(14)
C(20)	4787(8)	7782(5)	9758(4)	47(2)
C(21)	4473(8)	10002(4)	7332(4)	41.4(14)
C(22)	4505(10)	10937(5)	7769(6)	58(2)
C(23)	5149(10)	10079(6)	6258(5)	61(2)
C(24)	7252(7)	9045(5)	7932(5)	41.9(14)
C(25)	8172(6)	8295(5)	8560(4)	38.2(13)
C(26)	8219(7)	8532(6)	9481(5)	53(2)
C(27)	8983(9)	7886(7)	10109(5)	64(2)
C(28)	9768(8)	6960(6)	9850(5)	56(2)
C(29)	9757(7)	6730(6)	8945(5)	47(2)
C(30)	8991(6)	7373(5)	8289(4)	37.3(13)
C(31)	9156(7)	7095(5)	7286(4)	39.2(13)
C(32)	8362(7)	6457(6)	5697(4)	47(2)
C(33)	7884(10)	7460(7)	5143(5)	68(2)
C(34)	7787(8)	5644(6)	5342(5)	59(2)
C(35)	7921(7)	5258(4)	7571(4)	38.7(13)
C(36)	7253(8)	5185(5)	8643(5)	45.1(15)
C(37)	9543(8)	4667(6)	7382(6)	57(2)

Table 4C. Bond lengths (Å) and angles (°) for (13).

Pd-C(7)	2.137(5)	Pd-C(8)	2.142(5)
Pd-P(2)	2.2937(14)	Pd-P(1)	2.3167(14)
P(1)-C(21)	1.838(6)	P(1)-C(24)	1.851(6)
P(1)-C(18)	1.864(5)	P(2)-C(35)	1.841(6)
P(2)-C(31)	1.856(6)	P(2)-C(32)	1.877(6)
O-C(9)	1.234(8)	C(1)-C(2)	1.367(8)
C(1)-C(6)	1.403(8)	C(2)-C(3)	1.391(9)
C(3)-C(4)	1.379(10)	C(4)-C(5)	1.393(9)
C(5)-C(6)	1.405(7)	C(6)-C(7)	1.472(8)
C(7)-C(8)	1.426(7)	C(8)-C(9)	1.469(8)
C(9)-C(10)	1.492(8)	C(10)-C(11)	1.337(9)
C(11)-C(12)	1.487(9)	C(12)-C(13)	1.384(9)
C(12)-C(17)	1.393(9)	C(13)-C(14)	1.398(10)
C(14)-C(15)	1.373(11)	C(15)-C(16)	1.386(10)
C(16)-C(17)	1.389(9)	C(18)-C(20)	1.528(8)
C(18)-C(19)	1.537(9)	C(21)-C(22)	1.530(9)
C(21)-C(23)	1.540(9)	C(24)-C(25)	1.498(9)
C(25)-C(30)	1.402(8)	C(25)-C(26)	1.420(9)
C(26)-C(27)	1.357(11)	C(27)-C(28)	1.393(11)
C(28)-C(29)	1.386(10)	C(29)-C(30)	1.382(9)
C(30)-C(31)	1.516(8)	C(32)-C(33)	1.516(11)
C(32)-C(34)	1.530(10)	C(35)-C(37)	1.528(9)
C(35)-C(36)	1.535(9)		
C(7)-Pd-C(8)	38.9(2)	C(7)-Pd-P(2)	104.82(15)
C(8)-Pd-P(2)	143.74(15)	C(7)-Pd-P(1)	150.8(2)
C(8)-Pd-P(1)	111.89(15)	P(2)-Pd-P(1)	104.35(5)
C(21)-P(1)-C(24)	100.6(3)	C(21)-P(1)-C(18)	104.9(3)
C(24)-P(1)-C(18)	104.2(3)	C(21)-P(1)-Pd	114.7(2)
C(24)-P(1)-Pd	117.8(2)	C(18)-P(1)-Pd	113.0(2)
C(35)-P(2)-C(31)	105.6(3)	C(35)-P(2)-C(32)	104.7(3)
C(31)-P(2)-C(32)	99.0(3)	C(35)-P(2)-Pd	115.3(2)
C(31)-P(2)-Pd	118.7(2)	C(32)-P(2)-Pd	111.5(2)
C(2)-C(1)-C(6)	121.9(5)	C(1)-C(2)-C(3)	120.9(6)
C(4)-C(3)-C(2)	119.1(6)	C(3)-C(4)-C(5)	120.0(6)
C(4)-C(5)-C(6)	121.7(6)	C(1)-C(6)-C(5)	116.4(5)
C(1)-C(6)-C(7)	123.7(5)	C(5)-C(6)-C(7)	119.9(5)
C(8)-C(7)-C(6)	121.1(5)	C(8)-C(7)-Pd	70.7(3)
C(6)-C(7)-Pd	118.5(4)	C(7)-C(8)-C(9)	119.7(5)
C(7)-C(8)-Pd	70.4(3)	C(9)-C(8)-Pd	105.8(4)
O-C(9)-C(8)	123.9(5)	O-C(9)-C(10)	120.6(5)
C(8)-C(9)-C(10)	115.5(5)	C(11)-C(10)-C(9)	122.0(6)
C(10)-C(11)-C(12)	127.0(6)	C(13)-C(12)-C(17)	118.9(6)
C(13)-C(12)-C(11)	119.8(6)	C(17)-C(12)-C(11)	121.3(6)
C(12)-C(13)-C(14)	120.4(7)	C(15)-C(14)-C(13)	120.5(7)
C(14)-C(15)-C(16)	119.3(6)	C(15)-C(16)-C(17)	120.7(7)
C(16)-C(17)-C(12)	120.2(6)	C(20)-C(18)-C(19)	109.4(5)
C(20)-C(18)-P(1)	110.7(4)	C(19)-C(18)-P(1)	110.8(4)
C(22)-C(21)-C(23)	111.4(6)	C(22)-C(21)-P(1)	116.4(5)
C(23)-C(21)-P(1)	109.7(5)	C(25)-C(24)-P(1)	114.8(4)
C(30)-C(25)-C(26)	118.2(6)	C(30)-C(25)-C(24)	123.7(5)
C(26)-C(25)-C(24)	118.1(6)	C(27)-C(26)-C(25)	122.2(7)
C(26)-C(27)-C(28)	119.7(7)	C(29)-C(28)-C(27)	118.5(7)
C(30)-C(29)-C(28)	123.1(7)	C(29)-C(30)-C(25)	118.3(6)
C(29)-C(30)-C(31)	119.3(6)	C(25)-C(30)-C(31)	122.2(6)
C(30)-C(31)-P(2)	118.2(4)	C(33)-C(32)-C(34)	110.8(6)
C(33)-C(32)-P(2)	108.6(5)	C(34)-C(32)-P(2)	111.7(5)
C(37)-C(35)-C(36)	111.6(6)	C(37)-C(35)-P(2)	115.7(5)

C(36)-C(35)-P(2)	112.0(4)

Table 4D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (13).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	22.2(2)	30.9(2)	23.9(2)	-8.74(15)	2.93(14)	-6.63(15)
P(1)	30.2(7)	29.4(7)	27.6(7)	-8.7(5)	1.6(5)	-7.0(5)
P(2)	20.6(7)	41.6(8)	27.3(7)	-15.3(6)	5.0(5)	-4.9(6)
O	57(3)	60(3)	32(2)	-3(2)	-5(2)	6(2)
C(1)	32(3)	33(3)	35(3)	-8(2)	-2(2)	-5(2)
C(2)	38(3)	45(3)	34(3)	-5(2)	3(3)	-5(3)
C(3)	53(4)	32(3)	58(4)	-7(3)	-6(3)	-4(3)
C(4)	44(4)	33(3)	59(4)	-22(3)	-6(3)	-2(3)
C(5)	34(3)	42(3)	31(3)	-12(2)	-2(2)	-3(2)
C(6)	23(3)	37(3)	32(3)	-17(2)	-3(2)	-4(2)
C(7)	28(3)	38(3)	23(2)	-11(2)	2(2)	-7(2)
C(8)	22(3)	32(3)	31(3)	-6(2)	0(2)	-6(2)
C(9)	31(3)	39(3)	41(3)	-13(2)	-10(2)	0(2)
C(10)	26(3)	47(3)	39(3)	-4(3)	-7(2)	-2(2)
C(11)	44(4)	41(3)	44(3)	-8(3)	-4(3)	-8(3)
C(12)	32(3)	37(3)	47(3)	-4(3)	-6(3)	-7(2)
C(13)	52(4)	45(4)	49(4)	-5(3)	-13(3)	-9(3)
C(14)	49(4)	45(4)	70(5)	0(3)	-21(4)	-4(3)
C(15)	38(4)	45(4)	73(5)	-15(3)	-9(3)	-1(3)
C(16)	47(4)	49(4)	54(4)	-17(3)	-7(3)	-6(3)
C(17)	41(4)	39(3)	51(4)	-7(3)	-11(3)	-6(3)
C(18)	45(3)	36(3)	24(3)	-11(2)	-1(2)	-9(2)
C(19)	35(3)	43(3)	40(3)	-13(3)	9(3)	-2(3)
C(20)	49(4)	52(4)	32(3)	0(3)	2(3)	-4(3)
C(21)	51(4)	34(3)	39(3)	1(2)	-4(3)	-13(3)
C(22)	75(5)	32(3)	67(5)	-11(3)	-8(4)	-11(3)
C(23)	81(6)	56(4)	41(4)	5(3)	-3(4)	-16(4)
C(24)	32(3)	44(3)	53(4)	-12(3)	-1(3)	-16(3)
C(25)	24(3)	54(4)	40(3)	-19(3)	0(2)	-11(2)
C(26)	32(3)	76(5)	60(4)	-44(4)	-2(3)	-12(3)
C(27)	48(4)	110(7)	44(4)	-37(4)	-8(3)	-19(4)
C(28)	37(4)	87(6)	49(4)	-11(4)	-13(3)	-14(4)
C(29)	26(3)	67(4)	50(4)	-17(3)	-5(3)	-10(3)
C(30)	21(3)	56(4)	39(3)	-19(3)	1(2)	-13(2)
C(31)	26(3)	54(4)	38(3)	-20(3)	4(2)	-8(3)
C(32)	31(3)	83(5)	27(3)	-26(3)	12(2)	-12(3)
C(33)	73(6)	95(6)	34(4)	-5(4)	7(4)	-27(5)
C(34)	45(4)	90(6)	45(4)	-41(4)	6(3)	-8(4)
C(35)	32(3)	41(3)	44(3)	-17(3)	-5(3)	-3(2)
C(36)	43(4)	44(3)	47(4)	-6(3)	-5(3)	-6(3)
C(37)	40(4)	53(4)	75(5)	-20(4)	-8(4)	4(3)

Table 4E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (13).

	x	y	z	U
H(1)	3334(6)	5846(4)	8598(4)	40
H(2)	3128(7)	4271(5)	9289(4)	49
H(3)	3403(8)	2988(5)	8349(5)	58
H(4)	4042(7)	3298(4)	6695(5)	54
H(5)	4248(7)	4895(4)	5988(4)	43
H(7)	4155(69)	6672(44)	6061(6)	36
H(8)	2217(53)	7304(44)	7653(25)	35
H(10)	1025(6)	9081(5)	7535(5)	46
H(11)	1155(8)	10009(5)	5681(5)	52
H(13)	-1066(8)	11352(5)	5459(5)	58
H(14)	-2806(8)	12729(5)	6003(6)	65
H(15)	-3000(8)	13109(5)	7545(6)	63
H(16)	-1496(8)	12078(5)	8566(5)	59
H(17)	187(7)	10674(5)	8050(5)	52
H(18)	4760(7)	9295(4)	9500(4)	41
H(19A)	2411(7)	9780(14)	8958(29)	62
H(19B)	2194(8)	9109(34)	9953(5)	62
H(19C)	2292(9)	8652(21)	8990(30)	62
H(20A)	5879(9)	7589(18)	9711(32)	70
H(20B)	4413(53)	7301(9)	9487(24)	70
H(20C)	4317(50)	7802(11)	10424(9)	70
H(21)	3389(8)	9978(4)	7378(4)	50
H(22A)	4144(61)	10846(17)	8453(9)	87
H(22B)	3855(51)	11503(9)	7480(30)	87
H(22C)	5535(14)	11053(24)	7650(35)	87
H(23A)	5092(61)	9484(20)	5998(10)	91
H(23B)	6201(21)	10146(43)	6171(6)	91
H(23C)	4580(42)	10656(25)	5927(8)	91
H(24A)	7814(7)	9063(5)	7275(5)	50
H(24B)	7141(7)	9703(5)	8140(5)	50
H(26)	7705(7)	9158(6)	9661(5)	63
H(27)	8981(9)	8062(7)	10717(5)	76
H(28)	10294(8)	6501(6)	10280(5)	67
H(29)	10295(7)	6108(6)	8769(5)	56
H(31A)	10112(7)	6619(5)	7158(4)	47
H(31B)	9251(7)	7694(5)	6837(4)	47
H(32A)	7954(7)	6489(6)	6379(4)	57
H(32B)	9472(7)	6293(6)	5620(4)	57
H(33A)	8311(63)	7956(12)	5351(35)	102
H(33B)	6785(11)	7646(24)	5258(38)	102
H(33C)	8248(66)	7420(15)	4464(7)	102
H(34A)	6688(9)	5765(26)	5487(39)	89
H(34B)	8192(55)	5001(8)	5659(32)	89
H(34C)	8118(58)	5651(30)	4656(8)	89
H(35)	7311(7)	4918(4)	7277(4)	46
H(36A)	6215(19)	5550(31)	8735(5)	68
H(36B)	7852(33)	5466(33)	8979(7)	68
H(36C)	7271(52)	4492(6)	8891(9)	68
H(37A)	10178(16)	4918(28)	7717(33)	85
H(37B)	9934(24)	4736(34)	6701(7)	85
H(37C)	9548(12)	3970(9)	7608(37)	85

Table 5A. Crystal data, structure solution and refinement for (14).

Identification code	exti21
Chemical formula	$C_{66.5}H_{86}OP_2Pd$
Formula weight	1069.70
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 9.9570(4) Å α = 85.618(2)°
	b = 12.5908(5) Å β = 88.919(2)°
	c = 47.5159(19) Å γ = 77.405(2)°
Volume	5796.6(4) $Å^3$
Z	4
Density (calculated)	1.226 g/cm^3
Absorption coefficient μ	0.416 mm^{-1}
F(000)	2276
Reflections for cell refinement	27019 (θ range 2.02 to 28.48°)
Crystal colour	orange
Crystal size	0.60 × 0.42 × 0.19 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	0.86 to 28.60°
Index ranges	$-13 \le h \le 13$, $-15 \le k \le 16$, $-63 \le \ell \le 35$
Intensity decay	0%
Reflections collected	35204
Independent reflections	25488 (R_{int} = 0.0204)
Reflections with I>2σ(I)	21914
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.923 and 0.668
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0275, 15.3744
Data / restraints / parameters	25488 / 591 / 1283
Final R indices [I>2σ(I)]	R1 = 0.0645, wR2 = 0.1405
R indices (all data)	R1 = 0.0763, wR2 = 0.1454
Goodness-of-fit on F^2	1.272
Extinction coefficient	0.00044(7)
Largest and mean shift/esd	0.004 and 0.000
Largest diff. peak and hole	0.888 and -1.633 $eÅ^{-3}$

Crystal Data For [*o*-$C_6H_4(CH_2PCy_2)_2Pd(dba)$] (14)

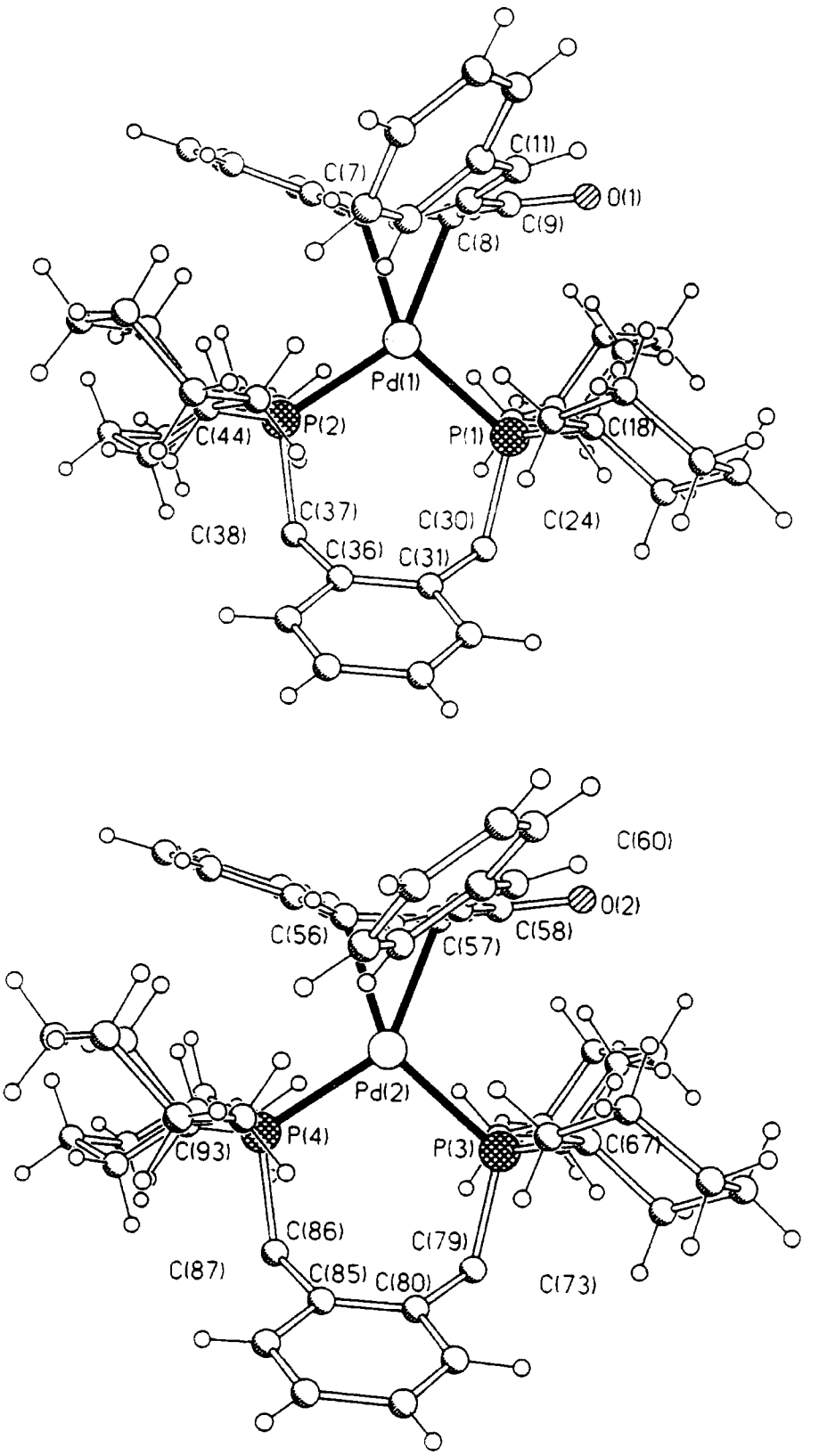


Table 5B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (14). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	Y	z	U(eq)
Pd(1)	7283.9(3)	3903.8(2)	1288.63(6)	16.11(7)
P(1)	8105.5(10)	2394.3(8)	1597.1(2)	17.9(2)
P(2)	4957.7(10)	3961.1(8)	1257.7(2)	17.67(19)
O(1)	10775(3)	4439(2)	1451.3(7)	28.0(6)
C(1)	7910(5)	4312(4)	547.8(9)	30.4(10)
C(2)	7525(5)	4308(5)	267.8(10)	41.1(12)
C(3)	6542(6)	5151(5)	145.8(10)	45.8(14)
C(4)	5937(5)	6007(5)	302.8(10)	43.1(13)
C(5)	6326(5)	6027(4)	579.7(9)	31.0(10)
C(6)	7312(4)	5174(3)	710.2(9)	23.5(8)
C(7)	7670(4)	5212(3)	1010.1(8)	19.6(8)
C(8)	8949(4)	4617(3)	1130.3(8)	20.1(8)
C(9)	9588(4)	4898(3)	1376.5(8)	19.3(8)
C(10)	8791(4)	5782(3)	1544.1(8)	20.9(8)
C(11)	9385(4)	6257(3)	1731.2(9)	22.6(8)
C(12)	8678(4)	7144(3)	1899.5(8)	22.1(8)
C(13)	7281(4)	7279(3)	1967.4(9)	26.7(9)
C(14)	6618(5)	8144(4)	2116.7(9)	30.8(10)
C(15)	7326(5)	8908(4)	2196.9(10)	32.4(10)
C(16)	8707(5)	8778(4)	2135.8(10)	33.2(10)
C(17)	9382(4)	7905(3)	1988.4(10)	28.7(9)
C(18)	9054(4)	2695(3)	1899.4(8)	20.2(8)
C(19)	8266(4)	3696(3)	2046.1(8)	20.9(8)
C(20)	9215(4)	4041(4)	2254.7(9)	26.4(9)
C(21)	9755(4)	3107(4)	2476.9(9)	29.0(9)
C(22)	10489(4)	2081(4)	2339.5(9)	28.1(9)
C(23)	9599(4)	1746(3)	2119.7(9)	23.7(8)
C(24)	9362(4)	1313(3)	1424.6(9)	23.5(8)
C(25)	10753(4)	1644(3)	1377.6(10)	26.3(9)
C(26)	11759(5)	833(4)	1211.1(12)	38.3(12)
C(27)	11150(5)	662(5)	934.1(13)	51.0(15)
C(28)	9803(5)	283(5)	979.4(13)	48.7(14)
C(29)	8779(5)	1112(4)	1145.6(10)	33.9(10)
C(30)	6886(4)	1577(3)	1748.7(9)	22.1(8)
C(31)	5679(4)	2209(3)	1911.2(8)	18.8(8)
C(32)	5719(4)	2160(3)	2206.7(9)	24.8(9)
C(33)	4639(4)	2704(3)	2364.3(9)	26.1(9)
C(34)	3456(4)	3288(3)	2228.5(9)	26.0(9)
C(35)	3373(4)	3324(3)	1938.2(9)	22.9(8)
C(36)	4472(4)	2807(3)	1774.3(8)	19.1(8)
C(37)	4270(4)	2868(3)	1460.2(8)	22.2(8)
C(38)	4385(4)	3796(3)	897.2(8)	20.6(8)
C(39)	5318(4)	2779(4)	781.6(9)	28.0(9)
C(40)	4951(5)	2667(4)	475.3(10)	35.0(10)
C(41)	3436(5)	2649(4)	443.5(11)	40.7(12)
C(42)	2509(5)	3644(4)	562.5(10)	36.0(11)
C(43)	2861(4)	3754(4)	867.6(9)	28.8(9)
C(44)	3836(4)	5223(3)	1379.9(8)	20.5(8)
C(45)	3598(5)	6170(4)	1150.6(10)	31.5(10)
C(46)	2650(6)	7192(4)	1266.2(11)	43.4(13)
C(47)	3227(6)	7521(4)	1529.8(12)	44.0(13)

C(48)	3549(5)	6577(4)	1755.0(10)	31.9(10)
C(49)	4476(4)	5566(3)	1639.7(9)	23.7(8)
Pd(2)	2094.5(3)	4720.3(2)	6316.20(6)	16.54(7)
P(3)	2871.8(10)	3419.6(8)	6682.1(2)	17.8(2)
P(4)	-217.7(10)	4726.5(8)	6285.6(2)	18.5(2)
O(2)	5531(3)	5402(2)	6450.5(7)	28.2(7)
C(50)	2898(5)	4681(4)	5573.3(10)	34.4(10)
C(51)	2589(6)	4487(5)	5300.1(11)	48.0(14)
C(52)	1578(6)	5221(6)	5147.4(11)	50.8(15)
C(53)	881(6)	6150(5)	5267.9(10)	48.0(14)
C(54)	1199(5)	6358(4)	5537.7(10)	34.8(10)
C(55)	2212(4)	5618(4)	5697.8(9)	26.9(9)
C(56)	2501(4)	5861(3)	5986.0(8)	20.3(8)
C(57)	3768(4)	5361(3)	6127.7(8)	20.4(8)
C(58)	4347(4)	5801(3)	6361.0(9)	21.7(8)
C(59)	3487(4)	6748(3)	6496.1(9)	22.6(8)
C(60)	4012(4)	7276(3)	6683.9(9)	24.5(8)
C(61)	3234(4)	8181(3)	6840.8(9)	24.1(8)
C(62)	1809(5)	8349(4)	6877.1(11)	34.2(11)
C(63)	1097(5)	9210(4)	7020.4(11)	36.8(11)
C(64)	1781(5)	9926(4)	7133.3(10)	34.1(10)
C(65)	3193(5)	9769(4)	7099.8(10)	33.0(10)
C(66)	3913(5)	8907(4)	6955.8(9)	28.6(9)
C(67)	3770(4)	3903(3)	6964.7(8)	19.2(8)
C(68)	2956(4)	4966(3)	7077.6(8)	20.5(8)
C(69)	3865(4)	5419(3)	7271.6(9)	24.6(8)
C(70)	4425(4)	4590(4)	7516.2(9)	26.9(9)
C(71)	5184(4)	3508(3)	7410.8(9)	26.1(9)
C(72)	4297(4)	3055(3)	7210.9(9)	23.8(8)
C(73)	4161(4)	2243(3)	6555.5(9)	22.6(8)
C(74)	5555(4)	2548(3)	6493.2(9)	24.8(9)
C(75)	6578(5)	1627(4)	6360.5(11)	34.3(11)
C(76)	5993(5)	1261(4)	6101.7(12)	44.1(13)
C(77)	4641(5)	918(4)	6171.4(11)	40.1(12)
C(78)	3604(5)	1854(4)	6294.3(11)	34.7(11)
C(79)	1655(4)	2667(3)	6866.6(9)	22.0(8)
C(80)	388(4)	3367(3)	6994.3(8)	19.7(8)
C(81)	355(4)	3508(4)	7280.9(9)	25.2(9)
C(82)	-777(4)	4128(4)	7410.7(9)	28.2(9)
C(83)	-1923(4)	4610(3)	7250.6(9)	26.3(9)
C(84)	-1940(4)	4446(3)	6966.7(9)	24.2(8)
C(85)	-794(4)	3841(3)	6832.5(8)	20.2(8)
C(86)	-897(4)	3713(3)	6520.9(8)	22.1(8)
C(87)	-762(4)	4390(3)	5939.4(9)	24.1(8)
C(88)	142(5)	3306(4)	5857.7(9)	29.6(9)
C(89)	-183(5)	3049(4)	5560.2(10)	39.5(11)
C(90)	-1711(5)	3066(5)	5527.4(11)	44.3(13)
C(91)	-2607(5)	4132(5)	5609.9(10)	39.8(12)
C(92)	-2291(4)	4373(4)	5910.0(9)	31.3(10)
C(93)	-1364(4)	6029(3)	6369.9(9)	22.2(8)
C(94)	-1599(5)	6896(4)	6122.4(10)	34.5(10)
C(95)	-2598(6)	7931(4)	6208.0(12)	47.7(13)
C(96)	-2092(6)	8376(4)	6463.5(13)	51.3(15)
C(97)	-1758(5)	7528(4)	6707.9(11)	36.4(11)
C(98)	-767(4)	6498(3)	6618.0(9)	25.9(9)
C(111)	13508(5)	96(4)	2541.2(10)	35.1(10)
C(112)	13116(5)	-278(4)	2805.3(12)	41.5(12)
C(113)	12267(5)	-1035(4)	2828.8(12)	44.5(12)
C(114)	11844(5)	-1401(4)	2584.0(12)	44.2(12)
C(115)	12236(5)	-1028(4)	2318.2(12)	39.2(11)
C(116)	13080(4)	-265(3)	2293.8(10)	32.6(10)
C(117)	13458(5)	177(4)	2008.6(12)	44.1(12)

C(121)	17485(7)	-1512(5)	793.5(19)	78(2)
C(122)	17734(7)	-1678(5)	1080(2)	82(2)
C(123)	16771(7)	-1189(6)	1275.1(18)	82(2)
C(124)	15538(7)	-545(6)	1175.5(16)	77(2)
C(125)	15265(6)	-393(5)	887.1(16)	66.4(17)
C(126)	16237(7)	-863(5)	690.7(16)	68.9(17)
C(127)	15960(12)	-687(8)	379.5(19)	111(3)
C(131)	8650(11)	2808(10)	-434(2)	153(4)
C(132)	9713(11)	3341(10)	-402(3)	168(5)
C(133)	10550(11)	3067(12)	-168(3)	150(4)
C(134)	10392(11)	2186(10)	23(3)	134(4)
C(135)	9396(10)	1604(9)	1(2)	125(3)
C(136)	8541(10)	1922(9)	-243(2)	139(4)
C(137)	7504(13)	1326(13)	-283(4)	218(7)
C(141)	6599(11)	-1766(9)	5122(2)	127(4)
C(142)	6488(14)	-2461(12)	5354(3)	164(5)
C(143)	5377(15)	-2967(12)	5397(3)	185(6)
C(144)	4461(12)	-2870(10)	5177(3)	152(5)
C(145)	4536(9)	-2181(8)	4940(2)	113(3)
C(146)	5589(10)	-1635(7)	4912.4(19)	97(2)
C(147)	5753(17)	-968(12)	4652(3)	185(6)
C(151)	1786(12)	-902(8)	5634(3)	126(3)
C(152)	2540(10)	-1004(7)	5877(3)	122(4)
C(153)	2019(12)	-598(8)	6128(2)	120(3)
C(154)	694(13)	-8(8)	6137(2)	121(3)
C(155)	-115(9)	106(8)	5902(3)	116(3)
C(156)	397(12)	-321(8)	5651(2)	124(3)
C(157)	-406(22)	-248(15)	5394(4)	270(10)

Table 5C. Bond lengths (Å) and angles (°) for (14).

Pd(1)-C(7)	2.130(4)	Pd(1)-C(8)	2.149(4)
Pd(1)-P(2)	2.3087(10)	Pd(1)-P(1)	2.3177(10)
P(1)-C(18)	1.840(4)	P(1)-C(30)	1.858(4)
P(1)-C(24)	1.865(4)	P(2)-C(38)	1.856(4)
P(2)-C(44)	1.857(4)	P(2)-C(37)	1.864(4)
O(1)-C(9)	1.242(5)	C(1)-C(2)	1.392(6)
C(1)-C(6)	1.399(6)	C(2)-C(3)	1.377(8)
C(3)-C(4)	1.380(8)	C(4)-C(5)	1.382(7)
C(5)-C(6)	1.401(6)	C(6)-C(7)	1.482(6)
C(7)-C(8)	1.433(6)	C(8)-C(9)	1.445(6)
C(9)-C(10)	1.493(5)	C(10)-C(11)	1.324(6)
C(11)-C(12)	1.468(6)	C(12)-C(17)	1.398(6)
C(12)-C(13)	1.399(6)	C(13)-C(14)	1.383(6)
C(14)-C(15)	1.389(7)	C(15)-C(16)	1.376(7)
C(16)-C(17)	1.389(6)	C(18)-C(23)	1.538(5)
C(18)-C(19)	1.540(5)	C(19)-C(20)	1.531(6)
C(20)-C(21)	1.530(6)	C(21)-C(22)	1.526(6)
C(22)-C(23)	1.523(6)	C(24)-C(29)	1.518(6)
C(24)-C(25)	1.539(5)	C(25)-C(26)	1.522(6)
C(26)-C(27)	1.509(8)	C(27)-C(28)	1.525(7)
C(28)-C(29)	1.544(6)	C(30)-C(31)	1.522(5)
C(31)-C(32)	1.402(6)	C(31)-C(36)	1.412(5)
C(32)-C(33)	1.384(6)	C(33)-C(34)	1.387(6)
C(34)-C(35)	1.380(6)	C(35)-C(36)	1.401(5)
C(36)-C(37)	1.504(5)	C(38)-C(43)	1.539(5)
C(38)-C(39)	1.541(6)	C(39)-C(40)	1.532(6)
C(40)-C(41)	1.525(7)	C(41)-C(42)	1.526(7)
C(42)-C(43)	1.521(6)	C(44)-C(49)	1.532(6)
C(44)-C(45)	1.535(6)	C(45)-C(46)	1.551(6)
C(46)-C(47)	1.510(8)	C(47)-C(48)	1.521(7)
C(48)-C(49)	1.533(6)	Pd(2)-C(56)	2.138(4)
Pd(2)-C(57)	2.156(4)	Pd(2)-P(4)	2.3078(10)
Pd(2)-P(3)	2.3166(10)	P(3)-C(67)	1.839(4)
P(3)-C(79)	1.862(4)	P(3)-C(73)	1.866(4)
P(4)-C(93)	1.849(4)	P(4)-C(87)	1.849(4)
P(4)-C(86)	1.861(4)	O(2)-C(58)	1.245(5)
C(50)-C(51)	1.392(7)	C(50)-C(55)	1.396(6)
C(51)-C(52)	1.383(8)	C(52)-C(53)	1.382(9)
C(53)-C(54)	1.384(7)	C(54)-C(55)	1.406(6)
C(55)-C(56)	1.473(6)	C(56)-C(57)	1.436(6)
C(57)-C(58)	1.458(6)	C(58)-C(59)	1.490(6)
C(59)-C(60)	1.331(6)	C(60)-C(61)	1.475(6)
C(61)-C(62)	1.397(6)	C(61)-C(66)	1.397(6)
C(62)-C(63)	1.379(6)	C(63)-C(64)	1.386(7)
C(64)-C(65)	1.384(7)	C(65)-C(66)	1.384(6)
C(67)-C(68)	1.536(5)	C(67)-C(72)	1.540(5)
C(68)-C(69)	1.527(6)	C(69)-C(70)	1.528(6)
C(70)-C(71)	1.523(6)	C(71)-C(72)	1.531(6)
C(73)-C(78)	1.525(6)	C(73)-C(74)	1.537(5)
C(74)-C(75)	1.533(5)	C(75)-C(76)	1.515(7)
C(76)-C(77)	1.524(7)	C(77)-C(78)	1.533(6)
C(79)-C(80)	1.518(5)	C(80)-C(81)	1.386(6)
C(80)-C(85)	1.411(6)	C(81)-C(82)	1.387(6)
C(82)-C(83)	1.382(6)	C(83)-C(84)	1.381(6)
C(84)-C(85)	1.399(5)	C(85)-C(86)	1.509(6)
C(87)-C(88)	1.536(6)	C(87)-C(92)	1.536(6)
C(88)-C(89)	1.530(6)	C(89)-C(90)	1.528(7)
C(90)-C(91)	1.515(8)	C(91)-C(92)	1.533(6)

C(93)-C(94)	1.528(6)	C(93)-C(98)	1.542(6)
C(94)-C(95)	1.534(7)	C(95)-C(96)	1.514(8)
C(96)-C(97)	1.507(8)	C(97)-C(98)	1.533(6)
C(111)-C(112)	1.386(7)	C(111)-C(116)	1.398(6)
C(112)-C(113)	1.403(6)	C(113)-C(114)	1.389(7)
C(114)-C(115)	1.393(7)	C(115)-C(116)	1.405(6)
C(116)-C(117)	1.499(7)	C(121)-C(122)	1.382(9)
C(121)-C(126)	1.403(8)	C(122)-C(123)	1.396(9)
C(123)-C(124)	1.385(8)	C(124)-C(125)	1.392(9)
C(125)-C(126)	1.400(8)	C(126)-C(127)	1.500(10)
C(131)-C(132)	1.388(12)	C(131)-C(136)	1.407(11)
C(132)-C(133)	1.377(12)	C(133)-C(134)	1.415(12)
C(134)-C(135)	1.366(11)	C(135)-C(136)	1.429(10)
C(136)-C(137)	1.425(12)	C(141)-C(142)	1.371(12)
C(141)-C(146)	1.405(10)	C(142)-C(143)	1.397(12)
C(143)-C(144)	1.381(12)	C(144)-C(145)	1.379(11)
C(145)-C(146)	1.373(10)	C(146)-C(147)	1.470(11)
C(151)-C(152)	1.372(11)	C(151)-C(156)	1.421(11)
C(152)-C(153)	1.381(11)	C(153)-C(154)	1.367(11)
C(154)-C(155)	1.373(11)	C(155)-C(156)	1.385(11)
C(156)-C(157)	1.459(12)		

C(7)-Pd(1)-C(8)	39.14(15)	C(7)-Pd(1)-P(2)	106.20(11)
C(8)-Pd(1)-P(2)	145.26(11)	C(7)-Pd(1)-P(1)	149.53(11)
C(8)-Pd(1)-P(1)	110.40(11)	P(2)-Pd(1)-P(1)	104.19(4)
C(18)-P(1)-C(30)	105.71(18)	C(18)-P(1)-C(24)	104.20(18)
C(30)-P(1)-C(24)	100.03(18)	C(18)-P(1)-Pd(1)	113.74(13)
C(30)-P(1)-Pd(1)	119.12(13)	C(24)-P(1)-Pd(1)	112.24(14)
C(38)-P(2)-C(44)	107.25(18)	C(38)-P(2)-C(37)	99.86(18)
C(44)-P(2)-C(37)	102.28(18)	C(38)-P(2)-Pd(1)	113.70(12)
C(44)-P(2)-Pd(1)	114.22(13)	C(37)-P(2)-Pd(1)	117.87(13)
C(2)-C(1)-C(6)	120.8(5)	C(3)-C(2)-C(1)	120.5(5)
C(2)-C(3)-C(4)	119.6(5)	C(3)-C(4)-C(5)	120.4(5)
C(4)-C(5)-C(6)	121.3(5)	C(1)-C(6)-C(5)	117.5(4)
C(1)-C(6)-C(7)	122.9(4)	C(5)-C(6)-C(7)	119.6(4)
C(8)-C(7)-C(6)	122.6(3)	C(8)-C(7)-Pd(1)	71.2(2)
C(6)-C(7)-Pd(1)	115.6(3)	C(7)-C(8)-C(9)	125.1(4)
C(7)-C(8)-Pd(1)	69.7(2)	C(9)-C(8)-Pd(1)	105.6(2)
O(1)-C(9)-C(8)	122.4(4)	O(1)-C(9)-C(10)	119.2(4)
C(8)-C(9)-C(10)	118.4(3)	C(11)-C(10)-C(9)	122.2(4)
C(10)-C(11)-C(12)	125.3(4)	C(17)-C(12)-C(13)	118.0(4)
C(17)-C(12)-C(11)	120.4(4)	C(13)-C(12)-C(11)	121.6(4)
C(14)-C(13)-C(12)	120.8(4)	C(13)-C(14)-C(15)	120.3(4)
C(16)-C(15)-C(14)	119.6(4)	C(15)-C(16)-C(17)	120.3(4)
C(16)-C(17)-C(12)	120.9(4)	C(23)-C(18)-C(19)	110.2(3)
C(23)-C(18)-P(1)	117.2(3)	C(19)-C(18)-P(1)	112.4(3)
C(20)-C(19)-C(18)	109.8(3)	C(21)-C(20)-C(19)	110.7(3)
C(22)-C(21)-C(20)	111.2(3)	C(23)-C(22)-C(21)	112.3(3)
C(22)-C(23)-C(18)	111.4(3)	C(29)-C(24)-C(25)	110.4(3)
C(29)-C(24)-P(1)	109.4(3)	C(25)-C(24)-P(1)	110.9(3)
C(26)-C(25)-C(24)	112.3(4)	C(27)-C(26)-C(25)	111.5(4)
C(26)-C(27)-C(28)	111.2(5)	C(27)-C(28)-C(29)	110.0(4)
C(24)-C(29)-C(28)	112.5(4)	C(31)-C(30)-P(1)	115.2(3)
C(32)-C(31)-C(36)	118.2(4)	C(32)-C(31)-C(30)	119.8(4)
C(36)-C(31)-C(30)	121.9(3)	C(33)-C(32)-C(31)	122.0(4)
C(32)-C(33)-C(34)	119.5(4)	C(35)-C(34)-C(33)	119.7(4)
C(34)-C(35)-C(36)	121.7(4)	C(35)-C(36)-C(31)	118.9(4)
C(35)-C(36)-C(37)	117.7(3)	C(31)-C(36)-C(37)	123.3(3)
C(36)-C(37)-P(2)	114.8(3)	C(43)-C(38)-C(39)	110.3(3)
C(43)-C(38)-P(2)	116.0(3)	C(39)-C(38)-P(2)	109.3(3)
C(40)-C(39)-C(38)	110.9(4)	C(41)-C(40)-C(39)	111.9(4)
C(40)-C(41)-C(42)	111.2(4)	C(43)-C(42)-C(41)	111.7(4)

C(42)-C(43)-C(38)	111.1(3)	C(49)-C(44)-C(45)	109.3(3)
C(49)-C(44)-P(2)	109.6(3)	C(45)-C(44)-P(2)	112.6(3)
C(44)-C(45)-C(46)	109.8(4)	C(47)-C(46)-C(45)	112.0(4)
C(46)-C(47)-C(48)	111.8(4)	C(47)-C(48)-C(49)	111.5(4)
C(44)-C(49)-C(48)	111.3(3)	C(56)-Pd(2)-C(57)	39.07(15)
C(56)-Pd(2)-P(4)	106.02(11)	C(57)-Pd(2)-P(4)	145.02(11)
C(56)-Pd(2)-P(3)	150.02(11)	C(57)-Pd(2)-P(3)	110.96(11)
P(4)-Pd(2)-P(3)	103.88(4)	C(67)-P(3)-C(79)	105.25(18)
C(67)-P(3)-C(73)	104.12(18)	C(79)-P(3)-C(73)	99.47(18)
C(67)-P(3)-Pd(2)	114.64(13)	C(79)-P(3)-Pd(2)	119.88(13)
C(73)-P(3)-Pd(2)	111.41(14)	C(93)-P(4)-C(87)	107.19(19)
C(93)-P(4)-C(86)	102.15(18)	C(87)-P(4)-C(86)	99.79(18)
C(93)-P(4)-Pd(2)	113.84(13)	C(87)-P(4)-Pd(2)	114.54(13)
C(86)-P(4)-Pd(2)	117.63(13)	C(51)-C(50)-C(55)	121.1(5)
C(52)-C(51)-C(50)	120.2(5)	C(53)-C(52)-C(51)	119.5(5)
C(52)-C(53)-C(54)	120.6(5)	C(53)-C(54)-C(55)	120.8(5)
C(50)-C(55)-C(54)	117.7(4)	C(50)-C(55)-C(56)	123.2(4)
C(54)-C(55)-C(56)	119.1(4)	C(57)-C(56)-C(55)	122.1(4)
C(57)-C(56)-Pd(2)	71.2(2)	C(55)-C(56)-Pd(2)	115.6(3)
C(55)-C(57)-C(58)	125.2(4)	C(56)-C(57)-Pd(2)	69.8(2)
C(58)-C(57)-Pd(2)	104.2(2)	O(2)-C(58)-C(57)	121.8(4)
O(2)-C(58)-C(59)	119.5(4)	C(57)-C(58)-C(59)	118.7(3)
C(60)-C(59)-C(58)	121.5(4)	C(59)-C(60)-C(61)	125.7(4)
C(62)-C(61)-C(66)	118.0(4)	C(62)-C(61)-C(60)	121.7(4)
C(66)-C(61)-C(60)	120.3(4)	C(63)-C(62)-C(61)	120.9(4)
C(62)-C(63)-C(64)	120.7(4)	C(65)-C(64)-C(63)	119.1(4)
C(66)-C(65)-C(64)	120.5(4)	C(65)-C(66)-C(61)	120.9(4)
C(68)-C(67)-C(72)	110.3(3)	C(68)-C(67)-P(3)	113.3(3)
C(72)-C(67)-P(3)	115.7(3)	C(69)-C(68)-C(67)	110.0(3)
C(68)-C(69)-C(70)	111.4(3)	C(71)-C(70)-C(69)	111.5(3)
C(70)-C(71)-C(72)	111.9(3)	C(71)-C(72)-C(67)	110.5(3)
C(78)-C(73)-C(74)	111.0(3)	C(78)-C(73)-P(3)	109.3(3)
C(74)-C(73)-P(3)	111.3(3)	C(75)-C(74)-C(73)	111.8(3)
C(76)-C(75)-C(74)	112.2(4)	C(75)-C(76)-C(77)	110.9(4)
C(76)-C(77)-C(78)	110.4(4)	C(73)-C(78)-C(77)	112.0(4)
C(80)-C(79)-P(3)	115.9(3)	C(81)-C(80)-C(85)	118.4(4)
C(81)-C(80)-C(79)	119.5(4)	C(85)-C(80)-C(79)	122.0(4)
C(80)-C(81)-C(82)	122.3(4)	C(83)-C(82)-C(81)	119.1(4)
C(84)-C(83)-C(82)	119.8(4)	C(83)-C(84)-C(85)	121.5(4)
C(84)-C(85)-C(80)	118.8(4)	C(84)-C(85)-C(86)	118.0(4)
C(80)-C(85)-C(86)	123.3(3)	C(85)-C(86)-P(4)	114.9(3)
C(88)-C(87)-C(92)	110.2(4)	C(88)-C(87)-P(4)	109.9(3)
C(92)-C(87)-P(4)	116.4(3)	C(89)-C(88)-C(87)	111.7(4)
C(90)-C(89)-C(88)	111.5(4)	C(91)-C(90)-C(89)	111.6(4)
C(90)-C(91)-C(92)	111.5(4)	C(91)-C(92)-C(87)	110.8(4)
C(94)-C(93)-C(98)	108.4(3)	C(94)-C(93)-P(4)	113.8(3)
C(98)-C(93)-P(4)	110.0(3)	C(93)-C(94)-C(95)	110.3(4)
C(96)-C(95)-C(94)	111.9(4)	C(97)-C(96)-C(95)	112.5(4)
C(96)-C(97)-C(98)	111.1(4)	C(97)-C(98)-C(93)	110.9(4)
C(112)-C(111)-C(116)	121.6(4)	C(111)-C(112)-C(113)	119.9(5)
C(114)-C(113)-C(112)	118.8(5)	C(113)-C(114)-C(115)	121.5(4)
C(114)-C(115)-C(116)	119.9(5)	C(111)-C(116)-C(115)	118.3(5)
C(111)-C(116)-C(117)	121.3(4)	C(115)-C(116)-C(117)	120.3(5)
C(122)-C(121)-C(126)	120.5(7)	C(121)-C(122)-C(123)	121.3(7)
C(124)-C(123)-C(122)	118.6(7)	C(123)-C(124)-C(125)	120.5(7)
C(124)-C(125)-C(126)	121.1(6)	C(125)-C(126)-C(121)	117.9(7)
C(125)-C(126)-C(127)	121.4(7)	C(121)-C(126)-C(127)	120.7(7)
C(132)-C(131)-C(136)	119.0(10)	C(133)-C(132)-C(131)	119.5(12)
C(132)-C(133)-C(134)	119.7(12)	C(135)-C(134)-C(133)	123.9(11)
C(134)-C(135)-C(136)	114.5(10)	C(131)-C(136)-C(137)	119.6(11)
C(131)-C(136)-C(135)	123.1(10)	C(137)-C(136)-C(135)	117.3(12)
C(142)-C(141)-C(146)	117.2(10)	C(141)-C(142)-C(143)	122.9(11)

C(144)-C(143)-C(142)	117.3(12)	C(145)-C(144)-C(143)	121.1(11)
C(146)-C(145)-C(144)	119.8(10)	C(145)-C(146)-C(141)	121.1(9)
C(145)-C(146)-C(147)	120.7(10)	C(141)-C(146)-C(147)	118.1(10)
C(152)-C(151)-C(156)	115.7(10)	C(151)-C(152)-C(153)	123.9(10)
C(154)-C(153)-C(152)	119.4(10)	C(153)-C(154)-C(155)	119.1(10)
C(154)-C(155)-C(156)	121.6(9)	C(155)-C(156)-C(151)	120.2(9)
C(155)-C(156)-C(157)	124.6(13)	C(151)-C(156)-C(157)	115.2(13)

Table 5D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (14).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	12.55(14)	17.81(14)	18.15(14)	-0.96(11)	0.79(10)	-3.87(10)
P(1)	14.0(4)	17.3(5)	22.1(5)	-0.9(4)	1.3(4)	-3.0(4)
P(2)	13.5(4)	21.6(5)	18.5(5)	-0.7(4)	0.0(4)	-5.2(4)
O(1)	15.3(14)	30.7(16)	37.5(17)	-5.1(13)	-2.2(12)	-3.0(12)
C(1)	28(2)	39(2)	26(2)	-2.6(19)	2.1(18)	-10.3(19)
C(2)	45(3)	60(3)	24(2)	-12(2)	8(2)	-21(3)
C(3)	48(3)	77(4)	18(2)	5(2)	-1(2)	-26(3)
C(4)	39(3)	58(3)	31(3)	17(2)	-7(2)	-14(2)
C(5)	30(2)	37(2)	27(2)	3.6(19)	-3.7(18)	-10.2(19)
C(6)	21.3(19)	29(2)	22(2)	4.1(16)	1.5(15)	-11.1(16)
C(7)	20.3(19)	20.4(19)	19.5(19)	-1.4(15)	1.7(15)	-7.6(15)
C(8)	16.9(18)	20.5(19)	24(2)	-1.1(15)	4.3(15)	-6.1(15)
C(9)	16.7(18)	18.1(18)	24(2)	1.1(15)	2.9(15)	-7.3(15)
C(10)	17.7(18)	23.1(19)	22.7(19)	-2.3(16)	0.0(15)	-6.0(15)
C(11)	20.4(19)	23(2)	25(2)	1.6(16)	0.2(16)	-7.6(16)
C(12)	24(2)	22.8(19)	19.2(19)	-0.1(15)	-0.5(15)	-5.8(16)
C(13)	28(2)	27(2)	28(2)	-3.6(17)	2.7(17)	-12.2(18)
C(14)	31(2)	30(2)	29(2)	1.8(18)	7.9(18)	-3.8(18)
C(15)	41(3)	23(2)	30(2)	-1.9(18)	5(2)	-0.1(19)
C(16)	38(3)	25(2)	38(3)	-5.3(19)	-6(2)	-10.0(19)
C(17)	25(2)	26(2)	36(2)	-3.5(18)	-3.7(18)	-7.7(17)
C(18)	14.9(18)	20.8(19)	24(2)	2.3(15)	0.1(15)	-3.3(15)
C(19)	15.5(18)	21.9(19)	25(2)	0.2(16)	0.5(15)	-3.9(15)
C(20)	21(2)	30(2)	30(2)	-7.1(18)	2.5(17)	-7.2(17)
C(21)	26(2)	38(2)	23(2)	-3.1(18)	-2.1(17)	-7.0(19)
C(22)	19(2)	36(2)	26(2)	3.8(18)	-1.5(16)	-3.1(17)
C(23)	17.8(19)	24(2)	28(2)	4.2(17)	-1.8(16)	-4.0(16)
C(24)	20.5(19)	18.5(19)	31(2)	-4.2(16)	5.1(16)	-3.0(15)
C(25)	18.3(19)	24(2)	35(2)	-6.1(18)	3.2(17)	-1.9(16)
C(26)	23(2)	34(3)	57(3)	-12(2)	11(2)	-1.6(19)
C(27)	39(3)	61(4)	56(4)	-32(3)	22(3)	-9(3)
C(28)	40(3)	59(3)	53(3)	-35(3)	13(2)	-15(3)
C(29)	27(2)	38(3)	40(3)	-16(2)	6.9(19)	-8.1(19)
C(30)	17.8(18)	19.5(19)	28(2)	4.1(16)	4.1(15)	-4.1(15)
C(31)	17.3(18)	20.5(18)	20.6(19)	0.6(15)	1.3(14)	-9.4(15)
C(32)	21(2)	31(2)	25(2)	5.8(17)	-3.0(16)	-14.4(17)
C(33)	32(2)	33(2)	19.3(19)	-0.8(17)	2.6(16)	-19.4(18)
C(34)	25(2)	30(2)	27(2)	-6.7(17)	9.0(17)	-12.4(17)
C(35)	18.2(19)	26(2)	25(2)	-0.6(16)	1.4(15)	-8.3(16)
C(36)	16.9(18)	20.4(18)	21.5(19)	-0.5(15)	0.5(14)	-8.0(15)
C(37)	19.5(19)	29(2)	20.1(19)	1.8(16)	0.2(15)	-9.9(16)
C(38)	18.0(18)	27(2)	17.7(18)	1.4(15)	-0.7(14)	-8.4(16)
C(39)	26(2)	31(2)	27(2)	-4.0(18)	-0.8(17)	-5.3(18)
C(40)	36(3)	41(3)	29(2)	-10(2)	2.8(19)	-7(2)
C(41)	45(3)	54(3)	29(2)	-7(2)	-5(2)	-23(2)
C(42)	26(2)	58(3)	26(2)	-1(2)	-6.4(18)	-14(2)
C(43)	21(2)	42(3)	25(2)	-1.1(19)	-4.2(16)	-10.1(18)
C(44)	15.1(18)	22.6(19)	24(2)	-3.5(16)	1.9(15)	-4.6(15)
C(45)	35(2)	27(2)	29(2)	0.2(18)	3.9(19)	0.5(19)
C(46)	48(3)	27(2)	47(3)	2(2)	-1(2)	9(2)
C(47)	52(3)	26(2)	53(3)	-9(2)	6(3)	-3(2)

C(48)	31(2)	32(2)	34(2)	-14.2(19)	3.3(19)	-7.0(19)
C(49)	22(2)	26(2)	25(2)	-7.4(17)	2.2(16)	-7.2(16)
Pd(2)	13.15(14)	17.65(14)	19.33(15)	-1.41(11)	1.29(10)	-4.59(11)
P(3)	14.7(4)	16.7(5)	21.7(5)	-0.7(4)	2.1(4)	-3.0(4)
P(4)	14.5(4)	21.7(5)	20.4(5)	-2.4(4)	0.4(4)	-6.0(4)
O(2)	15.6(14)	32.6(16)	37.1(17)	-7.2(13)	-1.9(12)	-5.5(12)
C(50)	31(2)	42(3)	30(2)	-5(2)	2.3(19)	-9(2)
C(51)	48(3)	66(4)	37(3)	-18(3)	11(2)	-21(3)
C(52)	49(3)	87(5)	23(2)	-4(3)	2(2)	-30(3)
C(53)	39(3)	81(4)	24(2)	14(3)	-7(2)	-20(3)
C(54)	33(2)	46(3)	26(2)	4(2)	-1.1(19)	-13(2)
C(55)	25(2)	37(2)	21(2)	1.8(18)	2.8(16)	-14.8(18)
C(56)	19.5(19)	22.6(19)	19.7(19)	0.6(15)	3.3(15)	-7.8(15)
C(57)	18.3(18)	23.1(19)	20.4(19)	-2.7(15)	7.1(15)	-6.5(15)
C(58)	16.3(18)	25(2)	25(2)	1.8(16)	4.4(15)	-10.0(15)
C(59)	18.6(19)	21.5(19)	29(2)	0.9(16)	3.3(16)	-9.0(15)
C(60)	22(2)	25(2)	29(2)	-0.6(17)	3.0(16)	-9.2(16)
C(61)	27(2)	23(2)	24(2)	-1.0(16)	2.3(16)	-10.5(17)
C(62)	30(2)	36(2)	42(3)	-13(2)	9(2)	-18(2)
C(63)	34(2)	34(2)	45(3)	-8(2)	13(2)	-11(2)
C(64)	40(3)	27(2)	35(3)	-5.6(19)	7(2)	-7(2)
C(65)	41(3)	27(2)	34(2)	-5.1(19)	-6(2)	-12(2)
C(66)	27(2)	30(2)	31(2)	-2.0(18)	-5.0(18)	-9.5(18)
C(67)	14.8(17)	20.3(18)	22.4(19)	0.3(15)	-0.2(14)	-4.3(15)
C(68)	18.8(18)	18.5(18)	23.2(19)	2.4(15)	1.9(15)	-3.1(15)
C(69)	23(2)	26(2)	26(2)	-5.3(17)	2.0(16)	-5.5(16)
C(70)	26(2)	34(2)	23(2)	-2.5(18)	-1.3(16)	-10.2(18)
C(71)	20(2)	30(2)	28(2)	3.0(17)	-2.7(16)	-6.4(17)
C(72)	19.3(19)	22(2)	29(2)	0.6(16)	-3.3(16)	-3.0(16)
C(73)	18.9(19)	19.5(19)	28(2)	-2.8(16)	4.9(16)	-1.3(15)
C(74)	20(2)	21.0(19)	32(2)	-6.3(17)	5.5(17)	-2.1(16)
C(75)	29(2)	26(2)	46(3)	-8(2)	13(2)	0.6(18)
C(76)	43(3)	43(3)	45(3)	-19(2)	19(2)	-2(2)
C(77)	41(3)	38(3)	42(3)	-21(2)	6(2)	-5(2)
C(78)	29(2)	32(2)	44(3)	-16(2)	4(2)	-5.1(19)
C(79)	19.1(19)	20.4(19)	26(2)	2.4(16)	5.1(15)	-5.8(15)
C(80)	16.9(18)	18.9(18)	25(2)	0.4(15)	3.8(15)	-9.0(15)
C(81)	23(2)	35(2)	21(2)	2.6(17)	-0.2(16)	-16.1(18)
C(82)	28(2)	38(2)	24(2)	-6.4(18)	4.6(17)	-17.9(19)
C(83)	23(2)	30(2)	30(2)	-10.4(18)	9.4(17)	-10.9(17)
C(84)	16.4(18)	27(2)	31(2)	-1.2(17)	0.5(16)	-7.4(16)
C(85)	21.5(19)	22.4(19)	19.6(19)	-2.0(15)	3.1(15)	-11.3(16)
C(86)	22.1(19)	24(2)	23(2)	-1.7(16)	1.5(15)	-11.7(16)
C(87)	20.5(19)	32(2)	22(2)	0.2(17)	0.8(15)	-10.1(17)
C(88)	29(2)	35(2)	27(2)	-8.0(18)	2.2(18)	-9.1(19)
C(89)	42(3)	48(3)	33(3)	-16(2)	2(2)	-13(2)
C(90)	49(3)	66(4)	28(2)	-13(2)	-2(2)	-32(3)
C(91)	28(2)	70(4)	26(2)	-5(2)	-4.1(19)	-22(2)
C(92)	22(2)	51(3)	23(2)	-4(2)	-0.3(17)	-14(2)
C(93)	15.6(18)	25(2)	26(2)	-1.4(16)	0.7(15)	-4.2(15)
C(94)	29(2)	32(2)	39(3)	4(2)	-3(2)	-1.9(19)
C(95)	48(3)	36(3)	52(3)	3(2)	-1(3)	6(2)
C(96)	56(3)	23(2)	71(4)	-7(3)	4(3)	0(2)
C(97)	30(2)	30(2)	49(3)	-12(2)	5(2)	-5.3(19)
C(98)	19.5(19)	24(2)	36(2)	-6.0(18)	1.9(17)	-7.9(16)
C(111)	26(2)	27(2)	53(3)	0(2)	-12(2)	-6.3(18)
C(112)	27(2)	35(3)	59(3)	4(2)	-10(2)	-1(2)
C(113)	25(2)	34(3)	70(3)	2(2)	1(2)	2.0(19)
C(114)	25(2)	31(3)	77(4)	-5(2)	4(2)	-8(2)
C(115)	24(2)	30(2)	65(3)	-10(2)	1(2)	-6.5(18)
C(116)	19(2)	23(2)	54(3)	-3(2)	-3.9(19)	-1.7(16)
C(117)	34(3)	44(3)	54(3)	3(2)	-4(2)	-9(2)

C(121)	52(4)	39(3)	141(6)	-8(4)	12(4)	-7(3)
C(122)	50(4)	41(3)	153(7)	26(4)	-10(4)	-15(3)
C(123)	71(4)	59(4)	113(6)	41(4)	-5(4)	-21(3)
C(124)	60(4)	69(5)	98(5)	32(4)	8(4)	-17(3)
C(125)	43(3)	51(4)	100(5)	12(4)	1(3)	-7(3)
C(126)	65(4)	42(3)	102(5)	-2(3)	-1(3)	-18(3)
C(127)	148(9)	92(7)	91(5)	-16(5)	-10(6)	-18(6)
C(131)	102(7)	201(11)	115(8)	-70(6)	-25(7)	78(7)
C(132)	74(6)	205(10)	187(11)	-59(9)	18(7)	64(6)
C(133)	79(6)	206(12)	149(11)	-65(8)	30(6)	17(8)
C(134)	80(6)	166(11)	151(10)	-88(7)	-7(7)	9(6)
C(135)	89(6)	151(8)	120(7)	-80(6)	-26(5)	30(5)
C(136)	93(6)	159(9)	156(9)	-114(6)	-44(6)	31(6)
C(137)	130(11)	271(16)	275(18)	-186(14)	-18(10)	-30(10)
C(141)	132(8)	123(9)	128(8)	-43(6)	-45(7)	-16(7)
C(142)	147(10)	183(14)	130(9)	-2(8)	-41(9)	35(9)
C(143)	139(11)	166(12)	195(12)	38(10)	51(9)	61(9)
C(144)	97(8)	108(9)	240(15)	-8(8)	69(8)	-8(7)
C(145)	74(5)	105(7)	165(9)	-52(6)	7(6)	-14(5)
C(146)	116(7)	78(6)	95(6)	-5(5)	-2(5)	-15(5)
C(147)	268(18)	148(12)	120(9)	33(8)	21(10)	-22(11)
C(151)	143(8)	70(6)	181(10)	-30(7)	54(7)	-53(6)
C(152)	89(6)	50(5)	230(12)	2(7)	21(6)	-30(5)
C(153)	137(8)	72(6)	154(8)	48(6)	-19(7)	-50(5)
C(154)	141(8)	88(7)	141(8)	20(6)	33(6)	-54(6)
C(155)	66(5)	83(6)	200(10)	4(7)	21(5)	-27(5)
C(156)	148(8)	79(7)	156(8)	15(6)	-32(7)	-52(6)
C(157)	378(22)	201(17)	254(15)	38(14)	-184(17)	-119(16)

Table 5E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (14).

	x	y	z	U
H(1)	8587	3724	629	36
H(2)	7944	3718	160	49
H(3)	6282	5144	-45	55
H(4)	5250	6586	220	52
H(5)	5916	6631	684	37
H(7)	7209(41)	5881(26)	1093(9)	24
H(8)	9495(40)	4098(30)	1010(8)	24
H(10)	7826	6011	1516	25
H(11)	10348	6004	1759	27
H(13)	6782	6770	1910	32
H(14)	5674	8217	2165	37
H(15)	6861	9516	2293	39
H(16)	9200	9289	2195	40
H(17)	10335	7824	1947	34
H(18)	9891	2914	1816	24
H(19A)	7931	4306	1903	25
H(19B)	7458	3514	2148	25
H(20A)	9999	4253	2151	32
H(20B)	8703	4682	2349	32
H(21A)	10401	3334	2604	35
H(21B)	8976	2945	2592	35
H(22A)	11346	2213	2248	34
H(22B)	10747	1475	2487	34
H(23A)	8812	1503	2215	28
H(23B)	10147	1123	2023	28
H(24)	9508	623	1550	28
H(25A)	10599	2374	1275	32
H(25B)	11162	1696	1563	32
H(26A)	12610	1107	1174	46
H(26B)	12008	126	1325	46
H(27A)	11815	109	835	61
H(27B)	10981	1354	813	61
H(28A)	9982	-441	1085	58
H(28B)	9402	213	795	58
H(29A)	8529	1812	1029	41
H(29B)	7928	837	1182	41
H(32	6513	1740	2302	30
H(33	4707	2678	2564	31
H(34	2706	3661	2335	31
H(35	2550	3710	1847	27
H(38	4535	4442	775	25
H(39A)	6292	2837	792	34
H(39B)	5211	2120	900	34
H(40A)	5162	3285	354	42
H(40B)	5524	1984	410	42
H(41A)	3250	1977	544	49
H(41B)	3223	2636	241	49
H(42A)	2610	4310	446	43
H(42B)	1538	3582	551	43
H(43A)	2669	3125	987	35
H(43B)	2273	4428	934	35
H(44)	2924	5060	1436	25

H(45A)	3167	5959	984	38
H(45B)	4491	6341	1091	38
H(46A)	2532	7806	1119	52
H(46B)	1732	7036	1309	52
H(47A)	2553	8132	1606	53
H(47B)	4078	7781	1481	53
H(48A)	2679	6393	1825	38
H(48B	4012	6801	1916	38
H(49A	5384	5726	1588	28
H(49B	4623	4957	1788	28
H(50)	3588	4167	5677	41
H(51)	3074	3848	5218	58
H(52)	1365	5088	4961	61
H(53)	177	6650	5164	58
H(54)	726	7010	5616	42
H(56)	2023(41)	6581(24)	6032(9)	24
H(57)	4406(39)	4783(29)	6042(9)	24
H(59)	2543	6981	6447	27
H(60)	4971	7051	6720	29
H(62)	1325	7863	6802	41
H(63)	127	9313	7042	44
H(64)	1287	10517	7232	41
H(65)	3671	10256	7176	40
H(66)	4882	8808	6935	34
H(67)	4612	4090	6874	23
H(68A)	2635	5509	6918	25
H(68B)	2138	4825	7183	25
H(69A)	3324	6092	7348	30
H(69B)	4643	5611	7162	30
H(70A)	5061	4888	7630	32
H(70B	3654	4467	7640	32
H(71A	5456	2973	7574	31
H(71B)	6033	3613	7311	31
H(72A)	3504	2863	7316	29
H(72B)	4846	2383	7136	29
H(73)	4297	1633	6707	27
H(74A)	5415	3215	6363	30
H(74B)	5945	2711	6671	30
H(75A)	7428	1882	6307	41
H(75B)	6829	998	6502	41
H(76A)	6664	639	6030	53
H(76B)	5836	1865	5952	53
H(77A)	4811	274	6310	48
H(77B)	4258	710	5998	48
H(78A)	3376	2472	6149	42
H(78B)	2746	1608	6345	42
H(81)	1135	3169	7392	30
H(82)	-764	4221	7607	34
H(83)	-2697	5052	7336	32
H(84)	-2748	4752	6860	29
H(87)	-573	4968	5797	29
H(88A)	1123	3344	5867	36
H(88B)	-7	2709	5995	36
H(89A)	81	3593	5421	47
H(89B)	365	2320	5521	47
H(90A)	-1900	2961	5329	53
H(90B)	-1947	2454	5647	53
H(91A)	-3587	4095	5598	48
H(91B)	-2452	4734	5475	48
H(92A)	-2526	3807	6047	38
H(92B)	-2862	5088	5954	38
H(93)	-2276	5877	6430	27

H(94A)	-1983	6610	5961	41
H(94B)	-711	7074	6063	41
H(95A)	-2710	8495	6048	57
H(95B)	-3510	7764	6251	57
H(96A)	-1258	8655	6411	62
H(96B)	-2808	8997	6523	62
H(97A)	-2618	7336	6782	44
H(97B)	-1336	7832	6861	44
H(98A)	-598	5943	6780	31
H(98B)	124	6676	6561	31

Table 6A. Crystal data, structure solution and refinement for (18).

Identification code	extis1
Chemical formula	$C_{49}H_{42}OP_2Pd$
Formula weight	815.17
Temperature	160(2) K
Radiation and wavelength	synchrotron, 0.68890 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 8.6608(2) Å $\alpha = 90^\circ$
	b = 32.6232(8) Å $\beta = 95.309(2)^\circ$
	c = 13.8956(3) Å $\gamma = 90^\circ$
Volume	3909.26(16) $Å^3$
Z	4
Density (calculated)	1.385 g/cm^3
Absorption coefficient μ	0.594 mm^{-1}
F(000)	1680
Reflections for cell refinement	15976 (θ range 1.55 to 27.24°)
Crystal colour	yellow
Crystal size	0.22 × 0.12 × 0.06 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.21 to 27.24°
Index ranges	$-9 \le h \le 10$, $-40 \le k \le 30$, $-18 \le \ell \le 17$
Intensity decay	50%
Reflections collected	20772
Independent reflections	8326 (R_{int} = 0.0264)
Reflections with I>2σ(I)	7093
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.972 and 0.937
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0479, 0.0000
Data / restraints / parameters	8326 / 0 / 485
Final R indices [I>2σ(I)]	R1 = 0.0264, wR2 = 0.0712
R indices (all data)	R1 = 0.0326, wR2 = 0.0778
Goodness-of-fit on F^2	1.051
Extinction coefficient	0.0009(2)
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	0.478 and -0.671 $eÅ^{-3}$

The Crystal Structure of [*o*-$C_6H_4(CH_2PPh_2)_2Pd(dba)$] (18)

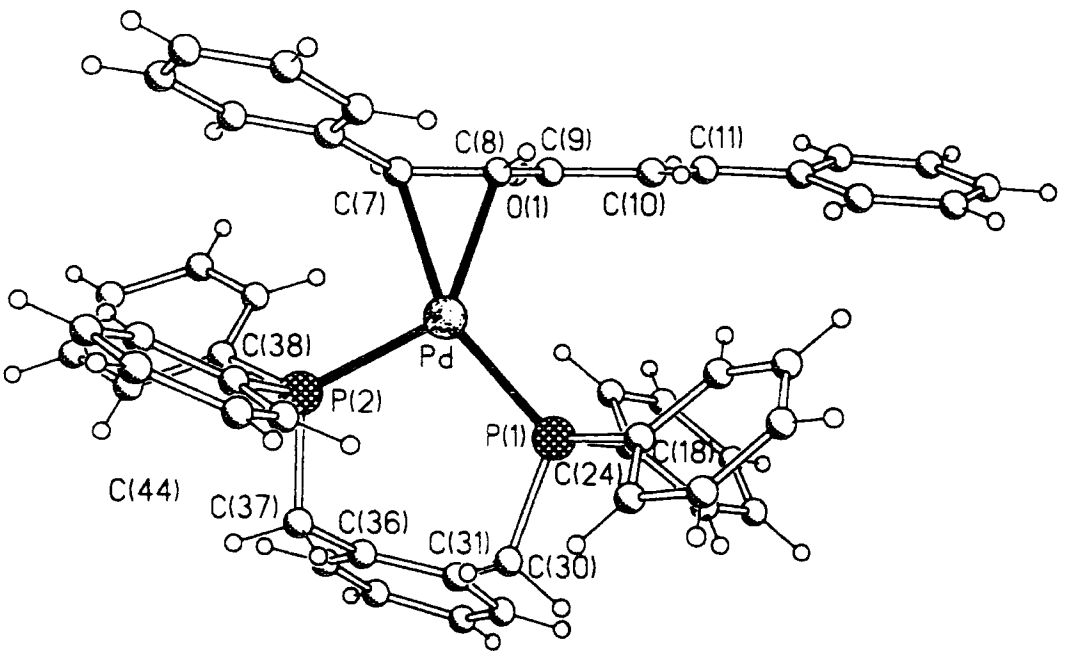


Table 6B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (18). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	2592.78(15)	1297.76(4)	9459.73(10)	16.25(6)
O(1)	5121.8(17)	1294.9(4)	7788.0(11)	29.5(3)
C(1)	6391(2)	1381.0(7)	11404.6(16)	31.2(5)
C(2)	6937(3)	1297.0(8)	12350.6(18)	42.1(6)
C(3)	6659(3)	924.3(9)	12760.9(18)	46.7(6)
C(4)	5833(3)	630.5(8)	12214.3(18)	43.9(6)
C(5)	5279(2)	711.3(7)	11269.9(16)	32.9(5)
C(6)	5541(2)	1087.9(6)	10838.2(14)	22.6(4)
C(7)	5011(2)	1184.9(6)	9826.0(14)	21.0(4)
C(8)	4455(2)	895.5(6)	9118.5(14)	22.2(4)
C(9)	4562(2)	978.4(6)	8096.6(14)	23.7(4)
C(10)	3950(2)	650.7(6)	7419.0(15)	27.7(4)
C(11)	4017(2)	680.8(6)	6469.5(15)	29.6(5)
C(12)	3388(2)	393.2(6)	5722.0(15)	30.4(5)
C(13)	2395(3)	75.1(7)	5912.1(17)	34.8(5)
C(14)	1788(3)	-184.8(7)	5186.9(18)	42.1(6)
C(15)	2167(3)	-123.5(8)	4245.8(18)	45.3(6)
C(16)	3149(3)	187.8(8)	4043.9(17)	45.2(6)
C(17)	3764(3)	446.8(7)	4779.5(16)	37.4(5)
P(1)	174.3(5)	1177.56(14)	8664.6(3)	16.35(10)
P(2)	2212.6(5)	1823.21(15)	10499.4(3)	19.21(11)
C(18)	-573(2)	658.1(5)	8793.8(14)	20.0(4)
C(19)	-1606(2)	556.3(6)	9463.2(16)	30.9(5)
C(20)	-2067(3)	150.6(7)	9562.1(19)	41.2(6)
C(21)	-1513(3)	-153.1(7)	9005.4(19)	40.2(6)
C(22)	-490(3)	-55.4(7)	8343.8(19)	43.3(6)
C(23)	-27(3)	346.2(6)	8237.8(16)	34.6(5)
C(24)	-48(2)	1247.8(5)	7355.4(13)	19.0(4)
C(25)	-1412(2)	1133.5(6)	6811.6(14)	22.9(4)
C(26)	-1596(2)	1206.3(6)	5819.7(15)	27.2(4)
C(27)	-418(3)	1395.4(7)	5379.5(15)	31.2(5)
C(28)	938(3)	1509.7(7)	5913.0(15)	31.7(5)
C(29)	1130(2)	1437.6(6)	6904.4(14)	23.7(4)
C(30)	-1430(2)	1503.3(5)	9016.5(13)	18.1(4)
C(31)	-1146(2)	1946.0(6)	8776.3(13)	18.9(4)
C(32)	-1758(2)	2096.2(6)	7881.5(14)	24.5(4)
C(33)	-1448(3)	2491.5(6)	7588.9(15)	31.3(5)
C(34)	-502(3)	2744.8(6)	8182.6(17)	32.9(5)
C(35)	65(2)	2606.0(6)	9086.2(16)	28.4(5)
C(36)	-254(2)	2212.2(6)	9404.7(14)	20.0(4)
C(37)	312(2)	2085.6(6)	10419.2(14)	22.2(4)
C(38)	3562(2)	2254.2(6)	10507.3(15)	24.1(4)
C(39)	4598(2)	2269.5(6)	9798.8(16)	29.1(5)
C(40)	5680(3)	2586.1(7)	9798.0(19)	37.7(5)
C(41)	5713(3)	2888.6(7)	10491(2)	42.1(6)
C(42)	4663(3)	2886.1(7)	11180.1(19)	40.5(6)
C(43)	3587(2)	2572.1(6)	11186.4(16)	31.9(5)
C(44)	2284(2)	1627.6(6)	11738.4(14)	24.5(4)
C(45)	3319(3)	1754.8(7)	12499.7(15)	34.8(5)
C(46)	3260(3)	1580.2(9)	13413.0(17)	45.2(6)
C(47)	2202(3)	1280.7(7)	13558.0(18)	42.2(6)

C(48)	1179(3)	1145.5(7)	12802.9(17)	37.4(5)
C(49)	1237(3)	1317.2(6)	11895.8(16)	30.9(5)

Table 6C. Bond lengths (Å) and angles (°) for (18).

Pd-C(7)	2.1407(19)	Pd-C(8)	2.1654(19)
Pd-P(2)	2.2852(5)	Pd-P(1)	2.3094(5)
O(1)-C(9)	1.234(2)	C(1)-C(2)	1.383(3)
C(1)-C(6)	1.403(3)	C(2)-C(3)	1.374(3)
C(3)-C(4)	1.381(4)	C(4)-C(5)	1.380(3)
C(5)-C(6)	1.395(3)	C(6)-C(7)	1.473(3)
C(7)-C(8)	1.415(3)	C(8)-C(9)	1.457(3)
C(9)-C(10)	1.489(3)	C(10)-C(11)	1.330(3)
C(11)-C(12)	1.467(3)	C(12)-C(13)	1.389(3)
C(12)-C(17)	1.390(3)	C(13)-C(14)	1.383(3)
C(14)-C(15)	1.392(3)	C(15)-C(16)	1.370(4)
C(16)-C(17)	1.394(3)	P(1)-C(24)	1.8260(19)
P(1)-C(18)	1.8287(18)	P(1)-C(30)	1.8503(18)
P(2)-C(38)	1.828(2)	P(2)-C(44)	1.832(2)
P(2)-C(37)	1.8495(19)	C(18)-C(23)	1.387(3)
C(18)-C(19)	1.389(3)	C(19)-C(20)	1.393(3)
C(20)-C(21)	1.371(3)	C(21)-C(22)	1.372(3)
C(22)-C(23)	1.382(3)	C(24)-C(29)	1.391(3)
C(24)-C(25)	1.393(3)	C(25)-C(26)	1.393(3)
C(26)-C(27)	1.382(3)	C(27)-C(28)	1.381(3)
C(28)-C(29)	1.392(3)	C(30)-C(31)	1.508(2)
C(31)-C(32)	1.395(3)	C(31)-C(36)	1.411(3)
C(32)-C(33)	1.386(3)	C(33)-C(34)	1.382(3)
C(34)-C(35)	1.382(3)	C(35)-C(36)	1.395(3)
C(36)-C(37)	1.507(3)	C(38)-C(39)	1.393(3)
C(38)-C(43)	1.401(3)	C(39)-C(40)	1.395(3)
C(40)-C(41)	1.378(3)	C(41)-C(42)	1.380(3)
C(42)-C(43)	1.386(3)	C(44)-C(45)	1.385(3)
C(44)-C(49)	1.390(3)	C(45)-C(46)	1.396(3)
C(46)-C(47)	1.368(4)	C(47)-C(48)	1.381(4)
C(48)-C(49)	1.385(3)		

C(7)-Pd-C(8)	38.37(7)	C(7)-Pd-P(2)	100.00(5)
C(8)-Pd-P(2)	138.32(5)	C(7)-Pd-P(1)	155.30(5)
C(8)-Pd-P(1)	116.94(5)	P(2)-Pd-P(1)	104.623(17)
C(2)-C(1)-C(6)	120.9(2)	C(3)-C(2)-C(1)	120.8(2)
C(2)-C(3)-C(4)	119.2(2)	C(5)-C(4)-C(3)	120.5(2)
C(4)-C(5)-C(6)	121.4(2)	C(5)-C(6)-C(1)	117.17(19)
C(5)-C(6)-C(7)	123.46(19)	C(1)-C(6)-C(7)	119.35(19)
C(8)-C(7)-C(6)	125.17(18)	C(8)-C(7)-Pd	71.76(11)
C(6)-C(7)-Pd	118.39(13)	C(7)-C(8)-C(9)	120.33(18)
C(7)-C(8)-Pd	69.87(11)	C(9)-C(8)-Pd	102.52(12)
O(1)-C(9)-C(8)	123.81(18)	O(1)-C(9)-C(10)	120.61(18)
C(8)-C(9)-C(10)	115.58(18)	C(11)-C(10)-C(9)	121.9(2)
C(10)-C(11)-C(12)	127.4(2)	C(13)-C(12)-C(17)	118.5(2)
C(13)-C(12)-C(11)	122.7(2)	C(17)-C(12)-C(11)	118.8(2)
C(14)-C(13)-C(12)	121.3(2)	C(13)-C(14)-C(15)	119.3(2)
C(16)-C(15)-C(14)	120.3(2)	C(15)-C(16)-C(17)	120.1(2)
C(12)-C(17)-C(16)	120.5(2)	C(24)-P(1)-C(18)	102.03(8)
C(24)-P(1)-C(30)	100.29(8)	C(18)-P(1)-C(30)	103.01(8)
C(24)-P(1)-Pd	117.57(6)	C(18)-P(1)-Pd	115.08(6)
C(30)-P(1)-Pd	116.49(6)	C(38)-P(2)-C(44)	107.24(9)
C(38)-P(2)-C(37)	102.08(9)	C(44)-P(2)-C(37)	99.81(9)
C(38)-P(2)-Pd	116.84(7)	C(44)-P(2)-Pd	109.79(6)
C(37)-P(2)-Pd	119.25(6)	C(23)-C(18)-C(19)	118.12(18)
C(23)-C(18)-P(1)	118.91(15)	C(19)-C(18)-P(1)	122.88(15)
C(18)-C(19)-C(20)	120.1(2)	C(21)-C(20)-C(19)	120.8(2)
C(20)-C(21)-C(22)	119.5(2)	C(21)-C(22)-C(23)	120.2(2)

C(22)-C(23)-C(18)	121.3(2)	C(29)-C(24)-C(25)	119.68(17)
C(29)-C(24)-P(1)	119.37(14)	C(25)-C(24)-P(1)	120.86(14)
C(24)-C(25)-C(26)	120.30(18)	C(27)-C(26)-C(25)	119.5(2)
C(28)-C(27)-C(26)	120.58(19)	C(27)-C(28)-C(29)	120.21(19)
C(24)-C(29)-C(28)	119.72(19)	C(31)-C(30)-P(1)	110.49(12)
C(32)-C(31)-C(36)	118.46(17)	C(32)-C(31)-C(30)	118.56(17)
C(36)-C(31)-C(30)	122.95(17)	C(33)-C(32)-C(31)	121.38(19)
C(34)-C(33)-C(32)	120.10(19)	C(35)-C(34)-C(33)	119.21(19)
C(34)-C(35)-C(36)	121.7(2)	C(35)-C(36)-C(31)	118.95(18)
C(35)-C(36)-C(37)	119.51(17)	C(31)-C(36)-C(37)	121.51(17)
C(36)-C(37)-P(2)	113.19(13)	C(39)-C(38)-C(43)	118.62(18)
C(39)-C(38)-P(2)	118.46(15)	C(43)-C(38)-P(2)	122.92(16)
C(38)-C(39)-C(40)	120.2(2)	C(41)-C(40)-C(39)	120.0(2)
C(40)-C(41)-C(42)	120.5(2)	C(41)-C(42)-C(43)	119.7(2)
C(42)-C(43)-C(38)	120.8(2)	C(45)-C(44)-C(49)	118.91(19)
C(45)-C(44)-P(2)	125.22(17)	C(49)-C(44)-P(2)	115.83(16)
C(44)-C(45)-C(46)	119.8(2)	C(47)-C(46)-C(45)	120.4(2)
C(46)-C(47)-C(48)	120.5(2)	C(47)-C(48)-C(49)	119.2(2)
C(48)-C(49)-C(44)	121.1(2)		

Table 6D. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (18).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	14.53(9)	18.15(8)	16.01(9)	-3.00(5)	1.12(5)	-0.46(5)
O(1)	26.3(8)	35.6(8)	26.5(8)	-0.8(6)	2.0(6)	-5.2(6)
C(1)	24.8(11)	37.5(12)	30.2(12)	-2.7(9)	-2.8(9)	-1.7(9)
C(2)	37.2(14)	55.1(16)	32.2(13)	-7.2(11)	-7.4(11)	-3.1(11)
C(3)	43.1(15)	67.3(18)	27.7(13)	8.2(12)	-7.5(11)	6.5(13)
C(4)	41.9(14)	49.1(15)	40.4(14)	14.8(12)	2.0(11)	3.2(11)
C(5)	29.1(12)	36.2(12)	33.0(12)	3.4(9)	0.7(9)	-2.4(9)
C(6)	14.3(9)	29.5(10)	24.3(10)	-1.9(8)	2.9(8)	2.9(8)
C(7)	15.2(9)	24.9(9)	23.2(10)	0.2(8)	3.6(8)	-0.2(7)
C(8)	19.7(10)	21.6(9)	25.6(10)	-1.7(8)	3.3(8)	2.1(7)
C(9)	15.2(9)	28.6(10)	27.2(11)	-4.3(8)	2.0(8)	4.9(8)
C(10)	28.2(11)	26.4(10)	28.2(11)	-5.7(8)	1.2(9)	3.9(8)
C(11)	26.4(11)	32.6(11)	29.5(11)	-3.7(9)	1.2(9)	5.3(9)
C(12)	30.7(11)	32.5(11)	26.8(11)	-4.4(9)	-2.6(9)	12.0(9)
C(13)	40.2(13)	34.9(12)	28.2(12)	-7.3(9)	-2.2(10)	7.1(10)
C(14)	51.8(15)	33.0(12)	39.5(14)	-5.9(10)	-6.8(12)	3.1(11)
C(15)	61.6(17)	38.8(13)	32.5(13)	-15.6(10)	-11.0(12)	11.6(12)
C(16)	64.8(17)	46.2(14)	23.7(12)	-5.9(10)	-1.2(12)	16.6(13)
C(17)	44.0(14)	38.3(12)	29.3(12)	-1.8(10)	0.1(11)	7.9(10)
P(1)	15.8(2)	17.2(2)	16.1(2)	-1.77(17)	1.62(18)	-1.38(17)
P(2)	18.7(2)	21.0(2)	17.6(2)	-4.44(18)	-0.16(19)	0.31(18)
C(18)	19.3(9)	19.0(9)	21.1(10)	0.5(7)	-1.4(8)	-1.5(7)
C(19)	27.0(11)	25.0(10)	42.0(13)	2.6(9)	10.0(10)	0.6(8)
C(20)	30.7(12)	31.0(12)	63.6(17)	13.0(11)	13.3(12)	-5.7(9)
C(21)	36.5(13)	19.8(10)	62.9(17)	6.7(10)	-3.0(12)	-6.8(9)
C(22)	58.5(17)	23.1(11)	49.0(15)	-10.2(10)	8.0(13)	-2.1(11)
C(23)	47.2(14)	25.0(10)	33.4(12)	-5.1(9)	12.9(11)	-3.4(9)
C(24)	22.5(10)	17.4(9)	17.0(9)	-1.1(7)	2.0(8)	2.5(7)
C(25)	22.8(10)	24.1(9)	22.0(10)	-3.0(8)	2.8(8)	-0.4(8)
C(26)	30.3(11)	27.6(10)	22.6(11)	-3.6(8)	-3.6(9)	3.0(8)
C(27)	42.1(13)	33.8(11)	17.8(10)	4.3(8)	2.9(9)	2.8(9)
C(28)	34.5(12)	36.0(12)	25.9(11)	6.0(9)	9.4(9)	-4.8(9)
C(29)	22.7(10)	25.3(9)	23.0(10)	1.1(8)	2.7(8)	-1.2(8)
C(30)	15.4(9)	20.4(9)	18.6(9)	-1.3(7)	2.5(7)	-0.9(7)
C(31)	15.6(9)	20.6(9)	21.0(10)	-1.6(7)	3.6(7)	2.1(7)
C(32)	26.2(10)	25.3(10)	21.5(10)	-1.4(8)	-0.1(8)	3.8(8)
C(33)	35.7(12)	30.6(11)	27.5(11)	8.7(9)	3.1(9)	6.5(9)
C(34)	34.8(12)	21.9(10)	42.8(13)	8.2(9)	7.4(10)	0.5(9)
C(35)	24.1(10)	22.3(10)	38.6(12)	-2.8(9)	2.1(9)	-1.4(8)
C(36)	15.2(9)	21.6(9)	23.3(10)	-3.7(7)	2.7(7)	2.8(7)
C(37)	18.8(9)	24.7(9)	23.0(10)	-7.9(8)	1.2(8)	1.7(7)
C(38)	20.2(10)	21.0(9)	29.8(11)	-1.4(8)	-4.1(8)	0.2(7)
C(39)	27.6(11)	23.1(10)	36.5(12)	0.9(9)	1.9(9)	-1.0(8)
C(40)	28.8(12)	29.9(11)	54.9(16)	8.4(11)	7.3(11)	-2.2(9)
C(41)	32.4(13)	25.4(11)	66.0(18)	6.0(11)	-9.4(12)	-7.1(9)
C(42)	36.0(13)	27.2(11)	54.7(16)	-11.6(11)	-15.3(12)	1.0(9)
C(43)	27.9(11)	29.7(11)	36.6(12)	-10.3(9)	-5.4(9)	2.7(9)
C(44)	26.6(10)	29.2(10)	17.8(10)	-4.2(8)	3.2(8)	8.2(8)
C(45)	32.0(12)	47.8(13)	23.5(11)	-2.8(10)	-2.9(9)	0.5(10)
C(46)	48.3(15)	62.7(17)	23.3(12)	0.4(11)	-4.1(11)	7.0(13)
C(47)	58.9(17)	45.0(14)	23.7(12)	6.2(10)	9.5(11)	21.1(12)

C(48)	54.6(15)	26.3(11)	33.2(13)	2.5(9)	14.3(11)	5.0(10)
C(49)	43.9(13)	24.0(10)	24.7(11)	-3.1(8)	2.1(10)	1.1(9)

Table 6E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (18).

	x	y	z	U
H(1)	6595	1641	11134	37
H(2)	7511	1500	12722	51
H(3)	7031	869	13413	56
H(4)	5644	371	12490	53
H(5)	4708	506	10906	39
H(7)	5460(3)	1383(7)	9588(16)	25
H(8)	4320(2)	619(7)	9320(15)	27
H(10)	3498	413	7673	33
H(11)	4532	915	6250	36
H(13)	2127	35	6553	42
H(14)	1118	-403	5329	51
H(15)	1745	-298	3742	54
H(16)	3410	227	3401	54
H(17)	4446	662	4635	45
H(19)	-1998	764	9854	37
H(20)	-2775	84	10021	49
H(21)	-1834	-429	9077	48
H(22)	-98	-265	7957	52
H(23)	678	410	7775	42
H(25)	-2221	1005	7118	28
H(26)	-2524	1127	5449	33
H(27)	-543	1447	4704	37
H(28)	1743	1638	5603	38
H(29)	2061	1518	7271	28
H(30A)	-2419	1411	8670	22
H(30B)	-1516	1475	9719	22
H(32)	-2401	1924	7464	29
H(33)	-1886	2588	6979	38
H(34)	-245	3011	7972	40
H(35)	689	2784	9502	34
H(37A)	-463	1900	10670	27
H(37B)	395	2332	10836	27
H(39)	4567	2063	9314	35
H(40)	6394	2593	9319	45
H(41)	6466	3101	10495	51
H(42)	4678	3099	11648	49
H(43)	2857	2572	11657	38
H(45)	4066	1960	12401	42
H(46)	3960	1670	13937	54
H(47)	2170	1165	14183	51
H(48)	445	937	12905	45
H(49)	549	1221	11372	37

Table 7A. Crystal data, structure solution and refinement for (21).

Identification code	exti26
Chemical formula	$C_{44}H_{40}OP_2Pd$
Formula weight	753.10
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.1401(4) Å α = 90° b = 41.0250(16) Å β = 92.380(2)° c = 9.7145(4) Å γ = 90°
Volume	3639.5(3) $Å^3$
Z	4
Density (calculated)	1.374 g/cm^3
Absorption coefficient μ	0.631 mm^{-1}
F(000)	1552
Reflections for cell refinement	19783 (θ range 1.98 to 28.68°)
Crystal colour	orange
Crystal size	0.31 × 0.20 × 0.06 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	0.99 to 28.69°
Index ranges	$-12 \le h \le 11$, $-53 \le k \le 50$, $-12 \le \ell \le 13$
Intensity decay	0%
Reflections collected	29743
Independent reflections	8641 (R_{int} = 0.0409)
Reflections with I>2σ(I)	7241
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.928 and 0.802
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0125, 4.0594
Data / restraints / parameters	8641 / 0 / 440
Final R indices [I>2σ(I)]	R1 = 0.0464, wR2 = 0.0767
R indices (all data)	R1 = 0.0623, wR2 = 0.0810
Goodness-of-fit on F^2	1.202
Extinction coefficient	0.00066(9)
Largest and mean shift/esd	0.000 and 0.000
Largest diff. peak and hole	0.469 and -0.809 $eÅ^{-3}$

The Crystal Structure of [1,3-$C_3H_6(PPh_2)_2$ Pd (dba)] (21)

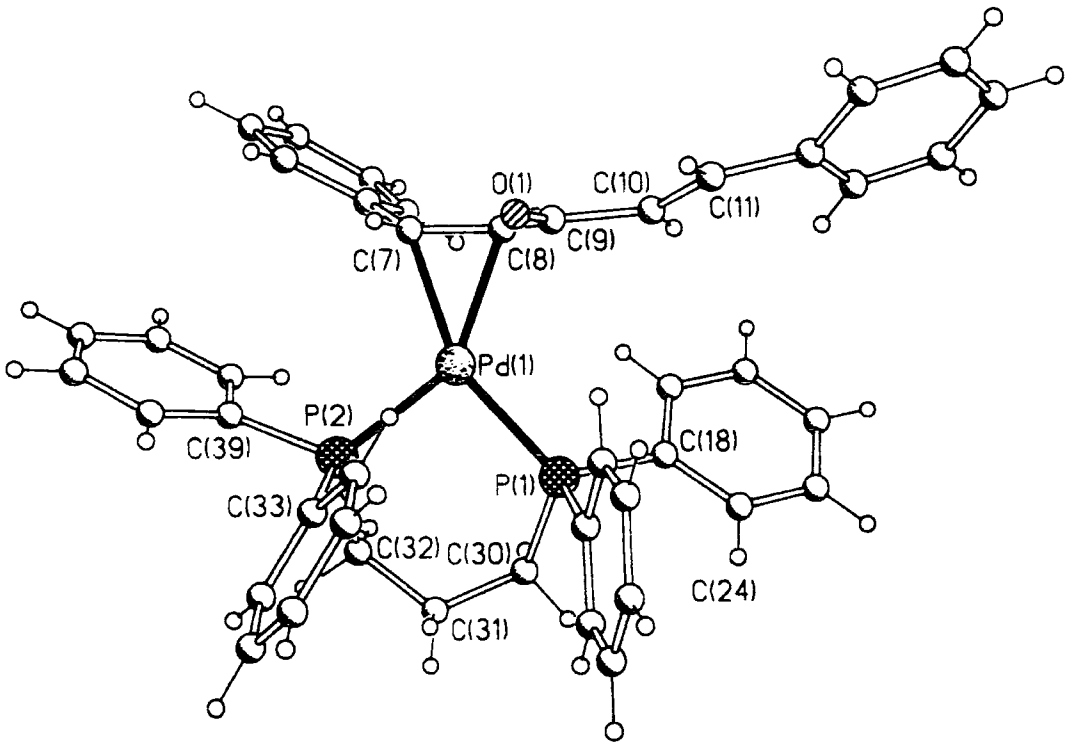


Table 7B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (21). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	1520.7(2)	1173.20(5)	4749.9(2)	19.13(6)
P(1)	3438.1(8)	1501.15(18)	5465.2(7)	21.87(15)
P(2)	2863.3(8)	706.25(18)	4767.7(8)	22.40(15)
O(1)	-1190(2)	1343.1(5)	6841(2)	32.4(5)
C(1)	-1797(4)	664.1(9)	2431(4)	42.5(8)
C(2)	-2221(5)	576.4(11)	1088(5)	62.5(13)
C(3)	-1864(5)	772.0(12)	-1(4)	64.7(13)
C(4)	-1016(4)	1043.9(10)	232(4)	51.3(10)
C(5)	-579(4)	1131.0(8)	1571(3)	36.0(7)
C(6)	-991(3)	947.5(7)	2698(3)	28.2(6)
C(7)	-677(3)	1054.6(7)	4138(3)	23.6(6)
C(8)	-601(3)	1390.9(7)	4481(3)	22.7(6)
C(9)	-893(3)	1515.0(7)	5845(3)	24.6(6)
C(10)	-905(3)	1877.4(7)	5928(3)	27.6(6)
C(11)	-1505(3)	2039.9(7)	6944(3)	30.0(7)
C(12)	-1737(3)	2393.8(8)	7000(3)	30.4(7)
C(13)	-2728(4)	2519.7(8)	7907(3)	36.7(8)
C(14)	-3061(4)	2849.2(9)	7924(4)	43.9(9)
C(15)	-2394(4)	3057.9(9)	7046(4)	44.6(9)
C(16)	-1378(4)	2941.1(9)	6153(4)	45.4(9)
C(17)	-1051(4)	2610.7(8)	6134(4)	39.9(8)
C(18)	3381(3)	1932.8(7)	4999(3)	25.6(6)
C(19)	4219(4)	2166.8(8)	5698(3)	37.8(8)
C(20)	4170(5)	2489.8(8)	5279(4)	48.7(10)
C(21)	3287(4)	2581.6(9)	4168(4)	47.6(9)
C(22)	2452(4)	2352.6(9)	3458(4)	49.9(10)
C(23)	2492(4)	2028.4(8)	3884(3)	37.9(8)
C(24)	3780(3)	1503.1(7)	7327(3)	23.8(6)
C(25)	2567(4)	1534.8(7)	8141(3)	30.3(7)
C(26)	2735(4)	1536.5(9)	9563(3)	42.7(8)
C(27)	4106(5)	1499.6(10)	10184(4)	52.3(10)
C(28)	5304(5)	1464.6(10)	9399(4)	53.0(10)
C(29)	5165(4)	1468.7(8)	7975(3)	36.5(7)
C(30)	5178(3)	1378.2(7)	4743(3)	28.5(6)
C(31)	5612(3)	1019.7(8)	4932(4)	34.8(7)
C(32)	4690(3)	769.1(8)	4093(4)	34.5(7)
C(33)	3280(3)	564.3(7)	6513(3)	28.9(6)
C(34)	4437(4)	355.3(9)	6859(4)	45.9(9)
C(35)	4793(5)	283.1(10)	8222(5)	58.7(12)
C(36)	3987(5)	413.6(11)	9254(4)	59.4(12)
C(37)	2825(5)	615.8(9)	8930(4)	48.2(9)
C(38)	2472(4)	691.6(8)	7566(3)	32.6(7)
C(39)	2175(3)	349.7(7)	3823(3)	27.0(6)
C(40)	1873(5)	56.7(9)	4429(4)	53.5(10)
C(41)	1219(6)	-195.6(10)	3652(5)	70.4(14)
C(42)	893(4)	-153.7(9)	2286(4)	51.5(10)
C(43)	1194(4)	134.2(10)	1665(4)	48.7(9)
C(44)	1824(4)	388.1(8)	2435(3)	38.7(8)

Table 7C. Bond lengths (Å) and angles (°) for (21).

Pd(1)-C(7)	2.128(3)	Pd(1)-C(8)	2.141(3)
Pd(1)-P(2)	2.2747(8)	Pd(1)-P(1)	2.2942(7)
P(1)-C(24)	1.823(3)	P(1)-C(18)	1.828(3)
P(1)-C(30)	1.836(3)	P(2)-C(33)	1.818(3)
P(2)-C(39)	1.825(3)	P(2)-C(32)	1.837(3)
O(1)-C(9)	1.236(3)	C(1)-C(2)	1.393(5)
C(1)-C(6)	1.395(4)	C(2)-C(3)	1.378(7)
C(3)-C(4)	1.372(6)	C(4)-C(5)	1.391(4)
C(5)-C(6)	1.393(4)	C(6)-C(7)	1.482(4)
C(7)-H(7)	0.97(3)	C(7)-C(8)	1.421(4)
C(8)-H(8)	0.94(3)	C(8)-C(9)	1.455(4)
C(9)-C(10)	1.489(4)	C(10)-C(11)	1.329(4)
C(11)-C(12)	1.468(4)	C(12)-C(13)	1.389(4)
C(12)-C(17)	1.392(5)	C(13)-C(14)	1.386(5)
C(14)-C(15)	1.370(5)	C(15)-C(16)	1.382(5)
C(16)-C(17)	1.388(5)	C(18)-C(23)	1.383(4)
C(18)-C(19)	1.388(4)	C(19)-C(20)	1.386(5)
C(20)-C(21)	1.373(5)	C(21)-C(22)	1.377(5)
C(22)-C(23)	1.393(5)	C(24)-C(25)	1.394(4)
C(24)-C(29)	1.398(4)	C(25)-C(26)	1.383(4)
C(26)-C(27)	1.377(5)	C(27)-C(28)	1.368(6)
C(28)-C(29)	1.384(5)	C(30)-C(31)	1.533(4)
C(31)-C(32)	1.541(4)	C(33)-C(38)	1.388(4)
C(33)-C(34)	1.392(4)	C(34)-C(35)	1.383(5)
C(35)-C(36)	1.376(6)	C(36)-C(37)	1.373(6)
C(37)-C(38)	1.387(4)	C(39)-C(40)	1.371(5)
C(39)-C(44)	1.382(4)	C(40)-C(41)	1.400(5)
C(41)-C(42)	1.359(6)	C(42)-C(43)	1.360(6)
C(43)-C(44)	1.393(5)		

C(7)-Pd(1)-C(8)	38.88(11)	C(7)-Pd(1)-P(2)	108.20(8)
C(8)-Pd(1)-P(2)	146.92(8)	C(7)-Pd(1)-P(1)	156.83(8)
C(8)-Pd(1)-P(1)	117.96(8)	P(2)-Pd(1)-P(1)	94.96(3)
C(24)-P(1)-C(18)	104.11(13)	C(24)-P(1)-C(30)	105.37(14)
C(18)-P(1)-C(30)	100.82(13)	C(24)-P(1)-Pd(1)	113.60(9)
C(18)-P(1)-Pd(1)	118.64(10)	C(30)-P(1)-Pd(1)	112.72(10)
C(33)-P(2)-C(39)	105.46(14)	C(33)-P(2)-C(32)	102.67(15)
C(39)-P(2)-C(32)	103.45(13)	C(33)-P(2)-Pd(1)	111.65(10)
C(39)-P(2)-Pd(1)	119.79(10)	C(32)-P(2)-Pd(1)	112.16(11)
C(2)-C(1)-C(6)	121.0(4)	C(3)-C(2)-C(1)	120.2(4)
C(4)-C(3)-C(2)	119.8(4)	C(3)-C(4)-C(5)	120.1(4)
C(4)-C(5)-C(6)	121.3(3)	C(5)-C(6)-C(1)	117.5(3)
C(5)-C(6)-C(7)	122.2(3)	C(1)-C(6)-C(7)	120.2(3)
H(7)-C(7)-C(8)	117.6(18)	H(7)-C(7)-C(6)	115.2(18)
C(8)-C(7)-C(6)	121.0(3)	H(7)-C(7)-Pd(1)	104.4(18)
C(8)-C(7)-Pd(1)	71.06(16)	C(6)-C(7)-Pd(1)	118.33(19)
H(8)-C(8)-C(7)	120.5(18)	H(8)-C(8)-C(9)	114.0(18)
C(7)-C(8)-C(9)	123.0(3)	H(8)-C(8)-Pd(1)	112.9(18)
C(7)-C(8)-Pd(1)	70.06(16)	C(9)-C(8)-Pd(1)	103.55(18)
O(1)-C(9)-C(8)	124.6(3)	O(1)-C(9)-C(10)	121.7(3)
C(8)-C(9)-C(10)	113.6(2)	C(11)-C(10)-C(9)	123.0(3)
C(10)-C(11)-C(12)	126.0(3)	C(13)-C(12)-C(17)	117.9(3)
C(13)-C(12)-C(11)	119.3(3)	C(17)-C(12)-C(11)	122.7(3)
C(14)-C(13)-C(12)	121.3(3)	C(15)-C(14)-C(13)	119.9(3)
C(14)-C(15)-C(16)	120.1(3)	C(15)-C(16)-C(17)	119.8(4)
C(16)-C(17)-C(12)	120.9(3)	C(23)-C(18)-C(19)	118.8(3)
C(23)-C(18)-P(1)	118.6(2)	C(19)-C(18)-P(1)	122.6(2)
C(20)-C(19)-C(18)	120.4(3)	C(21)-C(20)-C(19)	120.3(3)

C(20)-C(21)-C(22)	120.1(3)	C(21)-C(22)-C(23)	119.7(3)
C(18)-C(23)-C(22)	120.7(3)	C(25)-C(24)-C(29)	118.8(3)
C(25)-C(24)-P(1)	117.1(2)	C(29)-C(24)-P(1)	124.1(2)
C(26)-C(25)-C(24)	120.6(3)	C(27)-C(26)-C(25)	119.9(3)
C(28)-C(27)-C(26)	120.1(3)	C(27)-C(28)-C(29)	120.9(4)
C(28)-C(29)-C(24)	119.7(3)	C(31)-C(30)-P(1)	116.2(2)
C(30)-C(31)-C(32)	116.4(3)	C(31)-C(32)-P(2)	113.0(2)
C(38)-C(33)-C(34)	118.4(3)	C(38)-C(33)-P(2)	118.0(2)
C(34)-C(33)-P(2)	123.4(3)	C(35)-C(34)-C(33)	120.6(4)
C(36)-C(35)-C(34)	120.1(4)	C(37)-C(36)-C(35)	120.0(4)
C(36)-C(37)-C(38)	120.1(4)	C(37)-C(38)-C(33)	120.7(3)
C(40)-C(39)-C(44)	118.4(3)	C(40)-C(39)-P(2)	123.9(3)
C(44)-C(39)-P(2)	117.4(2)	C(39)-C(40)-C(41)	120.4(4)
C(42)-C(41)-C(40)	120.3(4)	C(41)-C(42)-C(43)	120.2(4)
C(42)-C(43)-C(44)	119.8(4)	C(39)-C(44)-C(43)	120.9(3)

Table 7D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (21).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	15.97(10)	20.48(10)	20.85(10)	-1.67(9)	-0.04(7)	-0.94(9)
P(1)	19.4(3)	23.7(4)	22.4(4)	-1.5(3)	-0.2(3)	-3.8(3)
P(2)	17.6(3)	21.4(4)	28.1(4)	-3.4(3)	0.3(3)	0.1(3)
O(1)	33.2(12)	35.9(12)	28.4(11)	2.1(9)	5.3(9)	2.3(10)
C(1)	32.7(18)	42(2)	53(2)	-16.1(17)	1.9(16)	-5.0(15)
C(2)	46(2)	66(3)	74(3)	-43(3)	-11(2)	-3(2)
C(3)	54(3)	88(3)	50(2)	-39(2)	-20(2)	19(2)
C(4)	53(2)	68(3)	32.0(18)	-10.4(18)	-4.6(17)	24(2)
C(5)	37.2(18)	40.0(19)	30.6(16)	-7.7(14)	-3.3(13)	3.2(15)
C(6)	17.9(14)	31.5(16)	35.0(16)	-9.3(13)	-1.3(12)	1.5(12)
C(7)	14.3(13)	26.7(15)	29.7(15)	-0.6(12)	-0.3(11)	-0.9(11)
C(8)	17.2(14)	27.3(15)	23.4(14)	-1.4(12)	-1.9(11)	2.2(11)
C(9)	15.4(13)	28.8(15)	29.2(15)	-3.1(12)	-3.1(11)	3.7(11)
C(10)	24.7(15)	28.3(16)	29.4(15)	-2.7(12)	-3.1(12)	1.6(12)
C(11)	30.8(17)	30.4(16)	28.6(15)	-3.9(12)	-3.0(13)	1.8(13)
C(12)	27.2(16)	32.5(17)	30.6(15)	-8.9(13)	-9.0(12)	1.8(13)
C(13)	36.9(19)	35.6(18)	37.3(18)	-10.9(14)	-2.3(14)	3.7(14)
C(14)	44(2)	41(2)	46(2)	-18.8(17)	-6.2(17)	9.6(16)
C(15)	53(2)	30.4(18)	49(2)	-12.9(16)	-23.0(18)	5.0(16)
C(16)	58(2)	33.1(19)	44(2)	-4.5(15)	-10.2(18)	-8.0(17)
C(17)	43(2)	35.0(19)	41.5(19)	-9.2(15)	-1.3(16)	-1.0(15)
C(18)	27.8(15)	26.4(15)	22.8(14)	1.6(11)	1.7(12)	-4.4(12)
C(19)	53(2)	31.7(18)	28.1(16)	1.1(13)	-4.8(15)	-8.6(16)
C(20)	79(3)	25.7(18)	42(2)	-2.4(15)	1.3(19)	-10.3(18)
C(21)	63(3)	26.8(18)	54(2)	12.6(16)	10.6(19)	4.2(17)
C(22)	47(2)	49(2)	53(2)	26.3(18)	-8.0(18)	-2.4(18)
C(23)	32.4(18)	41(2)	39.6(18)	8.6(15)	-6.2(14)	-12.1(15)
C(24)	24.7(15)	19.4(14)	26.8(14)	0.5(11)	-5.4(11)	-4.5(11)
C(25)	32.1(17)	30.9(17)	28.0(15)	-0.3(12)	0.5(13)	-5.5(13)
C(26)	51(2)	48(2)	29.7(17)	-1.9(15)	4.7(15)	-7.3(17)
C(27)	71(3)	60(3)	24.4(17)	0.8(16)	-12.9(18)	0(2)
C(28)	52(2)	64(3)	41(2)	-3.3(18)	-21.3(18)	8(2)
C(29)	29.4(17)	41.7(19)	37.4(17)	-3.8(15)	-7.7(14)	1.0(14)
C(30)	20.3(15)	30.6(16)	35.0(16)	-4.9(13)	4.9(12)	-7.3(12)
C(31)	18.6(15)	30.9(17)	55(2)	-9.0(15)	4.7(14)	-1.3(12)
C(32)	23.6(16)	32.2(17)	48.5(19)	-10.5(15)	10.5(14)	-0.4(13)
C(33)	24.3(15)	25.6(15)	36.2(16)	-0.2(13)	-7.3(13)	-0.2(12)
C(34)	33.9(19)	45(2)	58(2)	5.8(18)	-10.1(17)	8.7(16)
C(35)	46(2)	53(3)	75(3)	28(2)	-24(2)	5(2)
C(36)	67(3)	61(3)	48(2)	23(2)	-23(2)	-13(2)
C(37)	66(3)	45(2)	33.2(18)	7.1(16)	-2.7(18)	-5.8(19)
C(38)	38.4(18)	28.3(16)	30.7(16)	6.4(13)	-3.3(14)	-2.7(14)
C(39)	20.2(15)	23.0(15)	38.1(16)	-7.5(12)	2.4(12)	0.9(11)
C(40)	75(3)	31(2)	53(2)	0.0(16)	-10(2)	-15.7(19)
C(41)	103(4)	31(2)	75(3)	-3(2)	-9(3)	-27(2)
C(42)	47(2)	42(2)	65(3)	-25.0(19)	2.7(19)	-7.5(18)
C(43)	49(2)	51(2)	45(2)	-20.5(18)	-2.7(17)	-6.4(18)
C(44)	45(2)	32.6(18)	38.3(18)	-8.0(14)	0.0(15)	-2.7(15)

Table 7E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (21).

	x	y	z	U
H(1)	-2060	529	3175	51
H(2)	-2759	381	922	75
H(3)	-2204	719	-911	78
H(4)	-727	1173	-522	62
H(5)	11	1319	1720	43
H(7)	-987(33)	905(8)	4840(31)	28
H(8)	-645(33)	1551(7)	3785(31)	27
H(10)	-462	1998	5221	33
H(11)	-1814	1916	7705	36
H(13)	-3187	2377	8527	44
H(14)	-3752	2930	8544	53
H(15)	-2629	3283	7051	54
H(16)	-906	3087	5553	54
H(17)	-349	2532	5522	48
H(19)	4830	2105	6470	45
H(20)	4749	2648	5762	58
H(21)	3251	2803	3888	57
H(22)	1851	2415	2682	60
H(23)	1903	1871	3403	46
H(25)	1616	1555	7715	36
H(26)	1905	1563	10110	51
H(27)	4221	1498	11161	63
H(28)	6245	1437	9837	64
H(29)	6007	1448	7440	44
H(30A)	5127	1427	3744	34
H(30B)	5967	1515	5168	34
H(31A)	5557	965	5921	42
H(31B)	6647	995	4686	42
H(32A)	5217	558	4097	41
H(32B)	4581	844	3126	41
H(34)	4987	261	6152	55
H(35)	5595	143	8448	70
H(36)	4234	364	10190	71
H(37)	2264	704	9643	58
H(38)	1668	832	7349	39
H(40)	2108	25	5381	64
H(41)	1002	-397	4082	84
H(42)	453	-326	1764	62
H(43)	975	162	707	58
H(44)	2016	590	2001	46

Table 8A. Crystal data, structure solution and refinement for (22).

Identification code	exti28
Chemical formula	$C_{57}H_{52}O_2P_2Pd$
Formula weight	937.33
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 14.7553(13) Å α = 90°
	b = 18.6845(17) Å β = 102.678(2)°
	c = 17.6057(16) Å γ = 90°
Volume	4735.5(7) $Å^3$
Z	4
Density (calculated)	1.315 g/cm^3
Absorption coefficient μ	0.501 mm^{-1}
F(000)	1944
Reflections for cell refinement	10324 (θ range 1.61 to 28.02°)
Crystal colour	yellow
Crystal size	0.52 x 0.09 x 0.04 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	1.41 to 25.00°
Index ranges	$-19 \le h \le 19$, $-23 \le k \le 23$, $-23 \le \ell \le 22$
Intensity decay	0%
Reflections collected	28416
Independent reflections	8332 (R_{int} = 0.0870)
Reflections with I>2σ(I)	5725
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.928 and 0.803
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0424, 13.5441
Data / restraints / parameters	8332 / 248 / 609
Final R indices [I>2σ(I)]	R1 = 0.0693, wR2 = 0.1273
R indices (all data)	R1 = 0.1160, wR2 = 0.1438
Goodness-of-fit on F^2	1.091
Extinction coefficient	0.00078(14)
Largest and mean shift/esd	0.003 and 0.000
Largest diff. peak and hole	1.139 and -0.364 $eÅ^{-3}$

The Crystal Structure of $[(PPh_3)_2Pd(dba)]$ (22)

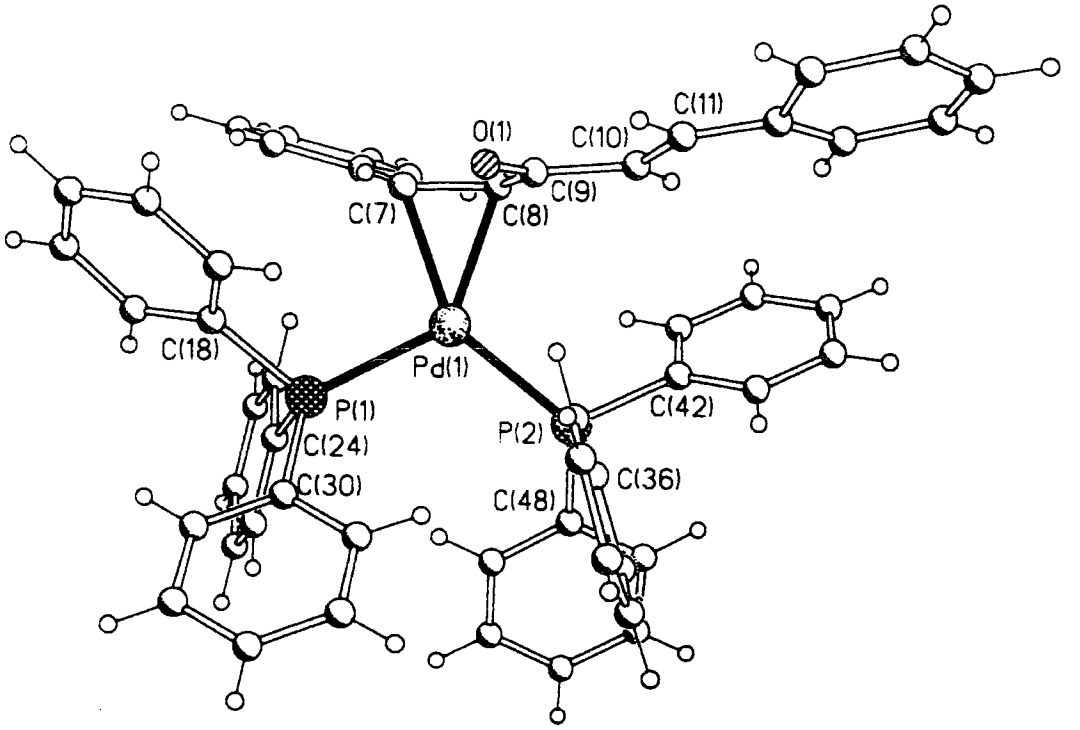


Table 8B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (22). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	3622.9(3)	3125.8(2)	5945.1(3)	21.42(15)
P(1)	2370.9(11)	3426.2(8)	6490.0(9)	24.2(4)
P(2)	3711.1(10)	1923.0(8)	5623.9(8)	23.6(3)
O(1)	5708(3)	3523(2)	7058(3)	44.7(12)
C(1)	3479(5)	4570(3)	4595(4)	36.1(16)
C(2)	2952(5)	5048(4)	4096(4)	42.2(17)
C(3)	2590(5)	5647(4)	4376(4)	41.7(18)
C(4)	2787(4)	5770(3)	5173(4)	35.7(16)
C(5)	3323(4)	5288(3)	5682(4)	28.0(14)
C(6)	3682(4)	4675(3)	5398(3)	25.7(14)
C(7)	4244(4)	4174(3)	5954(3)	24.2(14)
C(8)	4854(4)	3666(3)	5753(4)	28.2(14)
C(9)	5603(4)	3372(3)	6365(4)	31.9(15)
C(10)	6265(4)	2883(3)	6101(4)	37.4(17)
C(11)	7045(5)	2683(3)	6577(5)	55(2)
C(12)	7795(14)	2238(13)	6510(16)	54(5)
C(13)	7781(15)	1905(13)	5807(16)	67(5)
C(14)	8578(17)	1492(12)	5708(18)	80(6)
C(15)	9324(17)	1436(15)	6271(19)	83(7)
C(16)	9380(13)	1798(12)	6981(19)	77(6)
C(17)	8610(15)	2206(12)	7095(17)	65(5)
C(12X)	7810(2)	2230(2)	6240(2)	62(8)
C(13X)	7600(2)	1870(2)	5530(2)	79(8)
C(14X)	8220(2)	1376(17)	5350(2)	82(7)
C(15X)	9060(2)	1249(14)	5870(2)	82(8)
C(16X)	9274(19)	1615(16)	6570(2)	72(7)
C(17X)	8650(2)	2108(16)	6760(2)	66(7)
C(18)	2541(4)	4273(3)	7032(3)	25.4(14)
C(19)	3374(4)	4359(3)	7574(3)	30.2(15)
C(20)	3572(5)	4978(3)	7999(4)	38.4(17)
C(21)	2942(5)	5535(3)	7887(4)	44.2(19)
C(22)	2105(5)	5458(3)	7361(4)	44.3(19)
C(23)	1900(5)	4828(3)	6937(4)	33.4(15)
C(24)	1270(4)	3555(3)	5799(3)	28.1(14)
C(25)	1243(4)	4046(3)	5193(4)	31.3(15)
C(26)	433(4)	4163(4)	4644(4)	39.3(17)
C(27)	-352(5)	3794(4)	4681(5)	55(2)
C(28)	-338(5)	3301(4)	5265(5)	61(2)
C(29)	464(4)	3182(4)	5824(4)	46.2(19)
C(30)	2086(4)	2843(3)	7247(3)	29.3(14)
C(31)	2484(5)	2184(3)	7375(4)	38.8(17)
C(32)	2316(5)	1756(4)	7974(4)	52(2)
C(33)	1755(5)	1986(4)	8445(4)	49.2(19)
C(34)	1356(6)	2647(4)	8326(5)	62(2)
C(35)	1534(5)	3073(4)	7735(4)	55(2)
C(36)	4117(4)	1372(3)	6496(3)	24.4(14)
C(37)	3771(4)	700(3)	6606(4)	31.2(15)
C(38)	4032(4)	348(3)	7310(4)	34.4(16)
C(39)	4639(5)	670(3)	7919(4)	36.5(16)
C(40)	5018(5)	1327(3)	7819(4)	37.3(16)
C(41)	4755(4)	1681(3)	7113(3)	30.1(15)

C(42)	4499(4)	1687(3)	4994(3)	23.6(13)
C(43)	4418(4)	2068(3)	4294(3)	29.3(15)
C(44)	4964(5)	1881(4)	3777(4)	40.7(17)
C(45)	5588(5)	1329(4)	3934(4)	41.4(18)
C(46)	5677(5)	956(4)	4626(4)	43.4(18)
C(47)	5130(4)	1130(3)	5150(4)	34.6(16)
C(48)	2663(4)	1445(3)	5138(3)	27.5(14)
C(49)	2668(5)	878(3)	4625(3)	32.7(15)
C(50)	1851(5)	510(4)	4312(4)	44.3(18)
C(51)	1028(5)	707(4)	4491(4)	51(2)
C(52)	1014(5)	1284(4)	4981(4)	55(2)
C(53)	1815(5)	1654(4)	5295(4)	42.0(18)
C(54)	8467(12)	1029(8)	3138(9)	172(6)
C(55)	9146(11)	929(7)	2664(9)	165(6)
C(56)	9338(8)	145(6)	2577(6)	132(4)
C(57)	8963(13)	-160(6)	3197(8)	176(6)
C(58)	8400(11)	341(9)	3479(10)	187(6)

Table 8C. Bond lengths (Å) and angles (°) for (22).

Pd(1)-C(7)	2.160(5)	Pd(1)-C(8)	2.169(6)
Pd(1)-P(2)	2.3280(15)	Pd(1)-P(1)	2.3295(16)
P(1)-C(24)	1.819(6)	P(1)-C(18)	1.835(6)
P(1)-C(30)	1.840(6)	P(2)-C(48)	1.828(6)
P(2)-C(42)	1.828(6)	P(2)-C(36)	1.836(6)
O(1)-C(9)	1.229(7)	C(1)-C(2)	1.369(9)
C(1)-C(6)	1.394(8)	C(2)-C(3)	1.377(9)
C(3)-C(4)	1.389(9)	C(4)-C(5)	1.387(8)
C(5)-C(6)	1.399(8)	C(6)-C(7)	1.472(8)
C(7)-C(8)	1.405(8)	C(8)-C(9)	1.469(9)
C(9)-C(10)	1.484(9)	C(10)-C(11)	1.321(9)
C(11)-C(12)	1.410(18)	C(11)-C(12X)	1.62(2)
C(12)-C(13)	1.38(2)	C(12)-C(17)	1.403(19)
C(13)-C(14)	1.45(2)	C(14)-C(15)	1.31(2)
C(15)-C(16)	1.41(3)	C(16)-C(17)	1.42(2)
C(12X)-C(13X)	1.3900	C(12X)-C(17X)	1.3900
C(13X)-C(14X)	1.3900	C(14X)-C(15X)	1.3900
C(15X)-C(16X)	1.3900	C(16X)-C(17X)	1.3900
C(18)-C(23)	1.389(8)	C(18)-C(19)	1.390(8)
C(19)-C(20)	1.373(8)	C(20)-C(21)	1.380(9)
C(21)-C(22)	1.379(9)	C(22)-C(23)	1.392(9)
C(24)-C(29)	1.387(8)	C(24)-C(25)	1.401(8)
C(25)-C(26)	1.380(8)	C(26)-C(27)	1.360(9)
C(27)-C(28)	1.378(10)	C(28)-C(29)	1.380(9)
C(30)-C(31)	1.361(8)	C(30)-C(35)	1.377(9)
C(31)-C(32)	1.388(9)	C(32)-C(33)	1.364(9)
C(33)-C(34)	1.364(10)	C(34)-C(35)	1.379(9)
C(36)-C(37)	1.384(8)	C(36)-C(41)	1.397(8)
C(37)-C(38)	1.382(8)	C(38)-C(39)	1.376(9)
C(39)-C(40)	1.377(9)	C(40)-C(41)	1.386(8)
C(42)-C(47)	1.383(8)	C(42)-C(43)	1.404(8)
C(43)-C(44)	1.386(8)	C(44)-C(45)	1.371(9)
C(45)-C(46)	1.385(9)	C(46)-C(47)	1.391(8)
C(48)-C(49)	1.393(8)	C(48)-C(53)	1.396(8)
C(49)-C(50)	1.393(9)	C(50)-C(51)	1.369(10)
C(51)-C(52)	1.384(10)	C(52)-C(53)	1.376(9)
C(54)-C(58)	1.433(12)	C(54)-C(55)	1.450(13)
C(55)-C(56)	1.505(12)	C(56)-C(57)	1.446(12)
C(57)-C(58)	1.411(13)		

C(7)-Pd(1)-C(8)	37.9(2)	C(7)-Pd(1)-P(2)	146.12(16)
C(8)-Pd(1)-P(2)	108.55(16)	C(7)-Pd(1)-P(1)	98.77(16)
C(8)-Pd(1)-P(1)	135.99(16)	P(2)-Pd(1)-P(1)	115.11(6)
C(24)-P(1)-C(18)	103.5(3)	C(24)-P(1)-C(30)	104.5(3)
C(18)-P(1)-C(30)	99.3(3)	C(24)-P(1)-Pd(1)	115.4(2)
C(18)-P(1)-Pd(1)	113.03(19)	C(30)-P(1)-Pd(1)	118.9(2)
C(48)-P(2)-C(42)	100.6(3)	C(48)-P(2)-C(36)	101.8(3)
C(42)-P(2)-C(36)	103.8(3)	C(48)-P(2)-Pd(1)	119.9(2)
C(42)-P(2)-Pd(1)	117.18(17)	C(36)-P(2)-Pd(1)	111.34(18)
C(2)-C(1)-C(6)	121.6(6)	C(1)-C(2)-C(3)	120.7(6)
C(2)-C(3)-C(4)	119.0(6)	C(5)-C(4)-C(3)	120.6(6)
C(4)-C(5)-C(6)	120.5(6)	C(1)-C(6)-C(5)	117.6(6)
C(1)-C(6)-C(7)	123.2(5)	C(5)-C(6)-C(7)	119.1(5)
C(8)-C(7)-C(6)	124.2(5)	C(8)-C(7)-Pd(1)	71.4(3)
C(6)-C(7)-Pd(1)	113.3(4)	C(7)-C(8)-C(9)	119.2(5)
C(7)-C(8)-Pd(1)	70.8(3)	C(9)-C(8)-Pd(1)	103.5(4)
O(1)-C(9)-C(8)	123.5(6)	O(1)-C(9)-C(10)	120.3(6)
C(8)-C(9)-C(10)	116.2(6)	C(11)-C(10)-C(9)	121.1(7)

C(10)-C(11)-C(12)	134.8(13)	C(10)-C(11)-C(12X)	119.4(15)
C(13)-C(12)-C(17)	118.7(14)	C(13)-C(12)-C(11)	118.9(17)
C(17)-C(12)-C(11)	121.7(16)	C(12)-C(13)-C(14)	119.7(17)
C(15)-C(14)-C(13)	121.3(19)	C(14)-C(15)-C(16)	120.5(17)
C(15)-C(16)-C(17)	119.5(17)	C(12)-C(17)-C(16)	120.1(17)
C(13X)-C(12X)-C(17X)	120.0	C(13X)-C(12X)-C(11)	123.0(19)
C(17X)-C(12X)-C(11)	115.7(19)	C(12X)-C(13X)-C(14X)	120.0
C(15X)-C(14X)-C(13X)	120.0	C(14X)-C(15X)-C(16X)	120.0
C(17X)-C(16X)-C(15X)	120.0	C(16X)-C(17X)-C(12X)	120.0
C(23)-C(18)-C(19)	118.1(6)	C(23)-C(18)-P(1)	124.7(5)
C(19)-C(18)-P(1)	117.2(4)	C(20)-C(19)-C(18)	121.5(6)
C(19)-C(20)-C(21)	120.0(6)	C(22)-C(21)-C(20)	119.6(6)
C(21)-C(22)-C(23)	120.3(6)	C(18)-C(23)-C(22)	120.4(6)
C(29)-C(24)-C(25)	118.1(6)	C(29)-C(24)-P(1)	124.0(5)
C(25)-C(24)-P(1)	117.9(5)	C(26)-C(25)-C(24)	120.8(6)
C(27)-C(26)-C(25)	120.1(6)	C(26)-C(27)-C(28)	120.1(7)
C(27)-C(28)-C(29)	120.6(7)	C(28)-C(29)-C(24)	120.2(6)
C(31)-C(30)-C(35)	118.1(6)	C(31)-C(30)-P(1)	119.8(5)
C(35)-C(30)-P(1)	121.9(5)	C(30)-C(31)-C(32)	120.3(6)
C(33)-C(32)-C(31)	120.9(7)	C(34)-C(33)-C(32)	119.4(7)
C(33)-C(34)-C(35)	119.4(7)	C(30)-C(35)-C(34)	121.8(7)
C(37)-C(36)-C(41)	118.2(5)	C(37)-C(36)-P(2)	124.3(5)
C(41)-C(36)-P(2)	117.3(4)	C(38)-C(37)-C(36)	121.3(6)
C(39)-C(38)-C(37)	119.8(6)	C(38)-C(39)-C(40)	120.2(6)
C(39)-C(40)-C(41)	119.9(6)	C(40)-C(41)-C(36)	120.6(6)
C(47)-C(42)-C(43)	118.6(5)	C(47)-C(42)-P(2)	123.4(5)
C(43)-C(42)-P(2)	117.9(4)	C(44)-C(43)-C(42)	120.0(6)
C(45)-C(44)-C(43)	121.2(6)	C(44)-C(45)-C(46)	119.1(6)
C(45)-C(46)-C(47)	120.6(6)	C(42)-C(47)-C(46)	120.5(6)
C(49)-C(48)-C(53)	118.3(6)	C(49)-C(48)-P(2)	123.4(5)
C(53)-C(48)-P(2)	118.3(5)	C(48)-C(49)-C(50)	120.3(6)
C(51)-C(50)-C(49)	120.7(6)	C(50)-C(51)-C(52)	119.2(7)
C(53)-C(52)-C(51)	120.9(7)	C(52)-C(53)-C(48)	120.5(6)
C(58)-C(54)-C(55)	104.2(10)	C(54)-C(55)-C(56)	110.7(10)
C(57)-C(56)-C(55)	101.2(9)	C(58)-C(57)-C(56)	110.9(10)
C(57)-C(58)-C(54)	110.3(11)		

Table 8D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (22).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	26.1(3)	16.3(2)	21.8(2)	-1.1(2)	5.04(18)	1.6(2)
P(1)	29.0(9)	20.1(7)	23.7(9)	0.9(6)	6.5(7)	2.4(7)
P(2)	29.6(9)	18.6(7)	22.5(8)	-2.7(7)	5.4(7)	0.3(7)
O(1)	50(3)	40(3)	38(3)	-2(2)	-4(2)	7(2)
C(1)	48(4)	30(4)	32(4)	2(3)	12(3)	-3(3)
C(2)	55(5)	40(4)	33(4)	6(3)	11(4)	-5(4)
C(3)	44(4)	37(4)	41(4)	25(3)	2(4)	-1(3)
C(4)	32(4)	22(3)	53(5)	4(3)	9(3)	6(3)
C(5)	23(3)	24(3)	37(4)	1(3)	7(3)	-3(3)
C(6)	27(3)	19(3)	31(4)	1(3)	5(3)	-7(3)
C(7)	30(4)	20(3)	21(3)	-2(3)	2(3)	-7(3)
C(8)	30(4)	24(3)	33(4)	-2(3)	11(3)	-3(3)
C(9)	27(4)	23(3)	46(4)	-1(3)	8(3)	-5(3)
C(10)	28(4)	21(3)	63(5)	0(3)	8(4)	-7(3)
C(11)	37(4)	26(4)	101(7)	-4(4)	14(4)	-3(3)
C(12)	29(6)	25(7)	114(15)	15(9)	29(8)	-8(5)
C(13)	61(9)	37(9)	113(13)	17(9)	45(8)	2(8)
C(14)	71(12)	44(10)	140(15)	22(10)	53(10)	16(9)
C(15)	63(10)	54(13)	151(18)	40(11)	65(10)	19(9)
C(16)	38(7)	40(11)	155(17)	34(11)	29(10)	5(7)
C(17)	41(7)	34(8)	122(15)	25(9)	22(9)	5(6)
C(12X)	44(10)	35(13)	120(2)	10(13)	46(11)	-7(9)
C(13X)	65(13)	49(13)	136(19)	-9(14)	52(12)	2(11)
C(14X)	67(15)	51(13)	146(19)	-4(14)	60(12)	3(13)
C(15X)	72(14)	34(14)	160(2)	13(13)	60(14)	5(11)
C(16X)	68(12)	23(14)	140(2)	29(13)	53(14)	11(9)
C(17X)	46(9)	40(12)	127(18)	25(12)	51(12)	6(8)
C(18)	35(4)	21(3)	24(3)	4(3)	17(3)	0(3)
C(19)	35(4)	30(3)	27(4)	-1(3)	10(3)	1(3)
C(20)	45(4)	40(4)	30(4)	-8(3)	10(3)	-13(3)
C(21)	73(6)	25(4)	40(4)	-12(3)	25(4)	-3(4)
C(22)	60(5)	30(4)	50(5)	-1(3)	28(4)	13(3)
C(23)	41(4)	28(3)	33(4)	-5(3)	12(3)	4(3)
C(24)	27(4)	28(3)	31(4)	0(3)	10(3)	2(3)
C(25)	29(4)	36(4)	30(4)	-1(3)	10(3)	-1(3)
C(26)	34(4)	43(4)	42(4)	9(3)	11(3)	6(3)
C(27)	29(4)	68(5)	60(5)	14(4)	-12(4)	2(4)
C(28)	28(4)	55(5)	94(7)	25(5)	-1(4)	-8(4)
C(29)	31(4)	34(4)	72(5)	22(4)	8(4)	4(3)
C(30)	38(4)	25(3)	27(3)	-3(3)	10(3)	-1(3)
C(31)	53(5)	33(4)	35(4)	10(3)	20(4)	14(3)
C(32)	66(5)	36(4)	61(5)	21(4)	26(4)	10(4)
C(33)	66(5)	50(5)	36(4)	13(4)	20(4)	-12(4)
C(34)	99(7)	38(5)	68(6)	4(4)	58(5)	8(4)
C(35)	86(6)	28(4)	62(5)	9(4)	41(5)	15(4)
C(36)	29(4)	20(3)	27(3)	-1(3)	12(3)	5(3)
C(37)	40(4)	20(3)	34(4)	-2(3)	11(3)	1(3)
C(38)	44(4)	22(3)	41(4)	3(3)	18(4)	3(3)
C(39)	47(4)	31(4)	35(4)	8(3)	17(3)	16(3)
C(40)	43(4)	34(4)	30(4)	-1(3)	-1(3)	10(3)
C(41)	39(4)	22(3)	27(4)	1(3)	5(3)	4(3)

C(42)	29(3)	14(3)	29(3)	-1(2)	9(3)	-2(2)
C(43)	39(4)	21(3)	27(4)	-4(3)	5(3)	-2(3)
C(44)	60(5)	40(4)	25(3)	2(3)	16(3)	-12(4)
C(45)	46(4)	42(4)	43(4)	-7(3)	25(4)	-6(3)
C(46)	44(4)	46(4)	42(4)	0(3)	14(4)	15(3)
C(47)	41(4)	34(4)	29(4)	1(3)	10(3)	9(3)
C(48)	32(4)	27(3)	20(3)	2(3)	0(3)	-3(3)
C(49)	39(4)	34(4)	25(4)	-8(3)	8(3)	-3(3)
C(50)	53(5)	38(4)	38(4)	-12(3)	3(4)	-11(4)
C(51)	47(5)	62(5)	38(4)	-10(4)	1(4)	-21(4)
C(52)	34(4)	84(6)	54(5)	-6(5)	23(4)	-9(4)
C(53)	36(4)	48(4)	44(4)	-13(3)	12(3)	-6(3)
C(54)	200(16)	155(10)	138(13)	81(9)	-14(9)	15(10)
C(55)	178(15)	120(8)	170(14)	53(9)	-20(9)	-37(9)
C(56)	155(10)	96(7)	106(8)	44(6)	-57(7)	-33(7)
C(57)	301(19)	88(8)	124(11)	-11(8)	18(11)	-65(9)
C(58)	158(14)	181(14)	206(15)	70(12)	5(9)	-28(11)

Table 8E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (22).

	x	y	z	U
H(1)	3711	4155	4389	43
H(2)	2836	4966	3550	51
H(3)	2211	5971	4029	50
H(4)	2553	6187	5372	43
H(5)	3448	5376	6226	34
H(7)	4400(4)	4320(3)	6483(11)	29
H(8)	4930(4)	3630(3)	5234(13)	34
H(10)	6124	2710	5581	45
H(11)	7119	2887	7082	66
H(11X)	7158	2801	7115	66
H(13)	7252	1947	5390	80
H(14)	8560	1257	5226	96
H(15)	9829	1149	6198	100
H(16)	9928	1769	7380	92
H(17)	8647	2459	7569	78
H(13X)	7023	1956	5175	94
H(14X)	8076	1126	4868	99
H(15X)	9488	913	5745	98
H(16X)	9848	1529	6931	87
H(17X)	8795	2358	7239	79
H(19)	3816	3982	7652	36
H(20)	4143	5023	8371	46
H(21)	3085	5969	8169	53
H(22)	1665	5837	7289	53
H(23)	1319	4777	6580	40
H(25)	1789	4302	5160	38
H(26)	423	4501	4239	47
H(27)	-910	3877	4304	67
H(28)	-885	3041	5284	73
H(29)	464	2843	6226	55
H(31)	2879	2017	7054	47
H(32)	2596	1297	8056	63
H(33)	1643	1688	8852	59
H(34)	960	2812	8647	75
H(35)	1267	3537	7664	66
H(37)	3346	477	6190	37
H(38)	3794	-116	7373	41
H(39)	4797	438	8411	44
H(40)	5459	1539	8233	45
H(41)	5011	2137	7047	36
H(43)	3989	2452	4175	35
H(44)	4905	2142	3305	49
H(45)	5954	1203	3573	50
H(46)	6116	578	4745	52
H(47)	5190	865	5618	42
H(49)	3232	743	4487	39
H(50)	1864	118	3971	53
H(51)	474	451	4281	61
H(52)	444	1427	5101	66
H(53)	1790	2055	5622	50

Table 9A. Crystal data, structure solution and refinement for (24).

Identification code	exti44
Chemical formula	$C_{59}H_{54}O_{3.50}P_2Pd$
Formula weight	987.36
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, I2/a
Unit cell dimensions	a = 21.5459(15) Å α = 90° b = 21.2456(15) Å β = 111.643(2)° c = 23.0254(15) Å γ = 90°
Volume	9796.9(12) $Å^3$
Z	8
Density (calculated)	1.339 g/cm^3
Absorption coefficient μ	0.490 mm^{-1}
F(000)	4096
Reflections for cell refinement	12371 (θ range 2.21 to 28.66°)
Crystal colour	Orange
Crystal size	0.41 × 0.24 × 0.11 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	1.40 to 28.83°
Index ranges	$-27 \le h \le 24$, $-19 \le k \le 28$, $-29 \le \ell \le 25$
Intensity decay	0%
Reflections collected	30978
Independent reflections	11741 (R_{int} = 0.0471)
Reflections with I>2σ(I)	7813
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.9145 and 0.7807
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0573, 2.1794
Data / restraints / parameters	11741 / 0 / 601
Final R indices [I>2σ(I)]	R1 = 0.0455, wR2 = 0.0996
R indices (all data)	R1 = 0.0878, wR2 = 0.1158
Goodness-of-fit on F^2	1.016
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.962 and -0.506 $eÅ^{-3}$

The Crystal Structure of [{2,2-($C_6H_3O)_2PPh_2$}Pd(dba)] (24)

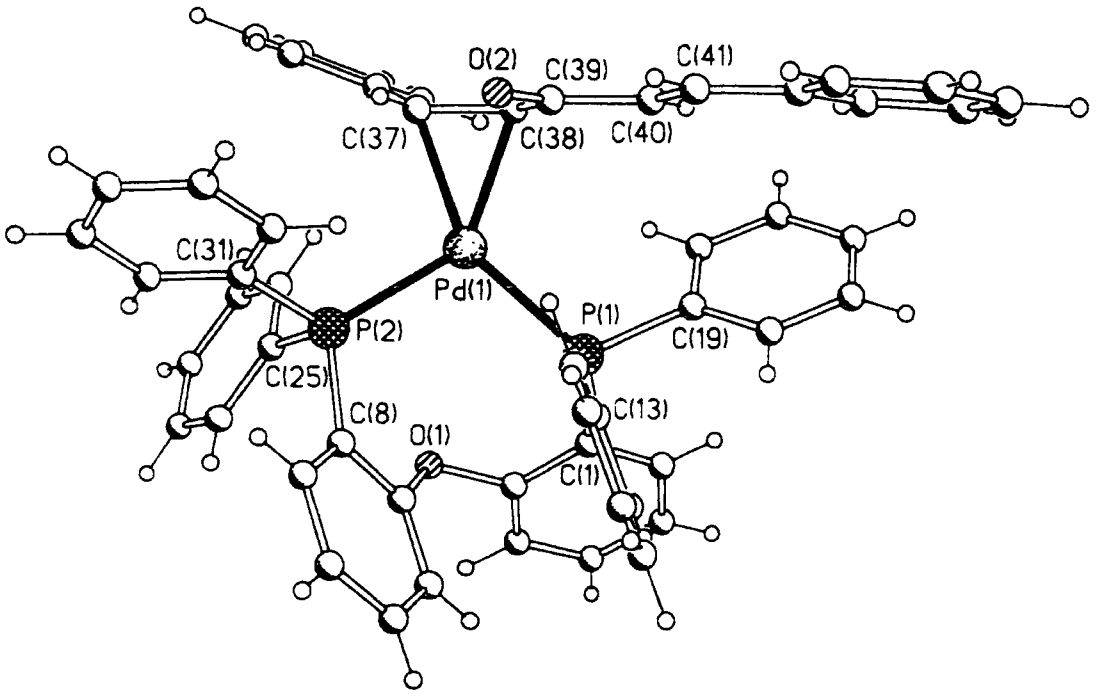


Table 9B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (24). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	4856.43(11)	6572.81(11)	2391.20(10)	22.17(8)
P(1)	4115.4(4)	5718.3(4)	2138.7(4)	24.24(18)
C(1)	4345.9(15)	4963.0(15)	2563.4(13)	25.7(7)
O(1)	5479.8(10)	5034.2(10)	2595.6(9)	28.2(5)
C(2)	4993.3(15)	4715.8(15)	2742.5(14)	26.7(7)
C(3)	5185.5(17)	4183.6(15)	3101.0(15)	32.6(8)
C(4)	4740.4(17)	3871.1(16)	3303.5(15)	35.1(8)
C(5)	4092.8(18)	4091.7(16)	3128.4(15)	36.6(8)
C(6)	3901.6(16)	4625.8(15)	2763.1(14)	31.5(7)
C(7)	5467.5(14)	4994.9(16)	1989.3(14)	27.3(7)
C(8)	5702.3(14)	5533.6(15)	1792.4(13)	26.3(7)
C(9)	5738.4(15)	5524.4(17)	1199.3(14)	32.2(8)
C(10)	5528.6(16)	4992.8(18)	823.3(15)	37.2(8)
C(11)	5287.8(16)	4478.8(18)	1025.4(15)	37.7(8)
C(12)	5261.9(15)	4465.5(16)	1622.9(15)	33.0(8)
C(13)	3833.6(14)	5489.5(15)	1315.0(14)	26.2(7)
C(14)	3653.2(15)	4877.8(16)	1107.1(15)	32.9(8)
C(15)	3418.0(16)	4739.8(18)	469.9(16)	40.3(9)
C(16)	3356.3(17)	5217.9(19)	45.4(15)	39.6(9)
C(17)	3527.1(18)	5822(2)	242.8(16)	44.9(9)
C(18)	3770.0(16)	5960.9(17)	877.0(15)	35.8(8)
C(19)	3323.0(15)	5869.9(14)	2247.7(14)	25.7(7)
C(20)	3360.3(16)	6154.1(16)	2803.9(15)	33.7(8)
C(21)	2792.4(18)	6233.1(17)	2942.3(17)	39.7(9)
C(22)	2180.4(17)	6037.5(18)	2524.8(18)	42.2(9)
C(23)	2134.4(16)	5769.5(17)	1967.7(17)	39.8(9)
C(24)	2704.8(15)	5683.9(16)	1829.4(15)	32.1(7)
P(2)	5831.0(4)	6229.5(4)	2288.4(4)	24.05(18)
C(25)	6560.0(14)	6033.6(15)	2981.4(13)	25.8(7)
C(26)	7031.5(16)	5592.5(18)	2976.9(16)	37.9(8)
C(27)	7580.5(17)	5466.4(19)	3513.9(17)	45.6(10)
C(28)	7662.2(18)	5792.8(19)	4058.3(18)	47.3(10)
C(29)	7200.9(18)	6231.6(19)	4067.7(16)	46.2(10)
C(30)	6646.1(16)	6353.2(17)	3527.1(15)	34.9(8)
C(31)	6150.2(15)	6799.0(15)	1870.8(14)	26.9(7)
C(32)	5685.6(16)	7147.4(16)	1399.9(14)	30.0(7)
C(33)	5889.2(17)	7571.6(16)	1047.5(15)	33.5(8)
C(34)	6556.4(18)	7659.3(17)	1168.9(15)	39.7(9)
C(35)	7027.4(18)	7321.9(19)	1644.8(16)	43.0(9)
C(36)	6829.0(16)	6891.7(18)	1993.6(15)	36.3(8)
C(37)	5071.8(15)	7551.3(15)	2624.4(15)	26.0(7)
C(38)	4380.8(15)	7446.7(15)	2470.2(15)	27.7(7)
C(39)	3913.2(15)	7547.6(15)	1828.8(15)	28.8(7)
O(2)	4097.3(11)	7723.8(11)	1404.0(10)	36.1(6)
C(40)	3195.8(15)	7430.4(15)	1699.0(15)	29.8(7)
C(41)	2735.9(16)	7527.6(18)	1135.3(15)	37.5(8)
C(42)	2014.7(16)	7416.3(17)	910.0(15)	34.4(8)
C(43)	1633.2(17)	7524(2)	284.4(16)	45.4(10)
C(44)	956.5(17)	7400.1(19)	41.5(16)	43.6(9)
C(45)	646.4(16)	7165.7(17)	420.1(16)	38.7(8)
C(46)	1013.1(17)	7067.3(17)	1044.7(16)	38.2(8)

C(47)	1687.5(16)	7192.9(16)	1287.4(15)	34.2(8)
C(48)	5556.3(14)	7671.6(15)	3259.7(14)	26.8(7)
C(49)	6136.4(16)	8013.5(16)	3339.5(16)	35.0(8)
C(50)	6614.2(17)	8115.8(19)	3934.0(18)	45.7(9)
C(51)	6522.7(18)	7878(2)	4455.0(17)	47.6(10)
C(52)	5949.0(17)	7542(2)	4379.4(16)	45.0(10)
C(53)	5468.6(16)	7441.6(17)	3789.0(15)	35.7(8)
C(54)	5498(3)	8827(3)	40(3)	103(2)
C(55)	4880(5)	8990(4)	-14(4)	140(3)
C(56)	4499(3)	9093(5)	-643(3)	162(4)
C(57)	5027(3)	9318(3)	-934(2)	85.2(16)
C(58)	5665(3)	9184(3)	-398(3)	109(2)
C(59)	7861(9)	4203(7)	5633(8)	103(6)
C(60)	7278(7)	4009(6)	5354(5)	188(5)
C(61)	6922(5)	4198(5)	4755(10)	208(6)

Table 9C. Bond lengths (Å) and angles (°) for (24).

Pd(1)-C(37)	2.155(3)	Pd(1)-C(38)	2.161(3)
Pd(1)-P(2)	2.3160(8)	Pd(1)-P(1)	2.3449(8)
P(1)-C(13)	1.831(3)	P(1)-C(19)	1.843(3)
P(1)-C(1)	1.849(3)	C(1)-C(6)	1.402(4)
C(1)-C(2)	1.403(4)	O(1)-C(7)	1.389(3)
O(1)-C(2)	1.390(4)	C(2)-C(3)	1.371(4)
C(3)-C(4)	1.381(5)	C(4)-C(5)	1.384(5)
C(5)-C(6)	1.382(4)	C(7)-C(12)	1.377(4)
C(7)-C(8)	1.393(4)	C(8)-C(9)	1.396(4)
C(8)-P(2)	1.826(3)	C(9)-C(10)	1.393(5)
C(10)-C(11)	1.363(5)	C(11)-C(12)	1.398(5)
C(13)-C(14)	1.390(4)	C(13)-C(18)	1.392(4)
C(14)-C(15)	1.395(4)	C(15)-C(16)	1.382(5)
C(16)-C(17)	1.366(5)	C(17)-C(18)	1.389(5)
C(19)-C(24)	1.383(4)	C(19)-C(20)	1.391(4)
C(20)-C(21)	1.384(4)	C(21)-C(22)	1.379(5)
C(22)-C(23)	1.373(5)	C(23)-C(24)	1.390(4)
P(2)-C(25)	1.827(3)	P(2)-C(31)	1.830(3)
C(25)-C(30)	1.379(4)	C(25)-C(26)	1.385(4)
C(26)-C(27)	1.386(4)	C(27)-C(28)	1.386(5)
C(28)-C(29)	1.369(5)	C(29)-C(30)	1.396(4)
C(31)-C(32)	1.387(4)	C(31)-C(36)	1.397(4)
C(32)-C(33)	1.388(4)	C(33)-C(34)	1.372(5)
C(34)-C(35)	1.387(5)	C(35)-C(36)	1.384(5)
C(37)-C(38)	1.415(4)	C(37)-C(48)	1.473(4)
C(38)-C(39)	1.464(4)	C(39)-O(2)	1.241(4)
C(39)-C(40)	1.483(4)	C(40)-C(41)	1.327(4)
C(41)-C(42)	1.465(4)	C(42)-C(47)	1.389(4)
C(42)-C(43)	1.389(4)	C(43)-C(44)	1.381(5)
C(44)-C(45)	1.372(5)	C(45)-C(46)	1.378(5)
C(46)-C(47)	1.377(4)	C(48)-C(53)	1.389(4)
C(48)-C(49)	1.398(4)	C(49)-C(50)	1.393(5)
C(50)-C(51)	1.381(5)	C(51)-C(52)	1.382(5)
C(52)-C(53)	1.388(4)	C(54)-C(55)	1.336(9)
C(54)-C(58)	1.411(8)	C(55)-C(56)	1.394(9)
C(56)-C(57)	1.591(9)	C(57)-C(58)	1.497(7)
C(59)-C(61A)	1.150(19)	C(59)-C(60)	1.252(18)
C(60)-C(61)	1.367(14)	C(60)-C(61A)	1.875(13)
C(61)-C(59A)	1.150(19)	C(61)-C(60A)	1.875(13)

C(37)-Pd(1)-C(38)	38.28(11)	C(37)-Pd(1)-P(2)	102.08(8)
C(38)-Pd(1)-P(2)	139.05(9)	C(37)-Pd(1)-P(1)	150.84(8)
C(38)-Pd(1)-P(1)	112.67(9)	P(2)-Pd(1)-P(1)	106.92(3)
C(13)-P(1)-C(19)	102.56(14)	C(13)-P(1)-C(1)	103.83(14)
C(19)-P(1)-C(1)	99.29(13)	C(13)-P(1)-Pd(1)	113.43(10)
C(19)-P(1)-Pd(1)	114.28(10)	C(1)-P(1)-Pd(1)	121.01(10)
C(6)-C(1)-C(2)	115.9(3)	C(6)-C(1)-P(1)	122.3(2)
C(2)-C(1)-P(1)	121.6(2)	C(7)-O(1)-C(2)	118.6(2)
C(3)-C(2)-O(1)	117.4(3)	C(3)-C(2)-C(1)	122.2(3)
O(1)-C(2)-C(1)	120.2(3)	C(2)-C(3)-C(4)	120.4(3)
C(3)-C(4)-C(5)	119.3(3)	C(6)-C(5)-C(4)	119.8(3)
C(5)-C(6)-C(1)	122.2(3)	C(12)-C(7)-O(1)	123.2(3)
C(12)-C(7)-C(8)	123.0(3)	O(1)-C(7)-C(8)	113.8(3)
C(7)-C(8)-C(9)	117.7(3)	C(7)-C(8)-P(2)	116.8(2)
C(9)-C(8)-P(2)	124.9(3)	C(10)-C(9)-C(8)	119.8(3)
C(11)-C(10)-C(9)	121.0(3)	C(10)-C(11)-C(12)	120.7(3)
C(7)-C(12)-C(11)	117.8(3)	C(14)-C(13)-C(18)	118.9(3)
C(14)-C(13)-P(1)	123.3(2)	C(18)-C(13)-P(1)	117.8(3)

C(13)-C(14)-C(15)	120.4(3)	C(16)-C(15)-C(14)	119.5(3)
C(17)-C(16)-C(15)	120.8(3)	C(16)-C(17)-C(18)	120.0(3)
C(17)-C(18)-C(13)	120.5(3)	C(24)-C(19)-C(20)	118.6(3)
C(24)-C(19)-P(1)	123.9(2)	C(20)-C(19)-P(1)	117.3(2)
C(21)-C(20)-C(19)	120.6(3)	C(22)-C(21)-C(20)	120.2(3)
C(23)-C(22)-C(21)	119.8(3)	C(22)-C(23)-C(24)	120.2(3)
C(19)-C(24)-C(23)	120.6(3)	C(8)-P(2)-C(25)	104.19(14)
C(8)-P(2)-C(31)	101.92(14)	C(25)-P(2)-C(31)	103.94(14)
C(8)-P(2)-Pd(1)	112.62(10)	C(25)-P(2)-Pd(1)	120.15(10)
C(31)-P(2)-Pd(1)	112.09(10)	C(30)-C(25)-C(26)	119.2(3)
C(30)-C(25)-P(2)	117.8(2)	C(26)-C(25)-P(2)	123.0(2)
C(25)-C(26)-C(27)	120.7(3)	C(28)-C(27)-C(26)	119.5(3)
C(29)-C(28)-C(27)	120.3(3)	C(28)-C(29)-C(30)	120.0(3)
C(25)-C(30)-C(29)	120.3(3)	C(32)-C(31)-C(36)	118.9(3)
C(32)-C(31)-P(2)	117.4(2)	C(36)-C(31)-P(2)	123.7(2)
C(31)-C(32)-C(33)	120.7(3)	C(34)-C(33)-C(32)	120.2(3)
C(33)-C(34)-C(35)	119.8(3)	C(36)-C(35)-C(34)	120.5(3)
C(35)-C(36)-C(31)	120.0(3)	C(38)-C(37)-C(48)	124.8(3)
C(38)-C(37)-Pd(1)	71.09(18)	C(48)-C(37)-Pd(1)	115.1(2)
C(37)-C(38)-C(39)	119.9(3)	C(37)-C(38)-Pd(1)	70.63(17)
C(39)-C(38)-Pd(1)	102.2(2)	O(2)-C(39)-C(38)	122.5(3)
O(2)-C(39)-C(40)	120.3(3)	C(38)-C(39)-C(40)	117.2(3)
C(41)-C(40)-C(39)	121.2(3)	C(40)-C(41)-C(42)	129.3(3)
C(47)-C(42)-C(43)	117.5(3)	C(47)-C(42)-C(41)	123.4(3)
C(43)-C(42)-C(41)	119.0(3)	C(44)-C(43)-C(42)	121.4(3)
C(45)-C(44)-C(43)	120.0(3)	C(44)-C(45)-C(46)	119.5(3)
C(47)-C(46)-C(45)	120.5(3)	C(46)-C(47)-C(42)	121.0(3)
C(53)-C(48)-C(49)	118.1(3)	C(53)-C(48)-C(37)	122.3(3)
C(49)-C(48)-C(37)	119.5(3)	C(50)-C(49)-C(48)	120.7(3)
C(51)-C(50)-C(49)	120.4(3)	C(50)-C(51)-C(52)	119.2(3)
C(51)-C(52)-C(53)	120.8(3)	C(52)-C(53)-C(48)	120.8(3)
C(55)-C(54)-C(58)	107.5(5)	C(54)-C(55)-C(56)	108.8(7)
C(55)-C(56)-C(57)	104.3(6)	C(58)-C(57)-C(56)	100.2(5)
C(54)-C(58)-C(57)	107.1(5)	C(61A)-C(59)-C(60)	102.6(16)
C(59)-C(60)-C(61)	120.2(11)	C(59)-C(60)-C(61A)	36.8(8)
C(61)-C(60)-C(61A)	90.2(8)	C(59A)-C(61)-C(60)	123.3(15)
C(59A)-C(61)-C(60A)	40.7(10)	C(60)-C(61)-C(60A)	82.7(8)

Symmetry transformations used to generate equivalent atoms:

A: -x+3/2,y,-z+1

Table 9D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (24).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	17.90(12)	24.73(13)	25.10(13)	-0.89(10)	9.35(9)	-0.57(10)
P(1)	21.1(4)	25.8(4)	26.9(4)	1.0(3)	10.2(3)	-0.6(3)
C(1)	29.0(16)	25.7(17)	23.1(16)	-2.9(13)	10.4(13)	-0.7(13)
O(1)	27.6(11)	31.1(13)	26.0(11)	-0.1(9)	9.8(9)	-0.4(9)
C(2)	33.3(17)	25.1(17)	25.0(17)	-3.8(13)	14.5(14)	-1.5(14)
C(3)	33.4(18)	28.5(19)	35.1(19)	0.1(14)	11.9(15)	5.1(14)
C(4)	49(2)	24.2(18)	33.4(19)	3.6(14)	16.8(16)	3.1(16)
C(5)	49(2)	28.9(19)	38(2)	1.0(15)	24.1(17)	-5.0(16)
C(6)	33.4(18)	29.4(19)	32.7(18)	-1.0(14)	13.4(15)	-2.6(14)
C(7)	20.2(15)	36.3(19)	25.8(17)	-2.5(14)	9.0(13)	6.2(13)
C(8)	17.6(14)	34.6(19)	25.1(16)	-2.4(13)	6.1(12)	4.7(13)
C(9)	23.2(16)	45(2)	28.3(18)	1.1(15)	9.4(14)	5.3(15)
C(10)	30.2(18)	56(2)	24.6(17)	-8.4(16)	8.5(14)	9.4(17)
C(11)	29.9(18)	44(2)	34.4(19)	-15.8(16)	6.7(15)	5.4(16)
C(12)	25.2(16)	31.3(19)	40(2)	-3.7(15)	9.6(15)	5.6(14)
C(13)	18.8(15)	33.7(19)	26.3(16)	3.1(14)	8.8(13)	-0.8(13)
C(14)	30.6(17)	34(2)	31.0(18)	1.3(15)	7.3(14)	-3.2(15)
C(15)	35.0(19)	44(2)	40(2)	-9.3(17)	12.3(16)	-2.1(17)
C(16)	33.7(19)	58(3)	25.1(18)	-2.3(17)	7.8(15)	-3.5(17)
C(17)	46(2)	57(3)	31(2)	9.6(17)	12.9(17)	-4.8(19)
C(18)	38.2(19)	36(2)	32.5(19)	3.8(15)	12.2(16)	-5.3(15)
C(19)	25.9(16)	22.5(17)	31.2(18)	5.0(13)	13.3(14)	0.8(13)
C(20)	29.7(17)	34(2)	40(2)	-1.7(15)	15.4(15)	-2.8(15)
C(21)	48(2)	35(2)	47(2)	-1.7(17)	31.1(18)	1.9(17)
C(22)	29.0(19)	46(2)	62(3)	7.4(19)	28.6(18)	1.8(16)
C(23)	22.3(17)	40(2)	55(2)	3.5(18)	12.3(16)	-3.9(15)
C(24)	24.7(16)	35(2)	37.0(19)	1.2(15)	12.4(14)	0.6(14)
P(2)	18.6(4)	30.1(5)	24.0(4)	0.2(3)	8.6(3)	0.8(3)
C(25)	20.8(15)	33.2(19)	22.5(16)	4.5(13)	7.1(13)	2.0(13)
C(26)	30.1(18)	48(2)	34.7(19)	-0.3(16)	10.2(15)	8.5(16)
C(27)	26.0(18)	56(3)	49(2)	6.2(19)	7.1(17)	14.2(17)
C(28)	33(2)	52(3)	43(2)	9.6(19)	-1.5(17)	3.6(18)
C(29)	45(2)	55(3)	28.1(19)	-1.1(17)	1.5(17)	5.5(19)
C(30)	31.5(18)	41(2)	30.3(18)	0.4(15)	8.9(15)	3.6(15)
C(31)	25.9(16)	29.8(18)	28.1(17)	-1.1(13)	13.6(14)	1.0(13)
C(32)	27.1(16)	36(2)	29.0(17)	2.2(14)	12.5(14)	0.2(14)
C(33)	38.4(19)	36(2)	27.7(18)	1.7(14)	13.6(15)	3.9(15)
C(34)	52(2)	40(2)	34(2)	1.7(16)	24.7(18)	-8.3(18)
C(35)	33.8(19)	56(3)	45(2)	-1.7(18)	20.2(17)	-11.8(18)
C(36)	25.7(17)	51(2)	32.9(19)	2.6(16)	11.7(15)	-0.9(16)
C(37)	30.5(17)	21.5(16)	27.8(17)	-1.1(13)	12.7(14)	-1.5(13)
C(38)	26.2(17)	30.1(19)	28.4(17)	-0.8(14)	12.0(14)	4.2(14)
C(39)	27.4(17)	25.2(18)	36.4(19)	-4.5(14)	14.7(15)	3.8(13)
O(2)	28.4(12)	47.6(16)	31.7(13)	1.7(11)	10.5(10)	-3.8(11)
C(40)	29.5(17)	29.3(19)	31.4(18)	-1.4(14)	12.2(15)	3.6(14)
C(41)	30.6(18)	53(2)	31.4(19)	-2.2(16)	14.2(15)	-0.6(16)
C(42)	28.3(17)	42(2)	31.9(19)	-3.9(15)	10.6(15)	-1.4(15)
C(43)	28.5(18)	77(3)	32(2)	-1.0(19)	12.4(16)	0.6(18)
C(44)	29.3(19)	65(3)	31.1(19)	-5.0(18)	4.3(15)	5.7(17)
C(45)	24.0(17)	44(2)	44(2)	-8.2(17)	7.8(16)	3.2(15)
C(46)	33.8(19)	41(2)	42(2)	-1.8(16)	16.4(16)	-4.3(16)

C(47)	31.5(18)	37(2)	31.5(18)	-1.3(15)	8.3(15)	0.8(15)
C(48)	21.4(15)	26.3(18)	32.1(18)	-3.5(13)	9.3(14)	2.8(13)
C(49)	32.7(18)	34(2)	39(2)	-1.9(15)	13.1(16)	-3.6(15)
C(50)	28.9(19)	49(2)	52(2)	-7.0(19)	7.1(17)	-7.9(17)
C(51)	34(2)	67(3)	36(2)	-14.2(19)	6.6(17)	4.4(19)
C(52)	36(2)	67(3)	33(2)	-1.8(18)	13.9(17)	9.2(19)
C(53)	28.2(17)	48(2)	33.3(19)	-5.0(16)	13.5(15)	-0.7(15)
C(54)	101(4)	155(6)	70(4)	65(4)	52(3)	69(4)
C(55)	173(8)	128(7)	126(7)	25(5)	63(6)	14(6)
C(56)	87(5)	335(14)	57(4)	-40(6)	16(4)	-12(6)
C(57)	95(4)	95(4)	57(3)	16(3)	18(3)	1(3)
C(58)	67(4)	139(6)	104(5)	-7(4)	10(3)	5(4)
C(59)	110(13)	87(10)	157(14)	-30(9)	100(12)	-21(8)
C(60)	159(9)	303(16)	119(7)	-34(8)	72(6)	-117(11)
C(61)	115(8)	159(10)	303(19)	65(12)	21(11)	48(7)

Table 9E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (24).

	x	y	z	U
H(3)	5628	4029	3211	39
H(4)	4878	3508	3560	42
H(5)	3780	3876	3259	44
H(6)	3454	4769	2643	38
H(9)	5905	5880	1053	39
H(10)	5554	4989	420	45
H(11)	5136	4126	757	45
H(12)	5108	4104	1771	40
H(14)	3690	4552	1400	39
H(15)	3301	4320	329	48
H(16)	3193	5125	-389	48
H(17)	3480	6147	-54	54
H(18)	3893	6381	1013	43
H(20)	3779	6295	3091	40
H(21)	2824	6423	3326	48
H(22)	1792	6088	2622	51
H(23)	1712	5642	1676	48
H(24)	2669	5496	1444	38
H(26)	6978	5374	2602	46
H(27)	7898	5159	3509	55
H(28)	8040	5712	4427	57
H(29)	7258	6453	4442	55
H(30)	6326	6657	3535	42
H(32)	5223	7095	1318	36
H(33)	5566	7802	721	40
H(34)	6695	7950	928	48
H(35)	7489	7386	1732	52
H(36)	7154	6660	2316	44
H(37)	5178(15)	7728(15)	2314(14)	31
H(38)	4208(15)	7439(15)	2788(14)	33
H(40)	3063	7283	2025	36
H(41)	2898	7693	835	45
H(43)	1842	7686	18	55
H(44)	705	7477	-388	52
H(45)	183	7072	253	46
H(46)	799	6912	1310	46
H(47)	1933	7126	1720	41
H(49)	6206	8178	2985	42
H(50)	7005	8350	3981	55
H(51)	6850	7945	4860	57
H(52)	5883	7377	4736	54
H(53)	5075	7213	3746	43

Table 10A. Crystal data, structure solution and refinement for (25).

Identification code	exti40
Chemical formula	$C_{41}H_{58}OP_2Pt$
Formula weight	823.90
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 9.2623(5) Å α = 97.976(2)°
	b = 11.4476(6) Å β = 93.121(2)°
	c = 19.3459(11) Å γ = 112.309(2)°
Volume	1866.48(18) $Å^3$
Z	2
Density (calculated)	1.466 g/cm^3
Absorption coefficient μ	3.875 mm^{-1}
F(000)	840
Reflections for cell refinement	10194 (θ range 2.38 to 28.72°)
Crystal colour	Yellow
Crystal size	0.41 × 0.32 × 0.02 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	2.06 to 28.80°
Index ranges	$-12 \le h \le 12$, $-15 \le k \le 14$, $-22 \le \ell \le 25$
Intensity decay	0%
Reflections collected	14128
Independent reflections	8516 (R_{int} = 0.0402)
Reflections with I>2σ(I)	6808
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.492 and 0.302
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0385, 0.0000
Data / restraints / parameters	8516 / 86 / 455
Final R indices [I>2σ(I)]	R1 = 0.0406, wR2 = 0.0850
R indices (all data)	R1 = 0.0547, wR2 = 0.0880
Goodness-of-fit on F^2	0.941
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	2.969 and -2.053 $eÅ^{-3}$

The Crystal Structure of [o-$C_6H_4(CH_2PBu^t_2)_2$Pt(dba)] (25)

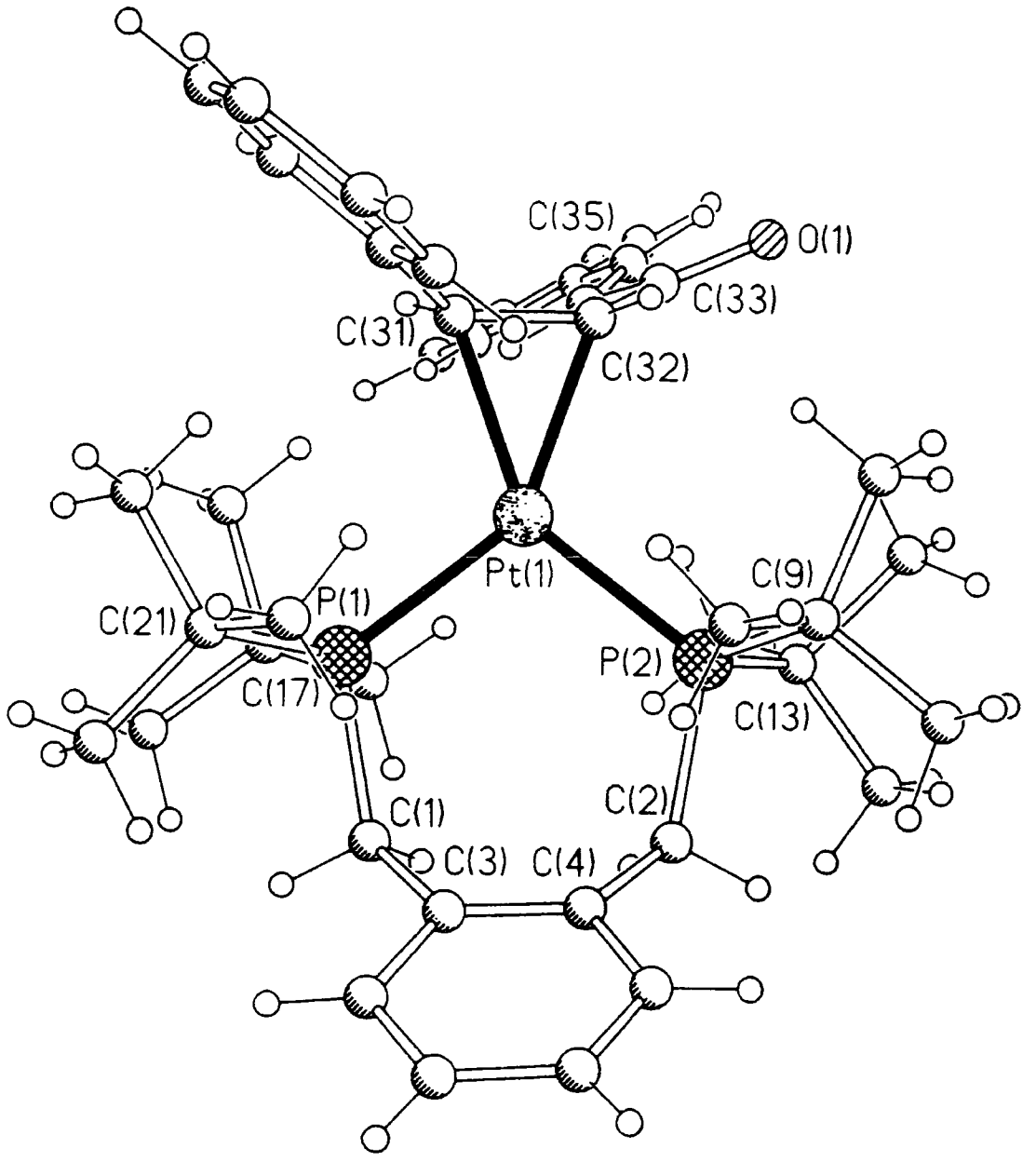


Table 10B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (25). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	3782.0(2)	6271.18(19)	7634.33(10)	20.11(7)
P(1)	1882.7(15)	6873.9(12)	8105.3(7)	22.2(3)
P(2)	2346.2(17)	4393.5(14)	6855.7(7)	29.1(3)
C(1)	-219(6)	5829(5)	7826(3)	30.0(13)
C(2)	183(7)	3721(5)	6830(3)	34.5(14)
C(3)	-850(6)	4445(5)	7938(3)	32.6(13)
C(4)	-619(7)	3489(5)	7488(3)	41.0(16)
C(5)	-1343(10)	2239(6)	7601(4)	73(3)
C(6)	-2228(11)	1905(7)	8146(4)	88(3)
C(7)	-2497(9)	2831(7)	8563(4)	71(3)
C(8)	-1829(7)	4092(6)	8464(3)	47.4(17)
C(9)	2945(10)	3085(6)	7092(4)	69(3)
C(10)	1962(9)	1738(5)	6667(3)	57(2)
C(11)	4673(11)	3399(9)	6975(8)	182(8)
C(12)	2725(16)	3054(8)	7879(4)	148(6)
C(13)	2463(7)	4452(7)	5884(3)	49.3(16)
C(14)	3952(12)	4090(11)	5707(6)	37(3)
C(15)	1116(14)	3309(10)	5432(6)	31(3)
C(16)	2658(15)	5677(10)	5757(6)	39(3)
C(14A)	4021(12)	5623(10)	5761(6)	38(3)
C(15A)	2068(18)	3374(10)	5331(6)	42(3)
C(16A)	1274(14)	5165(11)	5648(6)	37(3)
C(17)	1937(6)	8379(5)	7787(3)	28.6(12)
C(18)	3587(7)	9457(5)	7979(4)	44.0(16)
C(19)	1637(7)	8058(5)	6976(3)	35.5(14)
C(20)	715(7)	8884(6)	8055(3)	38.3(15)
C(21)	2026(6)	7106(5)	9095(3)	27.0(12)
C(22)	2216(7)	5896(5)	9286(3)	32.4(13)
C(23)	588(7)	7200(6)	9423(3)	38.5(15)
C(24)	3469(7)	8284(5)	9425(3)	35.3(14)
C(25)	6568(6)	7601(5)	8879(3)	25.1(12)
C(26)	7452(6)	8745(6)	9319(3)	35.2(14)
C(27)	7979(7)	8808(7)	10010(3)	45.1(17)
C(28)	7641(7)	7698(7)	10282(3)	48.5(18)
C(29)	6779(7)	6535(7)	9864(3)	41.2(16)
C(30)	6252(6)	6484(5)	9165(3)	31.3(13)
C(31)	6030(6)	7575(5)	8138(3)	26.7(12)
C(32)	6206(6)	6683(5)	7591(3)	27.3(12)
C(33)	6846(7)	7052(6)	6941(3)	34.4(14)
O(1)	7541(5)	6487(4)	6598(2)	40.1(10)
C(34)	6651(7)	8173(6)	6693(3)	42.9(16)
C(35)	7364(7)	8664(6)	6162(3)	42.3(16)
C(36)	7210(8)	9690(6)	5832(3)	45.8(17)
C(37)	7968(8)	9990(6)	5240(3)	46.9(17)
C(38)	7823(9)	10912(7)	4892(4)	66(2)
C(39)	6946(11)	11555(8)	5125(5)	80(3)
C(40)	6204(11)	11307(9)	5723(5)	84(3)
C(41)	6324(9)	10371(8)	6067(4)	66(2)

Table 10C. Bond lengths (Å) and angles (°) for (25).

Pt(1)-C(32)	2.121(5)	Pt(1)-C(31)	2.128(5)
Pt(1)-P(1)	2.3070(13)	Pt(1)-P(2)	2.3176(14)
P(1)-C(1)	1.858(5)	P(1)-C(21)	1.887(5)
P(1)-C(17)	1.892(5)	P(2)-C(2)	1.849(6)
P(2)-C(9)	1.885(6)	P(2)-C(13)	1.898(6)
C(1)-C(3)	1.518(8)	C(2)-C(4)	1.513(8)
C(3)-C(4)	1.391(8)	C(3)-C(8)	1.400(8)
C(4)-C(5)	1.385(8)	C(5)-C(6)	1.378(10)
C(6)-C(7)	1.350(11)	C(7)-C(8)	1.384(9)
C(9)-C(11)	1.538(13)	C(9)-C(10)	1.543(8)
C(9)-C(12)	1.550(13)	C(13)-C(16)	1.402(11)
C(13)-C(15A)	1.432(11)	C(13)-C(15)	1.536(12)
C(13)-C(14A)	1.610(11)	C(13)-C(14)	1.624(10)
C(13)-C(16A)	1.679(11)	C(17)-C(20)	1.537(7)
C(17)-C(18)	1.541(8)	C(17)-C(19)	1.546(8)
C(21)-C(24)	1.521(8)	C(21)-C(23)	1.539(7)
C(21)-C(22)	1.552(7)	C(25)-C(26)	1.383(8)
C(25)-C(30)	1.399(7)	C(25)-C(31)	1.484(7)
C(26)-C(27)	1.381(8)	C(27)-C(28)	1.374(9)
C(28)-C(29)	1.374(9)	C(29)-C(30)	1.399(8)
C(31)-C(32)	1.426(8)	C(32)-C(33)	1.467(8)
C(33)-O(1)	1.232(7)	C(33)-C(34)	1.499(8)
C(34)-C(35)	1.327(8)	C(35)-C(36)	1.461(8)
C(36)-C(41)	1.384(9)	C(36)-C(37)	1.392(8)
C(37)-C(38)	1.371(9)	C(38)-C(39)	1.345(11)
C(39)-C(40)	1.386(11)	C(40)-C(41)	1.373(10)
C(32)-Pt(1)-C(31)	39.2(2)	C(32)-Pt(1)-P(1)	147.89(16)
C(31)-Pt(1)-P(1)	108.84(15)	C(32)-Pt(1)-P(2)	108.40(16)
C(31)-Pt(1)-P(2)	147.26(15)	P(1)-Pt(1)-P(2)	103.69(5)
C(1)-P(1)-C(21)	103.3(3)	C(1)-P(1)-C(17)	99.3(2)
C(21)-P(1)-C(17)	110.4(2)	C(1)-P(1)-Pt(1)	118.83(19)
C(21)-P(1)-Pt(1)	114.39(16)	C(17)-P(1)-Pt(1)	109.47(18)
C(2)-P(2)-C(9)	104.4(3)	C(2)-P(2)-C(13)	98.2(3)
C(9)-P(2)-C(13)	109.5(3)	C(2)-P(2)-Pt(1)	118.22(18)
C(9)-P(2)-Pt(1)	108.6(2)	C(13)-P(2)-Pt(1)	116.9(2)
C(3)-C(1)-P(1)	119.8(4)	C(4)-C(2)-P(2)	122.0(4)
C(4)-C(3)-C(8)	118.5(6)	C(4)-C(3)-C(1)	122.1(5)
C(8)-C(3)-C(1)	119.1(6)	C(5)-C(4)-C(3)	117.8(6)
C(5)-C(4)-C(2)	118.5(6)	C(3)-C(4)-C(2)	123.1(5)
C(6)-C(5)-C(4)	123.5(7)	C(7)-C(6)-C(5)	118.2(7)
C(6)-C(7)-C(8)	120.5(7)	C(7)-C(8)-C(3)	121.3(7)
C(11)-C(9)-C(10)	107.4(6)	C(11)-C(9)-C(12)	110.8(8)
C(10)-C(9)-C(12)	108.4(7)	C(11)-C(9)-P(2)	109.7(7)
C(10)-C(9)-P(2)	114.6(4)	C(12)-C(9)-P(2)	106.0(5)
C(16)-C(13)-C(15A)	122.6(8)	C(16)-C(13)-C(15)	116.9(8)
C(15A)-C(13)-C(15)	34.7(6)	C(16)-C(13)-C(14A)	50.0(7)
C(15A)-C(13)-C(14A)	111.0(8)	C(15)-C(13)-C(14A)	137.5(8)
C(16)-C(13)-C(14)	112.7(8)	C(15A)-C(13)-C(14)	66.9(7)
C(15)-C(13)-C(14)	100.6(7)	C(14A)-C(13)-C(14)	64.3(6)
C(16)-C(13)-C(16A)	44.0(6)	C(15A)-C(13)-C(16A)	103.1(7)
C(15)-C(13)-C(16A)	79.3(7)	C(14A)-C(13)-C(16A)	93.0(7)
C(14)-C(13)-C(16A)	146.6(7)	C(16)-C(13)-P(2)	109.8(6)
C(15A)-C(13)-P(2)	126.2(7)	C(15)-C(13)-P(2)	111.2(6)
C(14A)-C(13)-P(2)	111.2(5)	C(14)-C(13)-P(2)	104.7(5)
C(16A)-C(13)-P(2)	106.4(5)	C(20)-C(17)-C(18)	108.9(5)
C(20)-C(17)-C(19)	108.3(4)	C(18)-C(17)-C(19)	107.0(5)
C(20)-C(17)-P(1)	115.1(4)	C(18)-C(17)-P(1)	110.5(4)

C(19)-C(17)-P(1)	106.8(3)	C(24)-C(21)-C(23)	108.2(4)
C(24)-C(21)-C(22)	108.9(4)	C(23)-C(21)-C(22)	107.6(5)
C(24)-C(21)-P(1)	111.0(4)	C(23)-C(21)-P(1)	116.1(4)
C(22)-C(21)-P(1)	104.8(3)	C(26)-C(25)-C(30)	116.5(5)
C(26)-C(25)-C(31)	121.1(5)	C(30)-C(25)-C(31)	122.4(5)
C(27)-C(26)-C(25)	122.7(6)	C(28)-C(27)-C(26)	119.8(6)
C(27)-C(28)-C(29)	119.8(6)	C(28)-C(29)-C(30)	119.9(6)
C(25)-C(30)-C(29)	121.3(5)	C(32)-C(31)-C(25)	119.7(5)
C(32)-C(31)-Pt(1)	70.1(3)	C(25)-C(31)-Pt(1)	122.2(4)
C(31)-C(32)-C(33)	122.6(5)	C(31)-C(32)-Pt(1)	70.7(3)
C(33)-C(32)-Pt(1)	117.0(4)	O(1)-C(33)-C(32)	122.7(5)
O(1)-C(33)-C(34)	119.2(5)	C(32)-C(33)-C(34)	118.1(5)
C(35)-C(34)-C(33)	121.5(6)	C(34)-C(35)-C(36)	127.8(6)
C(41)-C(36)-C(37)	117.8(6)	C(41)-C(36)-C(35)	123.7(6)
C(37)-C(36)-C(35)	118.5(6)	C(38)-C(37)-C(36)	121.3(7)
C(39)-C(38)-C(37)	120.0(7)	C(38)-C(39)-C(40)	120.4(7)
C(41)-C(40)-C(39)	119.8(8)	C(40)-C(41)-C(36)	120.6(7)

Table 10D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (25).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pt(1)	20.80(11)	20.55(11)	21.79(11)	8.84(7)	1.63(7)	9.53(8)
P(1)	20.9(7)	20.1(7)	29.3(8)	9.8(6)	2.7(6)	10.3(6)
P(2)	31.9(8)	29.4(8)	24.9(8)	0.0(6)	-5.1(6)	13.6(7)
C(1)	19(3)	32(3)	40(3)	14(3)	4(2)	9(2)
C(2)	38(3)	26(3)	26(3)	5(2)	0(3)	-2(3)
C(3)	23(3)	37(3)	29(3)	11(3)	0(2)	0(3)
C(4)	47(4)	26(3)	33(3)	10(3)	6(3)	-7(3)
C(5)	107(7)	26(4)	51(5)	0(3)	25(5)	-13(4)
C(6)	137(9)	31(4)	56(5)	12(4)	35(5)	-16(5)
C(7)	70(5)	56(5)	41(4)	7(4)	16(4)	-26(4)
C(8)	37(4)	47(4)	41(4)	11(3)	6(3)	-4(3)
C(9)	102(7)	43(4)	62(5)	-24(4)	-50(4)	49(4)
C(10)	102(6)	26(3)	40(4)	-3(3)	-22(4)	27(4)
C(11)	81(7)	70(6)	370(2)	-101(9)	-102(10)	65(6)
C(12)	323(17)	74(6)	69(6)	-27(5)	-110(9)	132(9)
C(13)	37(4)	75(4)	23(3)	-5(3)	3(3)	13(3)
C(14)	35(6)	36(7)	30(7)	7(5)	1(5)	4(5)
C(15)	45(7)	40(6)	17(6)	4(5)	5(6)	27(6)
C(16)	36(8)	51(6)	23(6)	9(5)	2(5)	8(6)
C(14A)	48(7)	37(6)	30(6)	4(5)	-1(5)	19(5)
C(15A)	70(10)	32(6)	26(7)	1(5)	-2(7)	24(6)
C(16A)	53(7)	34(6)	20(6)	13(5)	3(5)	11(6)
C(17)	31(3)	21(3)	37(3)	9(2)	-3(2)	13(2)
C(18)	43(4)	25(3)	68(5)	22(3)	1(3)	13(3)
C(19)	49(4)	26(3)	39(3)	15(3)	8(3)	20(3)
C(20)	50(4)	36(3)	41(4)	7(3)	1(3)	31(3)
C(21)	30(3)	35(3)	24(3)	7(2)	7(2)	20(3)
C(22)	35(3)	43(3)	28(3)	16(3)	6(2)	22(3)
C(23)	35(3)	50(4)	39(4)	9(3)	10(3)	25(3)
C(24)	37(3)	42(3)	33(3)	5(3)	5(3)	23(3)
C(25)	17(3)	29(3)	32(3)	11(2)	5(2)	10(2)
C(26)	28(3)	34(3)	45(4)	5(3)	3(3)	15(3)
C(27)	33(4)	56(4)	41(4)	-8(3)	1(3)	19(3)
C(28)	37(4)	77(5)	36(4)	10(4)	5(3)	27(4)
C(29)	34(4)	65(4)	39(4)	25(3)	11(3)	28(3)
C(30)	22(3)	33(3)	41(3)	11(3)	1(2)	11(2)
C(31)	19(3)	25(3)	36(3)	13(2)	0(2)	7(2)
C(32)	27(3)	30(3)	31(3)	14(2)	7(2)	14(3)
C(33)	26(3)	47(4)	39(3)	18(3)	8(3)	20(3)
O(1)	38(2)	53(3)	46(3)	25(2)	16(2)	29(2)
C(34)	38(4)	57(4)	54(4)	33(3)	22(3)	32(3)
C(35)	43(4)	54(4)	48(4)	29(3)	23(3)	30(3)
C(36)	53(4)	53(4)	49(4)	34(3)	21(3)	30(4)
C(37)	52(4)	48(4)	46(4)	27(3)	17(3)	18(3)
C(38)	72(6)	67(5)	68(5)	48(4)	23(4)	23(5)
C(39)	106(8)	67(6)	87(7)	53(5)	16(6)	43(5)
C(40)	116(8)	92(7)	97(7)	65(6)	50(6)	77(6)
C(41)	76(6)	80(6)	80(6)	53(5)	38(5)	54(5)

Table 10E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (25).

	x	y	z	U
H(1A)	-853	6247	8072	36
H(1B)	-427	5821	7318	36
H(2A)	-198	4296	6609	41
H(2B)	-217	2889	6505	41
H(5)	-1224	1577	7285	88
H(6)	-2637	1045	8227	106
H(7)	-3150	2616	8926	85
H(8)	-2040	4731	8759	57
H(10A)	2176	1093	6890	86
H(10B)	2245	1691	6186	86
H(10C)	843	1575	6656	86
H(11A)	5034	2801	7173	274
H(11B)	5319	4278	7207	274
H(11C)	4766	3318	6470	274
H(12A)	1650	2960	7951	223
H(12B)	3471	3855	8164	223
H(12C)	2913	2328	8018	223
H(14A)	3666	3171	5700	55
H(14B)	4842	4581	6069	55
H(14C)	4247	4300	5247	55
H(15A)	1251	3325	4934	46
H(15B)	110	3364	5521	46
H(15C)	1127	2508	5552	46
H(16A)	2695	5697	5254	59
H(16B)	3640	6312	6020	59
H(16C)	1773	5877	5909	59
H(14D)	4951	5462	5902	57
H(14E)	4073	6421	6043	57
H(14F)	3987	5699	5262	57
H(15D)	2118	3664	4876	63
H(15E)	1002	2758	5355	63
H(15F)	2814	2964	5383	63
H(16D)	1546	5476	5206	55
H(16E)	1400	5888	6016	55
H(16F)	180	4546	5583	55
H(18A)	4381	9124	7846	66
H(18B)	3764	9772	8487	66
H(18C)	3664	10162	7728	66
H(19A)	1741	8834	6787	53
H(19B)	575	7403	6831	53
H(19C)	2407	7733	6795	53
H(20A)	957	9182	8564	57
H(20B)	-334	8194	7951	57
H(20C)	742	9597	7821	57
H(22A)	2244	5928	9796	49
H(22B)	3198	5868	9136	49
H(22C)	1328	5127	9048	49
H(23A)	809	7374	9936	58
H(23B)	-323	6390	9275	58
H(23C)	363	7897	9265	58
H(24A)	3237	9052	9431	53
H(24B)	4346	8350	9150	53

H(24C)	3753	8209	9908	53
H(26)	7708	9521	9138	42
H(27)	8572	9615	10297	54
H(28)	8002	7736	10757	58
H(29)	6541	5766	10050	49
H(30)	5668	5674	8878	38
H(31)	6190(6)	8450(5)	8000(3)	32
H(32)	6440(6)	6030(5)	7680(3)	33
H(34)	6002	8541	6922	51
H(35)	8059	8304	5973	51
H(37)	8599	9547	5074	56
H(38)	8343	11096	4486	79
H(39)	6834	12184	4878	95
H(40)	5614	11784	5894	101
H(41)	5794	10189	6471	80

Table 11A. Crystal data, structure solution and refinement for (27).

Identification code	exti43
Chemical formula	$C_{30}H_{48}O_2P_2Pd$
Formula weight	609.02
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 8.725(3) Å α = 90° b = 16.465(6) Å β = 94.544(7)° c = 21.038(8) Å γ = 90°
Volume	3012.8(19) $Å^3$
Z	4
Density (calculated)	1.343 g/cm^3
Absorption coefficient μ	0.746 mm^{-1}
F(000)	1280
Reflections for cell refinement	6453 (θ range 2.31 to 27.67°)
Crystal colour	orange
Crystal size	0.28 × 0.18 × 0.06 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	1.57 to 25.00°
Index ranges	$-9 \le h \le 10$, $-19 \le k \le 14$, $-18 \le \ell \le 25$
Intensity decay	0%
Reflections collected	15281
Independent reflections	5301 (R_{int} = 0.1199)
Reflections with I>2σ(I)	3207
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.802 and 0.374
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0866, 0.0000
Data / restraints / parameters	5301 / 2 / 334
Final R indices [I>2σ(I)]	R1 = 0.0657, wR2 = 0.1516
R indices (all data)	R1 = 0.1137, wR2 = 0.1668
Goodness-of-fit on F^2	0.938
Largest and mean shift/esd	0.000 and 0.000
Largest diff. peak and hole	2.592 and -2.004 $eÅ^{-3}$

The Crystal Structure of [o–$C_6H_4(CH_2PBu^t_2)_2Pd(bq)$] (27)

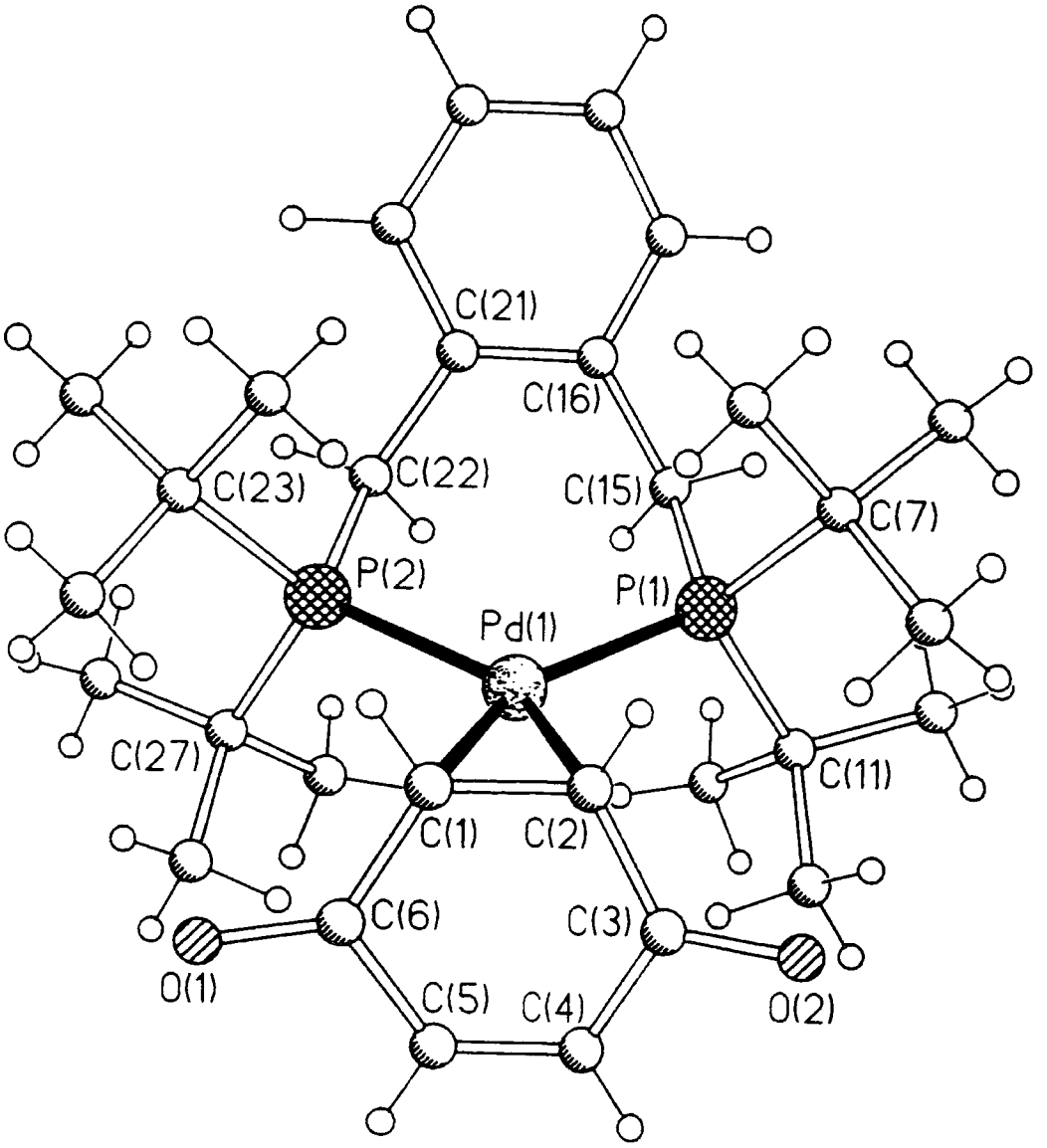


Table 11B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (27). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	6185.6(6)	8011.7(3)	1099.4(2)	19.4(2)
O(1)	3090(6)	9430(3)	1814(3)	43.0(15)
O(2)	2804(6)	7637(4)	-261(2)	42.5(15)
C(1)	3858(8)	8177(5)	1385(4)	28.9(19)
C(2)	3794(8)	7684(5)	827(3)	23.9(17)
C(3)	3274(8)	8055(5)	224(4)	31.2(19)
C(4)	3233(8)	8928(5)	178(4)	39(2)
C(5)	3312(9)	9389(6)	706(4)	42(2)
C(6)	3428(8)	9020(5)	1350(4)	34(2)
P(1)	7753(2)	7322.2(12)	414.3(8)	20.6(4)
P(2)	7931(2)	8578.7(11)	1895.1(8)	20.1(4)
C(7)	7083(9)	6234(5)	300(3)	31.9(19)
C(8)	8214(10)	5635(5)	22(4)	42(2)
C(9)	5563(9)	6212(5)	-135(4)	36(2)
C(10)	6719(10)	5930(4)	980(4)	36(2)
C(11)	7885(8)	7821(5)	-398(3)	29.0(19)
C(12)	6279(8)	8135(5)	-644(3)	30.7(19)
C(13)	8525(11)	7280(5)	-909(4)	45(2)
C(14)	8926(9)	8562(5)	-308(4)	37(2)
C(15)	9840(8)	7240(5)	678(3)	27.6(18)
C(16)	10335(7)	6879(4)	1327(3)	23.8(17)
C(17)	10938(9)	6096(5)	1357(4)	34(2)
C(18)	11519(9)	5747(5)	1929(4)	33(2)
C(19)	11543(9)	6196(5)	2479(4)	37(2)
C(20)	11017(8)	6979(5)	2454(3)	31.1(18)
C(21)	10384(8)	7338(5)	1891(3)	23.7(17)
C(22)	9957(8)	8233(4)	1881(3)	23.2(17)
C(23)	7366(8)	8300(5)	2726(3)	26.5(18)
C(24)	5966(8)	8794(5)	2893(3)	31.8(19)
C(25)	8658(10)	8421(5)	3277(3)	38(2)
C(26)	6939(10)	7411(5)	2696(4)	40(2)
C(27)	8215(8)	9715(4)	1824(3)	22.1(17)
C(28)	9129(10)	10103(5)	2401(4)	45(2)
C(29)	6639(8)	10128(5)	1720(4)	37(2)
C(30)	9042(9)	9889(5)	1235(4)	41(2)

Table 11C. Bond lengths (Å) and angles (°) for (27).

Pd(1)-C(1)	2.179(7)	Pd(1)-C(2)	2.187(7)
Pd(1)-P(1)	2.3556(19)	Pd(1)-P(2)	2.364(2)
O(1)-C(6)	1.241(9)	O(2)-C(3)	1.271(9)
C(1)-C(2)	1.425(10)	C(1)-C(6)	1.438(11)
C(2)-C(3)	1.448(11)	C(3)-C(4)	1.441(11)
C(4)-C(5)	1.343(11)	C(5)-C(6)	1.481(11)
P(1)-C(15)	1.866(7)	P(1)-C(7)	1.894(8)
P(1)-C(11)	1.908(7)	P(2)-C(22)	1.860(7)
P(2)-C(27)	1.895(7)	P(2)-C(23)	1.909(7)
C(7)-C(8)	1.541(10)	C(7)-C(9)	1.551(11)
C(7)-C(10)	1.573(10)	C(11)-C(14)	1.524(11)
C(11)-C(13)	1.535(10)	C(11)-C(12)	1.544(10)
C(15)-C(16)	1.520(10)	C(16)-C(17)	1.393(10)
C(16)-C(21)	1.406(10)	C(17)-C(18)	1.392(10)
C(18)-C(19)	1.372(11)	C(19)-C(20)	1.368(10)
C(20)-C(21)	1.398(10)	C(21)-C(22)	1.519(10)
C(23)-C(26)	1.511(11)	C(23)-C(24)	1.532(10)
C(23)-C(25)	1.565(10)	C(27)-C(30)	1.509(9)
C(27)-C(29)	1.534(10)	C(27)-C(28)	1.538(10)
C(1)-Pd(1)-C(2)	38.1(3)	C(1)-Pd(1)-P(1)	145.8(2)
C(2)-Pd(1)-P(1)	108.0(2)	C(1)-Pd(1)-P(2)	108.5(2)
C(2)-Pd(1)-P(2)	146.16(19)	P(1)-Pd(1)-P(2)	104.53(7)
C(2)-C(1)-C(6)	121.1(7)	C(2)-C(1)-Pd(1)	71.3(4)
C(6)-C(1)-Pd(1)	110.6(5)	C(1)-C(2)-C(3)	118.0(7)
C(1)-C(2)-Pd(1)	70.7(4)	C(3)-C(2)-Pd(1)	110.6(5)
O(2)-C(3)-C(4)	118.7(7)	O(2)-C(3)-C(2)	122.3(8)
C(4)-C(3)-C(2)	119.0(7)	C(5)-C(4)-C(3)	120.6(8)
C(4)-C(5)-C(6)	121.4(8)	O(1)-C(6)-C(1)	124.2(8)
O(1)-C(6)-C(5)	119.6(8)	C(1)-C(6)-C(5)	116.1(7)
C(15)-P(1)-C(7)	104.7(4)	C(15)-P(1)-C(11)	99.8(3)
C(7)-P(1)-C(11)	109.4(3)	C(15)-P(1)-Pd(1)	117.0(2)
C(7)-P(1)-Pd(1)	110.2(2)	C(11)-P(1)-Pd(1)	114.8(2)
C(22)-P(2)-C(27)	99.8(3)	C(22)-P(2)-C(23)	104.8(3)
C(27)-P(2)-C(23)	110.8(3)	C(22)-P(2)-Pd(1)	115.3(2)
C(27)-P(2)-Pd(1)	114.5(2)	C(23)-P(2)-Pd(1)	110.8(2)
C(8)-C(7)-C(9)	107.7(6)	C(8)-C(7)-C(10)	108.8(7)
C(9)-C(7)-C(10)	107.7(6)	C(8)-C(7)-P(1)	116.9(6)
C(9)-C(7)-P(1)	109.8(6)	C(10)-C(7)-P(1)	105.5(5)
C(14)-C(11)-C(13)	107.7(7)	C(14)-C(11)-C(12)	106.9(6)
C(13)-C(11)-C(12)	109.3(6)	C(14)-C(11)-P(1)	108.1(5)
C(13)-C(11)-P(1)	115.4(5)	C(12)-C(11)-P(1)	109.1(5)
C(16)-C(15)-P(1)	119.8(5)	C(17)-C(16)-C(21)	118.3(7)
C(17)-C(16)-C(15)	118.9(6)	C(21)-C(16)-C(15)	122.4(7)
C(18)-C(17)-C(16)	122.1(7)	C(19)-C(18)-C(17)	119.2(7)
C(20)-C(19)-C(18)	119.5(7)	C(19)-C(20)-C(21)	122.8(7)
C(20)-C(21)-C(16)	118.1(7)	C(20)-C(21)-C(22)	120.2(7)
C(16)-C(21)-C(22)	121.3(6)	C(21)-C(22)-P(2)	121.9(5)
C(26)-C(23)-C(24)	109.0(6)	C(26)-C(23)-C(25)	108.4(7)
C(24)-C(23)-C(25)	107.6(6)	C(26)-C(23)-P(2)	106.0(5)
C(24)-C(23)-P(2)	110.5(5)	C(25)-C(23)-P(2)	115.2(5)
C(30)-C(27)-C(29)	106.3(6)	C(30)-C(27)-C(28)	108.5(6)
C(29)-C(27)-C(28)	109.4(6)	C(30)-C(27)-P(2)	109.0(5)
C(29)-C(27)-P(2)	109.1(5)	C(28)-C(27)-P(2)	114.2(5)

Table 11D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (27).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	14.1(3)	26.5(4)	15.6(3)	-0.2(3)	-12.2(2)	-0.9(3)
O(1)	17(3)	53(4)	57(4)	-26(3)	-10(3)	3(3)
O(2)	26(3)	70(4)	29(3)	-7(3)	-20(3)	1(3)
C(1)	11(3)	45(6)	29(4)	-2(4)	-5(3)	-4(4)
C(2)	11(3)	30(5)	29(4)	-5(4)	-14(3)	-7(3)
C(3)	10(3)	49(6)	33(4)	-3(4)	-9(3)	-2(4)
C(4)	18(4)	49(7)	46(5)	15(5)	-20(4)	2(4)
C(5)	19(4)	44(6)	61(6)	7(5)	-16(4)	5(4)
C(6)	11(4)	40(6)	50(5)	-10(4)	-13(4)	0(4)
P(1)	18.0(10)	27.9(12)	13.9(9)	0.7(8)	-11.7(8)	0.1(8)
P(2)	16.1(9)	25.5(12)	16.3(9)	0.5(8)	-13.6(8)	-1.1(8)
C(7)	28(4)	43(5)	23(4)	-5(4)	-14(3)	-2(4)
C(8)	47(5)	33(5)	43(5)	-13(4)	-23(4)	10(4)
C(9)	44(5)	25(5)	35(5)	-3(4)	-23(4)	-8(4)
C(10)	50(5)	14(5)	40(5)	9(4)	-19(4)	-5(4)
C(11)	23(4)	42(6)	21(4)	5(3)	-6(3)	4(4)
C(12)	23(4)	45(6)	22(4)	5(4)	-11(3)	6(4)
C(13)	54(6)	59(6)	22(4)	9(4)	1(4)	20(5)
C(14)	26(4)	50(6)	32(4)	20(4)	-13(4)	-4(4)
C(15)	19(4)	45(5)	18(4)	2(3)	-8(3)	10(3)
C(16)	13(3)	33(5)	23(4)	-1(3)	-14(3)	4(3)
C(17)	33(5)	32(5)	33(4)	-9(4)	-20(4)	7(4)
C(18)	27(4)	26(5)	44(5)	9(4)	-14(4)	11(4)
C(19)	34(5)	50(6)	25(4)	13(4)	-12(4)	11(4)
C(20)	31(4)	35(5)	25(4)	4(4)	-14(3)	8(4)
C(21)	15(4)	29(5)	26(4)	7(3)	-9(3)	4(3)
C(22)	17(4)	35(5)	16(3)	-2(3)	-14(3)	1(3)
C(23)	27(4)	35(5)	16(4)	0(3)	-9(3)	-3(4)
C(24)	31(5)	45(5)	18(4)	5(4)	-9(3)	1(4)
C(25)	44(5)	54(6)	12(4)	4(4)	-17(4)	2(4)
C(26)	44(5)	45(6)	29(5)	17(4)	-2(4)	-6(4)
C(27)	18(4)	22(5)	24(4)	-2(3)	-17(3)	1(3)
C(28)	56(6)	22(5)	51(6)	-7(4)	-37(5)	-6(4)
C(29)	25(4)	30(5)	52(5)	5(4)	-13(4)	-3(4)
C(30)	36(5)	37(6)	50(5)	18(4)	-2(4)	4(4)

Table 11E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (27).

	x	y	z	U
H(1)	3860(8)	7920(4)	1789(16)	35
H(2)	3640(8)	7117(9)	880(3)	29
H(4)	3149	9179	-230	46
H(5)	3293	9964	666	51
H(8A)	7758	5091	0	64
H(8B)	9175	5623	297	64
H(8C)	8426	5811	-407	64
H(9A)	5780	6325	-576	54
H(9B)	4854	6623	8	54
H(9C)	5093	5673	-112	54
H(10A)	5872	6251	1130	54
H(10B)	7634	5995	1278	54
H(10C)	6424	5356	958	54
H(12A)	6349	8417	-1051	46
H(12B)	5900	8512	-332	46
H(12C)	5568	7676	-705	46
H(13A)	7889	6792	-970	68
H(13B)	9584	7124	-772	68
H(13C)	8512	7580	-1312	68
H(14A)	9996	8385	-225	55
H(14B)	8624	8883	54	55
H(14C)	8829	8895	-696	55
H(15A)	10329	6914	354	33
H(15B)	10282	7793	666	33
H(17)	10955	5789	975	41
H(18)	11893	5205	1938	40
H(19)	11922	5965	2875	45
H(20)	11086	7291	2835	37
H(22A)	10356	8469	1494	28
H(22B)	10543	8488	2251	28
H(24A)	5158	8756	2544	48
H(24B)	6264	9364	2959	48
H(24C)	5581	8579	3285	48
H(25A)	8295	8223	3678	57
H(25B)	8910	9000	3318	57
H(25C)	9576	8117	3181	57
H(26A)	6638	7233	3113	60
H(26B)	7824	7091	2581	60
H(26C)	6077	7330	2374	60
H(28A)	10107	9815	2486	68
H(28B)	8533	10065	2775	68
H(28C)	9331	10675	2309	68
H(29A)	6780	10713	1660	55
H(29B)	6056	10036	2093	55
H(29C)	6074	9899	1340	55
H(30A)	8919	10464	1121	62
H(30B)	8607	9552	882	62
H(30C)	10138	9764	1320	62

Table 12A. Crystal data, structure solution and refinement for (29).

Identification code	exti46
Chemical formula	$C_{26}H_{48}O_2P_2Pd$
Formula weight	560.98
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, C2/c
Unit cell dimensions	a = 14.4257(16) Å α = 90°
	b = 19.843(2) Å β = 91.218(3)°
	c = 18.835(2) Å γ = 90°
Volume	5390.2(10) Å^3
Z	8
Density (calculated)	1.383 g/cm^3
Absorption coefficient μ	0.827 mm^{-1}
F(000)	2368
Reflections for cell refinement	9529 (θ range 2.07 to 28.89°)
Crystal colour	orange
Crystal size	0.48 × 0.10 × 0.08 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	2.04 to 28.89°
Index ranges	$-13 \le h \le 19$, $-26 \le k \le 25$, $-22 \le \ell \le 24$
Intensity decay	0%
Reflections collected	17248
Independent reflections	6431 (R_{int} = 0.0404)
Reflections with I>2σ(I)	4812
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.8622 and 0.7462
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0380, 0.0000
Data / restraints / parameters	6431 / 0 / 298
Final R indices [I>2σ(I)]	R1 = 0.0356, wR2 = 0.0700
R indices (all data)	R1 = 0.0615, wR2 = 0.0774
Goodness-of-fit on F^2	0.988
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	1.159 and -0.623 eÅ^{-3}

The Crystal Structure of [1,4-C_4H_8(PBu^t_2)$_2$ Pd (BQ)] (29)

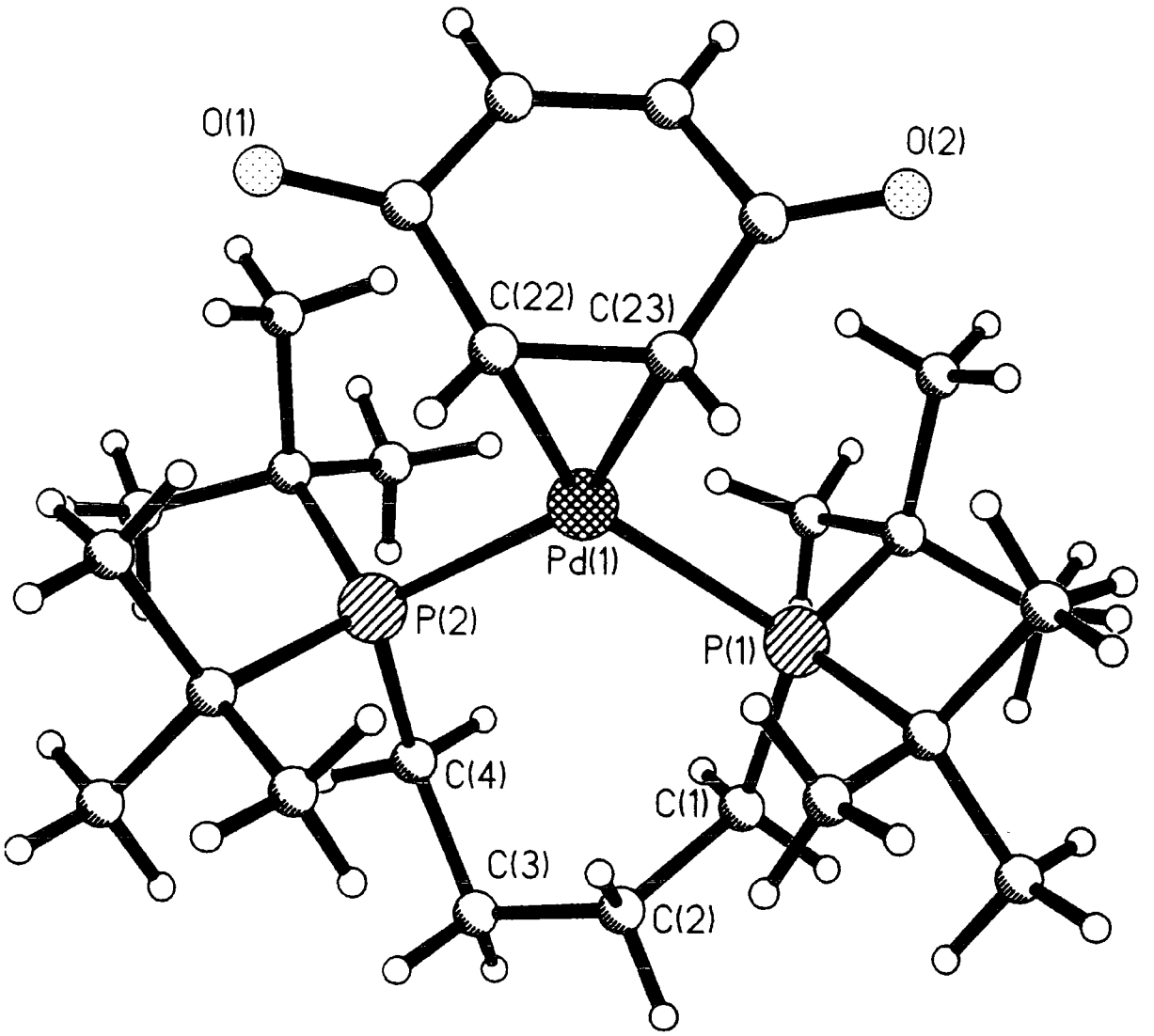


Table 12B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (29). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	7696.76(14)	4809.96(9)	1889.26(9)	15.87(6)
P(1)	7646.4(5)	5676.2(3)	1033.0(3)	18.95(15)
C(1)	7882(2)	5378.3(14)	127.7(13)	24.4(6)
C(2)	8712(2)	4897.6(14)	101.2(15)	28.2(6)
C(3)	8480(2)	4185.4(14)	-147.6(13)	26.8(6)
C(4)	7667.6(19)	3857.4(13)	230.4(12)	23.5(6)
P(2)	7662.4(5)	3798.0(3)	1215.1(3)	16.87(14)
C(5)	8614(2)	6313.0(14)	1193.0(14)	25.9(6)
C(6)	9482.7(19)	5933.5(14)	1468.1(15)	29.1(7)
C(7)	8887(2)	6700.4(16)	524.2(16)	39.3(8)
C(8)	8341(2)	6817.6(14)	1769.3(16)	34.9(7)
C(9)	6493.7(19)	6121.4(13)	905.1(14)	23.5(6)
C(10)	6520(2)	6752.7(15)	439.2(16)	36.0(7)
C(11)	6096(2)	6294.2(15)	1632.1(14)	32.3(7)
C(12)	5825(2)	5615.4(15)	555.2(15)	31.7(7)
C(13)	8703.9(18)	3255.9(13)	1446.4(13)	20.7(6)
C(14)	9546.5(19)	3730.5(14)	1498.2(14)	25.8(6)
C(15)	8926(2)	2702.7(14)	900.7(14)	28.8(7)
C(16)	8583(2)	2922.9(13)	2173.1(13)	25.6(6)
C(17)	6558.6(18)	3287.6(13)	1314.5(13)	21.3(6)
C(18)	6626(2)	2548.5(13)	1096.7(15)	29.5(7)
C(19)	6251(2)	3326.2(15)	2088.6(14)	32.4(7)
C(20)	5785.4(19)	3612.1(15)	859.2(16)	32.1(7)
O(1)	7455.9(19)	3626.0(11)	3586.0(10)	48.8(7)
O(2)	7064.0(16)	6239.8(10)	3228.6(10)	39.9(6)
C(21)	7342(2)	4192.9(15)	3339.4(14)	31.9(7)
C(22)	8054(2)	4583.7(14)	2995.8(14)	24.9(6)
C(23)	7959(2)	5286.2(14)	2902.2(13)	24.1(6)
C(24)	7122(2)	5628.7(15)	3139.6(13)	27.2(7)
C(25)	6328(2)	5189.0(17)	3306.0(15)	37.0(7)
C(26)	6437(2)	4533.0(18)	3404.8(15)	39.1(8)

Table 12C. Bond lengths (Å) and angles (°) for (29).

Pd(1)-C(23)	2.155(3)	Pd(1)-C(22)	2.183(3)
Pd(1)-P(1)	2.3572(7)	Pd(1)-P(2)	2.3759(7)
P(1)-C(1)	1.843(3)	P(1)-C(9)	1.894(3)
P(1)-C(5)	1.902(3)	C(1)-C(2)	1.533(4)
C(2)-C(3)	1.524(4)	C(3)-C(4)	1.529(4)
C(4)-P(2)	1.859(2)	P(2)-C(13)	1.891(3)
P(2)-C(17)	1.900(3)	C(5)-C(8)	1.534(4)
C(5)-C(7)	1.534(4)	C(5)-C(6)	1.543(4)
C(9)-C(10)	1.530(4)	C(9)-C(12)	1.532(4)
C(9)-C(11)	1.535(4)	C(13)-C(16)	1.533(3)
C(13)-C(14)	1.539(4)	C(13)-C(15)	1.542(4)
C(17)-C(18)	1.527(4)	C(17)-C(20)	1.534(4)
C(17)-C(19)	1.535(4)	O(1)-C(21)	1.227(3)
O(2)-C(24)	1.227(3)	C(21)-C(22)	1.450(4)
C(21)-C(26)	1.476(5)	C(22)-C(23)	1.411(4)
C(23)-C(24)	1.464(4)	C(24)-C(25)	1.478(4)
C(25)-C(26)	1.324(4)		
C(23)-Pd(1)-C(22)	37.97(10)	C(23)-Pd(1)-P(1)	106.75(8)
C(22)-Pd(1)-P(1)	143.75(8)	C(23)-Pd(1)-P(2)	147.67(8)
C(22)-Pd(1)-P(2)	109.77(8)	P(1)-Pd(1)-P(2)	104.52(3)
C(1)-P(1)-C(9)	102.15(12)	C(1)-P(1)-C(5)	102.18(13)
C(9)-P(1)-C(5)	110.46(12)	C(1)-P(1)-Pd(1)	113.29(9)
C(9)-P(1)-Pd(1)	116.19(8)	C(5)-P(1)-Pd(1)	111.36(9)
C(2)-C(1)-P(1)	112.90(18)	C(3)-C(2)-C(1)	114.8(2)
C(2)-C(3)-C(4)	114.7(2)	C(3)-C(4)-P(2)	120.72(19)
C(4)-P(2)-C(13)	104.24(12)	C(4)-P(2)-C(17)	98.82(12)
C(13)-P(2)-C(17)	109.73(12)	C(4)-P(2)-Pd(1)	118.63(9)
C(13)-P(2)-Pd(1)	110.50(8)	C(17)-P(2)-Pd(1)	113.95(8)
C(8)-C(5)-C(7)	109.2(2)	C(8)-C(5)-C(6)	107.4(2)
C(7)-C(5)-C(6)	107.4(2)	C(8)-C(5)-P(1)	110.34(19)
C(7)-C(5)-P(1)	113.8(2)	C(6)-C(5)-P(1)	108.50(18)
C(10)-C(9)-C(12)	108.2(2)	C(10)-C(9)-C(11)	110.1(2)
C(12)-C(9)-C(11)	106.6(2)	C(10)-C(9)-P(1)	115.0(2)
C(12)-C(9)-P(1)	107.01(18)	C(11)-C(9)-P(1)	109.56(18)
C(16)-C(13)-C(14)	108.2(2)	C(16)-C(13)-C(15)	108.5(2)
C(14)-C(13)-C(15)	107.6(2)	C(16)-C(13)-P(2)	110.25(18)
C(14)-C(13)-P(2)	106.80(17)	C(15)-C(13)-P(2)	115.23(18)
C(18)-C(17)-C(20)	107.6(2)	C(18)-C(17)-C(19)	108.9(2)
C(20)-C(17)-C(19)	106.8(2)	C(18)-C(17)-P(2)	115.31(19)
C(20)-C(17)-P(2)	108.80(18)	C(19)-C(17)-P(2)	109.09(18)
O(1)-C(21)-C(22)	124.6(3)	O(1)-C(21)-C(26)	120.0(3)
C(22)-C(21)-C(26)	115.4(3)	C(23)-C(22)-C(21)	121.1(3)
C(23)-C(22)-Pd(1)	69.96(15)	C(21)-C(22)-Pd(1)	112.4(2)
C(22)-C(23)-C(24)	119.9(3)	C(22)-C(23)-Pd(1)	72.08(15)
C(24)-C(23)-Pd(1)	110.10(19)	O(2)-C(24)-C(23)	124.0(3)
O(2)-C(24)-C(25)	119.9(3)	C(23)-C(24)-C(25)	116.0(3)
C(26)-C(25)-C(24)	121.3(3)	C(25)-C(26)-C(21)	122.7(3)

Table 12D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (29).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	15.79(11)	16.79(10)	14.99(10)	0.23(8)	-0.34(7)	0.58(9)
P(1)	16.9(4)	19.7(3)	20.2(3)	3.6(3)	0.3(3)	0.8(3)
C(1)	25.4(16)	29.8(15)	18.0(13)	5.5(11)	0.6(11)	4.4(12)
C(2)	21.6(15)	38.3(17)	24.8(14)	3.3(13)	5.6(12)	1.8(13)
C(3)	25.2(16)	39.3(17)	15.9(13)	-0.6(12)	2.9(11)	6.5(13)
C(4)	26.7(16)	25.7(15)	17.8(13)	-1.6(11)	-3.3(11)	5.5(12)
P(2)	15.2(4)	18.6(3)	16.7(3)	-1.6(3)	-1.4(3)	1.3(3)
C(5)	22.8(16)	22.6(14)	32.4(15)	4.6(12)	1.4(12)	-3.9(12)
C(6)	18.4(15)	31.6(16)	37.2(16)	2.6(13)	-2.2(13)	-6.5(13)
C(7)	29.3(19)	37.5(18)	51(2)	18.3(15)	0.7(15)	-7.3(15)
C(8)	30.9(18)	23.6(15)	50.0(19)	-6.4(14)	-1.9(15)	-5.2(13)
C(9)	18.5(15)	24.7(15)	27.2(14)	5.5(11)	-0.5(12)	6.4(12)
C(10)	28.0(18)	36.4(18)	43.6(18)	15.8(14)	0.8(14)	8.8(14)
C(11)	26.0(17)	38.6(18)	32.1(16)	-2.7(13)	0.4(13)	9.7(14)
C(12)	21.0(16)	39.5(18)	34.4(16)	3.4(14)	-1.7(13)	3.2(14)
C(13)	17.4(14)	21.9(14)	22.5(13)	-0.4(11)	-3.6(11)	3.2(11)
C(14)	19.0(15)	28.2(15)	30.0(15)	1.7(12)	-4.1(12)	1.1(12)
C(15)	24.0(16)	28.1(16)	34.2(16)	-2.5(13)	-1.9(13)	10.0(13)
C(16)	27.7(16)	22.7(15)	26.2(14)	2.1(11)	-7.4(12)	0.7(12)
C(17)	15.6(14)	22.4(14)	26.0(14)	-1.4(11)	-1.1(11)	-1.4(11)
C(18)	23.9(16)	25.6(15)	38.5(16)	-5.1(13)	-7.0(13)	-2.0(13)
C(19)	26.7(17)	36.0(17)	35.0(16)	-2.4(13)	8.2(13)	-8.1(14)
C(20)	16.8(16)	34.1(17)	45.2(18)	5.3(14)	-4.4(13)	0.2(13)
O(1)	94(2)	30.2(13)	22.1(11)	6.1(9)	2.7(12)	-3.5(13)
O(2)	53.3(16)	30.7(12)	35.7(12)	-10.2(9)	-2.5(11)	9.1(11)
C(21)	52(2)	30.0(17)	13.9(13)	-3.4(12)	2.7(13)	-4.4(15)
C(22)	30.4(17)	28.2(15)	15.8(13)	-1.8(11)	-3.6(12)	4.5(13)
C(23)	26.9(16)	29.7(16)	15.5(13)	-4.6(11)	-1.5(11)	-2.4(13)
C(24)	37.4(19)	27.9(16)	16.1(13)	-3.1(11)	-1.6(12)	2.7(13)
C(25)	29.0(18)	51(2)	31.2(16)	-9.1(15)	7.0(13)	2.0(16)
C(26)	43(2)	49(2)	25.7(16)	-3.7(14)	14.2(14)	-15.3(17)

Table 12E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (29).

	x	y	z	U
H(1A)	7325	5145	-65	29
H(1B)	8002	5772	-180	29
H(2A)	9176	5091	-221	34
H(2B)	9002	4871	582	34
H(3A)	9036	3899	-76	32
H(3B)	8334	4198	-664	32
H(4A)	7605	3393	43	28
H(4B)	7100	4104	81	28
H(6A)	9956	6260	1622	44
H(6B)	9726	5653	1087	44
H(6C)	9318	5647	1870	44
H(7A)	8347	6946	334	59
H(7B)	9105	6382	167	59
H(7C)	9383	7020	645	59
H(8A)	8886	7082	1917	52
H(8B)	8104	6573	2179	52
H(8C)	7859	7120	1580	52
H(10A)	5889	6926	367	54
H(10B)	6783	6639	-21	54
H(10C)	6906	7097	674	54
H(11A)	6508	6614	1879	48
H(11B)	6046	5882	1916	48
H(11C)	5480	6496	1566	48
H(12A)	5190	5791	573	48
H(12B)	5861	5185	810	48
H(12C)	5994	5547	59	48
H(14A)	10094	3475	1656	39
H(14B)	9424	4090	1840	39
H(14C)	9658	3929	1031	39
H(15A)	9492	2465	1051	43
H(15B)	9017	2909	435	43
H(15C)	8409	2383	869	43
H(16A)	8095	2580	2138	38
H(16B)	8410	3265	2521	38
H(16C)	9167	2710	2325	38
H(18A)	6016	2335	1135	44
H(18B)	7073	2317	1410	44
H(18C)	6831	2519	605	44
H(19A)	5691	3054	2146	49
H(19B)	6118	3796	2211	49
H(19C)	6747	3154	2403	49
H(20A)	5918	3549	355	48
H(20B)	5753	4095	965	48
H(20C)	5191	3400	966	48
H(22)	8620(2)	4391(14)	3007(14)	30
H(23)	8470(2)	5535(15)	2886(14)	29
H(25)	5728	5381	3343	44
H(26)	5912	4270	3523	47

Table 13A. Crystal data, structure solution and refinement for (32).

Identification code	exti50
Chemical formula	$C_{25}H_{46}O_2P_2Pd$
Formula weight	546.96
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	orthorhombic, Cmca
Unit cell dimensions	a = 19.5904(11) Å α = 90°
	b = 14.0585(8) Å β = 90°
	c = 18.8785(11) Å γ = 90°
Volume	5199.4(5) $Å^3$
Z	8
Density (calculated)	1.397 g/cm^3
Absorption coefficient μ	0.856 mm^{-1}
F(000)	2304
Reflections for cell refinement	13128 (θ range 2.08 to 28.59°)
Crystal colour	orange/red
Crystal size	0.46 x 0.34 x 0.16 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	2.08 to 28.77°
Index ranges	$-25 \le h \le 25$, $-18 \le k \le 15$, $-25 \le \ell \le 19$
Intensity decay	0%
Reflections collected	15942
Independent reflections	3267 (R_{int} = 0.0278)
Reflections with I>2σ(I)	3011
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.802 and 0.696
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0254, 5.4570
Data / restraints / parameters	3267 / 0 / 148
Final R indices [I>2σ(I)]	R1 = 0.0226, wR2 = 0.0534
R indices (all data)	R1 = 0.0262, wR2 = 0.0550
Goodness-of-fit on F^2	1.072
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.546 and -0.363 $eÅ^{-3}$

The Crystal Structure of [1,3-$C_3H_6(PBu^t_2)_2Pd(BQ)$] (32)

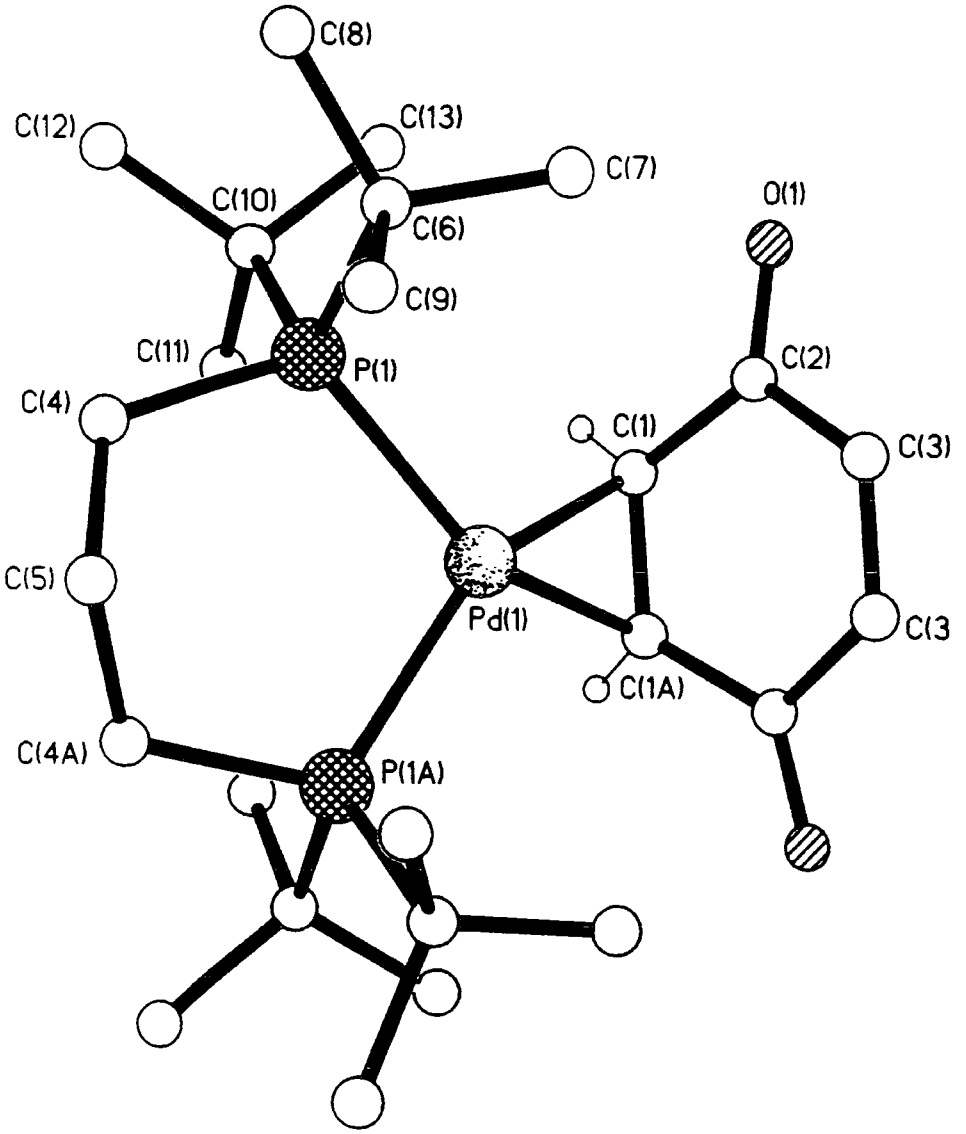


Table 13B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (32). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5000	2399.01(11)	6999.45(8)	13.13(6)
C(1)	4634.1(8)	3081.7(12)	7953.7(8)	20.2(3)
C(2)	4259.8(9)	2416.3(12)	8396.3(9)	25.8(4)
C(3)	4657.8(10)	1617.5(12)	8692.1(9)	30.6(4)
O(1)	3649.1(7)	2506.5(11)	8544.5(7)	39.2(3)
P(1)	4090.90(19)	2141.3(3)	6226.52(19)	14.29(8)
C(4)	4339.8(8)	2018.1(11)	5287.6(8)	18.5(3)
C(5)	5000	1476.4(16)	5118.0(11)	19.3(4)
C(6)	3553.9(8)	1050.8(10)	6411.4(8)	18.5(3)
C(7)	3456.1(9)	950.0(12)	7211.6(9)	26.8(4)
C(8)	2858.6(8)	1045.9(12)	6037.7(9)	26.8(3)
C(9)	3950.5(9)	177.5(11)	6154.4(9)	24.0(3)
C(10)	3533.5(8)	3241.0(11)	6181.8(8)	19.1(3)
C(11)	4023.1(9)	4097.3(11)	6153.5(9)	25.2(3)
C(12)	3065.3(9)	3298.5(12)	5530.2(9)	25.0(3)
C(13)	3092.7(8)	3325.2(12)	6848.0(9)	23.9(3)

Table 13C. Bond lengths (Å) and angles (°) for (32).

Pd(1)-C(1A)	2.1633(14)	Pd(1)-C(1)	2.1633(14)
Pd(1)-P(1)	2.3307(4)	Pd(1)-P(1A)	2.3307(4)
C(1)-C(1A)	1.434(3)	C(1)-C(2)	1.453(2)
C(2)-O(1)	1.235(2)	C(2)-C(3)	1.477(3)
C(3)-C(3A)	1.341(4)	P(1)-C(4)	1.8465(15)
P(1)-C(6)	1.8918(15)	P(1)-C(10)	1.8947(15)
C(4)-C(5)	1.5347(19)	C(5)-C(4A)	1.5347(19)
C(6)-C(7)	1.529(2)	C(6)-C(9)	1.532(2)
C(6)-C(8)	1.534(2)	C(10)-C(13)	1.530(2)
C(10)-C(12)	1.536(2)	C(10)-C(11)	1.540(2)
C(1A)-Pd(1)-C(1)	38.70(8)	C(1A)-Pd(1)-P(1)	147.51(4)
C(1)-Pd(1)-P(1)	109.70(4)	C(1A)-Pd(1)-P(1A)	109.70(4)
C(1)-Pd(1)-P(1A)	147.51(4)	P(1)-Pd(1)-P(1A)	99.658(19)
C(1A)-C(1)-C(2)	120.31(10)	C(1A)-C(1)-Pd(1)	70.65(4)
C(2)-C(1)-Pd(1)	111.13(11)	O(1)-C(2)-C(1)	123.57(17)
O(1)-C(2)-C(3)	120.25(17)	C(1)-C(2)-C(3)	116.15(15)
C(3A)-C(3)-C(2)	121.86(10)	C(4)-P(1)-C(6)	104.35(7)
C(4)-P(1)-C(10)	100.72(7)	C(6)-P(1)-C(10)	110.43(7)
C(4)-P(1)-Pd(1)	114.44(5)	C(6)-P(1)-Pd(1)	115.81(5)
C(10)-P(1)-Pd(1)	109.97(5)	C(5)-C(4)-P(1)	117.99(12)
C(4A)-C(5)-C(4)	114.86(18)	C(7)-C(6)-C(9)	107.59(13)
C(7)-C(6)-C(8)	110.03(13)	C(9)-C(6)-C(8)	107.53(13)
C(7)-C(6)-P(1)	109.08(10)	C(9)-C(6)-P(1)	108.01(10)
C(8)-C(6)-P(1)	114.37(11)	C(13)-C(10)-C(12)	108.49(13)
C(13)-C(10)-C(11)	108.63(13)	C(12)-C(10)-C(11)	107.63(13)
C(13)-C(10)-P(1)	110.59(11)	C(12)-C(10)-P(1)	115.00(10)
C(11)-C(10)-P(1)	106.28(10)		

Symmetry transformations used to generate equivalent atoms:

A: -x+1,y,z

Table 13D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (32).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	12.13(8)	15.29(8)	11.98(9)	-2.35(5)	0	0
C(1)	21.1(8)	23.8(8)	15.6(7)	-6.1(6)	-0.8(6)	2.7(6)
C(2)	24.6(8)	36.1(9)	16.7(8)	-10.7(6)	1.7(6)	-6.9(7)
C(3)	45.4(10)	25.7(8)	20.8(8)	-5.2(6)	3.0(7)	-9.4(8)
O(1)	22.6(6)	67.5(10)	27.4(7)	-11.2(6)	6.6(5)	-9.1(6)
P(1)	14.43(17)	14.68(18)	13.75(18)	-1.09(13)	-1.44(14)	-0.33(13)
C(4)	20.8(7)	20.1(7)	14.5(7)	-0.3(5)	-3.3(6)	0.7(6)
C(5)	23.0(11)	19.7(10)	15.1(10)	-3.5(8)	0	0
C(6)	18.4(7)	17.5(7)	19.8(7)	0.8(5)	-2.6(6)	-3.3(6)
C(7)	28.3(9)	29.0(9)	23.1(8)	2.7(6)	2.0(7)	-8.5(7)
C(8)	21.6(8)	24.2(8)	34.6(9)	0.2(7)	-8.7(7)	-5.2(6)
C(9)	25.8(8)	16.6(7)	29.6(9)	1.8(6)	-2.0(7)	-0.8(6)
C(10)	17.4(7)	16.9(7)	22.8(8)	-2.4(5)	-4.3(6)	1.2(6)
C(11)	25.7(8)	16.4(7)	33.4(9)	-0.1(6)	-2.0(7)	-0.1(6)
C(12)	24.4(8)	22.6(8)	27.9(9)	0.2(6)	-9.4(7)	4.3(7)
C(13)	18.9(7)	25.4(8)	27.3(8)	-5.1(6)	-1.0(6)	3.1(6)

Table 13E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (32).

	x	Y	z	U
H(1)	4400(10)	3615(14)	7818(10)	24
H(3)	4422	1089	8888	37
H(4A)	3961	1698	5036	22
H(4B)	4382	2665	5085	22
H(5A)	5000	873	5388	23
H(5B)	5000	1313	4608	23
H(7A)	3219	1512	7395	40
H(7B)	3903	893	7442	40
H(7C)	3184	380	7311	40
H 8A)	2635	431	6114	40
H(8B)	2924	1149	5529	40
H(8C)	2572	1555	6231	40
H(9A)	4407	178	6366	36
H(9B)	3991	197	5637	36
H(9C)	3707	-402	6295	36
H(11A)	3758	4688	6137	38
H(11B)	4310	4051	5729	38
H(11C)	4313	4097	6576	38
H(12A)	2718	2798	5558	37
H(12B)	3337	3212	5099	37
H(12C)	2842	3922	5517	37
H(13A)	3376	3219	7268	36
H(13B)	2728	2848	6832	36
H(13C)	2891	3963	6870	36

Table 14A. Crystal data, structure solution and refinement for (34).

Identification code	exti53
Chemical formula	$C_{43}H_{34}Cl_2O_3P_2Pd$
Formula weight	837.94
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 11.1250(8) Å α = 76.549(2)°
	b = 11.3119(8) Å β = 79.842(2)°
	c = 16.6951(12) Å γ = 64.592(2)°
Volume	1838.7(2) $Å^3$
Z	2
Density (calculated)	1.514 g/cm^3
Absorption coefficient μ	0.778 mm^{-1}
F(000)	852
Reflections for cell refinement	8682 (θ range 2.19 to 28.60°)
Crystal colour	orange
Crystal size	0.62 × 0.10 × 0.02 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	2.19 to 28.78°
Index ranges	$-14 \le h \le 14$, $-13 \le k \le 14$, $-21 \le \ell \le 21$
Intensity decay	0%
Reflections collected	13115
Independent reflections	8213 (R_{int} = 0.0340)
Reflections with I>2σ(I)	6325
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.862 and 0.706
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0451, 1.4770
Data / restraints / parameters	8213 / 4 / 466
Final R indices [I>2σ(I)]	R1 = 0.0506, wR2 = 0.1023
R indices (all data)	R1 = 0.0752, wR2 = 0.1131
Goodness-of-fit on F^2	1.021
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	1.164 and -1.209 $eÅ^{-3}$

The Crystal Structure of [{2,2'-$(C_6H_3O)_2PPh_2$}Pd(bq)] (34)

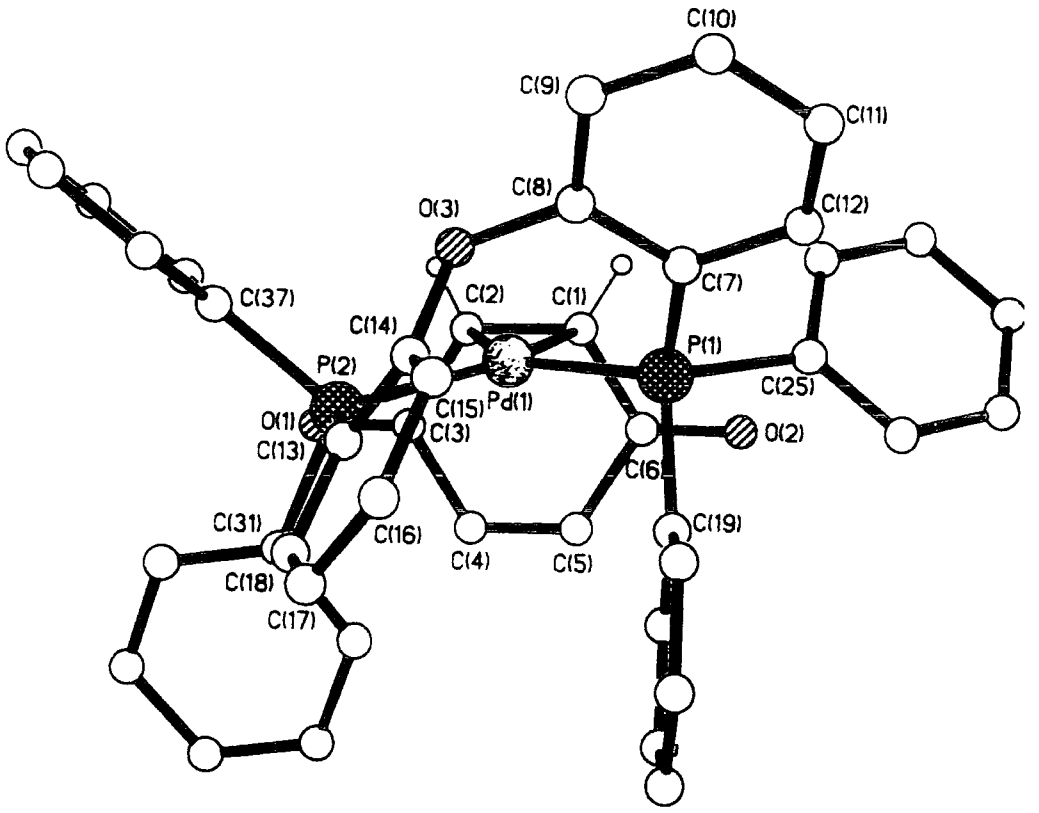


Table 14B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (34). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	10351.1(3)	3534.1(3)	3541.04(17)	17.11(9)
O(1)	13718(3)	1356(3)	2636.6(17)	32.6(7)
O(2)	10769(3)	1024(3)	5505.9(18)	35.5(7)
C(1)	11665(4)	2370(4)	4511(2)	22.6(8)
C(2)	12456(4)	2444(4)	3748(2)	22.7(8)
C(3)	12877(4)	1436(4)	3242(2)	26.9(9)
C(4)	12274(4)	455(4)	3487(3)	29.8(9)
C(5)	11538(4)	378(4)	4203(3)	33.1(10)
C(6)	11275(4)	1250(4)	4804(2)	25.8(9)
P(1)	8189.0(9)	4278.4(9)	4162.9(5)	16.6(2)
P(2)	10147.6(10)	4197.3(10)	2124.3(6)	20.2(2)
O(3)	8217(3)	6576(3)	2740.5(14)	21.3(6)
C(7)	7159(4)	6076(4)	4089(2)	18.4(8)
C(8)	7357(4)	7011(4)	3432(2)	19.9(8)
C(9)	6732(4)	8363(4)	3438(2)	26.7(9)
C(10)	5799(4)	8822(4)	4083(2)	28.5(9)
C(11)	5501(4)	7933(4)	4720(2)	24.1(9)
C(12)	6194(4)	6584(4)	4728(2)	20.8(8)
C(13)	8469(4)	5212(4)	1790(2)	21.7(8)
C(14)	7636(4)	6279(4)	2180(2)	22.3(8)
C(15)	6319(4)	7024(4)	2008(2)	28.2(9)
C(16)	5820(4)	6689(5)	1429(2)	34.6(10)
C(17)	6628(4)	5660(5)	1019(2)	34.3(11)
C(18)	7942(4)	4914(5)	1197(2)	29.8(10)
C(19)	7215(4)	3610(4)	3780(2)	16.6(7)
C(20)	7774(4)	2242(4)	3780(2)	22.6(8)
C(21)	7134(4)	1685(4)	3442(2)	23.8(8)
C(22)	5924(4)	2478(4)	3107(2)	28.9(9)
C(23)	5356(4)	3833(4)	3112(2)	27.6(9)
C(24)	5999(4)	4393(4)	3450(2)	21.8(8)
C(25)	8053(4)	3752(4)	5287(2)	19.0(8)
C(26)	8842(4)	3976(4)	5747(2)	24.5(9)
C(27)	8768(4)	3634(4)	6601(2)	29.6(10)
C(28)	7909(4)	3056(4)	7003(2)	30.6(10)
C(29)	7124(4)	2817(4)	6558(2)	29.4(9)
C(30)	7194(4)	3159(4)	5701(2)	22.5(8)
C(31)	10683(4)	2759(4)	1616(2)	23.8(9)
C(32)	10238(5)	1777(4)	1982(3)	35.0(10)
C(33)	10602(5)	662(5)	1630(3)	45.4(12)
C(34)	11416(5)	519(5)	917(3)	53.6(14)
C(35)	11862(5)	1492(6)	540(3)	52.3(14)
C(36)	11505(5)	2617(5)	884(3)	37.7(11)
C(37)	11135(4)	5108(4)	1543(2)	24.6(9)
C(38)	12512(4)	4527(5)	1613(2)	30.2(10)
C(39)	13304(5)	5175(5)	1165(3)	37.7(11)
C(40)	12746(5)	6388(5)	666(3)	41.9(12)
C(41)	11394(5)	6966(5)	602(3)	43.5(12)
C(42)	10581(5)	6341(4)	1039(2)	34.3(10)
C(43)	3997(6)	9546(8)	-1238(4)	91(2)
Cl(1)	4784.1(16)	8488.8(19)	-404.7(10)	79.3(5)
Cl(2)	2439.6(18)	9612(3)	-1297.1(10)	106.8(8)

Table 14C. Bond lengths (Å) and angles (°) for (34).

Pd(1)-C(1)	2.164(4)	Pd(1)-C(2)	2.175(4)
Pd(1)-P(1)	2.3152(10)	Pd(1)-P(2)	2.3294(10)
O(1)-C(3)	1.242(5)	O(2)-C(6)	1.228(5)
C(1)-C(2)	1.422(5)	C(1)-C(6)	1.463(6)
C(2)-C(3)	1.444(6)	C(3)-C(4)	1.476(6)
C(4)-C(5)	1.332(6)	C(5)-C(6)	1.475(6)
P(1)-C(19)	1.824(4)	P(1)-C(25)	1.833(4)
P(1)-C(7)	1.843(4)	P(2)-C(37)	1.828(4)
P(2)-C(13)	1.830(4)	P(2)-C(31)	1.832(4)
O(3)-C(14)	1.397(4)	O(3)-C(8)	1.400(4)
C(7)-C(8)	1.395(5)	C(7)-C(12)	1.404(5)
C(8)-C(9)	1.384(5)	C(9)-C(10)	1.382(6)
C(10)-C(11)	1.384(6)	C(11)-C(12)	1.381(5)
C(13)-C(14)	1.391(5)	C(13)-C(18)	1.401(5)
C(14)-C(15)	1.385(5)	C(15)-C(16)	1.387(5)
C(16)-C(17)	1.374(6)	C(17)-C(18)	1.384(6)
C(19)-C(24)	1.388(5)	C(19)-C(20)	1.399(5)
C(20)-C(21)	1.383(5)	C(21)-C(22)	1.387(6)
C(22)-C(23)	1.387(6)	C(23)-C(24)	1.388(5)
C(25)-C(26)	1.393(5)	C(25)-C(30)	1.394(5)
C(26)-C(27)	1.386(5)	C(27)-C(28)	1.378(6)
C(28)-C(29)	1.383(6)	C(29)-C(30)	1.390(5)
C(31)-C(32)	1.379(6)	C(31)-C(36)	1.387(5)
C(32)-C(33)	1.386(6)	C(33)-C(34)	1.359(7)
C(34)-C(35)	1.375(7)	C(35)-C(36)	1.391(6)
C(37)-C(42)	1.390(6)	C(37)-C(38)	1.398(6)
C(38)-C(39)	1.394(6)	C(39)-C(40)	1.371(7)
C(40)-C(41)	1.372(7)	C(41)-C(42)	1.388(6)
C(43)-Cl(1)	1.700(6)	C(43)-Cl(2)	1.722(7)
C(1)-Pd(1)-C(2)	38.26(14)	C(1)-Pd(1)-P(1)	107.13(11)
C(2)-Pd(1)-P(1)	145.31(11)	C(1)-Pd(1)-P(2)	146.79(11)
C(2)-Pd(1)-P(2)	109.01(11)	P(1)-Pd(1)-P(2)	105.66(3)
C(2)-C(1)-C(6)	120.2(4)	C(2)-C(1)-Pd(1)	71.3(2)
C(6)-C(1)-Pd(1)	101.9(2)	C(1)-C(2)-C(3)	121.2(4)
C(1)-C(2)-Pd(1)	70.4(2)	C(3)-C(2)-Pd(1)	101.9(2)
O(1)-C(3)-C(2)	123.2(4)	O(1)-C(3)-C(4)	120.2(4)
C(2)-C(3)-C(4)	116.6(4)	C(5)-C(4)-C(3)	121.7(4)
C(4)-C(5)-C(6)	122.8(4)	O(2)-C(6)-C(1)	123.1(4)
O(2)-C(6)-C(5)	120.9(4)	C(1)-C(6)-C(5)	115.9(4)
C(19)-P(1)-C(25)	104.62(16)	C(19)-P(1)-C(7)	105.84(16)
C(25)-P(1)-C(7)	99.87(16)	C(19)-P(1)-Pd(1)	110.23(12)
C(25)-P(1)-Pd(1)	114.67(12)	C(7)-P(1)-Pd(1)	120.07(12)
C(37)-P(2)-C(13)	103.72(18)	C(37)-P(2)-C(31)	103.90(18)
C(13)-P(2)-C(31)	102.09(17)	C(37)-P(2)-Pd(1)	116.77(12)
C(13)-P(2)-Pd(1)	117.46(12)	C(31)-P(2)-Pd(1)	111.09(13)
C(14)-O(3)-C(8)	114.0(3)	C(8)-C(7)-C(12)	116.2(3)
C(8)-C(7)-P(1)	122.3(3)	C(12)-C(7)-P(1)	121.3(3)
C(9)-C(8)-C(7)	122.3(3)	C(9)-C(8)-O(3)	118.4(3)
C(7)-C(8)-O(3)	119.3(3)	C(10)-C(9)-C(8)	119.5(4)
C(9)-C(10)-C(11)	120.1(4)	C(12)-C(11)-C(10)	119.5(4)
C(11)-C(12)-C(7)	122.2(4)	C(14)-C(13)-C(18)	118.0(4)
C(14)-C(13)-P(2)	118.7(3)	C(18)-C(13)-P(2)	123.2(3)
C(15)-C(14)-C(13)	121.9(3)	C(15)-C(14)-O(3)	122.0(4)
C(13)-C(14)-O(3)	116.1(3)	C(14)-C(15)-C(16)	118.8(4)
C(17)-C(16)-C(15)	120.6(4)	C(16)-C(17)-C(18)	120.4(4)
C(17)-C(18)-C(13)	120.4(4)	C(24)-C(19)-C(20)	118.9(3)
C(24)-C(19)-P(1)	123.5(3)	C(20)-C(19)-P(1)	117.4(3)

C(21)-C(20)-C(19)	120.4(4)	C(20)-C(21)-C(22)	120.3(4)
C(23)-C(22)-C(21)	119.7(4)	C(22)-C(23)-C(24)	120.1(4)
C(19)-C(24)-C(23)	120.6(4)	C(26)-C(25)-C(30)	118.9(3)
C(26)-C(25)-P(1)	117.8(3)	C(30)-C(25)-P(1)	123.4(3)
C(27)-C(26)-C(25)	121.0(4)	C(28)-C(27)-C(26)	119.6(4)
C(27)-C(28)-C(29)	120.3(4)	C(28)-C(29)-C(30)	120.3(4)
C(29)-C(30)-C(25)	120.0(4)	C(32)-C(31)-C(36)	119.0(4)
C(32)-C(31)-P(2)	117.8(3)	C(36)-C(31)-P(2)	123.2(3)
C(31)-C(32)-C(33)	120.9(4)	C(34)-C(33)-C(32)	120.1(5)
C(33)-C(34)-C(35)	119.8(5)	C(34)-C(35)-C(36)	120.9(5)
C(31)-C(36)-C(35)	119.4(4)	C(42)-C(37)-C(38)	119.0(4)
C(42)-C(37)-P(2)	123.1(3)	C(38)-C(37)-P(2)	117.9(3)
C(39)-C(38)-C(37)	119.7(4)	C(40)-C(39)-C(38)	120.7(4)
C(39)-C(40)-C(41)	119.7(4)	C(40)-C(41)-C(42)	120.8(5)
C(41)-C(42)-C(37)	120.0(4)	Cl(1)-C(43)-Cl(2)	114.5(4)

Table 14D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (34).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	17.29(15)	19.75(16)	15.91(14)	-3.27(10)	-1.99(10)	-8.74(12)
O(1)	26.2(15)	38.8(19)	30.5(15)	-12.3(13)	6.0(13)	-11.0(14)
O(2)	34.9(17)	28.4(17)	33.8(17)	3.7(13)	1.8(13)	-10.3(14)
C(1)	22(2)	21(2)	24.0(19)	-4.6(16)	-6.3(16)	-6.5(17)
C(2)	19(2)	17(2)	33(2)	0.5(16)	-8.8(16)	-8.9(17)
C(3)	18(2)	29(2)	30(2)	-5.2(17)	-7.0(17)	-4.5(18)
C(4)	27(2)	24(2)	41(2)	-11.4(18)	-2.0(19)	-10.0(19)
C(5)	25(2)	22(2)	50(3)	-3.7(19)	-6(2)	-8.0(19)
C(6)	17.8(19)	21(2)	32(2)	1.5(17)	-7.3(17)	-3.0(17)
P(1)	18.0(5)	16.9(5)	16.7(4)	-2.6(4)	-2.0(4)	-8.9(4)
P(2)	23.2(5)	25.1(6)	15.9(4)	-4.5(4)	-0.9(4)	-13.1(5)
O(3)	26.3(14)	23.2(15)	16.8(12)	-1.4(10)	-3.7(11)	-12.7(12)
C(7)	20.4(19)	17(2)	20.7(18)	-4.7(15)	-4.6(15)	-8.6(16)
C(8)	19.3(19)	23(2)	22.6(18)	-5.4(15)	-5.7(15)	-10.5(17)
C(9)	34(2)	20(2)	28(2)	2.4(16)	-12.0(18)	-13.1(19)
C(10)	27(2)	21(2)	35(2)	-10.6(18)	-8.3(18)	-2.7(19)
C(11)	21(2)	22(2)	31(2)	-8.3(17)	-4.4(16)	-6.8(18)
C(12)	21.2(19)	20(2)	23.7(19)	-3.0(15)	-4.1(15)	-10.3(17)
C(13)	25(2)	28(2)	16.6(17)	-2.1(15)	-0.4(15)	-17.2(18)
C(14)	28(2)	30(2)	14.7(17)	-1.0(15)	-4.6(15)	-17.7(19)
C(15)	30(2)	30(2)	23(2)	-1.9(17)	-4.0(17)	-10(2)
C(16)	31(2)	47(3)	26(2)	-3(2)	-10.3(18)	-14(2)
C(17)	36(2)	52(3)	23(2)	-9(2)	-9.4(18)	-22(2)
C(18)	28(2)	45(3)	20.7(19)	-10.8(18)	-2.2(17)	-17(2)
C(19)	20.8(19)	20(2)	13.6(16)	-6.6(14)	2.9(14)	-11.9(16)
C(20)	23(2)	23(2)	22.6(19)	-3.1(16)	-1.6(16)	-10.4(18)
C(21)	27(2)	20(2)	30(2)	-12.9(16)	5.4(17)	-14.2(18)
C(22)	30(2)	41(3)	27(2)	-11.2(19)	-1.0(17)	-23(2)
C(23)	24(2)	33(3)	28(2)	-3.3(18)	-6.5(17)	-12(2)
C(24)	20.8(19)	22(2)	22.4(18)	-4.4(15)	-0.6(15)	-8.4(17)
C(25)	22.7(19)	15.3(19)	16.7(17)	-4.7(14)	2.5(15)	-6.1(16)
C(26)	28(2)	25(2)	22.6(19)	-8.3(16)	-0.7(16)	-11.9(18)
C(27)	38(2)	29(2)	24(2)	-8.2(17)	-8.4(18)	-12(2)
C(28)	42(3)	20(2)	18.6(19)	-3.9(16)	0.5(18)	-3(2)
C(29)	35(2)	22(2)	27(2)	-5.1(17)	6.4(18)	-10.1(19)
C(30)	22(2)	19(2)	27(2)	-6.1(16)	-0.6(16)	-7.7(17)
C(31)	24(2)	31(2)	20.9(18)	-8.0(16)	-3.4(16)	-12.6(19)
C(32)	44(3)	36(3)	32(2)	-10.7(19)	5(2)	-24(2)
C(33)	60(3)	38(3)	50(3)	-12(2)	-5(3)	-28(3)
C(34)	52(3)	47(3)	72(4)	-39(3)	0(3)	-18(3)
C(35)	56(3)	64(4)	51(3)	-41(3)	20(3)	-31(3)
C(36)	46(3)	49(3)	32(2)	-22(2)	12(2)	-30(2)
C(37)	29(2)	35(2)	18.1(18)	-8.3(16)	4.1(16)	-21(2)
C(38)	35(2)	41(3)	25(2)	-8.3(18)	1.6(18)	-26(2)
C(39)	38(3)	57(3)	33(2)	-13(2)	3(2)	-33(3)
C(40)	62(3)	61(4)	27(2)	-10(2)	7(2)	-50(3)
C(41)	63(3)	45(3)	32(2)	1(2)	0(2)	-37(3)
C(42)	40(3)	38(3)	28(2)	-1.9(19)	-1.8(19)	-21(2)
C(43)	72(4)	94(6)	51(4)	15(3)	21(3)	-6(4)
Cl(1)	59.7(10)	100.0(14)	71.7(10)	14.8(9)	-8.3(8)	-40.4(10)
Cl(2)	71.6(11)	190(2)	40.4(8)	-14.8(11)	-6.4(8)	-37.8(14)

Table 14E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (34).

	x	y	z	U
H(1)	11560(4)	2890(4)	4900(2)	27
H(2)	12820(4)	3000(4)	3660(2)	27
H(4)	12414	-137	3125	36
H(5)	11166	-267	4332	40
H(9)	6942	8971	3002	32
H(10)	5361	9749	4089	34
H(11)	4825	8248	5148	29
H(12)	6012	5980	5180	25
H(15)	5767	7751	2280	34
H(16)	4911	7176	1315	42
H(17)	6283	5460	611	41
H(18)	8491	4196	916	36
H(20)	8598	1692	4012	27
H(21)	7524	756	3440	29
H(22)	5486	2093	2875	35
H(23)	4527	4379	2885	33
H(24)	5603	5322	3454	26
H(26)	9440	4369	5470	29
H(27)	9307	3797	6908	36
H(28)	7856	2820	7589	37
H(29)	6534	2417	6839	35
H(30)	6656	2990	5398	27
H(32)	9675	1865	2483	42
H(33)	10282	-2	1888	54
H(34)	11676	-251	680	64
H(35)	12421	1395	37	63
H(36)	11821	3283	621	45
H(38)	12905	3693	1963	36
H(39)	14242	4773	1206	45
H(40)	13294	6825	367	50
H(41)	11010	7804	254	52
H(42)	9645	6755	993	41
H(43A)	4565	9273	-1747	109
H(43B)	3906	10451	-1223	109

Table 15A. Crystal data, structure solution and refinement for (35).

Identification code	exti54
Chemical formula	$C_{46}H_{38}Cl_2O_3P_2Pd$
Formula weight	878.00
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 8.8641(6) Å α = 90°
	b = 18.4696(12) Å β = 99.155(2)°
	c = 24.3678(16) Å γ = 90°
Volume	3938.6(5) Å^3
Z	4
Density (calculated)	1.481 g/cm^3
Absorption coefficient μ	0.730 mm^{-1}
F(000)	1792
Reflections for cell refinement	11065 (θ range 2.20 to 28.81°)
Crystal colour	orange
Crystal size	0.41 × 0.18 × 0.02 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	2.02 to 26.00°
Index ranges	$-10 \le h \le 8$, $-22 \le k \le 22$, $-25 \le \ell \le 30$
Intensity decay	0%
Reflections collected	21584
Independent reflections	7678 (R_{int} = 0.0679)
Reflections with I>2σ(I)	5185
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.862 and 0.694
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0290, 0.3295
Data / restraints / parameters	7678 / 0 / 495
Final R indices [I>2σ(I)]	R1 = 0.0519, wR2 = 0.0852
R indices (all data)	R1 = 0.0964, wR2 = 0.0968
Goodness-of-fit on F^2	1.068
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.730 and -0.474 eÅ^{-3}

The Crystal Structure of [xantphosPd(bq)] (35)

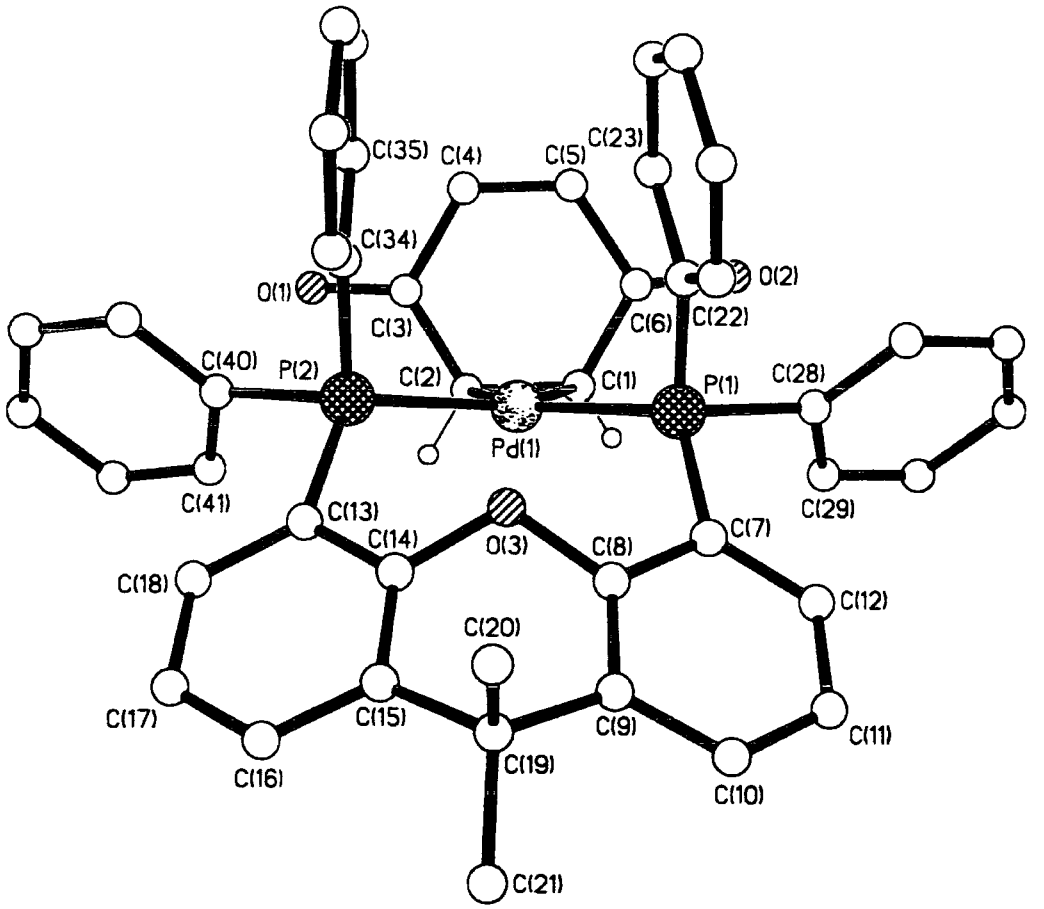


Table 15B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (35). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2575.4(4)	3659.67(16)	6178.86(12)	16.48(9)
O(1)	2455(4)	5084.4(16)	5003.7(12)	42.3(9)
O(2)	2911(4)	2207.1(16)	5111.8(13)	46.5(10)
C(1)	1605(6)	3249(2)	5377.5(18)	26.4(11)
C(2)	1489(5)	4008(2)	5362.6(17)	25.3(10)
C(3)	2619(6)	4436(2)	5123.3(17)	29.5(11)
C(4)	3992(5)	4052(2)	5002.2(16)	31.3(12)
C(5)	4106(6)	3327(3)	5029.2(17)	33.7(12)
C(6)	2854(6)	2867(2)	5175.1(17)	31.3(12)
P(1)	3455.1(12)	2656.0(5)	6737.3(4)	17.0(3)
P(2)	3454.8(12)	4700.2(5)	6686.1(4)	16.0(2)
O(3)	3553(3)	3699.6(13)	7608.2(10)	17.0(6)
C(7)	2855(4)	2499(2)	7410.6(16)	17.3(9)
C(8)	2888(4)	3079(2)	7776.6(16)	15.8(9)
C(9)	2318(5)	3062(2)	8277.1(16)	18.1(9)
C(10)	1762(5)	2401(2)	8427.2(17)	21.7(10)
C(11)	1768(5)	1795(2)	8092.2(17)	25.2(10)
C(12)	2298(5)	1840(2)	7587.2(17)	23.0(10)
C(13)	2892(5)	4903(2)	7367.5(16)	18.1(10)
C(14)	2909(4)	4344(2)	7750.5(16)	16.5(9)
C(15)	2322(4)	4400(2)	8245.8(16)	17.6(9)
C(16)	1720(5)	5071(2)	8355.6(17)	22.5(10)
C(17)	1730(5)	5648(2)	7999.1(16)	22.7(10)
C(18)	2312(5)	5569(2)	7506.0(16)	19.4(10)
C(19)	2446(4)	3742(2)	8635.9(15)	19.3(9)
C(20)	4035(5)	3747(2)	9001.9(16)	27.1(10)
C(21)	1199(5)	3762(2)	9008.4(17)	29.1(11)
C(22)	5532(5)	2669(2)	6912.2(17)	19.7(10)
C(23)	6361(5)	2852(2)	6491.1(19)	28.5(11)
C(24)	7955(5)	2883(2)	6602(2)	32.9(12)
C(25)	8706(5)	2743(2)	7130(2)	33.7(12)
C(26)	7892(5)	2562(2)	7547(2)	35.1(12)
C(27)	6314(5)	2524(2)	7435.6(17)	26.9(11)
C(28)	3041(5)	1765(2)	6422.2(16)	19.2(10)
C(29)	1590(5)	1635(2)	6130.9(17)	25.9(11)
C(30)	1207(6)	955(2)	5900.0(17)	34.4(12)
C(31)	2290(7)	409(2)	5962(2)	40.7(14)
C(32)	3722(6)	529(2)	6250.1(19)	36.4(12)
C(33)	4093(5)	1200(2)	6480.9(17)	26.8(11)
C(34)	5534(5)	4712(2)	6808.6(16)	18.9(10)
C(35)	6276(5)	4693(2)	6343.6(18)	25.9(11)
C(36)	7840(5)	4693(2)	6401.1(19)	29.3(11)
C(37)	8710(5)	4699(2)	6927(2)	33.6(12)
C(38)	7979(5)	4722(2)	7391(2)	35.9(12)
C(39)	6415(5)	4726(2)	7333.5(18)	27.5(11)
C(40)	2967(5)	5570(2)	6339.5(15)	18.3(9)
C(41)	1452(5)	5668(2)	6099.3(16)	23.2(10)
C(42)	947(6)	6342(3)	5896.2(16)	32.8(11)
C(43)	1953(7)	6910(3)	5921.1(17)	39.4(14)
C(44)	3469(6)	6811(2)	6137.5(19)	38.2(13)
C(45)	3988(5)	6140(2)	6355.2(17)	26.3(11)

C(46)	6431(6)	1427(2)	5483.4(19)	39.6(12)
Cl(1)	7583.7(17)	2066.2(7)	5207.6(6)	55.6(4)
Cl(2)	6674.5(17)	557.4(7)	5221.6(5)	47.6(4)

Table 15C. Bond lengths (Å) and angles (°) for (35).

Pd(1)-C(1)	2.143(4)	Pd(1)-C(2)	2.165(4)
Pd(1)-P(2)	2.3499(11)	Pd(1)-P(1)	2.3576(11)
O(1)-C(3)	1.235(5)	O(2)-C(6)	1.230(5)
C(1)-C(2)	1.405(6)	C(1)-C(6)	1.463(7)
C(2)-C(3)	1.468(6)	C(3)-C(4)	1.478(6)
C(4)-C(5)	1.343(6)	C(5)-C(6)	1.485(6)
P(1)-C(22)	1.823(4)	P(1)-C(7)	1.827(4)
P(1)-C(28)	1.828(4)	P(2)-C(34)	1.820(4)
P(2)-C(40)	1.834(4)	P(2)-C(13)	1.846(4)
O(3)-C(8)	1.380(4)	O(3)-C(14)	1.387(4)
C(7)-C(8)	1.392(5)	C(7)-C(12)	1.406(5)
C(8)-C(9)	1.393(5)	C(9)-C(10)	1.386(5)
C(9)-C(19)	1.525(5)	C(10)-C(11)	1.386(5)
C(11)-C(12)	1.388(5)	C(13)-C(14)	1.390(5)
C(13)-C(18)	1.396(5)	C(14)-C(15)	1.392(5)
C(15)-C(16)	1.391(5)	C(15)-C(19)	1.536(5)
C(16)-C(17)	1.376(5)	C(17)-C(18)	1.389(5)
C(19)-C(21)	1.538(5)	C(19)-C(20)	1.543(5)
C(22)-C(27)	1.377(5)	C(22)-C(23)	1.395(6)
C(23)-C(24)	1.397(6)	C(24)-C(25)	1.376(6)
C(25)-C(26)	1.377(6)	C(26)-C(27)	1.384(6)
C(28)-C(29)	1.387(6)	C(28)-C(33)	1.392(5)
C(29)-C(30)	1.396(6)	C(30)-C(31)	1.384(6)
C(31)-C(32)	1.367(7)	C(32)-C(33)	1.378(6)
C(34)-C(39)	1.389(5)	C(34)-C(35)	1.398(5)
C(35)-C(36)	1.371(6)	C(36)-C(37)	1.387(6)
C(37)-C(38)	1.391(6)	C(38)-C(39)	1.371(6)
C(40)-C(45)	1.385(5)	C(40)-C(41)	1.388(6)
C(41)-C(42)	1.389(5)	C(42)-C(43)	1.371(6)
C(43)-C(44)	1.375(7)	C(44)-C(45)	1.397(6)
C(46)-Cl(2)	1.754(4)	C(46)-Cl(1)	1.763(5)
C(1)-Pd(1)-C(2)	38.06(15)	C(1)-Pd(1)-P(2)	145.08(13)
C(2)-Pd(1)-P(2)	107.59(12)	C(1)-Pd(1)-P(1)	107.21(13)
C(2)-Pd(1)-P(1)	145.26(12)	P(2)-Pd(1)-P(1)	106.73(4)
C(2)-C(1)-C(6)	121.9(4)	C(2)-C(1)-Pd(1)	71.8(2)
C(6)-C(1)-Pd(1)	105.2(3)	C(1)-C(2)-C(3)	119.7(4)
C(1)-C(2)-Pd(1)	70.1(2)	C(3)-C(2)-Pd(1)	107.0(3)
O(1)-C(3)-C(2)	123.6(4)	O(1)-C(3)-C(4)	119.2(4)
C(2)-C(3)-C(4)	117.1(4)	C(5)-C(4)-C(3)	121.8(5)
C(4)-C(5)-C(6)	121.9(5)	O(2)-C(6)-C(1)	124.6(5)
O(2)-C(6)-C(5)	119.4(5)	C(1)-C(6)-C(5)	116.0(4)
C(22)-P(1)-C(7)	102.69(18)	C(22)-P(1)-C(28)	103.78(18)
C(7)-P(1)-C(28)	99.59(18)	C(22)-P(1)-Pd(1)	110.71(13)
C(7)-P(1)-Pd(1)	121.77(13)	C(28)-P(1)-Pd(1)	116.06(13)
C(34)-P(2)-C(40)	102.91(19)	C(34)-P(2)-C(13)	105.16(18)
C(40)-P(2)-C(13)	99.15(17)	C(34)-P(2)-Pd(1)	109.80(13)
C(40)-P(2)-Pd(1)	116.09(13)	C(13)-P(2)-Pd(1)	121.61(13)
C(8)-O(3)-C(14)	115.1(3)	C(8)-C(7)-C(12)	116.3(4)
C(8)-C(7)-P(1)	118.3(3)	C(12)-C(7)-P(1)	125.4(3)
O(3)-C(8)-C(7)	114.5(3)	O(3)-C(8)-C(9)	120.8(3)
C(7)-C(8)-C(9)	124.7(4)	C(10)-C(9)-C(8)	116.5(4)
C(10)-C(9)-C(19)	124.8(4)	C(8)-C(9)-C(19)	118.6(3)
C(11)-C(10)-C(9)	121.3(4)	C(10)-C(11)-C(12)	120.5(4)
C(11)-C(12)-C(7)	120.5(4)	C(14)-C(13)-C(18)	117.2(4)
C(14)-C(13)-P(2)	118.5(3)	C(18)-C(13)-P(2)	124.0(3)
O(3)-C(14)-C(13)	115.4(3)	O(3)-C(14)-C(15)	120.4(3)
C(13)-C(14)-C(15)	124.1(4)	C(16)-C(15)-C(14)	116.2(4)

C(16)-C(15)-C(19)	125.2(4)	C(14)-C(15)-C(19)	118.5(3)
C(17)-C(16)-C(15)	121.8(4)	C(16)-C(17)-C(18)	120.4(4)
C(17)-C(18)-C(13)	120.2(4)	C(9)-C(19)-C(15)	107.8(3)
C(9)-C(19)-C(21)	111.3(3)	C(15)-C(19)-C(21)	111.0(3)
C(9)-C(19)-C(20)	108.2(3)	C(15)-C(19)-C(20)	108.8(3)
C(21)-C(19)-C(20)	109.5(3)	C(27)-C(22)-C(23)	118.8(4)
C(27)-C(22)-P(1)	123.7(3)	C(23)-C(22)-P(1)	117.5(3)
C(22)-C(23)-C(24)	120.2(4)	C(25)-C(24)-C(23)	119.8(4)
C(24)-C(25)-C(26)	120.2(5)	C(25)-C(26)-C(27)	120.0(4)
C(22)-C(27)-C(26)	121.1(4)	C(29)-C(28)-C(33)	118.3(4)
C(29)-C(28)-P(1)	118.6(3)	C(33)-C(28)-P(1)	123.1(3)
C(28)-C(29)-C(30)	120.6(4)	C(31)-C(30)-C(29)	119.4(4)
C(32)-C(31)-C(30)	120.6(4)	C(31)-C(32)-C(33)	119.8(4)
C(32)-C(33)-C(28)	121.3(4)	C(39)-C(34)-C(35)	118.6(4)
C(39)-C(34)-P(2)	123.9(3)	C(35)-C(34)-P(2)	117.5(3)
C(36)-C(35)-C(34)	121.1(4)	C(35)-C(36)-C(37)	119.9(4)
C(36)-C(37)-C(38)	119.3(4)	C(39)-C(38)-C(37)	120.7(4)
C(38)-C(39)-C(34)	120.4(4)	C(45)-C(40)-C(41)	119.8(4)
C(45)-C(40)-P(2)	123.2(3)	C(41)-C(40)-P(2)	116.7(3)
C(40)-C(41)-C(42)	120.2(4)	C(43)-C(42)-C(41)	119.9(4)
C(42)-C(43)-C(44)	120.3(4)	C(43)-C(44)-C(45)	120.3(4)
C(40)-C(45)-C(44)	119.4(4)	Cl(2)-C(46)-Cl(1)	111.2(3)

Table 15D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (35).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	15.32(17)	17.29(16)	16.74(17)	-0.19(15)	2.30(12)	-1.16(16)
O(1)	70(3)	26.4(19)	34(2)	8.8(15)	19.3(18)	7.4(18)
O(2)	85(3)	19.7(18)	39(2)	-11.9(15)	25.1(19)	-2.7(18)
C(1)	31(3)	30(3)	16(2)	-1(2)	0(2)	-10(2)
C(2)	27(3)	30(3)	18(2)	2(2)	0(2)	6(2)
C(3)	44(3)	29(3)	16(2)	-6(2)	3(2)	0(2)
C(4)	41(3)	36(3)	20(3)	-1(2)	13(2)	-6(2)
C(5)	38(3)	38(3)	26(3)	-3(2)	10(2)	2(2)
C(6)	53(4)	28(3)	14(2)	-2(2)	6(2)	-4(2)
P(1)	14.8(6)	16.3(6)	20.3(6)	-0.7(4)	4.4(5)	0.5(5)
P(2)	14.8(6)	17.0(6)	16.2(6)	1.0(4)	2.4(5)	-1.5(5)
O(3)	18.6(15)	13.3(13)	20.8(14)	1.1(12)	8.4(11)	-0.4(13)
C(7)	12(2)	17(2)	23(2)	4.0(18)	3.1(18)	1.5(18)
C(8)	7(2)	20(2)	19(2)	3.6(18)	0.4(17)	-0.9(17)
C(9)	15(2)	21(2)	19(2)	3.8(18)	4.1(18)	-2.2(18)
C(10)	22(3)	22(2)	22(2)	4.8(19)	7.8(19)	-2.4(19)
C(11)	26(3)	20(2)	32(3)	7(2)	9(2)	-3(2)
C(12)	23(3)	20(2)	25(2)	2.7(19)	5(2)	2(2)
C(13)	16(2)	14(2)	23(2)	1.8(18)	0.6(18)	-2.6(18)
C(14)	12(2)	14(2)	23(2)	-3.7(18)	0.2(18)	-2.1(18)
C(15)	14(2)	22(2)	17(2)	-2.5(18)	2.5(17)	-3.9(18)
C(16)	23(3)	26(2)	19(2)	-6.2(19)	6.3(19)	1(2)
C(17)	24(3)	18(2)	25(2)	-4.2(19)	-1.3(19)	1.7(19)
C(18)	22(3)	17(2)	19(2)	-1.3(18)	1.5(19)	-4.8(19)
C(19)	20(2)	22(2)	17(2)	-0.2(18)	8.1(17)	-0.5(19)
C(20)	35(3)	25(2)	20(2)	0.0(19)	0.6(19)	-3(2)
C(21)	36(3)	28(3)	28(3)	0(2)	17(2)	0(2)
C(22)	18(3)	15(2)	26(2)	-2.3(18)	4.9(19)	0.6(18)
C(23)	19(3)	30(3)	36(3)	2(2)	4(2)	-1(2)
C(24)	25(3)	27(3)	50(3)	4(2)	19(2)	0(2)
C(25)	19(3)	24(3)	58(3)	-5(2)	3(2)	-1(2)
C(26)	28(3)	33(3)	40(3)	-1(2)	-6(2)	4(2)
C(27)	20(3)	28(2)	32(3)	-1(2)	2(2)	0(2)
C(28)	19(3)	19(2)	21(2)	0.7(18)	8.7(19)	-0.1(19)
C(29)	27(3)	23(2)	28(3)	0(2)	5(2)	0(2)
C(30)	41(3)	31(3)	29(3)	-3(2)	3(2)	-15(3)
C(31)	63(4)	20(3)	44(3)	-11(2)	27(3)	-15(3)
C(32)	47(4)	20(2)	47(3)	-3(2)	25(3)	7(2)
C(33)	26(3)	23(3)	33(3)	0(2)	13(2)	2(2)
C(34)	18(2)	16(2)	22(2)	1.2(17)	1.8(19)	-4.1(18)
C(35)	18(3)	33(3)	28(3)	-3(2)	6(2)	-1(2)
C(36)	20(3)	30(3)	40(3)	2(2)	12(2)	-6(2)
C(37)	13(3)	31(3)	58(3)	3(2)	9(2)	-7(2)
C(38)	21(3)	49(3)	35(3)	7(2)	-6(2)	-7(2)
C(39)	23(3)	34(3)	25(3)	3(2)	1(2)	-5(2)
C(40)	28(3)	16(2)	12(2)	-0.5(17)	7.7(18)	0.3(19)
C(41)	24(3)	27(2)	19(2)	-2.4(19)	3.8(19)	6(2)
C(42)	42(3)	37(3)	19(2)	-2(2)	2(2)	15(3)
C(43)	70(4)	30(3)	22(3)	14(2)	19(3)	25(3)
C(44)	59(4)	19(3)	43(3)	3(2)	28(3)	-3(2)
C(45)	29(3)	25(3)	28(3)	-1.7(19)	12(2)	-6(2)

C(46)	48(3)	37(3)	37(3)	3(2)	19(2)	-1(3)
Cl(1)	62.4(10)	47.3(8)	63.3(9)	13.7(7)	28.7(8)	-4.0(7)
Cl(2)	59.7(10)	38.3(7)	40.5(8)	2.2(6)	-4.8(7)	0.3(7)

Table 15E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (35).

	x	y	z	U
H(1)	860(5)	3010(2)	5398(17)	32
H(2)	540(5)	4270(2)	5395(15)	30
H(4)	4815	4325	4902	38
H(5)	5014	3102	4953	40
H(10)	1369	2363	8767	26
H(11)	1407	1346	8209	30
H(12)	2284	1422	7359	28
H(16)	1291	5132	8686	27
H(17)	1336	6103	8091	27
H(18)	2316	5970	7262	23
H(20A)	4136	3322	9246	41
H(20B)	4151	4188	9228	41
H(20C)	4829	3733	8764	41
H(21A)	191	3783	8775	44
H(21B)	1343	4190	9248	44
H(21C)	1269	3325	9239	44
H(23)	5840	2954	6128	34
H(24)	8519	3001	6314	39
H(25)	9789	2772	7207	40
H(26)	8414	2463	7910	42
H(27)	5761	2396	7725	32
H(29)	851	2012	6088	31
H(30)	212	867	5702	41
H(31)	2036	-54	5804	49
H(32)	4460	152	6291	44
H(33)	5086	1278	6684	32
H(35)	5688	4680	5982	31
H(36)	8328	4689	6081	35
H(37)	9794	4688	6970	40
H(38)	8570	4736	7753	43
H(39)	5931	4737	7654	33
H(41)	760	5272	6074	28
H(42)	-96	6411	5740	39
H(43)	1601	7373	5788	47
H(44)	4168	7202	6139	46
H(45)	5030	6076	6513	32
H(46A)	6700	1420	5894	48
H(46B)	5345	1571	5388	48

Table 16A. Crystal data, structure solution and refinement for (40).

Identification code	exti34
Chemical formula	$C_{19}H_{22}O_7S_2$
Formula weight	426.49
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 7.8585(6) Å α = 90°
	b = 12.0834(10) Å β = 96.256(2)°
	c = 21.2594(17) Å γ = 90°
Volume	2006.7(3) Å^3
Z	4
Density (calculated)	1.412 g/cm^3
Absorption coefficient μ	0.304 mm^{-1}
F(000)	896
Reflections for cell refinement	7951 (θ range 1.93 to 28.20°)
Crystal colour	red
Crystal size	0.28 × 0.24 × 0.06 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.93 to 28.41°
Index ranges	$-10 \le h \le 10$, $-15 \le k \le 10$, $-28 \le \ell \le 28$
Intensity decay	0%
Reflections collected	12160
Independent reflections	4545 (R_{int} = 0.0377)
Reflections with I>2σ(I)	3407
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.894 and 0.529
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0504, 0.0000
Data / restraints / parameters	4545 / 0 / 264
Final R indices [I>2σ(I)]	R1 = 0.0356, wR2 = 0.0899
R indices (all data)	R1 = 0.0544, wR2 = 0.0969
Goodness-of-fit on F^2	1.016
Extinction coefficient	0.0015(7)
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.297 and -0.374 eÅ^{-3}

The Crystal Structure of $[dbaH]^+[MeSO_3]^-.MeSO3H$ (40)

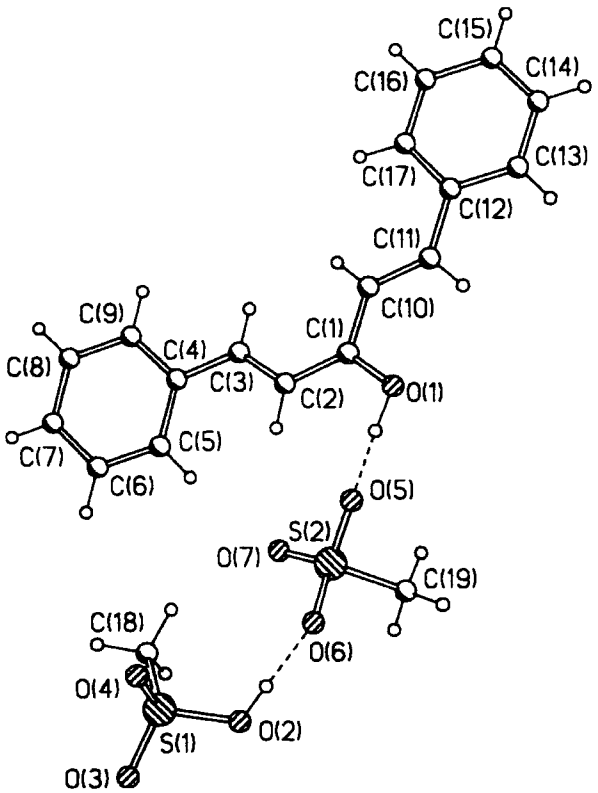


Table 16B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (40). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	12288.2(16)	5698.4(10)	6216.5(5)	28.5(3)
C(1)	12032(2)	5001.4(14)	5751.8(7)	21.1(3)
C(2)	11096(2)	4006.9(14)	5827.9(7)	22.6(4)
C(3)	10707.3(19)	3265.9(14)	5362.4(7)	21.9(3)
C(4)	9756(2)	2245.3(13)	5407.0(8)	22.1(3)
C(5)	9376(2)	1798.9(14)	5985.9(8)	25.7(4)
C(6)	8404(2)	848.4(15)	5993.1(9)	30.7(4)
C(7)	7789(2)	333.7(15)	5434.0(9)	36.7(5)
C(8)	8147(3)	765.9(16)	4858.7(9)	38.8(5)
C(9)	9147(2)	1702.7(15)	4845.6(8)	29.6(4)
C(10)	12705(2)	5293.9(13)	5171.9(7)	21.1(3)
C(11)	13598.3(19)	6232.9(14)	5107.2(7)	20.8(3)
C(12)	14171.8(19)	6635.5(13)	4519.7(7)	20.8(3)
C(13)	15177(2)	7588.5(14)	4536.7(8)	24.9(4)
C(14)	15679(2)	8034.6(15)	3983.3(8)	30.3(4)
C(15)	15181(2)	7535.0(15)	3408.2(8)	30.6(4)
C(16)	14186(2)	6588.0(15)	3384.3(8)	30.2(4)
C(17)	13683(2)	6135.0(14)	3933.1(7)	25.0(4)
S(1)	2552.5(6)	2720.3(4)	3488.28(19)	27.21(13)
O(2)	4129.0(17)	2052.1(11)	3769.8(6)	32.3(3)
O(3)	2124.9(18)	3442.0(11)	3981.1(6)	40.3(3)
O(4)	1267.2(17)	1987.1(12)	3211.1(6)	42.1(3)
C(18)	3322(2)	3522.1(16)	2894.0(8)	34.3(4)
S(2)	10974.2(6)	4423.3(4)	7625.86(18)	25.54(13)
O(5)	10760.9(18)	5348.5(11)	7187.3(6)	40.3(3)
O(6)	9893.3(18)	4593.8(11)	8137.0(6)	38.6(3)
O(7)	10736(2)	3374.3(11)	7322.3(6)	48.3(4)
C(19)	13078(3)	4513(3)	7978.3(12)	79.8(10)

Table 16C. Bond lengths (Å) and angles (°) for (40).

O(1)-C(1)	1.2970(19)	C(1)-C(2)	1.427(2)
C(1)-C(10)	1.438(2)	C(2)-C(3)	1.345(2)
C(3)-C(4)	1.451(2)	C(4)-C(9)	1.399(2)
C(4)-C(5)	1.405(2)	C(5)-C(6)	1.380(2)
C(6)-C(7)	1.381(3)	C(7)-C(8)	1.387(3)
C(8)-C(9)	1.380(3)	C(10)-C(11)	1.349(2)
C(11)-C(12)	1.457(2)	C(12)-C(13)	1.395(2)
C(12)-C(17)	1.401(2)	C(13)-C(14)	1.390(2)
C(14)-C(15)	1.381(3)	C(15)-C(16)	1.384(2)
C(16)-C(17)	1.385(2)	S(1)-O(4)	1.4222(13)
S(1)-O(3)	1.4310(13)	S(1)-O(2)	1.5438(14)
S(1)-C(18)	1.7513(18)	S(2)-O(7)	1.4255(14)
S(2)-O(5)	1.4536(13)	S(2)-O(6)	1.4649(12)
S(2)-C(19)	1.742(2)		

O(1)-C(1)-C(2)	119.99(14)	O(1)-C(1)-C(10)	116.88(15)
C(2)-C(1)-C(10)	123.13(15)	C(3)-C(2)-C(1)	123.77(15)
C(2)-C(3)-C(4)	126.54(15)	C(9)-C(4)-C(5)	118.79(16)
C(9)-C(4)-C(3)	118.24(15)	C(5)-C(4)-C(3)	122.94(15)
C(6)-C(5)-C(4)	119.98(16)	C(5)-C(6)-C(7)	120.48(17)
C(6)-C(7)-C(8)	120.25(18)	C(9)-C(8)-C(7)	119.83(18)
C(8)-C(9)-C(4)	120.63(17)	C(11)-C(10)-C(1)	122.58(15)
C(10)-C(11)-C(12)	125.54(15)	C(13)-C(12)-C(17)	118.61(15)
C(13)-C(12)-C(11)	118.73(15)	C(17)-C(12)-C(11)	122.58(15)
C(14)-C(13)-C(12)	120.70(16)	C(15)-C(14)-C(13)	120.04(17)
C(14)-C(15)-C(16)	119.89(16)	C(15)-C(16)-C(17)	120.53(16)
C(16)-C(17)-C(12)	120.24(16)	O(4)-S(1)-O(3)	118.04(8)
O(4)-S(1)-O(2)	109.78(8)	O(3)-S(1)-O(2)	106.11(8)
O(4)-S(1)-C(18)	109.35(9)	O(3)-S(1)-C(18)	108.56(9)
O(2)-S(1)-C(18)	104.08(8)	O(7)-S(2)-O(5)	113.16(8)
O(7)-S(2)-O(6)	113.75(8)	O(5)-S(2)-O(6)	109.39(8)
O(7)-S(2)-C(19)	108.76(13)	O(5)-S(2)-C(19)	105.41(13)
O(6)-S(2)-C(19)	105.78(10)		

Table 16D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (40).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
O(1)	37.7(7)	30.9(7)	18.0(6)	-3.5(5)	8.2(5)	-7.5(6)
C(1)	19.0(8)	26.5(9)	17.6(8)	1.5(7)	0.7(6)	2.1(7)
C(2)	22.6(8)	28.7(9)	17.0(8)	3.9(7)	5.1(6)	1.3(7)
C(3)	19.7(8)	27.9(9)	18.5(8)	3.8(7)	4.3(6)	3.5(7)
C(4)	19.7(8)	23.0(8)	24.2(8)	0.1(7)	5.4(6)	3.2(7)
C(5)	25.4(9)	28.0(9)	24.0(9)	2.1(7)	3.6(7)	1.3(7)
C(6)	28.0(9)	32.3(10)	33.1(10)	7.3(8)	8.4(8)	-0.2(8)
C(7)	36.9(11)	25.9(10)	48.8(12)	-2.8(9)	11.7(9)	-7.1(8)
C(8)	47.3(12)	35.4(11)	34.7(11)	-12.4(9)	8.7(9)	-9.9(9)
C(9)	35.0(10)	29.8(9)	25.2(9)	-3.3(7)	9.5(8)	0.4(8)
C(10)	22.4(8)	24.8(8)	16.4(8)	1.3(6)	3.0(6)	1.9(7)
C(11)	18.1(8)	27.5(9)	16.8(8)	1.3(7)	1.3(6)	3.6(7)
C(12)	18.5(8)	24.7(8)	19.5(8)	4.4(7)	3.8(6)	4.4(7)
C(13)	23.0(8)	28.4(9)	22.9(9)	2.9(7)	1.1(7)	0.1(7)
C(14)	25.8(9)	31.8(10)	33.7(10)	8.2(8)	5.6(7)	-3.3(8)
C(15)	33.4(10)	35.3(10)	24.8(9)	11.7(8)	10.9(8)	6.0(8)
C(16)	40.6(10)	31.1(10)	19.6(9)	1.0(7)	6.5(8)	5.8(8)
C(17)	29.4(9)	23.7(9)	22.9(8)	2.6(7)	7.1(7)	0.2(7)
S(1)	33.4(2)	32.0(2)	17.5(2)	-4.96(18)	8.27(17)	-5.6(2)
O(2)	42.8(8)	35.7(7)	18.1(6)	-3.3(5)	2.2(5)	0.8(6)
O(3)	56.0(9)	42.8(8)	25.3(7)	-9.3(6)	18.4(6)	0.3(7)
O(4)	40.6(8)	47.9(8)	37.7(8)	-7.6(6)	4.3(6)	-16.2(7)
C(18)	43.7(11)	35.7(10)	25.9(9)	2.5(8)	15.2(8)	3.4(9)
S(2)	30.0(2)	30.8(2)	16.8(2)	-1.17(17)	6.60(17)	2.61(19)
O(5)	59.2(9)	35.0(7)	30.6(7)	6.5(6)	22.4(6)	7.5(7)
O(6)	54.0(9)	34.8(7)	31.9(7)	-1.6(6)	27.3(6)	-0.4(6)
O(7)	86.0(11)	35.0(8)	27.8(7)	-4.7(6)	24.0(7)	-10.3(8)
C(19)	39.1(13)	145(3)	52.8(15)	-25.7(17)	-6.0(11)	24.2(16)

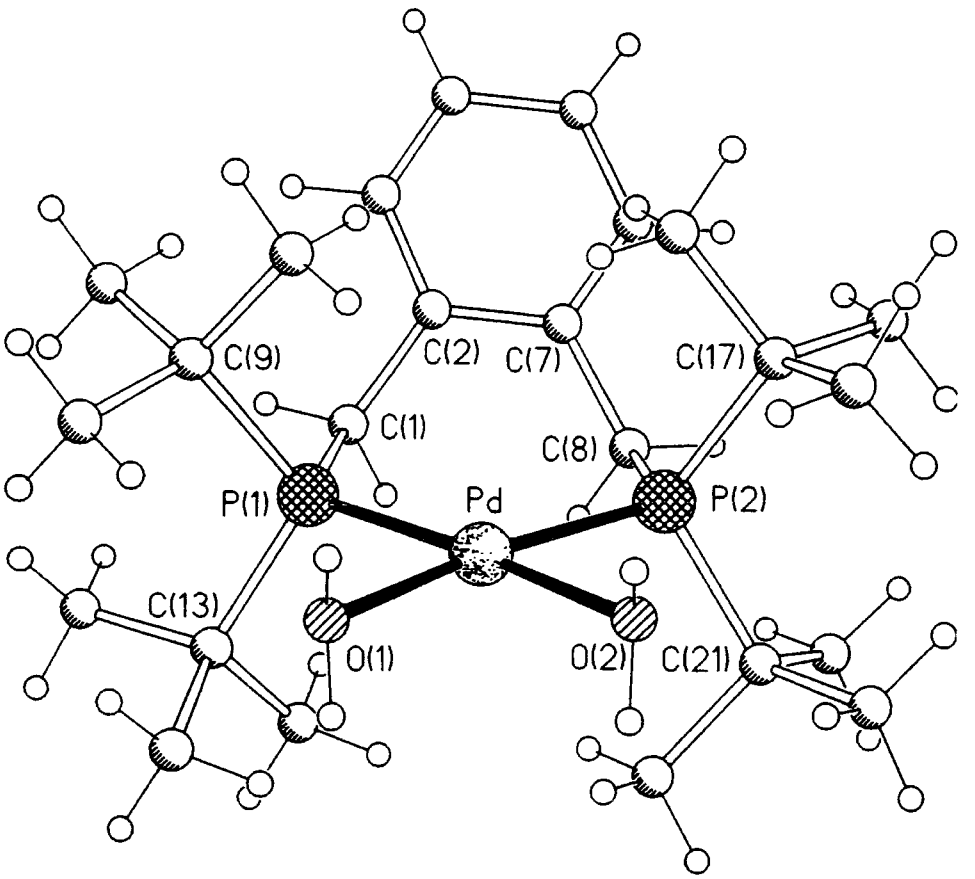
Table 16E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (40).

	x	y	z	U
H(1)	11730(3)	5490(2)	6592(13)	80(8)
H(2)	10727	3860	6230	27
H(3)	11095	3427	4964	26
H(5)	9787	2151	6372	31
H(6)	8157	546	6385	37
H(7)	7118	-319	5444	44
H(8)	7705	418	4475	47
H(9)	9426	1982	4452	35
H(10)	12514	4807	4821	25
H(11)	13877	6669	5476	25
H(13)	15522	7936	4931	30
H(14)	16365	8684	4001	36
H(15)	15521	7841	3030	37
H(16)	13845	6246	2988	36
H(17)	13005	5483	3912	30
H(2A)	4340(4)	1410(2)	3546(14)	97(10)
H(18A)	2402	3998	2698	51
H(18B)	3721	3035	2572	51
H(18C)	4275	3983	3079	51
H(19A)	13230	5205	8219	120
H(19B)	13861	4501	7650	120
H(19C)	13325	3884	8265	120

Table 17A. Crystal data, structure solution and refinement for (41).

Identification code	exti22
Chemical formula	$C_{38}H_{62}O_8P_2PdS_2$
Formula weight	879.34
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 14.6760(12) Å α = 90°
	b = 15.7127(13) Å β = 90.593(2)°
	c = 17.3890(14) Å γ = 90°
Volume	4009.7(6) Å^3
Z	4
Density (calculated)	1.457 g/cm^3
Absorption coefficient μ	0.696 mm^{-1}
F(000)	1848
Reflections for cell refinement	14707 (θ range 1.81 to 28.46°)
Crystal colour	yellow
Crystal size	0.60 x 0.50 x 0.13 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.75 to 28.46°
Index ranges	$-18 \le h \le 19$, $-20 \le k \le 20$, $-22 \le \ell \le 8$
Intensity decay	0%
Reflections collected	22881
Independent reflections	9170 (R_{int} = 0.0669)
Reflections with I>2σ(I)	6004
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.913 and 0.237
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.1184, 0.0000
Data / restraints / parameters	9170 / 7 / 474
Final R indices [I>2σ(I)]	R1 = 0.0667, wR2 = 0.1675
R indices (all data)	R1 = 0.1030, wR2 = 0.1890
Goodness-of-fit on F^2	0.959
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	2.619 and -2.323 eÅ^{-3}

The Crystal Structure of $[o\text{-}C_6H_4(CH_2PBu^t_2)_2Pd(OH_2)]^{2+}$ 2[OTs]$^-$ (41)
View 1



The Crystal Structure of $[o\text{-}C_6H_4(CH_2PBu^t_2)_2Pd(OH_2)]^{2+}$ 2[OTs]$^-$ (41)
View 2

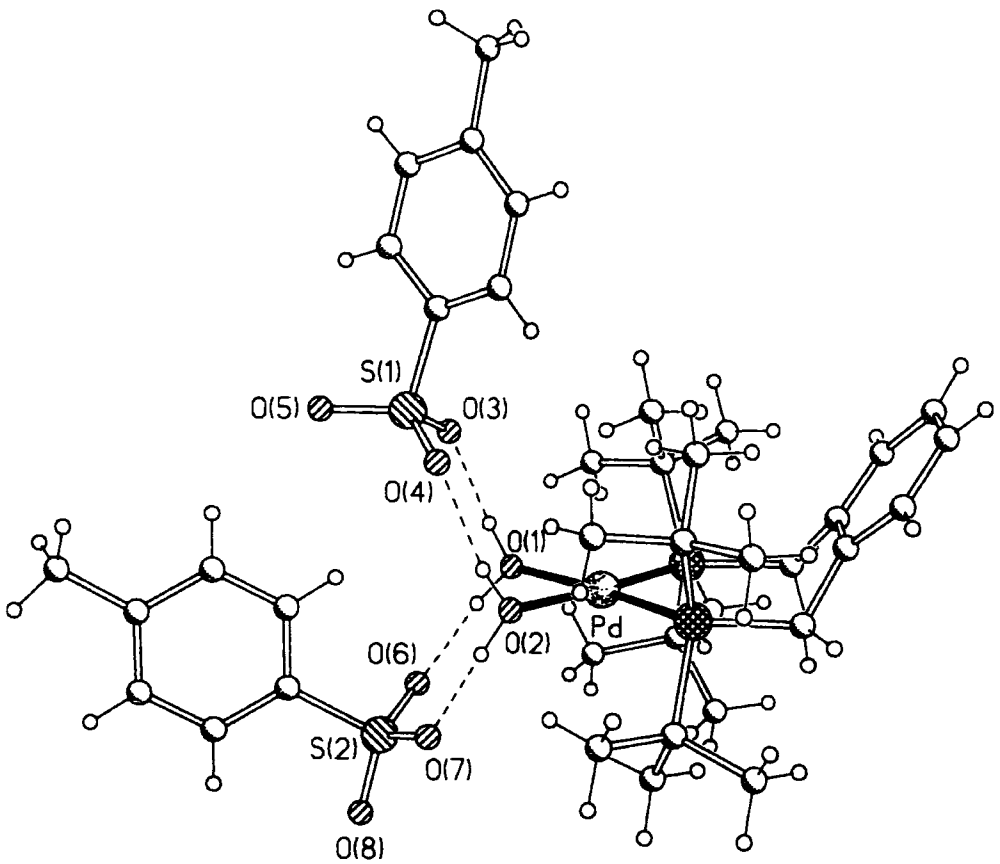


Table 17B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (41). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	4744.1(2)	5701.2(2)	2207.3(2)	18.61(13)
O(1)	5967(2)	6424(2)	2247(2)	23.8(8)
O(2)	4212(2)	6847(2)	1759(2)	24.3(8)
P(1)	5510.9(9)	4553.8(9)	2724.0(8)	20.9(3)
P(2)	3308.7(8)	5150.9(8)	2068.2(7)	20.2(3)
C(1)	4909(3)	3558(3)	2954(3)	23.1(11)
C(2)	4056(3)	3518(3)	3438(3)	22.5(11)
C(3)	4093(4)	3179(3)	4182(3)	29.1(12)
C(4)	3330(4)	3043(3)	4612(3)	29.1(12)
C(5)	2476(4)	3215(3)	4287(3)	28.5(12)
C(6)	2430(4)	3536(3)	3541(3)	26.7(12)
C(7)	3206(3)	3707(3)	3110(3)	22.8(11)
C(8)	3096(3)	4022(3)	2296(3)	23.5(11)
C(9)	6028(4)	4932(3)	3679(3)	26.7(11)
C(10)	6889(4)	5464(4)	3570(3)	32.0(13)
C(11)	6288(4)	4182(4)	4203(3)	33.6(13)
C(12)	5293(4)	5459(4)	4065(3)	29.6(12)
C(13)	6392(4)	4139(3)	2032(3)	27.2(12)
C(14)	6931(4)	4875(4)	1666(3)	34.5(13)
C(15)	5921(4)	3650(4)	1380(4)	36.9(14)
C(16)	7084(4)	3535(4)	2434(4)	42.3(15)
C(17)	2487(3)	5761(3)	2684(3)	23.9(11)
C(18)	2858(4)	5719(4)	3515(3)	32.4(13)
C(19)	1525(3)	5382(4)	2641(4)	34.3(13)
C(20)	2395(4)	6720(3)	2506(4)	37.9(14)
C(21)	3014(4)	5166(3)	1000(3)	26.6(12)
C(22)	2666(4)	6033(4)	723(3)	34.9(13)
C(23)	2297(4)	4488(4)	787(4)	42.0(16)
C(24)	3898(4)	4946(4)	572(3)	37.5(14)
S(1)	5127.6(10)	8249.6(9)	3367.1(8)	28.5(3)
O(3)	5826(3)	7576(3)	3348(2)	37.1(10)
O(4)	4325(3)	8011(3)	2902(2)	39.1(10)
O(5)	5478(4)	9079(3)	3188(2)	50.2(12)
C(25)	4759(3)	8310(3)	4332(3)	25.4(11)
C(26)	5228(4)	8860(3)	4826(3)	28.8(12)
C(27)	4930(4)	8961(4)	5573(3)	32.3(13)
C(28)	4165(4)	8533(4)	5845(3)	33.0(13)
C(29)	3701(4)	7993(3)	5332(3)	31.5(13)
C(30)	4006(3)	7882(3)	4593(3)	28.3(12)
C(31)	3856(5)	8678(4)	6651(3)	45.4(17)
S(2)	5853.0(10)	7465.3(9)	317.8(8)	31.3(3)
O(6)	6442(3)	7049(3)	894(2)	38.4(10)
O(7)	4895(3)	7217(2)	418(2)	34.2(9)
O(8)	6160(3)	7368(3)	-461(2)	44.2(11)
C(32)	5895(3)	8563(3)	543(3)	26.2(11)
C(33)	5696(4)	8842(4)	1287(3)	31.6(13)
C(34)	5693(4)	9697(4)	1455(3)	31.2(12)
C(35)	5891(3)	10303(4)	899(3)	29.1(12)
C(36)	6087(4)	10021(4)	162(3)	31.7(13)
C(37)	6089(3)	9166(4)	-12(3)	29.1(12)
C(38)	5884(4)	11239(4)	1091(4)	35.9(14)

Table 17C. Bond lengths (Å) and angles (°) for (41).

Pd-O(2)	2.109(4)	Pd-O(1)	2.125(3)
Pd-P(2)	2.2876(13)	Pd-P(1)	2.3030(14)
P(1)-C(1)	1.843(5)	P(1)-C(13)	1.891(5)
P(1)-C(9)	1.913(5)	P(2)-C(8)	1.845(5)
P(2)-C(17)	1.884(5)	P(2)-C(21)	1.903(5)
C(1)-C(2)	1.517(7)	C(2)-C(7)	1.398(7)
C(2)-C(3)	1.400(7)	C(3)-C(4)	1.370(8)
C(4)-C(5)	1.395(8)	C(5)-C(6)	1.392(8)
C(6)-C(7)	1.396(7)	C(7)-C(8)	1.507(7)
C(9)-C(12)	1.521(8)	C(9)-C(10)	1.529(7)
C(9)-C(11)	1.537(7)	C(13)-C(15)	1.528(8)
C(13)-C(14)	1.542(8)	C(13)-C(16)	1.552(8)
C(17)-C(19)	1.533(7)	C(17)-C(18)	1.539(7)
C(17)-C(20)	1.544(7)	C(21)-C(22)	1.531(8)
C(21)-C(23)	1.540(7)	C(21)-C(24)	1.540(8)
S(1)-O(5)	1.436(4)	S(1)-O(4)	1.470(4)
S(1)-O(3)	1.473(4)	S(1)-C(25)	1.771(6)
C(25)-C(30)	1.375(7)	C(25)-C(26)	1.395(7)
C(26)-C(27)	1.385(8)	C(27)-C(28)	1.396(8)
C(28)-C(29)	1.403(8)	C(28)-C(31)	1.495(8)
C(29)-C(30)	1.376(8)	S(2)-O(8)	1.440(4)
S(2)-O(6)	1.471(4)	S(2)-O(7)	1.471(4)
S(2)-C(32)	1.770(6)	C(32)-C(37)	1.385(7)
C(32)-C(33)	1.399(8)	C(33)-C(34)	1.375(8)
C(34)-C(35)	1.390(8)	C(35)-C(36)	1.389(8)
C(35)-C(38)	1.508(8)	C(36)-C(37)	1.377(8)
O(2)-Pd-O(1)	82.25(14)	O(2)-Pd-P(2)	86.92(10)
O(1)-Pd-P(2)	169.17(10)	O(2)-Pd-P(1)	172.03(10)
O(1)-Pd-P(1)	89.81(10)	P(2)-Pd-P(1)	101.01(5)
C(1)-P(1)-C(13)	100.2(2)	C(1)-P(1)-C(9)	105.2(2)
C(13)-P(1)-C(9)	113.1(2)	C(1)-P(1)-Pd	121.10(17)
C(13)-P(1)-Pd	110.85(18)	C(9)-P(1)-Pd	106.44(17)
C(8)-P(2)-C(17)	104.9(2)	C(8)-P(2)-C(21)	100.6(2)
C(17)-P(2)-C(21)	114.1(2)	C(8)-P(2)-Pd	119.88(16)
C(17)-P(2)-Pd	109.98(16)	C(21)-P(2)-Pd	107.34(17)
C(2)-C(1)-P(1)	123.8(4)	C(7)-C(2)-C(3)	118.9(5)
C(7)-C(2)-C(1)	120.2(5)	C(3)-C(2)-C(1)	120.3(5)
C(4)-C(3)-C(2)	122.7(5)	C(3)-C(4)-C(5)	119.0(5)
C(6)-C(5)-C(4)	118.8(5)	C(5)-C(6)-C(7)	122.6(5)
C(6)-C(7)-C(2)	118.0(5)	C(6)-C(7)-C(8)	119.2(4)
C(2)-C(7)-C(8)	122.6(5)	C(7)-C(8)-P(2)	120.1(4)
C(12)-C(9)-C(10)	110.4(5)	C(12)-C(9)-C(11)	109.2(5)
C(10)-C(9)-C(11)	107.0(4)	C(12)-C(9)-P(1)	106.0(3)
C(10)-C(9)-P(1)	112.6(4)	C(11)-C(9)-P(1)	111.7(4)
C(15)-C(13)-C(14)	107.5(5)	C(15)-C(13)-C(16)	108.4(5)
C(14)-C(13)-C(16)	107.9(5)	C(15)-C(13)-P(1)	109.8(4)
C(14)-C(13)-P(1)	111.2(4)	C(16)-C(13)-P(1)	111.9(4)
C(19)-C(17)-C(18)	110.2(4)	C(19)-C(17)-C(20)	106.9(4)
C(18)-C(17)-C(20)	105.0(4)	C(19)-C(17)-P(2)	111.6(4)
C(18)-C(17)-P(2)	106.8(3)	C(20)-C(17)-P(2)	115.9(4)
C(22)-C(21)-C(23)	108.3(4)	C(22)-C(21)-C(24)	109.1(5)
C(23)-C(21)-C(24)	107.8(5)	C(22)-C(21)-P(2)	112.9(4)
C(23)-C(21)-P(2)	112.0(4)	C(24)-C(21)-P(2)	106.6(3)
O(5)-S(1)-O(4)	113.5(3)	O(5)-S(1)-O(3)	113.3(3)
O(4)-S(1)-O(3)	110.9(2)	O(5)-S(1)-C(25)	105.7(3)
O(4)-S(1)-C(25)	106.5(3)	O(3)-S(1)-C(25)	106.2(2)
C(30)-C(25)-C(26)	119.6(5)	C(30)-C(25)-S(1)	122.8(4)

C(26)-C(25)-S(1)	117.5(4)	C(27)-C(26)-C(25)	119.3(5)
C(26)-C(27)-C(28)	121.7(5)	C(27)-C(28)-C(29)	117.6(5)
C(27)-C(28)-C(31)	119.8(6)	C(29)-C(28)-C(31)	122.6(6)
C(30)-C(29)-C(28)	120.7(5)	C(25)-C(30)-C(29)	121.1(5)
O(8)-S(2)-O(6)	114.0(3)	O(8)-S(2)-O(7)	113.1(3)
O(6)-S(2)-O(7)	110.9(2)	O(8)-S(2)-C(32)	107.5(3)
O(6)-S(2)-C(32)	105.3(2)	O(7)-S(2)-C(32)	105.3(2)
C(37)-C(32)-C(33)	118.5(5)	C(37)-C(32)-S(2)	121.3(4)
C(33)-C(32)-S(2)	120.1(4)	C(34)-C(33)-C(32)	120.2(5)
C(33)-C(34)-C(35)	121.4(5)	C(36)-C(35)-C(34)	118.0(5)
C(36)-C(35)-C(38)	121.2(5)	C(34)-C(35)-C(38)	120.8(5)
C(37)-C(36)-C(35)	121.1(5)	C(36)-C(37)-C(32)	120.9(5)

Table 17D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (41).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	12.94(19)	21.5(2)	21.1(2)	0.04(15)	-9.92(14)	-1.75(14)
O(1)	15.1(17)	25(2)	31(2)	-1.4(16)	-9.8(15)	-5.3(14)
O(2)	20.4(18)	24(2)	28(2)	-1.3(15)	-12.1(15)	0.7(14)
P(1)	14.7(6)	23.4(7)	24.3(7)	-0.4(5)	-8.0(5)	-0.9(5)
P(2)	13.9(6)	21.7(7)	24.9(7)	0.3(5)	-11.2(5)	-2.1(5)
C(1)	14(2)	24(3)	31(3)	0(2)	-7(2)	-1.0(19)
C(2)	17(2)	20(3)	30(3)	1(2)	-6(2)	-1.0(19)
C(3)	25(3)	22(3)	40(3)	6(2)	-17(2)	-1(2)
C(4)	39(3)	20(3)	28(3)	2(2)	-8(2)	-3(2)
C(5)	22(3)	19(3)	44(3)	4(2)	-1(2)	-1(2)
C(6)	19(3)	21(3)	40(3)	3(2)	-6(2)	0(2)
C(7)	22(3)	15(2)	31(3)	2(2)	-10(2)	-2.6(19)
C(8)	18(2)	26(3)	27(3)	2(2)	-9(2)	-4(2)
C(9)	21(3)	35(3)	25(3)	0(2)	-15(2)	2(2)
C(10)	25(3)	44(3)	27(3)	2(2)	-17(2)	-13(2)
C(11)	28(3)	38(3)	35(3)	8(2)	-16(2)	-2(2)
C(12)	27(3)	40(3)	21(3)	-2(2)	-10(2)	-2(2)
C(13)	19(3)	31(3)	31(3)	-3(2)	-3(2)	5(2)
C(14)	30(3)	35(3)	39(3)	-6(3)	6(3)	-6(2)
C(15)	30(3)	34(3)	46(4)	-11(3)	-5(3)	-2(2)
C(16)	28(3)	44(4)	55(4)	5(3)	2(3)	12(3)
C(17)	15(2)	27(3)	30(3)	-3(2)	-4(2)	-2(2)
C(18)	23(3)	44(4)	30(3)	-9(2)	-5(2)	0(2)
C(19)	13(3)	39(3)	51(4)	0(3)	-9(2)	-3(2)
C(20)	36(3)	30(3)	48(4)	-2(3)	6(3)	5(3)
C(21)	21(3)	30(3)	28(3)	-2(2)	-14(2)	-4(2)
C(22)	30(3)	40(3)	34(3)	6(3)	-19(3)	-1(3)
C(23)	43(4)	43(4)	40(4)	1(3)	-31(3)	-6(3)
C(24)	33(3)	44(4)	35(3)	-2(3)	-16(3)	6(3)
S(1)	31.0(7)	28.6(7)	25.8(7)	-1.2(5)	-11.3(6)	-2.5(6)
O(3)	26(2)	51(3)	34(2)	-9.5(19)	-9.1(18)	7.1(18)
O(4)	36(2)	51(3)	31(2)	-9.2(18)	-22.0(18)	4.1(19)
O(5)	84(4)	34(3)	33(2)	1.0(19)	0(2)	-14(2)
C(25)	20(3)	30(3)	26(3)	0(2)	-12(2)	3(2)
C(26)	23(3)	29(3)	34(3)	2(2)	-10(2)	-8(2)
C(27)	35(3)	35(3)	26(3)	-3(2)	-15(2)	1(3)
C(28)	33(3)	33(3)	33(3)	3(2)	-3(3)	15(2)
C(29)	18(3)	31(3)	45(3)	11(3)	-8(2)	3(2)
C(30)	15(2)	31(3)	39(3)	5(2)	-12(2)	2(2)
C(31)	53(4)	49(4)	35(3)	8(3)	8(3)	20(3)
S(2)	28.1(7)	33.9(8)	31.9(7)	4.4(6)	-2.1(6)	2.1(6)
O(6)	33(2)	42(3)	41(2)	14.2(19)	-0.4(19)	9.0(18)
O(7)	30(2)	37(2)	35(2)	4.2(17)	-6.3(18)	-7.7(17)
O(8)	50(3)	44(3)	39(2)	2(2)	8(2)	2(2)
C(32)	15(2)	34(3)	30(3)	4(2)	-9(2)	-2(2)
C(33)	24(3)	44(4)	27(3)	7(2)	-4(2)	-6(2)
C(34)	26(3)	38(3)	29(3)	2(2)	-11(2)	-3(2)
C(35)	12(2)	35(3)	39(3)	5(2)	-14(2)	-2(2)
C(36)	20(3)	38(3)	37(3)	14(3)	-7(2)	-6(2)
C(37)	15(2)	45(4)	27(3)	3(2)	-5(2)	-2(2)
C(38)	27(3)	42(4)	39(3)	6(3)	-13(3)	0(2)

Table 17E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (41).

	x	y	z	U
H(1X)	4467(30)	6980(32)	1294(27)	29
H(1Y)	4234(26)	7254(34)	2050(30)	29
H(2X)	6160(21)	6676(36)	1809(31)	29
H(2Y)	5912(25)	6824(37)	2593(27)	29
H(1A)	4753	3287	2456	28
H(1B)	5363	3182	3209	28
H(3)	4671	3039	4398	35
H(4)	3381	2834	5123	35
H(5)	1936	3116	4570	34
H(6)	1848	3643	3318	32
H(8A)	2465	3890	2129	28
H(8B)	3506	3678	1971	28
H(10A)	7356	5117	3321	38
H(10B)	7117	5657	4073	38
H(10C)	6748	5959	3248	38
H(11A)	6761	3840	3957	40
H(11B)	5749	3827	4291	40
H(11C)	6518	4399	4696	40
H(12A)	4746	5111	4131	36
H(12B)	5146	5954	3744	36
H(12C)	5515	5652	4570	36
H(14A)	7242	5201	2070	41
H(14B)	6511	5248	1382	41
H(14C)	7383	4642	1312	41
H(15A)	5571	3177	1595	44
H(15B)	6381	3427	1029	44
H(15C)	5509	4033	1099	44
H(16A)	7392	3839	2854	51
H(16B)	7535	3343	2060	51
H(16C)	6760	3041	2641	51
H(18A)	3472	5963	3535	39
H(18B)	2881	5125	3684	39
H(18C)	2457	6043	3854	39
H(19A)	1297	5412	2110	41
H(19B)	1120	5704	2977	41
H(19C)	1544	4786	2807	41
H(20A)	2999	6987	2528	46
H(20B)	1998	6987	2886	46
H(20C)	2131	6795	1991	46
H(22A)	3115	6473	854	42
H(22B)	2087	6162	973	42
H(22C)	2573	6018	164	42
H(23A)	2509	3928	960	50
H(23B)	2206	4480	228	50
H(23C)	1720	4625	1037	50
H(24A)	4124	4392	748	45
H(24B)	4358	5383	679	45
H(24C)	3773	4924	18	45
H(26)	5747	9163	4651	35
H(27)	5255	9331	5910	39
H(29)	3171	7701	5497	38
H(30)	3690	7504	4258	34

H(31A)	4239	8348	7007	68
H(31B)	3220	8497	6699	68
H(31C)	3906	9285	6776	68
H(33)	5562	8439	1677	38
H(34)	5552	9877	1961	37
H(36)	6222	10424	-228	38
H(37)	6225	8988	-521	35
H(38A)	5412	11352	1473	54
H(38B)	5755	11569	624	54
H(38C)	6480	11404	1302	54

Table 18A. Crystal data, structure solution and refinement for (42).

Identification code	exti6
Chemical formula	$C_{24}H_{48}B_2F_8O_2P_2Pd$
Formula weight	710.58
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 10.4611(7) Å α = 90°
	b = 15.3279(11) Å β = 99.040(2)°
	c = 19.3458(13) Å γ = 90°
Volume	3063.5(4) Å^3
Z	4
Density (calculated)	1.541 g/cm^3
Absorption coefficient μ	0.780 mm^{-1}
F(000)	1464
Reflections for cell refinement	12652 (θ range 1.33 to 26.39°)
Crystal colour	yellow
Crystal size	0.46 × 0.42 × 0.12 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.70 to 26.41°
Index ranges	$-12 \le h \le 12$, $-10 \le k \le 19$, $-24 \le \ell \le 24$
Reflections collected	16289
Independent reflections	6103 (R_{int} = 0.0429)
Reflections with I>2σ(I)	5484
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.711 and 0.600
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0321, 5.1549
Data / restraints / parameters	6099 / 7 / 377
Final R indices [I>2σ(I)]	R1 = 0.0311, wR2 = 0.0801
R indices (all data)	R1 = 0.0370, wR2 = 0.0875
Goodness-of-fit on F^2	1.101
Extinction coefficient	0.0008(2)
Largest and mean shift/esd	-0.001 and 0.000
Largest diff. peak and hole	1.380 and -0.637 eÅ^{-3}

The Crystal Structure of $[o\text{-}C_6H_4(CH_2PBu^t_2)_2Pd(OH_2)]^{2+}$ 2[BF4]$^-$ (42)

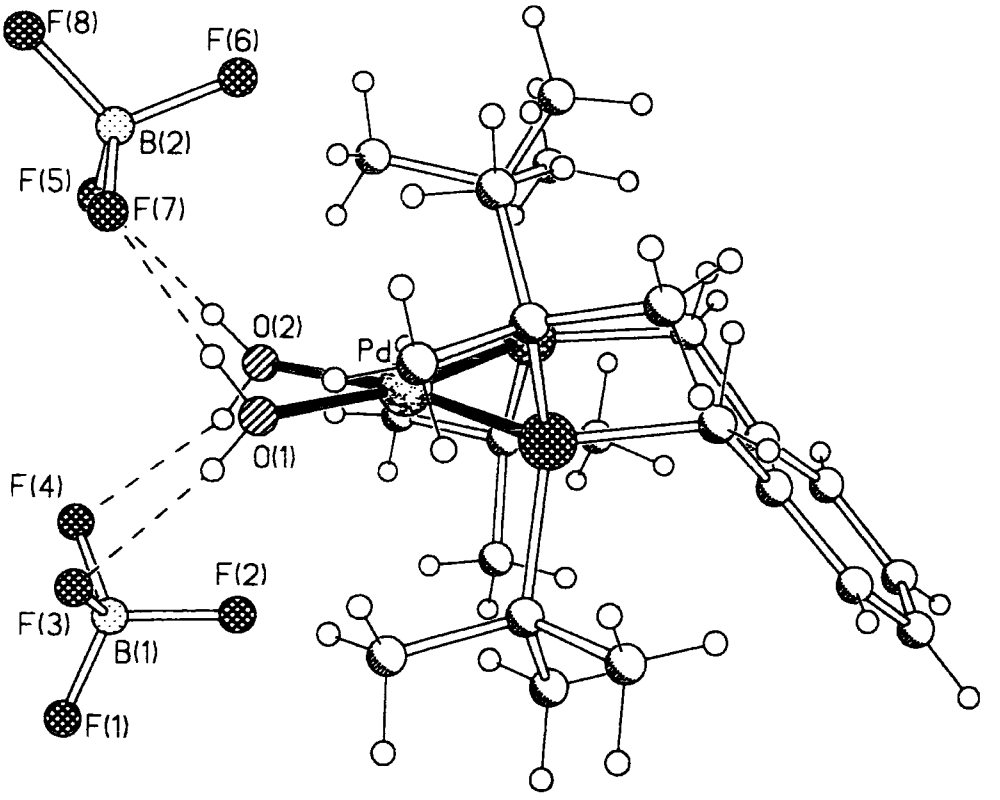


Table 18B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (42). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	5350.9(2)	2663.49(13)	3663.60(9)	16.88(8)
O(1)	4421(2)	3791.9(14)	4024.2(11)	26.9(4)
O(2)	3787(2)	2776.5(15)	2796.4(11)	26.6(4)
P(1)	6740.0(7)	2686.4(5)	4705.4(3)	18.96(15)
P(2)	6251.2(6)	1556.4(4)	3095.7(3)	16.43(14)
C(1)	5793(3)	2440(2)	5442.4(14)	26.3(6)
C(2)	6701(3)	2486(3)	6151(2)	38.8(8)
C(3)	4630(3)	3040(2)	5473(2)	35.5(7)
C(4)	5247(3)	1515(2)	5321(2)	32.0(7)
C(5)	7580(3)	3795(2)	4799.1(14)	24.4(6)
C(6)	6779(4)	4501(2)	5090(2)	39.4(8)
C(7)	8909(3)	3757(2)	5277(2)	32.7(7)
C(8)	7822(3)	4064(2)	4065.7(15)	30.1(6)
C(9)	8161(3)	1962(2)	4855.8(13)	22.8(6)
C(10)	8063(3)	981(2)	4813.3(14)	22.0(5)
C(11)	8313(3)	489(2)	5426.9(15)	28.4(6)
C(12)	8407(3)	-411(2)	5413(2)	32.5(7)
C(13)	8296(3)	-833(2)	4777(2)	31.5(7)
C(14)	8076(3)	-355(2)	4160(2)	28.4(6)
C(15)	7926(2)	547(2)	4168.7(14)	21.6(5)
C(16)	7796(3)	1058(2)	3490.2(13)	20.8(5)
C(17)	6732(3)	2009(2)	2255.1(13)	20.3(5)
C(18)	6987(3)	1266(2)	1760.2(14)	25.8(6)
C(19)	5699(3)	2618(2)	1860.5(14)	25.2(6)
C(20)	7980(3)	2544(2)	2444(2)	29.7(6)
C(21)	5026(3)	639(2)	2914.3(14)	21.4(5)
C(22)	3931(3)	838(2)	2310(2)	29.2(6)
C(23)	5665(3)	-226(2)	2748(2)	30.5(6)
C(24)	4432(3)	520(2)	3584.2(15)	28.9(6)
B(1)	1410(4)	2883(3)	3779(2)	45.2(10)
F(1)	303(2)	2583(2)	3951.1(13)	54.3(6)
F(2)	2436(2)	2308(2)	3957.3(15)	60.4(7)
F(3)	1795(3)	3675(2)	4074(2)	80.7(9)
F(4)	1287(3)	2980(2)	3046.1(14)	81.7(9)
B(2)	4571(4)	5038(2)	2536(2)	28.8(7)
F(5)	3636(2)	4418.9(13)	2262.8(10)	40.2(4)
F(6)	5788(2)	4677.5(13)	2531.1(11)	41.2(5)
F(7)	4434(2)	5197.6(13)	3234.9(10)	46.6(5)
F(8)	4422(2)	5794.7(14)	2164.1(11)	48.2(5)

Table 18C. Bond lengths (Å) and angles (°) for (42).

Pd-O(1)	2.154(2)	Pd-O(2)	2.159(2)
Pd-P(1)	2.2923(7)	Pd-P(2)	2.3018(7)
P(1)-C(9)	1.842(3)	P(1)-C(1)	1.897(3)
P(1)-C(5)	1.908(3)	P(2)-C(16)	1.842(3)
P(2)-C(21)	1.897(3)	P(2)-C(17)	1.907(3)
C(1)-C(4)	1.532(4)	C(1)-C(3)	1.534(4)
C(1)-C(2)	1.542(4)	C(5)-C(6)	1.529(4)
C(5)-C(8)	1.536(4)	C(5)-C(7)	1.545(4)
C(9)-C(10)	1.508(4)	C(10)-C(11)	1.396(4)
C(10)-C(15)	1.401(4)	C(11)-C(12)	1.383(5)
C(12)-C(13)	1.379(5)	C(13)-C(14)	1.388(4)
C(14)-C(15)	1.393(4)	C(15)-C(16)	1.516(4)
C(17)-C(20)	1.537(4)	C(17)-C(19)	1.537(4)
C(17)-C(18)	1.538(4)	C(21)-C(22)	1.534(4)
C(21)-C(24)	1.534(4)	C(21)-C(23)	1.542(4)
B(1)-F(1)	1.337(5)	B(1)-F(3)	1.375(5)
B(1)-F(2)	1.390(5)	B(1)-F(4)	1.410(5)
B(2)-F(8)	1.360(4)	B(2)-F(6)	1.389(4)
B(2)-F(7)	1.404(4)	B(2)-F(5)	1.405(4)
O(1)-Pd-O(2)	82.03(8)	O(1)-Pd-P(1)	87.66(6)
O(2)-Pd-P(1)	168.67(6)	O(1)-Pd-P(2)	170.47(6)
O(2)-Pd-P(2)	90.30(6)	P(1)-Pd-P(2)	100.40(2)
C(9)-P(1)-C(1)	105.36(13)	C(9)-P(1)-C(5)	99.99(13)
C(1)-P(1)-C(5)	113.14(13)	C(9)-P(1)-Pd	120.94(9)
C(1)-P(1)-Pd	108.90(9)	C(5)-P(1)-Pd	108.42(9)
C(16)-P(2)-C(21)	107.00(13)	C(16)-P(2)-C(17)	99.94(12)
C(21)-P(2)-C(17)	111.89(12)	C(16)-P(2)-Pd	120.44(9)
C(21)-P(2)-Pd	108.63(9)	C(17)-P(2)-Pd	108.72(9)
C(4)-C(1)-C(3)	106.4(3)	C(4)-C(1)-C(2)	110.0(3)
C(3)-C(1)-C(2)	108.6(3)	C(4)-C(1)-P(1)	107.2(2)
C(3)-C(1)-P(1)	114.8(2)	C(2)-C(1)-P(1)	109.7(2)
C(6)-C(5)-C(8)	109.2(3)	C(6)-C(5)-C(7)	107.5(2)
C(8)-C(5)-C(7)	107.4(2)	C(6)-C(5)-P(1)	113.2(2)
C(8)-C(5)-P(1)	106.9(2)	C(7)-C(5)-P(1)	112.4(2)
C(10)-C(9)-P(1)	123.1(2)	C(11)-C(10)-C(15)	118.6(3)
C(11)-C(10)-C(9)	119.4(3)	C(15)-C(10)-C(9)	121.2(2)
C(12)-C(11)-C(10)	121.8(3)	C(13)-C(12)-C(11)	119.3(3)
C(12)-C(13)-C(14)	119.9(3)	C(13)-C(14)-C(15)	121.2(3)
C(14)-C(15)-C(10)	119.1(3)	C(14)-C(15)-C(16)	119.8(2)
C(10)-C(15)-C(16)	120.6(3)	C(15)-C(16)-P(2)	121.8(2)
C(20)-C(17)-C(19)	107.4(2)	C(20)-C(17)-C(18)	108.6(2)
C(19)-C(17)-C(18)	108.5(2)	C(20)-C(17)-P(2)	108.6(2)
C(19)-C(17)-P(2)	112.7(2)	C(18)-C(17)-P(2)	110.8(2)
C(22)-C(21)-C(24)	108.3(2)	C(22)-C(21)-C(23)	108.0(2)
C(24)-C(21)-C(23)	108.6(2)	C(22)-C(21)-P(2)	113.3(2)
C(24)-C(21)-P(2)	106.5(2)	C(23)-C(21)-P(2)	112.0(2)
F(1)-B(1)-F(3)	114.1(4)	F(1)-B(1)-F(2)	112.6(3)
F(3)-B(1)-F(2)	107.0(3)	F(1)-B(1)-F(4)	110.0(4)
F(3)-B(1)-F(4)	107.4(4)	F(2)-B(1)-F(4)	105.2(4)
F(8)-B(2)-F(6)	111.4(3)	F(8)-B(2)-F(7)	109.9(3)
F(6)-B(2)-F(7)	107.9(3)	F(8)-B(2)-F(5)	111.3(3)
F(6)-B(2)-F(5)	108.2(3)	F(7)-B(2)-F(5)	108.0(3)

Table 18D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (42).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	18.91(12)	17.43(12)	14.79(11)	-1.14(7)	4.20(7)	-0.14(7)
O(1)	30.5(11)	23.6(11)	28.5(11)	-1.7(8)	10.6(9)	2.1(9)
O(2)	22.5(10)	32.5(12)	24.3(10)	-0.5(8)	2.0(8)	4.2(9)
P(1)	22.7(3)	20.3(3)	14.3(3)	-1.1(2)	4.3(3)	-2.0(3)
P(2)	18.9(3)	17.1(3)	13.8(3)	-0.3(2)	4.0(2)	-0.1(3)
C(1)	27.4(14)	36(2)	16.8(12)	0.9(11)	7.0(11)	-2.7(12)
C(2)	41(2)	59(2)	16.8(14)	0.9(14)	5.0(13)	-8(2)
C(3)	37(2)	42(2)	31(2)	0.5(14)	17.7(13)	3.4(15)
C(4)	33(2)	36(2)	29.6(15)	6.7(13)	12.8(13)	-2.5(14)
C(5)	32.4(15)	20.4(14)	20.2(13)	-2.3(11)	2.9(11)	-6.9(12)
C(6)	48(2)	28(2)	42(2)	-14.6(14)	8(2)	-3(2)
C(7)	38(2)	32(2)	26.0(14)	-2.3(12)	-1.8(12)	-14.0(14)
C(8)	38(2)	27(2)	24.6(14)	2.7(12)	2.4(12)	-9.6(13)
C(9)	20.7(13)	29.3(15)	18.0(12)	0.2(11)	1.6(10)	-1.9(11)
C(10)	17.7(12)	26.4(14)	21.9(13)	2.6(11)	3.2(10)	1.5(11)
C(11)	28.4(15)	34(2)	22.7(13)	4.6(12)	3.9(11)	2.8(13)
C(12)	29(2)	37(2)	32(2)	14.9(13)	5.1(12)	2.9(13)
C(13)	31(2)	24.1(15)	40(2)	7.6(13)	5.8(13)	5.7(12)
C(14)	28.6(15)	27(2)	28.9(15)	0.2(12)	2.6(12)	5.9(12)
C(15)	16.3(12)	25.4(14)	22.7(13)	3.2(11)	1.8(10)	2.0(11)
C(16)	21.0(13)	23.8(14)	18.2(12)	0.8(10)	4.9(10)	3.2(11)
C(17)	25.6(13)	20.6(13)	15.8(11)	-0.5(10)	6.1(10)	-2.1(11)
C(18)	34(2)	25.1(14)	19.9(13)	-1.9(11)	10.0(11)	1.7(12)
C(19)	33(2)	23.6(15)	20.1(13)	3.8(11)	7.6(11)	2.2(12)
C(20)	32(2)	36(2)	22.8(14)	1.8(12)	7.5(12)	-10.3(13)
C(21)	25.3(13)	19.2(13)	20.2(12)	0.8(10)	5.0(10)	-2.8(11)
C(22)	28.2(15)	28(2)	28.9(14)	1.9(12)	-2.3(12)	-7.6(12)
C(23)	37(2)	19.9(14)	34(2)	-3.3(12)	5.1(13)	-2.7(13)
C(24)	33(2)	28(2)	27.3(14)	3.0(12)	10.6(12)	-5.7(13)
B(1)	36(2)	44(2)	57(3)	6(2)	12(2)	-8(2)
F(1)	35.8(11)	66(2)	66.1(15)	-10.8(12)	24.1(11)	-12.8(11)
F(2)	43.4(12)	49.9(14)	91(2)	18.7(13)	20.5(12)	5.5(11)
F(3)	59(2)	53(2)	133(3)	-39(2)	26(2)	-14.4(13)
F(4)	59(2)	125(3)	62(2)	28(2)	9.3(13)	-9(2)
B(2)	34(2)	26(2)	27(2)	3.4(13)	5.9(13)	-2.2(14)
F(5)	35.4(10)	38.1(11)	45.0(11)	2.4(9)	-0.6(8)	-3.5(9)
F(6)	32.1(10)	39.0(11)	52.7(12)	-4.0(9)	7.4(9)	-0.1(8)
F(7)	79(2)	34.6(11)	29.8(10)	-0.5(8)	18.5(10)	4.7(10)
F(8)	66.1(14)	34.0(11)	44.9(11)	16.5(9)	9.4(10)	0.1(10)

Table 18E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (42).

	x	y	z	U
H(1A)	4392(33)	4194(19)	3769(16)	32
H(1B)	3692(24)	3689(23)	4042(18)	32
H(2A)	3708(33)	3221(18)	2595(17)	32
H(2B)	3113(27)	2699(23)	2904(19)	32
H(2C)	7034(20)	3082(5)	6228(7)	58
H(2D)	7426(14)	2082(13)	6147(5)	58
H(2E)	6221(8)	2325(17)	6528(2)	58
H(3A)	4926(4)	3647(3)	5523(13)	53
H(3B)	4213(15)	2879(11)	5874(8)	53
H(3C)	4009(11)	2979(12)	5040(6)	53
H(4A)	5959(3)	1103(3)	5308(12)	48
H(4B)	4657(17)	1495(4)	4874(6)	48
H(4C)	4776(19)	1357(6)	5702(6)	48
H(6A)	6713(21)	4367(9)	5579(4)	59
H(6B)	5910(9)	4519(11)	4814(8)	59
H(6C)	7200(13)	5068(3)	5065(12)	59
H(7A)	8809(5)	3483(14)	5723(5)	49
H(7B)	9247(11)	4349(2)	5363(10)	49
H(7C)	9513(7)	3413(13)	5048(6)	49
H(8A)	6990(3)	4147(15)	3760(4)	45
H(8B)	8315(19)	3606(7)	3872(5)	45
H(8C)	8313(20)	4611(8)	4097(2)	45
H(9A)	8734(3)	2142(2)	4519.7(13)	27
H(9B)	8629(3)	2102(2)	5328.4(13)	27
H(11)	8420(3)	780(2)	5865.9(15)	34
H(12)	8547(3)	-734(2)	5837(2)	39
H(13)	8371(3)	-1450(2)	4761(2)	38
H(14)	8025(3)	-649(2)	3725(2)	34
H(16A)	8063(3)	662(2)	3133.9(13)	25
H(16B)	8445(3)	1533(2)	3562.9(13)	25
H(18A)	7657(15)	879(8)	2002(4)	39
H(18B)	7277(20)	1512(2)	1344(5)	39
H(18C)	6187(6)	934(9)	1620(9)	39
H(19A)	5634(15)	3147(6)	2138(5)	38
H(19B)	4861(5)	2318(5)	1784(10)	38
H(19C)	5942(11)	2777(11)	1408(5)	38
H(20A)	7861(8)	2980(10)	2800(9)	44
H(20B)	8180(13)	2840(12)	2025(3)	44
H(20C)	8695(5)	2155(3)	2629(11)	44
H(22A)	4282(5)	867(15)	1870(2)	44
H(22B)	3532(15)	1399(7)	2395(6)	44
H(22C)	3277(11)	375(8)	2279(8)	44
H(23A)	6255(17)	-424(8)	3163(4)	46
H(23B)	6151(18)	-137(4)	2360(8)	46
H(23C)	4994(3)	-668(4)	2616(11)	46
H(24A)	5122(4)	406(15)	3979(3)	43
H(24B)	3830(17)	26(10)	3526(5)	43
H(24C)	3966(19)	1051(6)	3676(7)	43

Table 19A. Crystal data, structure solution and refinement for (43).

Identification code	exti9
Chemical formula	$C_{34}H_{30}B_2F_8O_2$
Formula weight	644.20
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 8.075(2) Å α = 101.297(7)°
	b = 8.426(2) Å β = 95.774(7)°
	c = 13.186(4) Å γ = 116.529(6)°
Volume	768.9(4) Å^3
Z	1
Density (calculated)	1.391 g/cm^3
Absorption coefficient μ	0.117 mm^{-1}
F(000)	332
Reflections for cell refinement	3003 (θ range 1.61 to 26.31°)
Crystal colour	orange
Crystal size	0.59 × 0.31 × 0.14 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.61 to 26.45°
Index ranges	$-9 \le h \le 10$, $-10 \le k \le 10$, $-16 \le \ell \le 16$
Intensity decay	1%
Reflections collected	4164
Independent reflections	2794 (R_{int} = 0.0781)
Reflections with I>2σ(I)	2443
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.986 and 0.393
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.1189, 0.5127
Data / restraints / parameters	2793 / 0 / 211
Final R indices [I>2σ(I)]	R1 = 0.0765, wR2 = 0.1900
R indices (all data)	R1 = 0.0853, wR2 = 0.2136
Goodness-of-fit on F^2	1.174
Extinction coefficient	0.075(17)
Largest and mean shift/esd	0.000 and 0.000
Largest diff. peak and hole	0.460 and -0.518 eÅ^{-3}

The Crystal Structure of $[dbaH]^+[BF_4]^-$ (43)

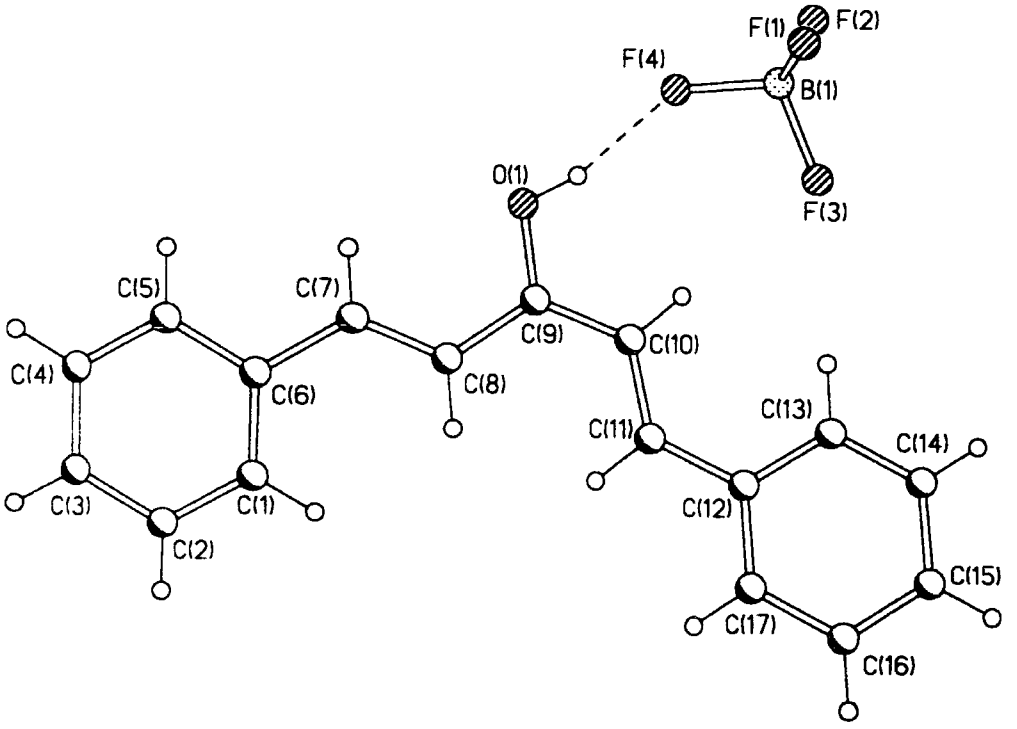


Table 19B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (43). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	9075(3)	1642(3)	1605(2)	35.7(5)
C(1)	16080(4)	5895(4)	1727(2)	33.1(6)
C(2)	17873(4)	6584(4)	1498(2)	35.9(7)
C(3)	18329(4)	5456(4)	802(2)	36.7(7)
C(4)	16995(4)	3631(4)	327(2)	36.7(7)
C(5)	15207(4)	2928(4)	559(2)	32.6(6)
C(6)	14726(3)	4047(4)	1258(2)	29.7(6)
C(7)	12815(3)	3270(4)	1455(2)	30.3(6)
C(8)	12107(3)	4178(4)	2077(2)	30.8(6)
C(9)	10186(3)	3318(3)	2215(2)	27.6(6)
C(10)	9441(3)	4176(3)	2931(2)	29.5(6)
C(11)	10549(3)	5795(3)	3676(2)	29.1(6)
C(12)	9938(3)	6741(3)	4464(2)	28.0(6)
C(13)	8011(4)	6119(4)	4521(2)	32.6(6)
C(14)	7530(4)	7089(4)	5298(2)	35.1(6)
C(15)	8928(4)	8666(4)	6048(2)	34.2(6)
C(16)	10828(4)	9291(4)	6001(2)	33.6(6)
C(17)	11327(4)	8340(3)	5216(2)	30.7(6)
B(1)	4358(4)	-120(4)	2517(3)	35.9(7)
F(1)	4427(3)	-1214(3)	3165(2)	55.8(6)
F(2)	2560(2)	-860(3)	1911(2)	60.4(6)
F(3)	4949(2)	1654(2)	3122.0(15)	44.9(5)
F(4)	5627(2)	-60(2)	1834.4(13)	42.3(5)

Table 19C. Bond lengths (Å) and angles (°) for (43).

O(1)-C(9)	1.313(3)	C(1)-C(2)	1.389(4)
C(1)-C(6)	1.403(4)	C(2)-C(3)	1.385(4)
C(3)-C(4)	1.387(4)	C(4)-C(5)	1.388(4)
C(5)-C(6)	1.396(4)	C(6)-C(7)	1.457(3)
C(7)-C(8)	1.351(4)	C(8)-C(9)	1.439(3)
C(9)-C(10)	1.418(4)	C(10)-C(11)	1.354(4)
C(11)-C(12)	1.446(4)	C(12)-C(17)	1.399(4)
C(12)-C(13)	1.418(3)	C(13)-C(14)	1.380(4)
C(14)-C(15)	1.393(4)	C(15)-C(16)	1.395(4)
C(16)-C(17)	1.386(4)	B(1)-F(2)	1.377(4)
B(1)-F(3)	1.385(4)	B(1)-F(1)	1.388(4)
B(1)-F(4)	1.421(3)		
C(2)-C(1)-C(6)	120.0(3)	C(3)-C(2)-C(1)	120.3(3)
C(2)-C(3)-C(4)	120.2(2)	C(3)-C(4)-C(5)	119.9(3)
C(4)-C(5)-C(6)	120.6(2)	C(5)-C(6)-C(1)	119.0(2)
C(5)-C(6)-C(7)	118.8(2)	C(1)-C(6)-C(7)	122.1(2)
C(8)-C(7)-C(6)	126.2(2)	C(7)-C(8)-C(9)	122.9(2)
O(1)-C(9)-C(10)	119.6(2)	O(1)-C(9)-C(8)	115.9(2)
C(10)-C(9)-C(8)	124.5(2)	C(11)-C(10)-C(9)	122.6(2)
C(10)-C(11)-C(12)	126.8(2)	C(17)-C(12)-C(13)	118.6(2)
C(17)-C(12)-C(11)	118.0(2)	C(13)-C(12)-C(11)	123.3(2)
C(14)-C(13)-C(12)	120.2(2)	C(13)-C(14)-C(15)	120.5(2)
C(14)-C(15)-C(16)	119.7(2)	C(17)-C(16)-C(15)	120.3(2)
C(16)-C(17)-C(12)	120.6(2)	F(2)-B(1)-F(3)	110.7(3)
F(2)-B(1)-F(1)	110.9(2)	F(3)-B(1)-F(1)	110.1(3)
F(2)-B(1)-F(4)	108.9(3)	F(3)-B(1)-F(4)	108.7(2)
F(1)-B(1)-F(4)	107.5(2)		

Table 19D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (43).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
O(1)	19.5(9)	25.8(10)	46.2(11)	5.7(8)	10.2(8)	-1.4(7)
C(1)	20.9(12)	28.7(14)	43.3(14)	9.9(11)	11.6(11)	5.4(10)
C(2)	17.2(13)	31.2(14)	49(2)	11.4(12)	9.2(11)	2.6(11)
C(3)	17.7(12)	39(2)	45.6(15)	13.2(12)	10.3(11)	6.1(11)
C(4)	22.8(13)	42(2)	40.0(14)	8.7(12)	13.3(11)	10.5(12)
C(5)	22.2(13)	29.4(14)	39.4(14)	8.6(11)	8.9(10)	6.4(11)
C(6)	17.0(12)	29.3(13)	37.9(13)	14.6(10)	9.7(10)	3.9(10)
C(7)	18.2(12)	27.1(13)	38.4(13)	12.2(10)	11.1(10)	2.4(10)
C(8)	16.2(12)	26.6(13)	39.0(13)	10.8(10)	9.2(10)	-0.3(10)
C(9)	16.3(11)	22.3(12)	35.8(12)	11.3(10)	8.0(9)	0.4(9)
C(10)	16.0(11)	25.4(13)	41.9(13)	14.5(10)	12.3(10)	2.3(10)
C(11)	16.7(11)	23.0(12)	42.5(14)	15.6(10)	12.1(10)	1.2(9)
C(12)	16.9(11)	21.5(12)	40.8(13)	14.4(10)	10.8(10)	1.8(9)
C(13)	19.6(13)	22.5(13)	46.1(14)	9.1(11)	10.5(10)	1.5(10)
C(14)	21.4(13)	27.9(14)	51(2)	13.8(12)	15.4(11)	5.3(11)
C(15)	30.3(14)	26.7(13)	44.3(14)	13.5(11)	15.7(11)	9.2(11)
C(16)	26.4(13)	21.8(12)	40.4(14)	8.9(10)	5.7(10)	1.3(10)
C(17)	21.3(12)	22.0(12)	42.2(14)	14.1(10)	11.3(10)	1.7(10)
B(1)	14.9(13)	24.5(15)	52(2)	4.2(13)	10.1(12)	-2.2(11)
F(1)	45.4(11)	34.9(10)	76.7(13)	24.0(9)	28.0(10)	3.7(8)
F(2)	16.9(9)	58.2(12)	74.5(13)	-9.6(10)	4.0(8)	3.4(8)
F(3)	26.2(9)	24.2(9)	66.4(11)	2.7(7)	15.8(8)	-0.4(7)
F(4)	20.3(8)	33.7(9)	55.3(10)	4.7(7)	16.3(7)	-0.6(7)

Table 19E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (43).

	x	y	z	U
H(1)	7978(13)	1265(19)	1723(21)	54
H(1A)	15771(4)	6676(4)	2201(2)	40
H(2)	18790(4)	7833(4)	1819(2)	43
H(3)	19558(4)	5933(4)	650(2)	44
H(4)	17305(4)	2863(4)	-157(2)	44
H(5)	14302(4)	1673(4)	240(2)	39
H(7)	11988(3)	2003(4)	1113(2)	36
H(8)	12914(3)	5439(4)	2440(2)	37
H(10)	8111(3)	3593(3)	2886(2)	35
H(11)	11866(3)	6368(3)	3681(2)	35
H(13)	7048(4)	5031(4)	4022(2)	39
H(14)	6234(4)	6678(4)	5321(2)	42
H(15)	8590(4)	9314(4)	6590(2)	41
H(16)	11784(4)	10372(4)	6508(2)	40
H(17)	12624(4)	8778(3)	5188(2)	37

Table 20A. Crystal data, structure solution and refinement for (44).

Identification code	exti20
Chemical formula	$C_{30}H_{58}O_8P_2PdS_2$
Formula weight	779.22
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	a = 9.8188(9) Å α = 90°
	b = 15.0712(14) Å β = 96.108(3)°
	c = 24.739(2) Å γ = 90°
Volume	3640.1(6) $Å^3$
Z	4
Density (calculated)	1.422 g/cm^3
Absorption coefficient μ	0.757 mm^{-1}
F(000)	1640
Reflections for cell refinement	9175 (θ range 2.14 to 28.13°)
Crystal colour	Pale Yellow
Crystal size	0.42 × 0.12 × 0.10 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.66 to 28.51°
Index ranges	$-13 \le h \le 12$, $-19 \le k \le 19$, $-17 \le \ell \le 33$
Reflections collected	22487
Independent reflections	8396 (R_{int} = 0.0731)
Reflections with I>2σ(I)	6062
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.855 and 0.659
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0267, 5.2091
Data / restraints / parameters	8396 / 0 / 398
Final R indices [I>2σ(I)]	R1 = 0.0430, wR2 = 0.0833
R indices (all data)	R1 = 0.0771, wR2 = 0.0977
Goodness-of-fit on F^2	1.051
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.657 and -1.089 $eÅ^{-3}$

The Crystal Structure of [o–$C_6H_4(CH_2PPr^i_2)_2Pd(CH_3SO_3)_2$] (44)

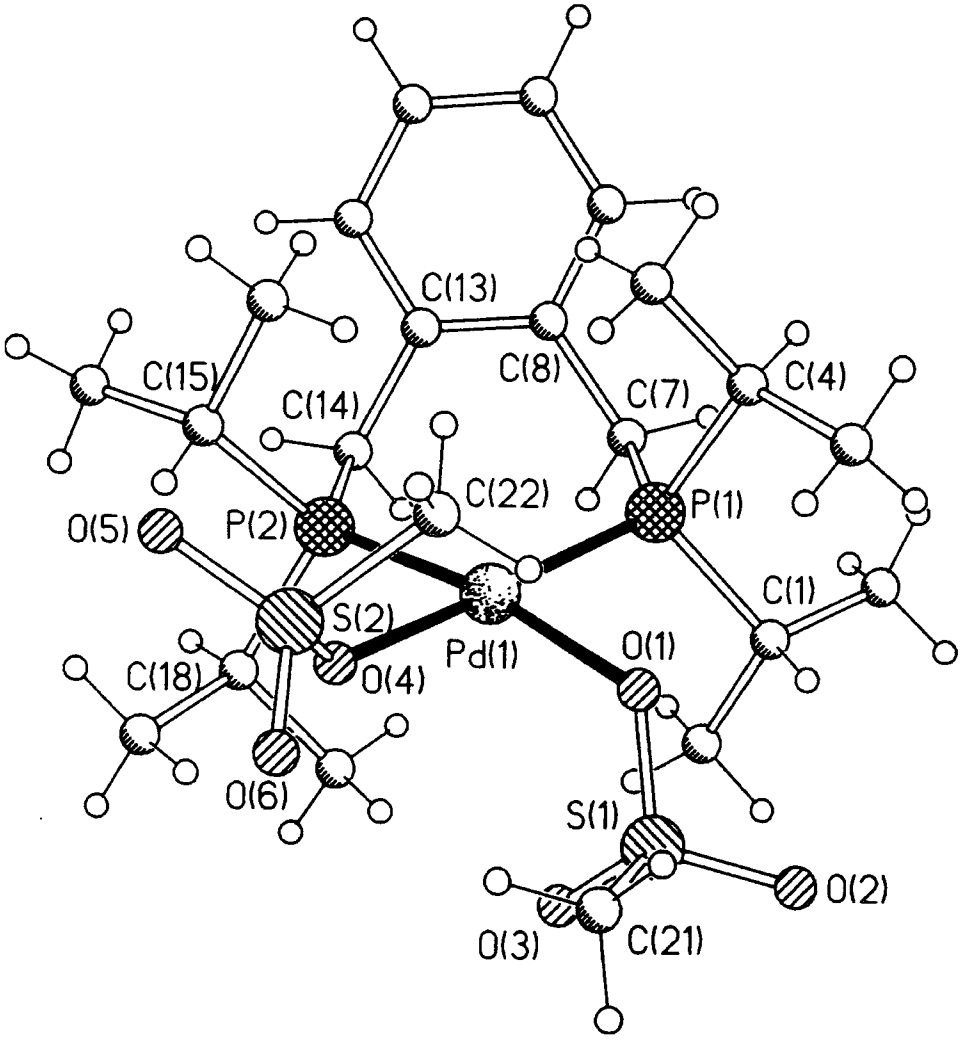


Table 20B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (44). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	-1587.1(2)	3803.71(16)	6458.34(10)	14.82(7)
P(1)	714.3(8)	3831.1(6)	6539.8(3)	16.60(17)
C(1)	1364(3)	4882(2)	6846.9(14)	21.9(7)
C(2)	868(4)	5007(3)	7405.7(15)	31.0(9)
C(3)	2936(4)	4960(3)	6876.0(17)	32.4(9)
C(4)	1298(3)	3763(2)	5856.0(13)	23.8(7)
C(5)	1208(4)	4655(3)	5560.0(16)	35.2(9)
C(6)	507(4)	3044(3)	5504.3(16)	38.4(10)
C(7)	1763(3)	3004(2)	6934.2(14)	22.8(7)
C(8)	1598(3)	2052(2)	6750.6(13)	21.9(7)
C(9)	2543(4)	1691(3)	6426.7(16)	30.4(9)
C(10)	2463(4)	813(3)	6273.0(16)	35.4(9)
C(11)	1455(4)	278(3)	6447.3(18)	37.6(10)
C(12)	517(4)	627(2)	6767.0(16)	32.3(9)
C(13)	561(3)	1517(2)	6915.2(14)	22.6(7)
C(14)	-494(3)	1883(2)	7259.1(14)	22.7(7)
P(2)	-1898.0(8)	2532.4(6)	6903.3(3)	18.01(18)
C(15)	-2964(4)	1777(2)	6458.2(15)	25.5(8)
C(16)	-2347(4)	1594(2)	5923.1(15)	30.1(8)
C(17)	-3311(4)	916(3)	6735.9(17)	35.9(9)
C(18)	-2864(3)	2796(2)	7484.8(14)	24.9(8)
C(19)	-4401(4)	2945(3)	7339.8(17)	41.5(11)
C(20)	-2219(5)	3592(3)	7798.0(16)	41.9(10)
O(1)	-1540(2)	5074.4(14)	6095.9(9)	21.3(5)
S(1)	-2038.7(9)	5871.4(6)	6376.7(4)	28.2(2)
O(2)	-1083(3)	6591.4(18)	6369.0(15)	51.7(9)
O(3)	-2443(3)	5645.7(19)	6903.7(11)	41.9(7)
C(21)	-3540(4)	6186(3)	5969(2)	44.9(11)
O(4)	-3748(2)	3825.6(16)	6247.6(9)	22.6(5)
S(2)	-4626.5(8)	3759.7(6)	5723.9(4)	25.14(19)
O(5)	-5220(3)	2887.0(19)	5650.1(12)	45.6(8)
O(6)	-5608(2)	4473.0(19)	5674.6(11)	38.7(7)
C(22)	-3543(4)	3922(3)	5208.7(14)	31.4(9)
O(7)	3053(3)	200(2)	5021.8(14)	56.5(9)
C(23)	1655(5)	373(4)	4878(2)	64.4(15)
C(24)	1579(7)	1023(5)	4425(3)	90(2)
C(25)	2922(8)	1487(5)	4517(4)	116(3)
C(26)	3807(6)	917(4)	4848(3)	89(2)
O(8)	1841(4)	3041(2)	8307.2(12)	58.9(9)
C(27)	3014(5)	2509(3)	8473.0(19)	53.8(12)
C(28)	2868(6)	2223(4)	9039.3(19)	60.2(14)
C(29)	2131(5)	3010(3)	9256.3(18)	53.4(13)
C(30)	1213(4)	3312(3)	8770.4(18)	41.5(10)

Table 20C. Bond lengths (Å) and angles (°) for (44).

Pd(1)-O(1)	2.117(2)	Pd(1)-O(4)	2.131(2)
Pd(1)-P(2)	2.2467(9)	Pd(1)-P(1)	2.2476(8)
P(1)-C(7)	1.830(3)	P(1)-C(1)	1.841(3)
P(1)-C(4)	1.846(3)	C(1)-C(2)	1.526(5)
C(1)-C(3)	1.542(5)	C(4)-C(5)	1.529(5)
C(4)-C(6)	1.546(5)	C(7)-C(8)	1.508(5)
C(8)-C(13)	1.393(5)	C(8)-C(9)	1.400(5)
C(9)-C(10)	1.377(6)	C(10)-C(11)	1.381(6)
C(11)-C(12)	1.381(6)	C(12)-C(13)	1.390(5)
C(13)-C(14)	1.513(5)	C(14)-P(2)	1.837(3)
P(2)-C(15)	1.833(4)	P(2)-C(18)	1.849(3)
C(15)-C(17)	1.524(5)	C(15)-C(16)	1.538(5)
C(18)-C(20)	1.529(5)	C(18)-C(19)	1.530(5)
O(1)-S(1)	1.496(2)	S(1)-O(2)	1.436(3)
S(1)-O(3)	1.443(3)	S(1)-C(21)	1.760(4)
O(4)-S(2)	1.482(2)	S(2)-O(6)	1.440(3)
S(2)-O(5)	1.442(3)	S(2)-C(22)	1.762(4)
O(7)-C(26)	1.403(6)	O(7)-C(23)	1.405(6)
C(23)-C(24)	1.486(8)	C(24)-C(25)	1.489(9)
C(25)-C(26)	1.419(9)	O(8)-C(30)	1.418(5)
O(8)-C(27)	1.427(5)	C(27)-C(28)	1.487(6)
C(28)-C(29)	1.518(6)	C(29)-C(30)	1.495(6)
O(1)-Pd(1)-O(4)	87.05(9)	O(1)-Pd(1)-P(2)	171.55(7)
O(4)-Pd(1)-P(2)	87.10(7)	O(1)-Pd(1)-P(1)	87.38(6)
O(4)-Pd(1)-P(1)	170.82(6)	P(2)-Pd(1)-P(1)	99.17(3)
C(7)-P(1)-C(1)	102.42(16)	C(7)-P(1)-C(4)	103.79(16)
C(1)-P(1)-C(4)	107.38(16)	C(7)-P(1)-Pd(1)	122.58(12)
C(1)-P(1)-Pd(1)	110.70(11)	C(4)-P(1)-Pd(1)	108.92(11)
C(2)-C(1)-C(3)	111.2(3)	C(2)-C(1)-P(1)	110.5(2)
C(3)-C(1)-P(1)	112.7(2)	C(5)-C(4)-C(6)	110.3(3)
C(5)-C(4)-P(1)	112.4(3)	C(6)-C(4)-P(1)	111.6(2)
C(8)-C(7)-P(1)	116.8(2)	C(13)-C(8)-C(9)	119.5(3)
C(13)-C(8)-C(7)	121.4(3)	C(9)-C(8)-C(7)	119.1(3)
C(10)-C(9)-C(8)	120.7(4)	C(9)-C(10)-C(11)	119.8(4)
C(12)-C(11)-C(10)	120.1(4)	C(11)-C(12)-C(13)	121.0(4)
C(12)-C(13)-C(8)	119.0(3)	C(12)-C(13)-C(14)	119.7(3)
C(8)-C(13)-C(14)	121.2(3)	C(13)-C(14)-P(2)	116.7(2)
C(15)-P(2)-C(14)	107.97(16)	C(15)-P(2)-C(18)	107.06(17)
C(14)-P(2)-C(18)	99.35(16)	C(15)-P(2)-Pd(1)	109.51(12)
C(14)-P(2)-Pd(1)	123.70(12)	C(18)-P(2)-Pd(1)	107.82(12)
C(17)-C(15)-C(16)	111.3(3)	C(17)-C(15)-P(2)	113.5(3)
C(16)-C(15)-P(2)	112.1(2)	C(20)-C(18)-C(19)	110.4(3)
C(20)-C(18)-P(2)	110.1(2)	C(19)-C(18)-P(2)	115.1(3)
S(1)-O(1)-Pd(1)	120.44(14)	O(2)-S(1)-O(3)	115.7(2)
O(2)-S(1)-O(1)	110.72(17)	O(3)-S(1)-O(1)	111.43(15)
O(2)-S(1)-C(21)	107.3(2)	O(3)-S(1)-C(21)	106.7(2)
O(1)-S(1)-C(21)	104.25(18)	S(2)-O(4)-Pd(1)	133.24(14)
O(6)-S(2)-O(5)	114.37(17)	O(6)-S(2)-O(4)	110.24(16)
O(5)-S(2)-O(4)	111.20(15)	O(6)-S(2)-C(22)	106.58(17)
O(5)-S(2)-C(22)	107.6(2)	O(4)-S(2)-C(22)	106.45(15)
C(26)-O(7)-C(23)	108.2(4)	O(7)-C(23)-C(24)	106.4(5)
C(23)-C(24)-C(25)	102.8(5)	C(26)-C(25)-C(24)	106.4(6)
O(7)-C(26)-C(25)	109.4(5)	C(30)-O(8)-C(27)	109.7(3)
O(8)-C(27)-C(28)	106.2(4)	C(27)-C(28)-C(29)	101.7(4)
C(30)-C(29)-C(28)	102.9(4)	O(8)-C(30)-C(29)	106.6(3)

Table 20D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (44).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	12.11(11)	17.86(13)	14.21(12)	1.62(11)	0.11(8)	1.24(10)
P(1)	12.6(4)	20.4(4)	16.4(4)	-0.5(4)	-0.5(3)	1.2(3)
C(1)	16.8(16)	21.7(17)	26.3(19)	-2.2(15)	-2.5(14)	0.0(13)
C(2)	30(2)	32(2)	30(2)	-9.1(17)	-1.1(16)	1.4(16)
C(3)	20.3(18)	33(2)	43(2)	-7.2(18)	-1.6(16)	-4.8(15)
C(4)	15.6(15)	38(2)	18.3(16)	-1.1(16)	3.9(13)	1.4(15)
C(5)	25.7(19)	54(3)	28(2)	13.6(19)	8.9(16)	11.0(18)
C(6)	29(2)	63(3)	23(2)	-14(2)	4.0(16)	-8.4(19)
C(7)	15.6(16)	27.7(19)	24.0(18)	-1.1(15)	-2.9(14)	1.5(13)
C(8)	22.4(17)	24.5(18)	17.7(17)	0.5(14)	-3.4(14)	6.6(14)
C(9)	27(2)	32(2)	33(2)	3.2(17)	4.2(16)	8.0(16)
C(10)	34(2)	40(2)	32(2)	-7.4(19)	1.8(18)	17.8(18)
C(11)	38(2)	26(2)	47(3)	-9.5(19)	-5.7(19)	8.8(17)
C(12)	33(2)	24.5(19)	37(2)	1.7(17)	-9.2(17)	1.5(16)
C(13)	21.2(17)	26.4(18)	18.6(17)	3.9(15)	-5.4(13)	5.1(14)
C(14)	22.6(17)	23.1(18)	21.4(18)	5.5(15)	-2.2(14)	2.0(14)
P(2)	16.4(4)	20.5(4)	17.0(4)	3.8(4)	0.7(3)	0.9(3)
C(15)	24.2(18)	23.3(18)	28(2)	3.8(15)	-0.4(15)	-3.2(14)
C(16)	35(2)	28.3(19)	26(2)	-1.4(16)	-3.5(16)	-3.8(16)
C(17)	39(2)	30(2)	38(2)	9.2(18)	-3.7(18)	-12.1(17)
C(18)	24.1(18)	33(2)	18.7(18)	3.3(15)	7.4(14)	2.4(15)
C(19)	25(2)	71(3)	31(2)	10(2)	13.6(17)	10(2)
C(20)	49(3)	52(3)	27(2)	-10.5(19)	16.3(19)	-3(2)
O(1)	20.2(12)	18.4(12)	25.2(13)	3.8(10)	1.6(10)	3.5(9)
S(1)	24.5(4)	20.9(4)	37.9(5)	-3.2(4)	-2.8(4)	4.3(3)
O(2)	42.3(17)	24.3(15)	86(3)	-6.4(16)	-5.3(17)	-7.6(13)
O(3)	48.4(18)	46.3(18)	31.0(15)	-10.4(14)	4.5(13)	12.4(14)
C(21)	35(2)	30(2)	66(3)	4(2)	-11(2)	15.3(18)
O(4)	15.6(11)	30.5(13)	21.8(12)	6.8(11)	2.1(9)	2.1(10)
S(2)	14.9(4)	30.9(5)	28.4(5)	8.6(4)	-3.1(3)	-2.1(4)
O(5)	38.1(16)	41.1(17)	53.0(19)	10.1(15)	-16.1(14)	-19.8(13)
O(6)	19.3(13)	53.4(18)	43.1(17)	16.6(14)	1.2(12)	12.4(12)
C(22)	27.7(19)	45(2)	21.3(18)	2.3(17)	-0.4(15)	6.7(17)
O(7)	55(2)	55(2)	62(2)	-5.3(18)	15.7(17)	-2.5(16)
C(23)	49(3)	86(4)	60(3)	-29(3)	13(3)	-16(3)
C(24)	81(5)	98(5)	85(5)	2(4)	-16(4)	3(4)
C(25)	92(5)	107(6)	146(7)	69(6)	6(5)	-28(5)
C(26)	62(4)	80(4)	125(6)	18(4)	16(4)	-21(3)
O(8)	80(2)	65(2)	29.5(17)	1.7(16)	-3.6(16)	27.5(19)
C(27)	70(3)	48(3)	45(3)	5(2)	15(2)	12(2)
C(28)	75(4)	66(3)	41(3)	18(3)	13(3)	30(3)
C(29)	77(4)	54(3)	30(2)	4(2)	8(2)	12(3)
C(30)	40(2)	37(2)	49(3)	2(2)	13(2)	-2.8(19)

Table 20E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (44).

	x	y	z	U
H(1)	965	5374	6609	26
H(2A)	1230	4529	7648	47
H(2B)	-135	4993	7371	47
H(2C)	1191	5580	7557	47
H(3A)	3212	5570	6970	49
H(3B)	3235	4806	6522	49
H(3C)	3360	4554	7154	49
H(4)	2285	3584	5903	29
H(5A)	256	4860	5519	53
H(5B)	1526	4585	5200	53
H(5C)	1785	5090	5771	53
H(6A)	564	2478	5700	58
H(6B)	911	2978	5161	58
H(6C)	-455	3220	5429	58
H(7A)	2737	3171	6930	27
H(7B)	1553	3039	7316	27
H(9)	3248	2055	6312	36
H(10)	3100	575	6048	42
H(11)	1406	-331	6347	45
H(12)	-170	254	6887	39
H(14A)	-14	2263	7546	27
H(14B)	-899	1380	7443	27
H(15)	-3852	2090	6358	31
H(16A)	-2171	2158	5746	45
H(16B)	-2993	1240	5682	45
H(16C)	-1486	1266	6000	45
H(17A)	-2494	538	6787	54
H(17B)	-4039	605	6509	54
H(17C)	-3623	1050	7090	54
H(18)	-2763	2275	7737	30
H(19A)	-4840	3034	7673	62
H(19B)	-4803	2425	7145	62
H(19C)	-4545	3471	7108	62
H(20A)	-2607	3649	8145	63
H(20B)	-2411	4133	7583	63
H(20C)	-1227	3506	7866	63
H(21A)	-3921	6721	6121	67
H(21B)	-4213	5705	5962	67
H(21C)	-3323	6308	5599	67
H(22A)	-3042	4480	5273	47
H(22B)	-4094	3945	4855	47
H(22C)	-2891	3429	5212	47
H(23A)	1235	622	5192	77
H(23B)	1164	-180	4761	77
H(24A)	809	1442	4444	108
H(24B)	1473	720	4068	108
H(25A)	3294	1600	4167	139
H(25B)	2819	2062	4703	139
H(26A)	4543	695	4639	106
H(26B)	4237	1247	5168	106
H(27A)	3864	2859	8460	65
H(27B)	3048	1988	8232	65

H(28A)	3772	2125	9249	72
H(28B)	2316	1674	9046	72
H(29A)	1596	2831	9555	64
H(29B)	2786	3482	9388	64
H(30A)	295	3039	8768	50
H(30B)	1110	3966	8774	50

Table 21A. Crystal data, structure solution and refinement for (45).

Identification code	exti49
Chemical formula	$C_{35}H_{64.67}Cl_{0.67}O_{10}P_2PdS_{2.67}$
Formula weight	923.06
Temperature	173(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 12.0373(5) Å α = 90°
	b = 18.6614(8) Å β = 105.443(2)°
	c = 19.5579(9) Å γ = 90°
Volume	4234.7(3) Å^3
Z	4
Density (calculated)	1.448 g/cm^3
Absorption coefficient μ	0.739 mm^{-1}
F(000)	1939
Reflections for cell refinement	11289 (θ range 2.41 to 28.60°)
Crystal colour	colourless
Crystal size	0.42 × 0.24 × 0.10 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.54 to 28.81°
Index ranges	$-7 \le h \le 16$, $-24 \le k \le 24$, $-25 \le \ell \le 26$
Intensity decay	0%
Reflections collected	25794
Independent reflections	10029 (R_{int} = 0.0450)
Reflections with I>2σ(I)	6890
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.888 and 0.738
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0448, 0.0000
Data / restraints / parameters	10029 / 70 / 509
Final R indices [I>2σ(I)]	R1 = 0.0428, wR2 = 0.0866
R indices (all data)	R1 = 0.0796, wR2 = 0.0977
Goodness-of-fit on F^2	1.023
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	0.640 and -0.502 eÅ^{-3}

The Crystal Structure of $[o\text{-}C_6H_4(CH_2PCy_2)_2Pd(H_2O)]^{2+}$ $2[CH_3SO_3]^-$ (45)

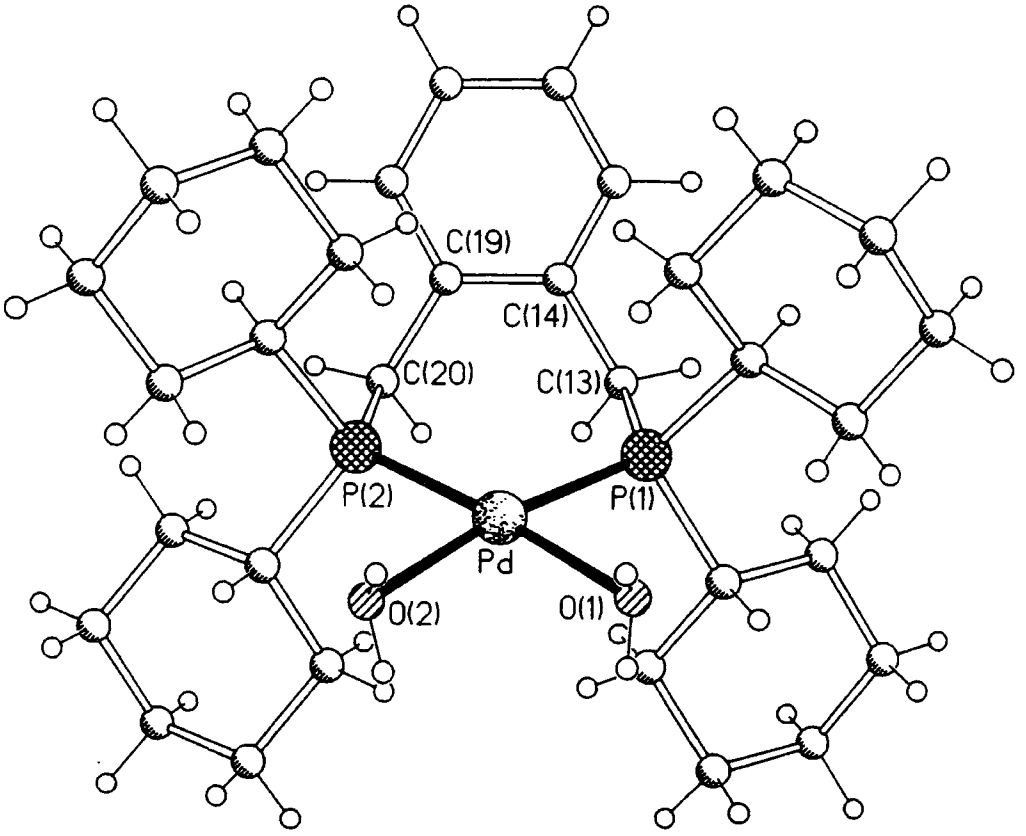


Table 21B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (45). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	5881.46(19)	2892.72(11)	7332.04(11)	19.71(7)
O(1)	6032.4(19)	2849.2(12)	8436.9(11)	28.3(5)
O(2)	5760.5(19)	1749.3(11)	7327.3(11)	27.2(5)
P(1)	6150.7(7)	4085.8(4)	7480.8(4)	22.77(18)
P(2)	5689.5(7)	2804.9(4)	6158.6(4)	21.44(17)
C(1)	7543(3)	4198.6(15)	8139.8(16)	27.6(7)
C(2)	8529(3)	3809.6(16)	7941.6(17)	30.5(7)
C(3)	9646(3)	3861.0(17)	8536.6(19)	39.0(9)
C(4)	9958(3)	4637(2)	8750(2)	50.6(10)
C(5)	8960(3)	5024(2)	8928(2)	55.3(12)
C(6)	7874(3)	4989.7(17)	8317(2)	43.1(9)
C(7)	5030(3)	4497.4(15)	7844.1(16)	25.2(7)
C(8)	5248(3)	4460.0(19)	8651.1(16)	36.5(8)
C(9)	4303(3)	4854.6(19)	8890.3(18)	40.9(9)
C(10)	3123(3)	4553(2)	8533.4(18)	41.5(9)
C(11)	2892(3)	4565.7(19)	7732.4(18)	38.8(9)
C(12)	3835(3)	4186.5(17)	7485.2(16)	30.3(7)
C(13)	6230(3)	4682.0(16)	6755.4(16)	29.0(7)
C(14)	5163(3)	4674.8(16)	6141.1(16)	26.3(7)
C(15)	4320(3)	5195.2(17)	6091.5(18)	36.9(8)
C(16)	3343(3)	5203.0(19)	5531.5(19)	43.2(10)
C(17)	3211(3)	4702.1(18)	5001.9(19)	41.6(9)
C(18)	4053(3)	4188.9(17)	5034.7(17)	36.4(8)
C(19)	5021(3)	4162.7(16)	5607.0(16)	28.4(7)
C(20)	5896(3)	3576.1(16)	5632.4(16)	29.5(7)
C(21)	4244(3)	2478.4(16)	5689.4(16)	28.2(7)
C(22)	3296(3)	2821.4(18)	5978.2(18)	35.5(8)
C(23)	2109(3)	2618(2)	5521(2)	56.5(11)
C(24)	1941(3)	1820(2)	5463(2)	53.3(11)
C(25)	2877(3)	1468.4(19)	5203.2(19)	42.5(9)
C(26)	4088(3)	1664.8(17)	5656.8(19)	38.0(8)
C(27)	6730(2)	2132.2(15)	6036.9(15)	23.3(6)
C(28)	6752(3)	2048.7(16)	5255.4(16)	30.3(7)
C(29)	7536(3)	1429.6(17)	5181.8(18)	37.4(8)
C(30)	8750(3)	1553(2)	5647(2)	46.6(10)
C(31)	8762(3)	1664(2)	6425.9(19)	44.5(10)
C(32)	7942(3)	2261.9(16)	6511.0(17)	32.3(8)
S(1)	8577.9(8)	1655.7(5)	8788.3(5)	39.2(2)
O(3)	8141(2)	2337.7(13)	8967.8(13)	46.6(6)
O(4)	7768(2)	1298.1(13)	8209.6(14)	51.5(7)
O(5)	8981(2)	1187.4(14)	9406.3(14)	61.2(8)
C(33)	9801(3)	1852(2)	8508(2)	55.0(11)
S(2)	3278.7(7)	1828.0(5)	8133.0(5)	33.5(2)
O(6)	4130(2)	2256.5(13)	8643.2(13)	45.6(6)
O(7)	3765(2)	1519.8(12)	7588.1(12)	41.7(6)
O(8)	2709(2)	1299.5(12)	8461.8(13)	44.8(6)
C(34)	2182(3)	2420(2)	7683(2)	49.5(10)
S(3)	9814.7(13)	1044.2(10)	11194.3(8)	40.1(5)
O(9)	10357(12)	1422(6)	11832(4)	60(3)
O(10)	9544(4)	1625(2)	10603(2)	69.5(15)
O(11)	8805(4)	678(3)	11156(2)	77.1(17)

C(36)	10854(7)	490(4)	10961(4)	66(2)
C(99)	10220(13)	563(6)	11071(7)	55(3)
Cl(1)	9382(3)	25.7(19)	11498.4(19)	69.0(12)
Cl(2)	10376(10)	1430(4)	11539(4)	75(2)

Table 21C. Bond lengths (Å) and angles (°) for (45).

Pd-O(1)	2.121(2)	Pd-O(2)	2.139(2)
Pd-P(2)	2.2505(8)	Pd-P(1)	2.2576(8)
O(1)-H(1Y)	0.769(18)	O(1)-H(1X)	0.780(18)
O(2)-H(2X)	0.793(18)	O(2)-H(2Y)	0.808(18)
P(1)-C(13)	1.825(3)	P(1)-C(1)	1.834(3)
P(1)-C(7)	1.851(3)	P(2)-C(20)	1.824(3)
P(2)-C(27)	1.833(3)	P(2)-C(21)	1.842(3)
C(1)-C(2)	1.526(4)	C(1)-C(6)	1.544(4)
C(2)-C(3)	1.529(4)	C(3)-C(4)	1.526(5)
C(4)-C(5)	1.520(5)	C(5)-C(6)	1.519(5)
C(7)-C(8)	1.531(4)	C(7)-C(12)	1.536(4)
C(8)-C(9)	1.529(4)	C(9)-C(10)	1.514(5)
C(10)-C(11)	1.516(4)	C(11)-C(12)	1.522(4)
C(13)-C(14)	1.507(4)	C(14)-C(15)	1.389(4)
C(14)-C(19)	1.392(4)	C(15)-C(16)	1.378(5)
C(16)-C(17)	1.373(5)	C(17)-C(18)	1.384(4)
C(18)-C(19)	1.385(4)	C(19)-C(20)	1.510(4)
C(21)-C(26)	1.529(4)	C(21)-C(22)	1.541(4)
C(22)-C(23)	1.518(5)	C(23)-C(24)	1.503(5)
C(24)-C(25)	1.505(5)	C(25)-C(26)	1.535(4)
C(27)-C(32)	1.525(4)	C(27)-C(28)	1.544(4)
C(28)-C(29)	1.523(4)	C(29)-C(30)	1.519(5)
C(30)-C(31)	1.534(5)	C(31)-C(32)	1.528(4)
S(1)-O(4)	1.446(2)	S(1)-O(3)	1.455(3)
S(1)-O(5)	1.465(2)	S(1)-C(33)	1.741(4)
S(2)-O(8)	1.446(2)	S(2)-O(6)	1.463(2)
S(2)-O(7)	1.463(2)	S(2)-C(34)	1.766(3)
S(3)-O(11)	1.379(4)	S(3)-O(9)	1.430(9)
S(3)-O(10)	1.555(4)	S(3)-C(36)	1.774(7)
C(99)-Cl(1)	1.782(16)	C(99)-Cl(2)	1.844(15)
O(1)-Pd-O(2)	87.33(9)	O(1)-Pd-P(2)	173.56(6)
O(2)-Pd-P(2)	86.25(6)	O(1)-Pd-P(1)	86.33(6)
O(2)-Pd-P(1)	172.67(6)	P(2)-Pd-P(1)	100.10(3)
H(1Y)-O(1)-H(1X)	115(3)	H(1Y)-O(1)-Pd	108.7(17)
H(1X)-O(1)-Pd	107.1(17)	H(2X)-O(2)-H(2Y)	108(3)
H(2X)-O(2)-Pd	104.9(16)	H(2Y)-O(2)-Pd	104.2(16)
C(13)-P(1)-C(1)	104.44(14)	C(13)-P(1)-C(7)	103.86(14)
C(1)-P(1)-C(7)	107.80(14)	C(13)-P(1)-Pd	122.44(10)
C(1)-P(1)-Pd	106.06(10)	C(7)-P(1)-Pd	111.37(10)
C(20)-P(2)-C(27)	105.47(14)	C(20)-P(2)-C(21)	103.44(15)
C(27)-P(2)-C(21)	107.24(14)	C(20)-P(2)-Pd	121.70(11)
C(27)-P(2)-Pd	107.10(9)	C(21)-P(2)-Pd	111.04(10)
C(2)-C(1)-C(6)	109.9(3)	C(2)-C(1)-P(1)	113.2(2)
C(6)-C(1)-P(1)	113.6(2)	C(1)-C(2)-C(3)	111.3(3)
C(4)-C(3)-C(2)	111.7(3)	C(5)-C(4)-C(3)	111.2(3)
C(6)-C(5)-C(4)	111.5(3)	C(5)-C(6)-C(1)	109.4(3)
C(8)-C(7)-C(12)	109.7(3)	C(8)-C(7)-P(1)	115.8(2)
C(12)-C(7)-P(1)	110.9(2)	C(9)-C(8)-C(7)	110.9(3)
C(10)-C(9)-C(8)	111.3(3)	C(9)-C(10)-C(11)	111.2(3)
C(10)-C(11)-C(12)	111.9(3)	C(11)-C(12)-C(7)	111.5(3)
C(14)-C(13)-P(1)	113.9(2)	C(15)-C(14)-C(19)	119.1(3)
C(15)-C(14)-C(13)	120.1(3)	C(19)-C(14)-C(13)	120.8(3)
C(16)-C(15)-C(14)	121.1(3)	C(17)-C(16)-C(15)	119.7(3)
C(16)-C(17)-C(18)	120.0(3)	C(17)-C(18)-C(19)	120.7(3)
C(18)-C(19)-C(14)	119.4(3)	C(18)-C(19)-C(20)	118.8(3)
C(14)-C(19)-C(20)	121.8(3)	C(19)-C(20)-P(2)	113.1(2)
C(26)-C(21)-C(22)	109.5(3)	C(26)-C(21)-P(2)	116.0(2)

C(22)-C(21)-P(2)	111.9(2)	C(23)-C(22)-C(21)	110.6(3)
C(24)-C(23)-C(22)	112.3(3)	C(23)-C(24)-C(25)	111.0(3)
C(24)-C(25)-C(26)	112.5(3)	C(21)-C(26)-C(25)	110.4(3)
C(32)-C(27)-C(28)	110.6(3)	C(32)-C(27)-P(2)	112.9(2)
C(28)-C(27)-P(2)	113.0(2)	C(29)-C(28)-C(27)	110.2(2)
C(30)-C(29)-C(28)	110.5(3)	C(29)-C(30)-C(31)	111.6(3)
C(32)-C(31)-C(30)	111.8(3)	C(27)-C(32)-C(31)	111.0(3)
O(4)-S(1)-O(3)	112.39(14)	O(4)-S(1)-O(5)	112.11(16)
O(3)-S(1)-O(5)	112.58(16)	O(4)-S(1)-C(33)	107.56(19)
O(3)-S(1)-C(33)	106.40(18)	O(5)-S(1)-C(33)	105.23(18)
O(8)-S(2)-O(6)	113.48(15)	O(8)-S(2)-O(7)	112.63(15)
O(6)-S(2)-O(7)	111.64(14)	O(8)-S(2)-C(34)	105.54(16)
O(6)-S(2)-C(34)	107.03(18)	O(7)-S(2)-C(34)	105.87(17)
O(11)-S(3)-O(9)	118.8(5)	O(11)-S(3)-O(10)	107.4(3)
O(9)-S(3)-O(10)	105.2(5)	O(11)-S(3)-C(36)	111.7(4)
O(9)-S(3)-C(36)	108.8(6)	O(10)-S(3)-C(36)	103.7(3)
Cl(1)-C(99)-Cl(2)	104.8(8)		

Table 21D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (45).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	20.48(12)	19.49(11)	19.11(12)	-0.03(9)	5.18(9)	-1.83(10)
O(1)	30.0(13)	32.0(12)	22.6(11)	0.9(9)	6.8(10)	-3.2(11)
O(2)	30.2(13)	25.6(11)	26.6(12)	0.2(9)	8.9(10)	-3.1(10)
P(1)	22.4(4)	21.4(4)	24.5(4)	-0.9(3)	6.4(3)	-3.0(3)
P(2)	22.2(4)	22.1(4)	20.5(4)	1.6(3)	6.4(3)	3.1(3)
C(1)	23.9(17)	26.5(16)	31.2(18)	-4.7(13)	5.4(14)	-5.4(13)
C(2)	26.0(17)	27.9(17)	37.5(19)	-3.3(14)	8.5(15)	-1.8(14)
C(3)	26.1(18)	39(2)	49(2)	-8.6(16)	4.8(17)	-1.2(16)
C(4)	24(2)	51(2)	70(3)	-13(2)	2(2)	-8.3(18)
C(5)	30(2)	43(2)	86(3)	-30(2)	4(2)	-11.9(18)
C(6)	28(2)	27.5(18)	69(3)	-13.6(17)	4.9(19)	-3.8(15)
C(7)	22.9(17)	23.0(15)	30.2(17)	-1.2(12)	7.5(14)	0.3(13)
C(8)	29.6(19)	48(2)	29.1(18)	-13.4(15)	2.9(16)	0.1(16)
C(9)	37(2)	50(2)	36(2)	-15.5(16)	9.1(17)	2.3(18)
C(10)	34(2)	53(2)	42(2)	-5.0(17)	17.2(18)	-4.7(17)
C(11)	21.7(18)	51(2)	42(2)	-2.9(17)	5.7(16)	-1.8(16)
C(12)	25.4(18)	37.1(18)	26.0(17)	-3.4(14)	3.0(14)	-4.5(14)
C(13)	34.6(19)	23.3(16)	32.4(18)	2.5(13)	14.5(15)	-0.8(14)
C(14)	31.0(18)	25.0(16)	27.1(17)	8.0(13)	15.2(15)	3.4(14)
C(15)	49(2)	31.8(18)	38(2)	7.1(15)	25.9(19)	11.3(16)
C(16)	43(2)	47(2)	48(2)	24.4(18)	26(2)	23.3(18)
C(17)	35(2)	45(2)	42(2)	19.9(17)	5.9(18)	8.0(17)
C(18)	45(2)	34.6(19)	28.4(18)	10.0(14)	7.9(17)	3.3(17)
C(19)	32.1(18)	28.4(17)	28.3(18)	10.4(13)	14.1(15)	5.5(14)
C(20)	34.5(19)	29.4(17)	27.0(17)	5.1(13)	12.1(15)	6.1(14)
C(21)	22.0(17)	36.8(18)	23.4(16)	-1.8(13)	2.0(14)	2.7(14)
C(22)	25.9(18)	44(2)	36.7(19)	-10.7(16)	9.0(15)	0.5(16)
C(23)	24(2)	67(3)	76(3)	-17(2)	9(2)	7.4(19)
C(24)	30(2)	61(2)	69(3)	-14(2)	13(2)	-12.0(19)
C(25)	35(2)	48(2)	42(2)	-14.4(17)	6.8(18)	-10.7(17)
C(26)	34(2)	36(2)	43(2)	-2.6(16)	8.2(17)	-2.7(16)
C(27)	23.7(16)	23.6(15)	23.7(15)	-0.4(12)	8.5(13)	1.9(13)
C(28)	31.1(18)	36.8(18)	24.8(16)	4.5(14)	10.5(14)	8.7(15)
C(29)	42(2)	40.0(19)	33.4(19)	1.7(15)	15.7(17)	14.4(17)
C(30)	33(2)	53(2)	58(3)	0.0(19)	20(2)	14.8(18)
C(31)	29(2)	53(2)	48(2)	-4.8(18)	2.9(18)	12.3(17)
C(32)	24.1(17)	34.6(19)	36.7(19)	-4.5(14)	5.6(15)	3.0(14)
S(1)	27.7(5)	42.5(5)	43.7(5)	6.3(4)	3.2(4)	-2.3(4)
O(3)	36.4(15)	54.7(16)	44.7(15)	-2.3(12)	3.7(12)	-0.9(12)
O(4)	35.1(15)	43.4(14)	63.7(18)	-1.5(13)	-8.3(13)	-0.4(12)
O(5)	47.4(17)	66.3(18)	62.4(18)	34.7(15)	1.3(14)	-3.4(15)
C(33)	42(2)	67(3)	58(3)	2(2)	17(2)	-7(2)
S(2)	27.3(5)	34.6(4)	39.0(5)	5.3(4)	9.8(4)	-1.3(4)
O(6)	35.3(14)	60.7(17)	42.0(15)	-6.6(12)	12.4(12)	-11.5(12)
O(7)	34.9(14)	48.8(15)	45.6(15)	-4.7(11)	17.9(12)	-5.5(12)
O(8)	42.3(15)	44.4(14)	51.3(16)	14.5(12)	18.3(13)	-3.2(12)
C(34)	38(2)	47(2)	64(3)	16.2(19)	15(2)	6.9(19)
S(3)	29.5(8)	52.7(11)	37.2(9)	-7.7(7)	7.2(7)	-5.8(8)
O(9)	43(3)	75(4)	55(5)	-15(4)	1(5)	-3(3)
O(10)	83(4)	59(3)	63(3)	12(2)	14(3)	6(3)
O(11)	60(3)	105(4)	68(3)	-24(3)	20(3)	-46(3)

C(36)	62(5)	73(5)	61(5)	-17(4)	12(4)	40(4)
C(99)	61(9)	24(6)	67(9)	-4(5)	-4(7)	23(6)
Cl(1)	63(2)	62(2)	83(3)	-13.3(18)	21.5(19)	3.4(17)
Cl(2)	79(4)	50(3)	92(6)	0(4)	16(5)	0(2)

Table 21E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (45).

	x	y	z	U
H(1X)	6606(19)	2649(16)	8613(11)	34
H(1Y)	5488(19)	2672(16)	8494(11)	34
H(2X)	6315(19)	1620(11)	7620(14)	33
H(2Y)	5200(2)	1669(11)	7473(16)	33
H(1)	7464	3973	8588	33
H(2A)	8649	4023	7503	37
H(2B)	8321	3299	7845	37
H(3A)	9557	3591	8955	47
H(3B)	10280	3638	8377	47
H(4A)	10637	4646	9168	61
H(4B)	10166	4888	8356	61
H(5A)	8806	4802	9354	66
H(5B)	9172	5531	9040	66
H(6A)	8010	5231	7895	52
H(6B)	7237	5240	8449	52
H(7)	5002	5017	7716	30
H(8A)	5270	3952	8801	44
H(8B)	6005	4678	8881	44
H(9A)	4449	4811	9411	49
H(9B)	4322	5370	8774	49
H(10A)	2527	4839	8674	50
H(10B)	3073	4054	8694	50
H(11A)	2836	5069	7567	47
H(11B)	2143	4330	7517	47
H(12A)	3681	4237	6964	36
H(12B)	3827	3669	7597	36
H(13A)	6364	5177	6941	35
H(13B)	6899	4542	6581	35
H(15)	4419	5552	6450	44
H(16)	2762	5553	5512	52
H(17)	2541	4708	4613	50
H(18)	3967	3851	4661	44
H(20A)	6678	3773	5835	35
H(20B)	5846	3416	5143	35
H(21)	4100	2645	5187	34
H(22A)	3381	2658	6471	43
H(22B)	3381	3349	5985	43
H(23A)	1516	2830	5726	68
H(23B)	2002	2822	5040	68
H(24A)	1182	1712	5131	64
H(24B)	1944	1622	5933	64
H(25A)	2800	1616	4706	51
H(25B)	2780	942	5209	51
H(26A)	4201	1473	6142	46
H(26B)	4674	1445	5450	46
H(27)	6470	1662	6184	28
H(28A)	5962	1958	4956	36
H(28B)	7034	2498	5090	36
H(29A)	7229	977	5322	45
H(29B)	7554	1385	4680	45
H(30A)	9084	1979	5475	56
H(30B)	9237	1134	5610	56

H(31A)	8535	1212	6617	53
H(31B)	9554	1784	6704	53
H(32A)	7917	2286	7012	39
H(32B)	8232	2727	6386	39
H(33A)	9590	2163	8090	83
H(33B)	10135	1406	8387	83
H(33C)	10368	2096	8891	83
H(34A)	1824	2644	8024	74
H(34B)	1598	2152	7330	74
H(34C)	2515	2791	7444	74

Table 22A. Crystal data, structure solution and refinement for (46).

Identification code	exti36
Chemical formula	$C_{28}H_{52}O_2P_2Pd$
Formula weight	589.04
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 7.2378(8) Å α = 97.694(3)°
	b = 9.2179(10) Å β = 90.882(3)°
	c = 22.177(3) Å γ = 101.133(3)°
Volume	1437.4(3) $Å^3$
Z	2
Density (calculated)	1.361 g/cm^3
Absorption coefficient μ	0.779 mm^{-1}
F(000)	624
Reflections for cell refinement	8276 (θ range 1.85 to 28.40°)
Crystal colour	pale blue
Crystal size	0.22 × 0.12 × 0.08 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.85 to 28.43°
Index ranges	$-9 \le h \le 9$, $-12 \le k \le 11$, $-29 \le \ell \le 25$
Intensity decay	0%
Reflections collected	10310
Independent reflections	6271 (R_{int} = 0.0221)
Reflections with I>2σ(I)	5601
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.862 and 0.747
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0338, 0.5525
Data / restraints / parameters	6271 / 0 / 311
Final R indices [I>2σ(I)]	R1 = 0.0312, wR2 = 0.0741
R indices (all data)	R1 = 0.0380, wR2 = 0.0771
Goodness-of-fit on F^2	1.082
Extinction coefficient	0.0014(4)
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.577 and -0.472 $eÅ^{-3}$

The Crystal Structure of [*o*-$C_6H_4(CH_2PPe'_2)_2Pd(O_2)$] (46)

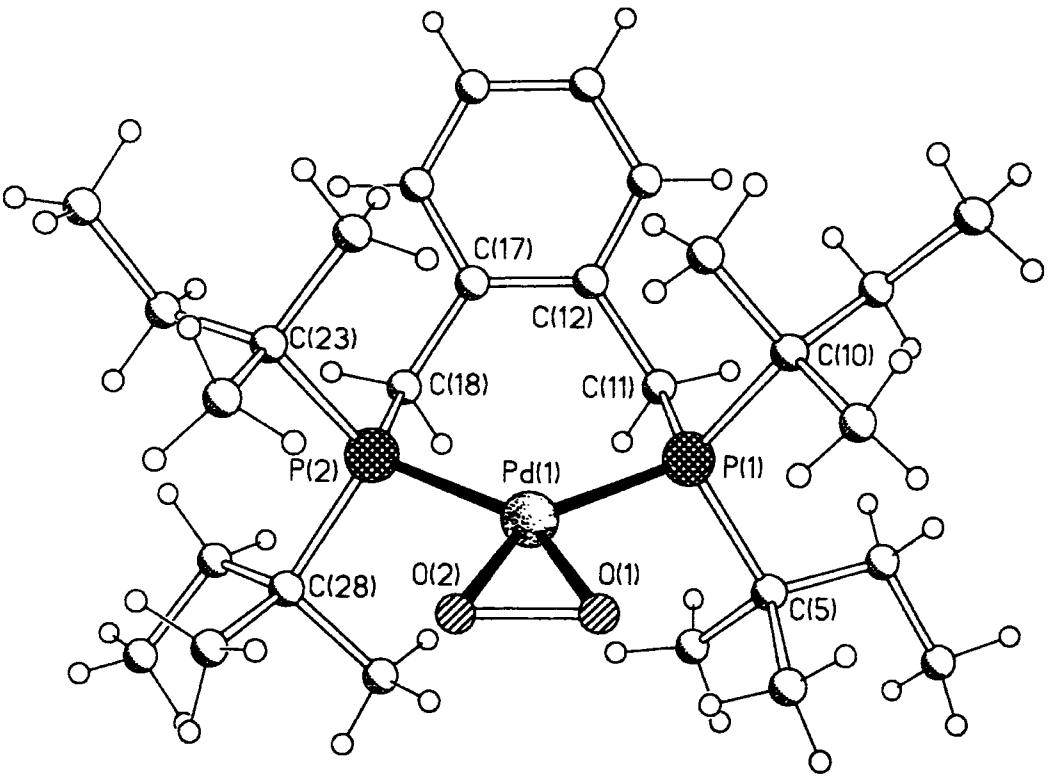


Table 22B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (46). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5244.9(2)	7102.6(2)	7464.70(8)	14.91(7)
P(1)	7116.8(9)	8310.5(7)	8290.3(3)	18.82(14)
P(2)	7296.4(8)	7179.5(7)	6691.1(3)	15.15(13)
O(1)	2597(2)	6451(2)	7741.5(8)	23.5(4)
O(2)	2748(2)	5965(2)	7100.1(8)	22.5(4)
C(1)	8227(6)	6668(5)	9959.0(15)	53.0(10)
C(2)	8004(5)	7740(4)	9500.0(14)	38.4(7)
C(3)	8499(5)	5883(4)	8596.5(15)	38.1(7)
C(4)	5245(4)	6022(4)	8903.6(14)	33.9(7)
C(5)	7231(4)	6962(3)	8861.3(12)	25.4(6)
C(6)	6490(6)	12253(4)	9456.3(17)	52.8(9)
C(7)	7412(4)	11075(4)	9109.9(15)	36.3(7)
C(8)	5732(4)	10786(3)	8093.0(14)	32.2(7)
C(9)	4190(4)	9395(3)	8896.0(14)	32.9(7)
C(10)	6088(4)	9965(3)	8629.9(13)	25.1(6)
C(11)	9645(3)	9044(3)	8206.2(12)	21.5(5)
C(12)	10259(3)	10132(3)	7760.5(12)	20.7(5)
C(13)	10916(4)	11650(3)	7977.7(14)	28.5(6)
C(14)	11630(4)	12677(3)	7601.1(16)	34.4(7)
C(15)	11767(4)	12199(3)	6995.3(15)	35.7(7)
C(16)	11179(4)	10697(3)	6769.0(14)	28.3(6)
C(17)	10374(3)	9651(3)	7140.7(12)	19.3(5)
C(18)	9806(3)	8038(3)	6855.6(11)	17.9(5)
C(19)	7228(4)	9138(3)	5050.5(13)	31.1(6)
C(20)	7652(4)	8182(3)	5525.3(12)	24.8(6)
C(21)	4349(4)	7498(3)	5889.8(13)	26.7(6)
C(22)	6417(4)	9793(3)	6395.3(13)	26.2(6)
C(23)	6415(3)	8191(3)	6082.8(12)	20.0(5)
C(24)	9295(4)	3544(3)	5662.5(14)	32.9(7)
C(25)	9234(4)	5104(3)	5990.2(12)	23.1(5)
C(26)	7670(4)	4399(3)	6937.3(12)	26.0(6)
C(27)	5648(4)	4398(3)	6018.8(13)	28.0(6)
C(28)	7486(4)	5191(3)	6377.8(12)	20.0(5)

Table 22C. Bond lengths (Å) and angles (°) for (46).

Pd(1)-O(2)	2.0038(17)	Pd(1)-O(1)	2.0254(17)
Pd(1)-P(1)	2.2854(7)	Pd(1)-P(2)	2.2856(7)
P(1)-C(11)	1.846(2)	P(1)-C(10)	1.896(3)
P(1)-C(5)	1.901(3)	P(2)-C(18)	1.846(2)
P(2)-C(28)	1.903(3)	P(2)-C(23)	1.907(3)
O(1)-O(2)	1.445(3)	C(1)-C(2)	1.538(5)
C(2)-C(5)	1.543(4)	C(3)-C(5)	1.545(4)
C(4)-C(5)	1.540(4)	C(6)-C(7)	1.512(4)
C(7)-C(10)	1.548(4)	C(8)-C(10)	1.538(4)
C(9)-C(10)	1.530(4)	C(11)-C(12)	1.512(3)
C(12)-C(17)	1.395(4)	C(12)-C(13)	1.404(4)
C(13)-C(14)	1.377(4)	C(14)-C(15)	1.368(4)
C(15)-C(16)	1.389(4)	C(16)-C(17)	1.400(4)
C(17)-C(18)	1.512(3)	C(19)-C(20)	1.524(4)
C(20)-C(23)	1.538(3)	C(21)-C(23)	1.538(4)
C(22)-C(23)	1.544(4)	C(24)-C(25)	1.531(4)
C(25)-C(28)	1.549(3)	C(26)-C(28)	1.538(4)
C(27)-C(28)	1.540(4)		
O(2)-Pd(1)-O(1)	42.04(7)	O(2)-Pd(1)-P(1)	150.56(5)
O(1)-Pd(1)-P(1)	108.59(6)	O(2)-Pd(1)-P(2)	106.59(5)
O(1)-Pd(1)-P(2)	148.62(6)	P(1)-Pd(1)-P(2)	102.79(2)
C(11)-P(1)-C(10)	106.03(12)	C(11)-P(1)-C(5)	101.14(12)
C(10)-P(1)-C(5)	111.60(13)	C(11)-P(1)-Pd(1)	120.40(9)
C(10)-P(1)-Pd(1)	108.13(9)	C(5)-P(1)-Pd(1)	109.38(9)
C(18)-P(2)-C(28)	100.68(11)	C(18)-P(2)-C(23)	106.57(11)
C(28)-P(2)-C(23)	111.99(12)	C(18)-P(2)-Pd(1)	119.76(8)
C(28)-P(2)-Pd(1)	108.69(8)	C(23)-P(2)-Pd(1)	108.96(8)
O(2)-O(1)-Pd(1)	68.18(9)	O(1)-O(2)-Pd(1)	69.78(9)
C(1)-C(2)-C(5)	114.5(3)	C(4)-C(5)-C(2)	110.0(2)
C(4)-C(5)-C(3)	107.2(2)	C(2)-C(5)-C(3)	110.1(3)
C(4)-C(5)-P(1)	108.66(18)	C(2)-C(5)-P(1)	113.6(2)
C(3)-C(5)-P(1)	106.99(18)	C(6)-C(7)-C(10)	114.2(3)
C(9)-C(10)-C(8)	108.3(2)	C(9)-C(10)-C(7)	111.0(2)
C(8)-C(10)-C(7)	108.4(2)	C(9)-C(10)-P(1)	109.12(19)
C(8)-C(10)-P(1)	105.74(18)	C(7)-C(10)-P(1)	113.98(19)
C(12)-C(11)-P(1)	120.28(18)	C(17)-C(12)-C(13)	118.3(2)
C(17)-C(12)-C(11)	121.7(2)	C(13)-C(12)-C(11)	119.7(2)
C(14)-C(13)-C(12)	122.5(3)	C(15)-C(14)-C(13)	119.1(3)
C(14)-C(15)-C(16)	119.9(3)	C(15)-C(16)-C(17)	121.7(3)
C(12)-C(17)-C(16)	118.4(2)	C(12)-C(17)-C(18)	123.5(2)
C(16)-C(17)-C(18)	117.9(2)	C(17)-C(18)-P(2)	120.35(17)
C(19)-C(20)-C(23)	115.8(2)	C(21)-C(23)-C(20)	110.4(2)
C(21)-C(23)-C(22)	106.0(2)	C(20)-C(23)-C(22)	112.0(2)
C(21)-C(23)-P(2)	110.53(17)	C(20)-C(23)-P(2)	111.74(17)
C(22)-C(23)-P(2)	105.96(17)	C(24)-C(25)-C(28)	114.7(2)
C(26)-C(28)-C(27)	107.9(2)	C(26)-C(28)-C(25)	108.4(2)
C(27)-C(28)-C(25)	111.5(2)	C(26)-C(28)-P(2)	105.80(17)
C(27)-C(28)-P(2)	109.60(18)	C(25)-C(28)-P(2)	113.25(17)

Table 22D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (46).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	10.40(9)	16.02(10)	18.22(11)	2.65(7)	0.90(6)	2.22(6)
P(1)	13.2(3)	23.4(3)	19.3(3)	1.3(3)	0.0(2)	3.4(2)
P(2)	12.7(3)	15.0(3)	18.0(3)	2.5(2)	2.0(2)	3.1(2)
O(1)	13.2(8)	29.5(10)	26.6(10)	4.4(8)	5.0(7)	0.9(7)
O(2)	15.4(8)	25.4(10)	23.7(10)	1.8(8)	-2.4(7)	-1.7(7)
C(1)	53(2)	73(3)	31.0(19)	19.1(18)	-10.7(16)	1.0(19)
C(2)	35.4(17)	52(2)	26.4(16)	9.9(14)	-2.7(13)	3.2(15)
C(3)	42.8(18)	41.2(18)	39.2(18)	18.9(15)	13.0(14)	20.5(15)
C(4)	27.8(15)	39.2(17)	34.4(17)	15.8(14)	-0.7(12)	-1.3(13)
C(5)	20.0(13)	33.3(15)	23.5(14)	7.0(12)	1.3(10)	4.6(11)
C(6)	55(2)	49(2)	50(2)	-6.5(18)	7.7(18)	9.5(18)
C(7)	29.7(15)	35.3(17)	39.0(18)	-14.4(14)	-4.3(13)	8.2(13)
C(8)	29.7(15)	33.1(16)	36.2(17)	-0.4(13)	0.7(12)	16.1(13)
C(9)	19.8(13)	41.2(18)	37.1(17)	-3.4(14)	2.8(12)	10.7(12)
C(10)	20.3(13)	26.0(14)	28.1(15)	-5.2(11)	0.8(11)	8.5(11)
C(11)	16.1(12)	25.8(14)	21.5(13)	0.4(11)	-1.6(10)	3.7(10)
C(12)	11.8(11)	18.7(13)	32.0(15)	4.6(11)	0.0(10)	2.8(9)
C(13)	20.1(13)	25.1(14)	37.3(17)	-5.0(12)	-2.3(12)	3.4(11)
C(14)	25.0(14)	17.8(14)	58(2)	2.7(14)	-3.8(14)	1.7(11)
C(15)	28.8(15)	24.8(15)	53(2)	17.2(15)	1.3(14)	-3.0(12)
C(16)	23.1(13)	27.8(15)	33.2(16)	10.7(12)	1.0(11)	-1.7(11)
C(17)	11.5(11)	19.1(13)	27.0(14)	3.5(11)	0.4(10)	2.4(9)
C(18)	13.6(11)	18.3(12)	21.8(13)	2.3(10)	3.7(9)	3.8(9)
C(19)	38.3(16)	34.7(16)	24.9(15)	11.7(13)	9.0(12)	12.4(13)
C(20)	24.0(13)	29.7(15)	24.5(14)	8.8(12)	6.9(11)	10.8(11)
C(21)	20.9(13)	35.2(16)	26.2(15)	7.6(12)	-2.2(11)	8.7(11)
C(22)	29.2(14)	22.3(14)	29.7(15)	5.7(12)	-0.3(11)	10.2(11)
C(23)	19.1(12)	21.6(13)	20.7(13)	5.2(10)	3.0(10)	5.5(10)
C(24)	40.5(17)	29.0(16)	31.4(16)	-1.4(13)	6.5(13)	15.9(13)
C(25)	26.5(13)	22.6(13)	22.1(14)	2.9(11)	5.1(11)	9.7(11)
C(26)	34.6(15)	19.9(13)	26.2(14)	4.7(11)	6.3(12)	10.3(11)
C(27)	24.2(13)	20.5(14)	36.5(16)	-1.8(12)	-2.0(12)	2.0(11)
C(28)	21.8(12)	15.9(12)	23.0(13)	2.1(10)	3.2(10)	5.6(10)

Table 22E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (46).

	x	y	z	U
H(1A)	9124	6045	9810	80
H(1B)	7003	6030	10007	80
H(1C)	8697	7247	10353	80
H(2A)	9247	8383	9459	46
H(2B)	7146	8396	9666	46
H(3A)	9820	6403	8636	57
H(3B)	8143	5540	8165	57
H(3C)	8338	5023	8820	57
H(4A)	5316	5227	9151	51
H(4B)	4737	5577	8494	51
H(4C)	4418	6662	9093	51
H(6A)	5504	11776	9704	79
H(6B)	5929	12778	9168	79
H(6C)	7439	12967	9721	79
H(7A)	7894	10505	9405	44
H(7B)	8506	11577	8903	44
H(8A)	5370	11734	8248	48
H(8B)	4715	10165	7823	48
H(8C)	6883	10983	7866	48
H(9A)	4401	8984	9271	49
H(9B)	3432	8615	8600	49
H(9C)	3522	10223	8988	49
H(11A)	10181	9531	8613	26
H(11B)	10249	8175	8094	26
H(13)	10866	11981	8401	34
H(14)	12023	13703	7760	41
H(15)	12263	12893	6730	43
H(16)	11328	10371	6351	34
H(18A)	10325	7429	7126	21
H(18B)	10455	7932	6467	21
H(19A)	7496	10192	5230	47
H(19B)	5897	8842	4915	47
H(19C)	8019	8996	4701	47
H(20A)	8986	8527	5670	30
H(20B)	7512	7138	5325	30
H(21A)	3643	7276	6251	40
H(21B)	4295	6573	5609	40
H(21C)	3794	8203	5687	40
H(22A)	5673	9749	6760	39
H(22B)	5864	10339	6113	39
H(22C)	7715	10306	6511	39
H(24A)	10498	3565	5464	49
H(24B)	8256	3233	5355	49
H(24C)	9171	2836	5959	49
H(25A)	9264	5793	5682	28
H(25B)	10382	5460	6259	28
H(26A)	8789	4922	7187	39
H(26B)	7791	3366	6803	39
H(26C)	6546	4403	7178	39
H(27A)	4567	4669	6236	42
H(27B)	5557	3315	5980	42
H(27C)	5652	4706	5613	42

Table 23A. Crystal data, structure solution and refinement for (47).

Identification code	exti41
Chemical formula	$C_{28}H_{46}O_2P_2Pd$
Formula weight	582.99
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 17.6034(13) Å α = 90°
	b = 7.2340(6) Å β = 91.244(2)°
	c = 21.7345(17) Å γ = 90°
Volume	2767.1(4) $Å^3$
Z	4
Density (calculated)	1.399 g/cm^3
Absorption coefficient μ	0.809 mm^{-1}
F(000)	1224
Reflections for cell refinement	9206 (θ range 2.18 to 28.80°)
Crystal colour	colourless
Crystal size	0.46 × 0.45 × 0.14 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	2.18 to 28.92°
Index ranges	$-13 \le h \le 22$, $-9 \le k \le 9$, $-29 \le \ell \le 28$
Intensity decay	0%
Reflections collected	17046
Independent reflections	6546 (R_{int} = 0.0613)
Reflections with I>2σ(I)	4507
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.8622 and 0.6176
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0326, 0.0000
Data / restraints / parameters	6546 / 0 / 310
Final R indices [I>2σ(I)]	R1 = 0.0384, wR2 = 0.0770
R indices (all data)	R1 = 0.0669, wR2 = 0.0825
Goodness-of-fit on F^2	0.924
Largest and mean shift/esd	0.002 and 0.000
Largest diff. peak and hole	1.296 and -1.594 $eÅ^{-3}$

The Crystal Structure of 2,3-[$C_{10}H_6(CH_2PBu^t_2)_2Pd(O_2)$] (47)

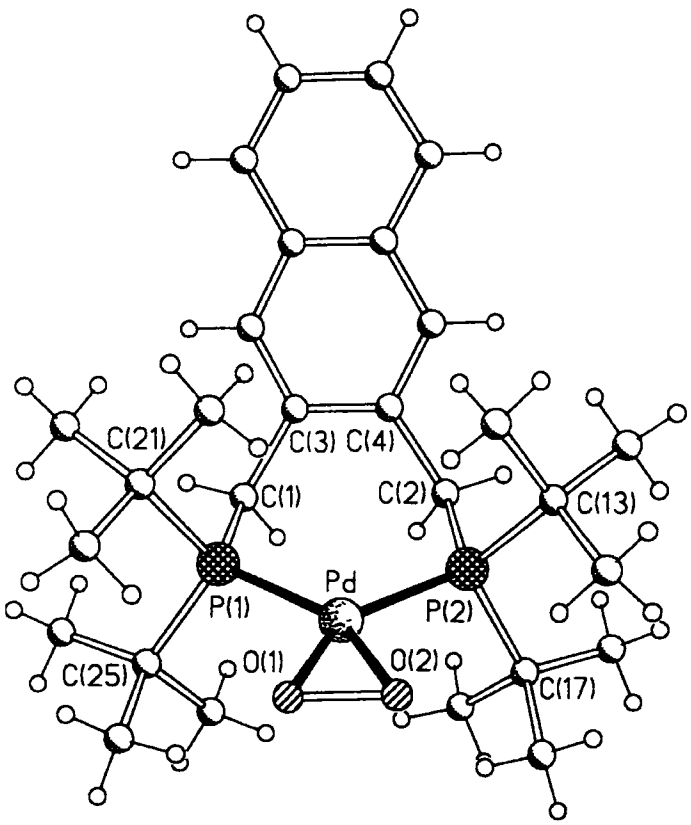


Table 23B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (47). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd	6837.71(13)	19320.1(3)	8036.16(10)	14.29(7)
O(1)	6786.0(13)	21740(3)	7572.3(10)	26.7(6)
O(2)	6220.5(12)	21654(3)	8041.0(10)	23.9(5)
P(1)	7801.9(4)	17592.4(12)	7655.5(4)	15.25(18)
P(2)	6358.6(4)	17391.2(12)	8762.7(4)	14.87(18)
C(1)	7990.8(17)	15222(4)	7936.6(14)	18.1(7)
C(2)	6756.4(17)	15056(4)	8890.0(14)	17.7(7)
C(3)	8169.3(17)	14815(4)	8603.0(14)	17.4(7)
C(4)	7587.3(17)	14726(4)	9053.2(14)	17.6(7)
C(5)	7776.8(18)	14115(5)	9636.6(14)	21.4(7)
C(6)	8521.9(19)	13562(5)	9815.4(14)	21.0(7)
C(7)	9096.5(18)	13649(4)	9373.3(15)	20.8(7)
C(8)	8895.1(17)	14277(4)	8775.6(14)	19.9(7)
C(9)	8706(2)	12865(5)	10410.8(15)	29.5(9)
C(10)	9425(2)	12293(5)	10550.6(16)	34.1(10)
C(11)	9995(2)	12364(5)	10108.2(17)	32.3(9)
C(12)	9833.7(19)	13032(5)	9535.8(16)	28.7(9)
C(13)	6386.4(18)	18559(5)	9539.4(13)	19.0(7)
C(14)	6032(2)	20493(5)	9496.5(15)	28.2(8)
C(15)	7231.6(19)	18846(5)	9716.9(15)	27.9(9)
C(16)	5991(2)	17448(5)	10042.4(14)	29.0(9)
C(17)	5352.5(17)	16746(5)	8516.5(14)	18.2(7)
C(18)	5023.1(19)	15060(5)	8851.2(16)	30.7(9)
C(19)	4813.9(18)	18388(5)	8577.8(16)	27.1(8)
C(20)	5391.5(19)	16240(5)	7831.5(14)	26.3(8)
C(21)	8710.5(17)	18925(4)	7802.4(15)	20.6(7)
C(22)	8689.8(18)	20731(5)	7430.3(16)	26.6(8)
C(23)	8712.0(18)	19435(5)	8492.5(14)	26.8(8)
C(24)	9445.3(18)	17875(5)	7668.7(16)	29.2(9)
C(25)	7642.4(18)	17149(5)	6803.4(14)	20.8(7)
C(26)	7007(2)	15743(5)	6732.2(15)	38.0(10)
C(27)	8336(2)	16424(7)	6474.6(17)	54.5(13)
C(28)	7377(2)	18925(5)	6482.4(16)	41.4(11)

Table 23C. Bond lengths (Å) and angles (°) for (47).

Pd-O(2)	2.008(2)	Pd-O(1)	2.021(2)
Pd-P(1)	2.2779(9)	Pd-P(2)	2.2825(9)
O(1)-O(2)	1.441(3)	P(1)-C(1)	1.848(3)
P(1)-C(21)	1.888(3)	P(1)-C(25)	1.894(3)
P(2)-C(2)	1.847(3)	P(2)-C(13)	1.887(3)
P(2)-C(17)	1.897(3)	C(1)-C(3)	1.504(4)
C(2)-C(4)	1.516(4)	C(3)-C(8)	1.380(4)
C(3)-C(4)	1.433(4)	C(4)-C(5)	1.377(4)
C(5)-C(6)	1.417(4)	C(6)-C(7)	1.412(5)
C(6)-C(9)	1.420(4)	C(7)-C(12)	1.410(4)
C(7)-C(8)	1.414(4)	C(9)-C(10)	1.360(5)
C(10)-C(11)	1.406(5)	C(11)-C(12)	1.359(5)
C(13)-C(14)	1.533(4)	C(13)-C(16)	1.535(4)
C(13)-C(15)	1.543(4)	C(17)-C(19)	1.528(4)
C(17)-C(20)	1.536(4)	C(17)-C(18)	1.539(4)
C(21)-C(24)	1.533(4)	C(21)-C(22)	1.537(4)
C(21)-C(23)	1.545(4)	C(25)-C(26)	1.517(5)
C(25)-C(27)	1.522(5)	C(25)-C(28)	1.530(5)
O(2)-Pd-O(1)	41.91(9)	O(2)-Pd-P(1)	150.56(7)
O(1)-Pd-P(1)	108.66(7)	O(2)-Pd-P(2)	107.59(7)
O(1)-Pd-P(2)	149.45(7)	P(1)-Pd-P(2)	101.85(3)
O(2)-O(1)-Pd	68.55(12)	O(1)-O(2)-Pd	69.54(12)
C(1)-P(1)-C(21)	105.78(14)	C(1)-P(1)-C(25)	100.84(14)
C(21)-P(1)-C(25)	111.02(15)	C(1)-P(1)-Pd	121.27(11)
C(21)-P(1)-Pd	107.07(10)	C(25)-P(1)-Pd	110.62(11)
C(2)-P(2)-C(13)	105.84(14)	C(2)-P(2)-C(17)	99.54(14)
C(13)-P(2)-C(17)	111.62(14)	C(2)-P(2)-Pd	121.20(11)
C(13)-P(2)-Pd	110.02(11)	C(17)-P(2)-Pd	108.18(10)
C(3)-C(1)-P(1)	122.2(2)	C(4)-C(2)-P(2)	122.7(2)
C(8)-C(3)-C(4)	118.2(3)	C(8)-C(3)-C(1)	119.3(3)
C(4)-C(3)-C(1)	121.9(3)	C(5)-C(4)-C(3)	118.7(3)
C(5)-C(4)-C(2)	118.6(3)	C(3)-C(4)-C(2)	122.2(3)
C(4)-C(5)-C(6)	123.2(3)	C(7)-C(6)-C(5)	118.2(3)
C(7)-C(6)-C(9)	118.9(3)	C(5)-C(6)-C(9)	122.8(3)
C(12)-C(7)-C(6)	119.0(3)	C(12)-C(7)-C(8)	122.9(3)
C(6)-C(7)-C(8)	118.1(3)	C(3)-C(8)-C(7)	123.5(3)
C(10)-C(9)-C(6)	120.3(3)	C(9)-C(10)-C(11)	120.7(3)
C(12)-C(11)-C(10)	120.1(3)	C(11)-C(12)-C(7)	121.0(3)
C(14)-C(13)-C(16)	109.3(3)	C(14)-C(13)-C(15)	106.3(3)
C(16)-C(13)-C(15)	110.0(3)	C(14)-C(13)-P(2)	110.6(2)
C(16)-C(13)-P(2)	113.5(2)	C(15)-C(13)-P(2)	106.9(2)
C(19)-C(17)-C(20)	108.1(3)	C(19)-C(17)-C(18)	109.5(3)
C(20)-C(17)-C(18)	107.1(3)	C(19)-C(17)-P(2)	111.2(2)
C(20)-C(17)-P(2)	105.7(2)	C(18)-C(17)-P(2)	114.9(2)
C(24)-C(21)-C(22)	109.4(3)	C(24)-C(21)-C(23)	108.6(3)
C(22)-C(21)-C(23)	107.9(3)	C(24)-C(21)-P(1)	115.5(2)
C(22)-C(21)-P(1)	109.6(2)	C(23)-C(21)-P(1)	105.6(2)
C(26)-C(25)-C(27)	108.5(3)	C(26)-C(25)-C(28)	107.4(3)
C(27)-C(25)-C(28)	108.4(3)	C(26)-C(25)-P(1)	107.8(2)
C(27)-C(25)-P(1)	114.5(2)	C(28)-C(25)-P(1)	109.9(2)

Table 23D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (47).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd	11.12(12)	13.59(13)	18.22(13)	0.96(11)	1.58(8)	-0.12(11)
O(1)	25.9(14)	19.1(14)	35.3(14)	11.5(11)	5.4(11)	0.1(10)
O(2)	20.2(13)	18.0(14)	33.5(13)	1.8(11)	2.9(10)	6.0(10)
P(1)	11.9(4)	15.0(5)	18.9(4)	-0.1(3)	2.4(3)	-0.5(3)
P(2)	12.8(4)	15.2(5)	16.7(4)	1.3(3)	2.4(3)	0.8(3)
C(1)	15.0(16)	16.5(19)	22.9(17)	-2.2(14)	2.1(13)	-0.5(13)
C(2)	15.0(16)	16.1(17)	21.8(17)	3.6(14)	-1.0(13)	-1.1(13)
C(3)	16.1(17)	12.5(17)	23.5(17)	-1.3(13)	-0.5(13)	1.0(13)
C(4)	13.4(16)	14.4(19)	24.8(18)	0.3(14)	-2.2(13)	-0.7(13)
C(5)	20.5(17)	21(2)	22.6(17)	1.3(15)	2.1(13)	1.9(15)
C(6)	24.0(19)	14.8(18)	24.1(18)	-1.0(14)	-3.4(14)	2.4(14)
C(7)	19.2(18)	14.2(18)	28.7(19)	-1.6(14)	-6.4(14)	1.9(14)
C(8)	16.0(16)	17.8(18)	26.0(17)	-4.5(15)	4.0(13)	1.9(15)
C(9)	32(2)	32(2)	25.0(19)	5.5(16)	-3.2(16)	2.0(17)
C(10)	37(2)	34(2)	30(2)	7.2(17)	-13.6(18)	4.7(18)
C(11)	24(2)	27(2)	45(2)	-0.4(19)	-13.5(18)	4.4(16)
C(12)	22.0(19)	24(2)	40(2)	-4.0(17)	-5.0(16)	4.1(16)
C(13)	21.5(18)	21.0(19)	14.6(16)	0.0(14)	4.1(13)	-2.1(14)
C(14)	34(2)	24(2)	26.4(18)	-5.7(16)	5.8(15)	4.3(17)
C(15)	30(2)	31(2)	23.3(18)	-5.8(16)	-0.8(15)	-1.4(16)
C(16)	37(2)	30(2)	19.8(18)	0.9(16)	8.0(16)	0.1(17)
C(17)	13.7(16)	19.1(19)	21.7(17)	3.2(14)	0.2(13)	-0.9(14)
C(18)	18.3(18)	35(2)	39(2)	10.2(17)	-2.1(16)	-10.2(16)
C(19)	14.6(18)	29(2)	38(2)	3.0(17)	2.1(15)	3.7(15)
C(20)	20.2(18)	29(2)	29.6(19)	1.4(16)	-4.6(15)	-2.7(15)
C(21)	13.1(16)	16.7(19)	32.2(19)	-3.7(15)	3.3(14)	-1.7(13)
C(22)	16.4(17)	21(2)	42(2)	4.4(17)	3.6(14)	-3.2(16)
C(23)	19.6(17)	25(2)	36(2)	-4.0(17)	-3.1(14)	-5.1(16)
C(24)	13.2(17)	28(2)	47(2)	-4.2(18)	3.5(16)	1.3(15)
C(25)	18.7(17)	25(2)	19.3(17)	-0.9(15)	4.9(13)	-1.7(14)
C(26)	47(2)	46(3)	20.8(18)	1.3(19)	-8.3(16)	-22(2)
C(27)	38(3)	98(4)	28(2)	-24(2)	6.2(19)	12(3)
C(28)	61(3)	41(3)	22.5(19)	8.1(18)	-8.6(19)	-9(2)

Table 23E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (47).

	x	y	z	U
H(1A)	7541	14468	7819	22
H(1B)	8420	14738	7698	22
H(2A)	6459	14483	9221	21
H(2B)	6644	14338	8511	21
H(5)	7389	14061	9934	26
H(8)	9280	14331	8477	24
H(9)	8325	12798	10713	35
H(10)	9543	11840	10952	41
H(11)	10494	11945	10209	39
H(12)	10223	13084	9241	34
H(14A)	5481	20382	9437	42
H(14B)	6246	21159	9148	42
H(14C)	6144	21174	9878	42
H(15A)	7271	19551	10101	42
H(15B)	7483	19528	9389	42
H(15C)	7478	17641	9773	42
H(16A)	6059	18080	10439	43
H(16B)	6215	16210	10069	43
H(16C)	5448	17346	9940	43
H(18A)	5039	15283	9296	46
H(18B)	5325	13961	8758	46
H(18C)	4496	14864	8712	46
H(19A)	5046	19491	8399	41
H(19B)	4716	18610	9014	41
H(19C)	4334	18119	8359	41
H(20A)	4884	15901	7677	39
H(20B)	5738	15194	7781	39
H(20C)	5578	17305	7600	39
H(22A)	9084	21571	7589	40
H(22B)	8191	21315	7468	40
H(22C)	8781	20460	6996	40
H(23A)	8668	18307	8739	40
H(23B)	8282	20252	8573	40
H(23C)	9188	20069	8603	40
H(24A)	9884	18669	7763	44
H(24B)	9448	17524	7233	44
H(24C)	9474	16760	7924	44
H(26A)	6868	15609	6295	57
H(26B)	6564	16163	6959	57
H(26C)	7179	14548	6896	57
H(27A)	8524	15306	6683	82
H(27B)	8735	17369	6483	82
H(27C)	8197	16129	6047	82
H(28A)	7784	19849	6506	62
H(28B)	6926	19404	6685	62
H(28C)	7252	18660	6050	62

Table 24A. Crystal data, structure solution and refinement for (48).

Identification code	exti23
Chemical formula	$C_{24}H_{44}O_2P_2Pd$
Formula weight	532.93
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 8.9816(5) Å α = 90°
	b = 19.8520(10) Å β = 102.1990(10)°
	c = 14.5897(8) Å γ = 90°
Volume	2542.6(2) Å^3
Z	4
Density (calculated)	1.392 g/cm^3
Absorption coefficient μ	0.873 mm^{-1}
F(000)	1120
Reflections for cell refinement	12132 (θ range 2.05 to 28.47°)
Crystal colour	Blue/Colourless
Crystal size	0.26 × 0.20 × 0.16 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.76 to 28.47°
Index ranges	$-11 \le h \le 12$, $-25 \le k \le 22$, $-10 \le \ell \le 19$
Reflections collected	15909
Independent reflections	5916 (R_{int} = 0.0343)
Reflections with I>2σ(I)	5338
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.831 and 0.717
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0215, 3.3628
Data / restraints / parameters	5916 / 0 / 275
Final R indices [I>2σ(I)]	R1 = 0.0309, wR2 = 0.0709
R indices (all data)	R1 = 0.0364, wR2 = 0.0748
Goodness-of-fit on F^2	1.143
Extinction coefficient	0.00112(15)
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.771 and -0.641 eÅ^{-3}

The Crystal Structure of [*o*-$C_6H_4(CH_2PBu^t_2)_2Pd(O_2)$] (48)

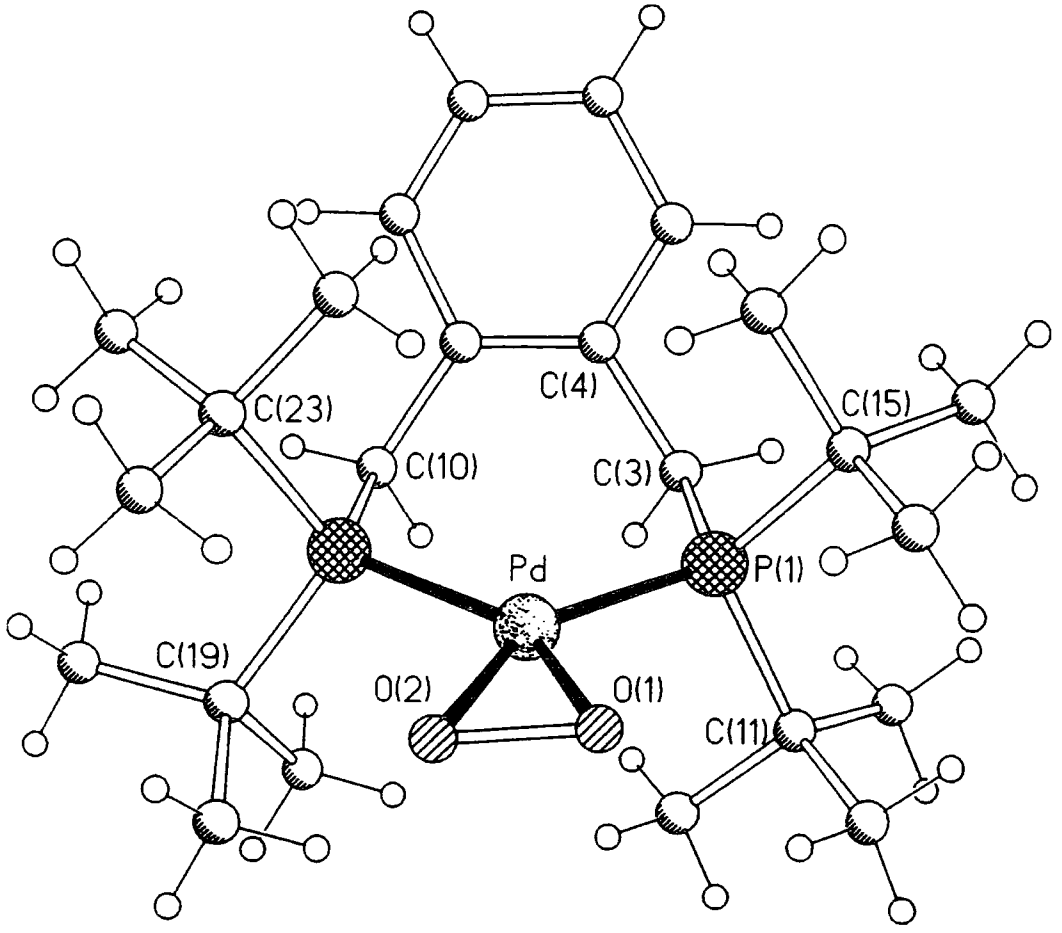


Table 24B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (48). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	24(3)	7622.7(12)	2195.0(16)	22.2(5)
C(2)	-1449(3)	7840.5(14)	1772.7(17)	29.7(5)
C(3)	-2652(3)	7400.3(15)	1501.2(19)	34.0(6)
C(4)	-2399(3)	6718.0(15)	1619.6(18)	32.2(6)
C(5)	-944(3)	6486.6(14)	1987.8(17)	27.9(5)
C(6)	284(3)	6923.7(12)	2288.3(15)	21.4(4)
C(7)	1858(3)	6621.9(12)	2610.9(15)	21.5(4)
P(1)	2731.8(6)	6581.6(3)	3873.1(4)	17.57(12)
C(8)	1641(3)	5909.2(12)	4373.7(16)	22.9(5)
C(9)	2405(3)	5745.3(14)	5397.1(17)	29.9(5)
C(10)	1427(3)	5255.4(13)	3798(2)	34.5(6)
C(11)	82(3)	6219.3(14)	4403(2)	32.5(6)
C(12)	4732(3)	6306.8(12)	3829.5(17)	23.7(5)
C(13)	5537(3)	6937.7(14)	3564.4(19)	30.6(5)
C(14)	5597(3)	6076.8(14)	4800.0(19)	32.3(6)
C(15)	4827(3)	5755.6(15)	3104(2)	39.0(7)
Pd(1)	2916.11(18)	7517.38(8)	4783.69(11)	16.69(6)
O(1)	3776(2)	7228.0(9)	6112.5(11)	26.0(4)
O(2)	3599(2)	7950.3(9)	6055.1(11)	27.9(4)
C(16)	3477(3)	9002.1(12)	3677.3(17)	28.1(5)
C(17)	4501(3)	8750.7(14)	3026.7(19)	32.5(6)
C(18)	4502(4)	9077.8(15)	4660.8(19)	38.5(7)
C(19)	2843(4)	9693.9(14)	3321(2)	39.3(7)
P(2)	1969.4(7)	8338.9(3)	3721.3(4)	20.33(12)
C(20)	300(3)	8723.6(13)	4140.8(18)	28.6(5)
C(21)	886(4)	9088.2(14)	5077.4(19)	36.3(6)
C(22)	-690(3)	9211.6(15)	3446(2)	38.0(6)
C(23)	-706(3)	8133.0(14)	4330(2)	34.7(6)
C(24)	1286(3)	8134.5(12)	2460.9(16)	22.7(5)

Table 24C. Bond lengths (Å) and angles (°) for (48).

C(1)-C(2)	1.404(3)	C(1)-C(6)	1.409(3)
C(1)-C(24)	1.510(3)	C(2)-C(3)	1.381(4)
C(3)-C(4)	1.378(4)	C(4)-C(5)	1.383(4)
C(5)-C(6)	1.399(3)	C(6)-C(7)	1.516(3)
C(7)-P(1)	1.845(2)	P(1)-C(12)	1.891(2)
P(1)-C(8)	1.892(2)	P(1)-Pd(1)	2.2694(6)
C(8)-C(10)	1.536(3)	C(8)-C(11)	1.538(4)
C(8)-C(9)	1.541(3)	C(12)-C(14)	1.533(3)
C(12)-C(13)	1.536(4)	C(12)-C(15)	1.538(4)
Pd(1)-O(1)	2.0130(16)	Pd(1)-O(2)	2.0187(16)
Pd(1)-P(2)	2.2865(6)	O(1)-O(2)	1.443(3)
C(16)-C(19)	1.535(4)	C(16)-C(17)	1.538(4)
C(16)-C(18)	1.540(3)	C(16)-P(2)	1.899(3)
P(2)-C(24)	1.857(2)	P(2)-C(20)	1.895(3)
C(20)-C(21)	1.538(4)	C(20)-C(23)	1.540(4)
C(20)-C(22)	1.541(4)		

C(2)-C(1)-C(6)	117.8(2)	C(2)-C(1)-C(24)	119.5(2)
C(6)-C(1)-C(24)	122.5(2)	C(3)-C(2)-C(1)	122.6(3)
C(4)-C(3)-C(2)	119.2(2)	C(3)-C(4)-C(5)	119.5(2)
C(4)-C(5)-C(6)	122.2(3)	C(5)-C(6)-C(1)	118.5(2)
C(5)-C(6)-C(7)	118.3(2)	C(1)-C(6)-C(7)	122.9(2)
C(6)-C(7)-P(1)	119.96(16)	C(7)-P(1)-C(12)	100.71(11)
C(7)-P(1)-C(8)	105.67(11)	C(12)-P(1)-C(8)	112.49(11)
C(7)-P(1)-Pd(1)	120.79(8)	C(12)-P(1)-Pd(1)	107.67(8)
C(8)-P(1)-Pd(1)	109.34(8)	C(10)-C(8)-C(11)	110.1(2)
C(10)-C(8)-C(9)	109.3(2)	C(11)-C(8)-C(9)	106.2(2)
C(10)-C(8)-P(1)	113.58(17)	C(11)-C(8)-P(1)	106.08(16)
C(9)-C(8)-P(1)	111.24(16)	C(14)-C(12)-C(13)	107.6(2)
C(14)-C(12)-C(15)	109.4(2)	C(13)-C(12)-C(15)	108.0(2)
C(14)-C(12)-P(1)	110.75(17)	C(13)-C(12)-P(1)	105.92(16)
C(15)-C(12)-P(1)	114.84(18)	O(1)-Pd(1)-O(2)	41.95(7)
O(1)-Pd(1)-P(1)	107.21(5)	O(2)-Pd(1)-P(1)	148.96(5)
O(1)-Pd(1)-P(2)	150.27(5)	O(2)-Pd(1)-P(2)	108.45(5)
P(1)-Pd(1)-P(2)	102.50(2)	O(2)-O(1)-Pd(1)	69.24(9)
O(1)-O(2)-Pd(1)	68.81(9)	C(19)-C(16)-C(17)	108.0(2)
C(19)-C(16)-C(18)	109.5(2)	C(17)-C(16)-C(18)	106.8(2)
C(19)-C(16)-P(2)	114.6(2)	C(17)-C(16)-P(2)	108.64(17)
C(18)-C(16)-P(2)	109.05(18)	C(24)-P(2)-C(20)	106.81(11)
C(24)-P(2)-C(16)	101.95(11)	C(20)-P(2)-C(16)	110.47(12)
C(24)-P(2)-Pd(1)	120.88(8)	C(20)-P(2)-Pd(1)	105.94(8)
C(16)-P(2)-Pd(1)	110.59(8)	C(21)-C(20)-C(23)	107.6(2)
C(21)-C(20)-C(22)	109.3(2)	C(23)-C(20)-C(22)	108.5(2)
C(21)-C(20)-P(2)	109.34(19)	C(23)-C(20)-P(2)	106.56(17)
C(22)-C(20)-P(2)	115.26(19)	C(1)-C(24)-P(2)	118.34(16)

Table 24D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (48).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
C(1)	21.8(11)	28.1(12)	15.9(10)	0.9(9)	2.3(8)	-1.2(9)
C(2)	27.8(12)	34.7(14)	23.8(12)	1.6(10)	-0.6(10)	6.3(11)
C(3)	22.3(12)	51.9(17)	25.2(13)	1.2(11)	-0.7(10)	2.1(11)
C(4)	25.0(12)	47.9(16)	21.6(12)	1.1(11)	0.7(9)	-10.4(12)
C(5)	28.3(12)	32.2(13)	21.5(11)	0.0(10)	1.6(9)	-5.3(10)
C(6)	22.6(11)	27.2(11)	14.1(10)	-0.1(8)	3.4(8)	-2.3(9)
C(7)	24.5(11)	24.2(11)	15.5(10)	-0.7(8)	3.5(8)	0.1(9)
P(1)	18.2(3)	18.3(3)	15.9(3)	-0.1(2)	3.1(2)	0.5(2)
C(8)	25.4(11)	21.9(11)	21.2(11)	2.4(9)	4.5(9)	-3.8(9)
C(9)	34.6(13)	31.4(13)	23.4(12)	7.7(10)	5.2(10)	-3.6(11)
C(10)	47.9(16)	24.0(12)	32.6(14)	-1.1(10)	10.9(12)	-8.1(11)
C(11)	27.4(13)	37.3(14)	34.6(14)	10.9(11)	10.8(11)	-0.9(11)
C(12)	19.4(11)	26.4(12)	25.9(12)	-1.4(9)	6.2(9)	4.1(9)
C(13)	22.6(12)	36.6(14)	34.4(14)	4.4(11)	9.8(10)	0.9(10)
C(14)	25.4(12)	35.2(14)	34.9(14)	5.8(11)	3.7(11)	7.9(11)
C(15)	33.4(14)	41.0(16)	45.2(17)	-13.8(13)	13.8(12)	7.8(12)
Pd(1)	18.63(10)	17.93(9)	13.41(9)	0.35(6)	3.13(6)	1.04(6)
O(1)	29.9(9)	29.9(9)	16.8(8)	5.3(7)	1.5(7)	0.9(7)
O(2)	36.3(10)	28.2(9)	17.8(8)	-5.6(7)	2.3(7)	2.2(7)
C(16)	36.7(14)	21.5(11)	23.4(12)	1.2(9)	0.4(10)	-5.2(10)
C(17)	31.1(13)	34.8(14)	31.9(13)	-1.4(11)	7.9(11)	-9.8(11)
C(18)	48.5(17)	35.4(15)	27.0(13)	0.0(11)	-2.1(12)	-17.0(13)
C(19)	55.1(18)	24.0(13)	39.9(15)	7.3(11)	12.4(14)	-1.8(12)
P(2)	26.2(3)	18.1(3)	16.2(3)	1.2(2)	3.2(2)	1.8(2)
C(20)	34.9(13)	27.0(12)	25.0(12)	1.5(10)	8.8(10)	10.9(10)
C(21)	51.5(17)	31.1(14)	28.2(13)	1.4(11)	13.1(12)	14.0(12)
C(22)	44.2(16)	36.9(15)	33.1(14)	5.5(12)	8.4(12)	16.9(13)
C(23)	35.7(14)	37.3(15)	35.6(14)	4.6(12)	17.9(12)	9.3(12)
C(24)	23.9(11)	24.0(11)	18.8(10)	2.2(9)	1.7(9)	0.1(9)

Table 24E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (48).

	x	y	z	U
H(2)	-1625	8309	1670	36
H(3)	-3642	7566	1236	41
H(4)	-3219	6409	1449	39
H(5)	-772	6015	2038	33
H(7A)	2560	6878	2303	26
H(7B)	1820	6156	2364	26
H(9A)	2709	6165	5739	45
H(9B)	3308	5465	5408	45
H(9C)	1685	5501	5695	45
H(10A)	2424	5053	3803	52
H(10B)	915	5356	3150	52
H(10C)	806	4939	4072	52
H(11A)	225	6605	4831	49
H(11B)	-555	5881	4623	49
H(11C)	-416	6369	3772	49
H(13A)	5564	7284	4046	46
H(13B)	4981	7109	2958	46
H(13C)	6580	6822	3520	46
H(14A)	6689	6055	4807	48
H(14B)	5235	5630	4937	48
H(14C)	5419	6398	5276	48
H(15A)	5898	5646	3124	59
H(15B)	4350	5918	2476	59
H(15C)	4294	5351	3249	59
H(17A)	5378	9052	3075	49
H(17B)	3919	8745	2378	49
H(17C)	4859	8294	3212	49
H(18A)	5329	9394	4633	58
H(18B)	4934	8638	4879	58
H(18C)	3897	9249	5096	58
H(19A)	2282	9888	3766	59
H(19B)	2156	9643	2707	59
H(19C)	3687	9993	3264	59
H(21A)	1423	9500	4966	54
H(21B)	1585	8792	5503	54
H(21C)	23	9205	5360	54
H(22A)	-1535	9375	3714	57
H(22B)	-1095	8976	2856	57
H(22C)	-68	9594	3326	57
H(23A)	-115	7838	4811	52
H(23B)	-1053	7876	3750	52
H(23C)	-1590	8309	4548	52
H(24B)	938	8559	2128	27
H(24A)	2170	7972	2217	27

Table 25A. Crystal data, structure solution and refinement for (50).

Identification code	exti45
Chemical formula	$C_{22.50}H_{46}Cl_2P_2Pd$
Formula weight	555.83
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 23.0537(16) Å α = 90°
	b = 14.7902(11) Å β = 98.175(2)°
	c = 16.1896(11) Å γ = 90°
Volume	5464.1(7) Å^3
Z	8
Density (calculated)	1.351 g/cm^3
Absorption coefficient μ	0.999 mm^{-1}
F(000)	2328
Reflections for cell refinement	25457 (θ range 2.15 to 28.80°)
Crystal colour	yellow
Crystal size	0.62 × 0.47 × 0.43 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.64 to 28.82°
Index ranges	$-30 \le h \le 23$, $-19 \le k \le 18$, $-11 \le \ell \le 21$
Intensity decay	0%
Reflections collected	28664
Independent reflections	12313 (R_{int} = 0.0232)
Reflections with I>2σ(I)	10752
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.7458 and 0.6610
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0000, 33.6548
Data / restraints / parameters	12313 / 72 / 551
Final R indices [I>2σ(I)]	R1 = 0.0637, wR2 = 0.1312
R indices (all data)	R1 = 0.0730, wR2 = 0.1342
Goodness-of-fit on F^2	1.312
Largest and mean shift/esd	0.000 and 0.000
Largest diff. peak and hole	1.037 and -1.301 eÅ^{-3}

The Crystal Structure of $[(Bu^t_2P(CH_2)_3PBu^t_2)Pd(Cl)_2]$ (50)

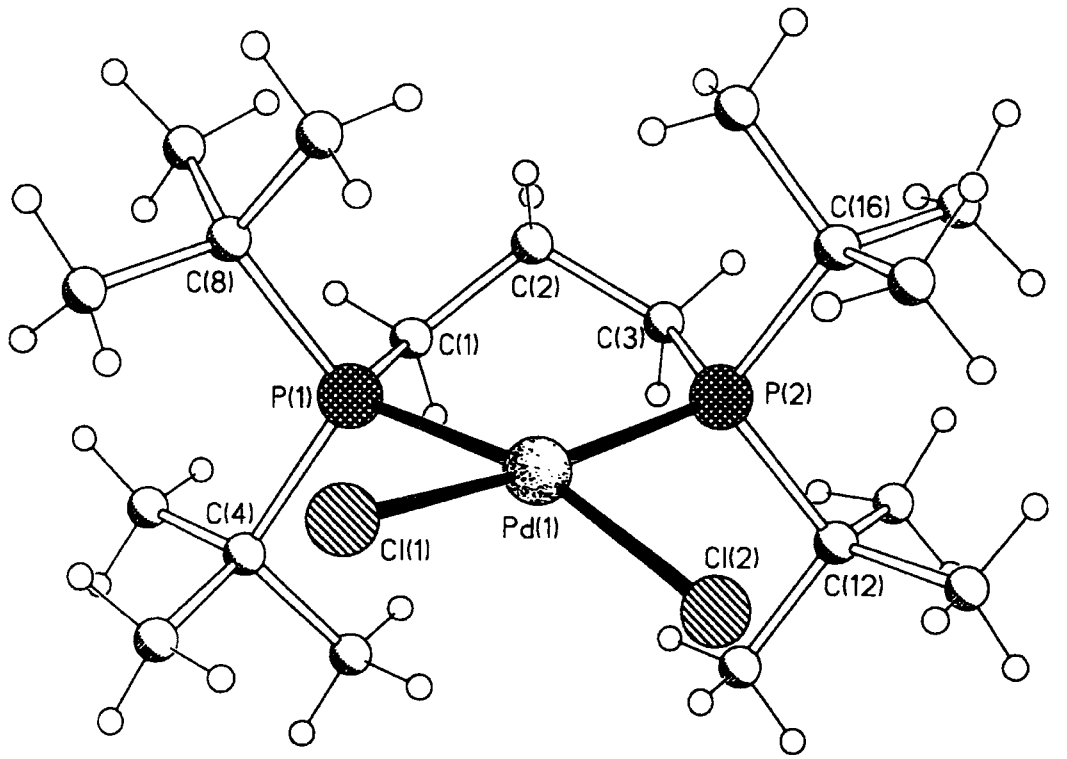


Table 25B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (50). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	281.68(17)	7318.4(2)	2448.4(2)	18.72(9)
Cl(1)	-459.9(6)	6221.1(9)	2111.8(10)	32.0(3)
Cl(2)	752.0(6)	6605.9(10)	1416.7(9)	30.4(3)
P(1)	-345.0(6)	8068.9(9)	3203.3(8)	20.5(3)
P(2)	1117.5(6)	8136.8(9)	2893.3(8)	20.2(3)
C(1)	-42(2)	9071(4)	3764(4)	26.5(11)
C(2)	579(2)	8957(4)	4230(3)	28.0(12)
C(3)	1034(2)	9052(4)	3629(3)	24.8(11)
C(4)	-959(2)	8611(4)	2467(3)	22.2(10)
C(5)	-1345(3)	9204(4)	2960(4)	31.7(13)
C(6)	-1358(3)	7955(4)	1919(4)	31.4(13)
C(7)	-667(3)	9209(4)	1864(4)	33.5(13)
C(8)	-625(2)	7350(4)	4047(3)	28.2(12)
C(9)	-157(3)	6635(4)	4338(4)	38.8(15)
C(10)	-1205(3)	6860(4)	3726(4)	35.4(14)
C(11)	-725(3)	7911(5)	4814(4)	41.7(16)
C(12)	1441(2)	8778(4)	2049(3)	26.4(11)
C(13)	1803(3)	9611(4)	2383(4)	33.7(13)
C(14)	915(3)	9116(4)	1431(4)	32.9(13)
C(15)	1837(3)	8195(4)	1576(4)	34.6(14)
C(16)	1692(2)	7382(4)	3493(4)	28.9(12)
C(17)	1452(3)	7067(5)	4288(4)	46.9(18)
C(18)	2274(3)	7884(5)	3766(4)	37.5(15)
C(19)	1821(3)	6532(4)	3018(4)	37.5(14)
Pd(2)	4744.17(17)	2187.3(2)	2668.3(3)	21.98(10)
Cl(3)	5512.6(6)	1149.4(9)	3046.8(11)	37.0(3)
Cl(4)	4261.0(7)	1412.6(13)	3640.7(12)	52.2(5)
P(5)	5336.9(7)	2927.6(10)	1850.4(12)	35.2(4)
P(6)	3893.3(6)	2980.1(9)	2259.9(9)	21.8(3)
C(20)	4990(3)	3875(5)	1223(5)	57(2)
C(21)	4359(4)	3735(5)	861(4)	54(2)
C(22)	3953(3)	3881(4)	1502(4)	28.3(12)
C(23)	5954(3)	3538(4)	2521(7)	69(3)
C(24)	5666(3)	4167(5)	3105(7)	83(4)
C(25)	6306(4)	4105(5)	1977(9)	114(5)
C(26)	6382(3)	2925(5)	3075(7)	68(3)
C(27)	5609(4)	2152(5)	1036(5)	56(2)
C(28)	5681(5)	2679(7)	219(7)	102(5)
C(29)	6194(3)	1701(5)	1356(6)	65(3)
C(30)	5139(3)	1424(5)	797(5)	50.6(19)
C(31)	3601(3)	3649(4)	3120(4)	28.2(12)
C(32)	3166(3)	4375(5)	2760(5)	51.0(19)
C(33)	3315(6)	3081(6)	3736(7)	99(4)
C(34)	4133(3)	4115(5)	3599(5)	53(2)
C(35)	3313(3)	2203(4)	1695(4)	33.9(13)
C(36)	3216(7)	1355(9)	2171(10)	43(4)
C(37)	2768(8)	2709(15)	1362(16)	54(6)
C(38)	3601(7)	1877(13)	910(10)	51(5)
C(36A)	2911(5)	1780(9)	2326(7)	36(3)
C(37A)	2883(7)	2652(13)	1026(9)	37(3)
C(38A)	3592(5)	1386(7)	1336(8)	36(3)

C(39)	2136(4)	3816(5)	-836(5)	59(2)
C(40)	2364(3)	4556(4)	-269(4)	36.3(14)
C(41)	2016(3)	4960(4)	248(4)	30.4(12)
C(42)	2224(4)	5640(5)	798(5)	55(2)
C(43)	2781(5)	5928(5)	850(5)	65(3)
C(44)	3151(4)	5516(6)	325(6)	64(3)
C(45)	2945(3)	4855(5)	-219(5)	50(2)

Table 25C. Bond lengths (Å) and angles (°) for (50).

Pd(1)-P(2)	2.3026(14)	Pd(1)-P(1)	2.3054(13)
Pd(1)-Cl(1)	2.3641(14)	Pd(1)-Cl(2)	2.3645(13)
P(1)-C(1)	1.824(5)	P(1)-C(4)	1.894(5)
P(1)-C(8)	1.914(6)	P(2)-C(3)	1.831(5)
P(2)-C(16)	1.892(6)	P(2)-C(12)	1.901(6)
C(1)-C(2)	1.530(8)	C(2)-C(3)	1.534(7)
C(4)-C(6)	1.531(7)	C(4)-C(7)	1.541(8)
C(4)-C(5)	1.550(7)	C(8)-C(9)	1.536(8)
C(8)-C(11)	1.537(8)	C(8)-C(10)	1.544(8)
C(12)-C(15)	1.537(7)	C(12)-C(13)	1.541(8)
C(12)-C(14)	1.542(8)	C(16)-C(19)	1.524(8)
C(16)-C(18)	1.541(8)	C(16)-C(17)	1.544(8)
Pd(2)-P(6)	2.3002(14)	Pd(2)-P(5)	2.3096(15)
Pd(2)-Cl(4)	2.3517(16)	Pd(2)-Cl(3)	2.3584(14)
P(5)-C(20)	1.845(6)	P(5)-C(23)	1.891(9)
P(5)-C(27)	1.918(8)	P(6)-C(22)	1.829(5)
P(6)-C(35)	1.897(6)	P(6)-C(31)	1.907(6)
C(20)-C(21)	1.501(12)	C(21)-C(22)	1.509(8)
C(23)-C(25)	1.530(12)	C(23)-C(26)	1.532(12)
C(23)-C(24)	1.542(12)	C(27)-C(29)	1.528(10)
C(27)-C(30)	1.537(12)	C(27)-C(28)	1.565(10)
C(31)-C(34)	1.519(9)	C(31)-C(33)	1.525(9)
C(31)-C(32)	1.527(9)	C(35)-C(37)	1.495(13)
C(35)-C(36)	1.505(13)	C(35)-C(37A)	1.514(12)
C(35)-C(38A)	1.523(11)	C(35)-C(38)	1.591(14)
C(35)-C(36A)	1.600(11)	C(39)-C(40)	1.477(10)
C(40)-C(41)	1.376(8)	C(40)-C(45)	1.401(9)
C(41)-C(42)	1.382(10)	C(42)-C(43)	1.343(12)
C(43)-C(44)	1.424(13)	C(44)-C(45)	1.356(12)

P(2)-Pd(1)-P(1)	98.09(5)	P(2)-Pd(1)-Cl(1)	168.11(5)
P(1)-Pd(1)-Cl(1)	88.03(5)	P(2)-Pd(1)-Cl(2)	90.45(5)
P(1)-Pd(1)-Cl(2)	166.88(5)	Cl(1)-Pd(1)-Cl(2)	85.44(5)
C(1)-P(1)-C(4)	99.7(2)	C(1)-P(1)-C(8)	103.9(3)
C(4)-P(1)-C(8)	112.7(2)	C(1)-P(1)-Pd(1)	115.47(18)
C(4)-P(1)-Pd(1)	109.80(16)	C(8)-P(1)-Pd(1)	114.30(18)
C(3)-P(2)-C(16)	103.5(3)	C(3)-P(2)-C(12)	100.8(2)
C(16)-P(2)-C(12)	110.2(3)	C(3)-P(2)-Pd(1)	115.56(18)
C(16)-P(2)-Pd(1)	110.14(19)	C(12)-P(2)-Pd(1)	115.73(18)
C(2)-C(1)-P(1)	114.9(4)	C(1)-C(2)-C(3)	110.7(5)
C(2)-C(3)-P(2)	119.3(4)	C(6)-C(4)-C(7)	106.1(5)
C(6)-C(4)-C(5)	108.4(4)	C(7)-C(4)-C(5)	109.7(5)
C(6)-C(4)-P(1)	115.5(4)	C(7)-C(4)-P(1)	106.6(4)
C(5)-C(4)-P(1)	110.4(4)	C(9)-C(8)-C(11)	107.7(5)
C(9)-C(8)-C(10)	108.4(5)	C(11)-C(8)-C(10)	107.7(5)
C(9)-C(8)-P(1)	107.9(4)	C(11)-C(8)-P(1)	112.4(4)
C(10)-C(8)-P(1)	112.5(4)	C(15)-C(12)-C(13)	107.1(5)
C(15)-C(12)-C(14)	109.0(5)	C(13)-C(12)-C(14)	107.8(5)
C(15)-C(12)-P(2)	113.6(4)	C(13)-C(12)-P(2)	113.2(4)
C(14)-C(12)-P(2)	105.9(4)	C(19)-C(16)-C(18)	108.6(5)
C(19)-C(16)-C(17)	106.9(5)	C(18)-C(16)-C(17)	107.9(5)
C(19)-C(16)-P(2)	113.6(4)	C(18)-C(16)-P(2)	112.4(4)
C(17)-C(16)-P(2)	107.3(4)	P(6)-Pd(2)-P(5)	98.25(5)
P(6)-Pd(2)-Cl(4)	88.57(5)	P(5)-Pd(2)-Cl(4)	171.87(7)
P(6)-Pd(2)-Cl(3)	170.03(5)	P(5)-Pd(2)-Cl(3)	88.49(6)
Cl(4)-Pd(2)-Cl(3)	85.34(6)	C(20)-P(5)-C(23)	100.7(4)
C(20)-P(5)-C(27)	103.5(4)	C(23)-P(5)-C(27)	112.8(4)
C(20)-P(5)-Pd(2)	115.5(2)	C(23)-P(5)-Pd(2)	110.8(3)

C(27)-P(5)-Pd(2)	112.8(2)	C(22)-P(6)-C(35)	103.5(3)
C(22)-P(6)-C(31)	100.3(3)	C(35)-P(6)-C(31)	111.6(3)
C(22)-P(6)-Pd(2)	114.93(19)	C(35)-P(6)-Pd(2)	110.11(19)
C(31)-P(6)-Pd(2)	115.45(19)	C(21)-C(20)-P(5)	115.5(5)
C(20)-C(21)-C(22)	111.9(6)	C(21)-C(22)-P(6)	118.0(4)
C(25)-C(23)-C(26)	108.1(7)	C(25)-C(23)-C(24)	109.3(7)
C(26)-C(23)-C(24)	107.2(9)	C(25)-C(23)-P(5)	110.4(8)
C(26)-C(23)-P(5)	115.0(5)	C(24)-C(23)-P(5)	106.6(5)
C(29)-C(27)-C(30)	109.6(6)	C(29)-C(27)-C(28)	108.0(7)
C(30)-C(27)-C(28)	107.0(8)	C(29)-C(27)-P(5)	112.8(6)
C(30)-C(27)-P(5)	107.8(5)	C(28)-C(27)-P(5)	111.6(5)
C(34)-C(31)-C(33)	108.0(7)	C(34)-C(31)-C(32)	108.3(5)
C(33)-C(31)-C(32)	108.3(6)	C(34)-C(31)-P(6)	105.4(4)
C(33)-C(31)-P(6)	115.0(4)	C(32)-C(31)-P(6)	111.5(4)
C(37)-C(35)-C(36)	115.1(12)	C(37)-C(35)-C(37A)	24.6(9)
C(36)-C(35)-C(37A)	127.0(11)	C(37)-C(35)-C(38A)	129.7(11)
C(36)-C(35)-C(38A)	68.7(8)	C(37A)-C(35)-C(38A)	110.1(9)
C(37)-C(35)-C(38)	106.7(12)	C(36)-C(35)-C(38)	105.4(10)
C(37A)-C(35)-C(38)	82.3(9)	C(38A)-C(35)-C(38)	37.5(7)
C(37)-C(35)-C(36A)	83.9(11)	C(36)-C(35)-C(36A)	37.5(7)
C(37A)-C(35)-C(36A)	104.4(8)	C(38A)-C(35)-C(36A)	104.4(7)
C(38)-C(35)-C(36A)	137.5(9)	C(37)-C(35)-P(6)	111.6(10)
C(36)-C(35)-P(6)	113.9(7)	C(37A)-C(35)-P(6)	115.0(9)
C(38A)-C(35)-P(6)	110.9(6)	C(38)-C(35)-P(6)	102.9(6)
C(36A)-C(35)-P(6)	111.3(6)	C(41)-C(40)-C(45)	117.6(7)
C(41)-C(40)-C(39)	120.9(7)	C(45)-C(40)-C(39)	121.5(7)
C(40)-C(41)-C(42)	121.9(7)	C(43)-C(42)-C(41)	120.9(8)
C(42)-C(43)-C(44)	118.3(8)	C(45)-C(44)-C(43)	120.8(7)
C(44)-C(45)-C(40)	120.6(7)		

Table 25D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (50).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	20.14(19)	18.67(17)	17.08(19)	-3.55(14)	1.76(15)	0.31(14)
Cl(1)	29.7(7)	24.0(6)	43.0(9)	-8.8(6)	7.7(6)	-5.5(5)
Cl(2)	30.8(7)	35.6(7)	25.2(7)	-13.0(6)	5.8(6)	0.3(5)
P(1)	21.4(6)	20.0(6)	20.5(7)	-2.6(5)	4.0(5)	-0.7(5)
P(2)	19.9(6)	23.5(6)	16.8(6)	-4.0(5)	0.7(5)	1.1(5)
C(1)	24(3)	29(3)	26(3)	-7(2)	5(2)	-1(2)
C(2)	27(3)	35(3)	22(3)	-9(2)	2(2)	-1(2)
C(3)	24(3)	26(3)	23(3)	-8(2)	-1(2)	-1(2)
C(4)	19(2)	28(3)	19(3)	-5(2)	0(2)	0.5(19)
C(5)	28(3)	29(3)	39(4)	-8(2)	9(3)	4(2)
C(6)	27(3)	33(3)	33(3)	-5(2)	-2(2)	0(2)
C(7)	32(3)	34(3)	33(3)	7(3)	1(3)	-3(2)
C(8)	26(3)	35(3)	25(3)	3(2)	8(2)	-1(2)
C(9)	37(3)	42(3)	38(4)	17(3)	10(3)	3(3)
C(10)	33(3)	41(3)	33(3)	6(3)	11(3)	-7(3)
C(11)	46(4)	54(4)	27(3)	-1(3)	13(3)	-3(3)
C(12)	26(3)	32(3)	23(3)	-6(2)	8(2)	-4(2)
C(13)	29(3)	34(3)	38(4)	-1(3)	6(3)	-7(2)
C(14)	33(3)	38(3)	28(3)	6(3)	5(3)	-1(2)
C(15)	32(3)	43(3)	32(3)	-7(3)	15(3)	-5(3)
C(16)	26(3)	31(3)	28(3)	-3(2)	-3(2)	6(2)
C(17)	48(4)	65(5)	28(3)	15(3)	6(3)	22(3)
C(18)	25(3)	51(4)	31(3)	-11(3)	-11(3)	9(3)
C(19)	39(3)	36(3)	35(4)	-3(3)	-4(3)	11(3)
Pd(2)	21.3(2)	16.55(17)	27.3(2)	7.11(15)	0.69(16)	0.60(14)
Cl(3)	31.9(7)	26.3(7)	50.0(10)	5.2(6)	-3.8(7)	9.3(5)
Cl(4)	33.8(8)	57.8(10)	65.0(12)	43.8(9)	7.2(8)	0.0(7)
P(5)	29.3(8)	19.6(6)	60.8(11)	12.2(7)	21.1(8)	4.7(6)
P(6)	21.9(6)	20.3(6)	22.5(7)	4.1(5)	0.4(5)	1.1(5)
C(20)	59(5)	35(3)	86(6)	42(4)	46(4)	20(3)
C(21)	90(6)	45(4)	32(4)	24(3)	28(4)	32(4)
C(22)	31(3)	24(3)	28(3)	6(2)	0(2)	6(2)
C(23)	32(4)	19(3)	159(9)	-6(4)	26(5)	-4(3)
C(24)	28(4)	43(4)	173(11)	-36(6)	1(5)	-2(3)
C(25)	48(5)	26(4)	284(17)	18(6)	77(8)	-2(3)
C(26)	28(4)	34(4)	138(9)	-21(5)	-3(4)	0(3)
C(27)	68(5)	38(4)	72(5)	25(4)	48(4)	23(3)
C(28)	138(10)	79(7)	114(9)	55(6)	104(8)	55(7)
C(29)	47(4)	31(3)	125(8)	11(4)	44(5)	11(3)
C(30)	63(5)	53(4)	38(4)	1(3)	16(4)	21(4)
C(31)	37(3)	24(3)	25(3)	-2(2)	10(2)	1(2)
C(32)	41(4)	57(4)	53(5)	-21(4)	0(3)	20(3)
C(33)	168(11)	38(4)	120(9)	8(5)	119(9)	5(5)
C(34)	54(4)	51(4)	46(4)	-22(3)	-16(4)	22(3)
C(35)	29(3)	30(3)	40(4)	0(2)	-5(3)	-4(2)
C(36)	45(9)	27(6)	54(9)	-3(6)	-3(7)	-6(6)
C(37)	31(9)	42(9)	80(16)	-1(11)	-27(10)	-2(7)
C(38)	47(9)	62(11)	39(9)	-19(8)	-4(7)	-18(7)
C(36A)	31(6)	38(7)	39(6)	11(5)	-3(5)	-9(5)
C(37A)	36(8)	38(7)	37(8)	8(6)	1(6)	-2(5)
C(38A)	41(6)	25(5)	38(7)	-3(5)	-4(5)	-8(4)

C(39)	95(7)	37(4)	42(4)	3(3)	-2(4)	17(4)
C(40)	46(4)	31(3)	30(3)	11(3)	0(3)	5(3)
C(41)	35(3)	31(3)	26(3)	9(2)	4(3)	5(2)
C(42)	93(6)	40(4)	35(4)	3(3)	12(4)	6(4)
C(43)	94(7)	45(4)	45(5)	10(4)	-28(5)	-19(4)
C(44)	46(4)	66(5)	70(6)	44(5)	-23(4)	-18(4)
C(45)	30(3)	62(5)	60(5)	39(4)	11(3)	11(3)

Table 25E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (50).

	x	y	z	U
H(1A)	-40	9573	3359	32
H(1B)	-304	9248	4170	32
H(2A)	618	8355	4498	34
H(2B)	653	9421	4673	34
H(3A)	1421	9148	3971	30
H(3B)	940	9610	3299	30
H(5A)	-1662	9477	2571	48
H(5B)	-1105	9682	3255	48
H(5C)	-1514	8828	3364	48
H(6A)	-1649	8298	1544	47
H(6B)	-1558	7559	2273	47
H(6C)	-1122	7588	1588	47
H(7A)	-422	8832	1555	50
H(7B)	-423	9667	2183	50
H(7C)	-970	9507	1471	50
H(9A)	-297	6243	4757	58
H(9B)	206	6935	4583	58
H(9C)	-82	6269	3859	58
H(10A)	-1295	6426	4146	53
H(10B)	-1164	6539	3207	53
H(10C)	-1522	7304	3619	53
H(11A)	-982	8424	4636	62
H(11B)	-348	8136	5096	62
H(11C)	-909	7531	5200	62
H(13A)	2114	9423	2827	51
H(13B)	1547	10049	2607	51
H(13C)	1978	9890	1929	51
H(14A)	1057	9457	982	49
H(14B)	669	9507	1725	49
H(14C)	685	8597	1195	49
H(15A)	1962	8550	1121	52
H(15B)	1619	7662	1345	52
H(15C)	2182	8002	1959	52
H(17A)	1070	6776	4132	70
H(17B)	1407	7591	4644	70
H(17C)	1726	6635	4592	70
H(18A)	2528	7512	4168	56
H(18B)	2194	8460	4026	56
H(18C)	2470	7999	3277	56
H(19A)	1985	6702	2514	56
H(19B)	1457	6192	2861	56
H(19C)	2104	6155	3374	56
H(20A)	5016	4423	1577	68
H(20B)	5217	3992	759	68
H(21A)	4308	3112	639	65
H(21B)	4254	4160	392	65
H(22A)	3556	3998	1200	34
H(22B)	4080	4437	1817	34
H(24A)	5971	4446	3509	124
H(24B)	5401	3815	3402	124
H(24C)	5444	4641	2774	124
H(25A)	6603	4455	2334	171

H(25B)	6042	4519	1632	171
H(25C)	6497	3705	1616	171
H(26A)	6554	2488	2725	103
H(26B)	6171	2602	3470	103
H(26C)	6693	3294	3383	103
H(28A)	5982	3147	345	153
H(28B)	5308	2962	-6	153
H(28C)	5799	2258	-193	153
H(29A)	6155	1348	1858	97
H(29B)	6495	2167	1492	97
H(29C)	6307	1301	924	97
H(30A)	5259	1033	362	76
H(30B)	4765	1714	588	76
H(30C)	5094	1059	1289	76
H(32A)	3021	4699	3217	76
H(32B)	2837	4089	2405	76
H(32C)	3362	4801	2428	76
H(33A)	3233	3463	4201	149
H(33B)	3580	2590	3951	149
H(33C)	2947	2825	3454	149
H(34A)	4347	4437	3208	79
H(34B)	4390	3662	3903	79
H(34C)	4005	4546	3996	79
H(36A)	3058	1513	2683	65
H(36B)	3589	1035	2314	65
H(36C)	2937	963	1825	65
H(37A)	2868	3209	1010	81
H(37B)	2586	2950	1827	81
H(37C)	2493	2300	1029	81
H(38A)	3350	1420	601	76
H(38B)	3988	1616	1099	76
H(38C)	3643	2395	545	76
H(36D)	2663	2254	2514	54
H(36E)	3160	1521	2808	54
H(36F)	2662	1304	2041	54
H(37D)	2584	2214	798	56
H(37E)	3092	2872	579	56
H(37F)	2695	3163	1269	56
H(38D)	3285	995	1048	53
H(38E)	3823	1048	1789	53
H(38F)	3849	1591	940	53
H(39A)	2443	3614	-1155	89
H(39B)	1798	4033	-1221	89
H(39C)	2016	3309	-509	89
H(41)	1621	4766	227	36
H(42)	1970	5907	1142	67
H(43)	2924	6395	1228	78
H(44)	3547	5706	357	76
H(45)	3196	4592	-570	60

Table 26A. Crystal data, structure solution and refinement for (52).

Identification code	exti51
Chemical formula	$C_{102.5}H_{213}Cl_{21}O_{16}P_8Pd_4$
Formula weight	3119.54
Temperature	180(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	orthorhombic, $Pca2_1$
Unit cell dimensions	a = 38.530(2) Å α = 90°
	b = 19.1969(9) Å β = 90°
	c = 20.3787(10) Å γ = 90°
Volume	15073.2(13) Å^3
Z	4
Density (calculated)	1.375 g/cm^3
Absorption coefficient μ	0.976 mm^{-1}
F(000)	6468
Reflections for cell refinement	40041 (θ range 2.11 to 28.85°)
Crystal colour	yellow
Crystal size	0.40 × 0.32 × 0.20 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.55 to 28.90°
Index ranges	$-40 \le h \le 51$, $-14 \le k \le 25$, $-23 \le \ell \le 26$
Intensity decay	0%
Reflections collected	91913
Independent reflections	33354 (R_{int} = 0.1008)
Reflections with I>2σ(I)	21570
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.802 and 0.388
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0685, 16.4146
Data / restraints / parameters	33354 / 287 / 1420
Final R indices [I>2σ(I)]	R1 = 0.0723, wR2 = 0.1407
R indices (all data)	R1 = 0.1329, wR2 = 0.1680
Goodness-of-fit on F^2	1.050
Absolute structure parameter	-0.04(2)
Extinction coefficient	0.00019(3)
Largest and mean shift/esd	0.060 and 0.001
Largest diff. peak and hole	1.411 and -1.387 eÅ^{-3}

Crystal Structure of [{($Bu^t_2P(CH_2)_3PBu^t_2$)$Pd(OAc)_2$}$_4$] (52)

One Palladium Centre Only

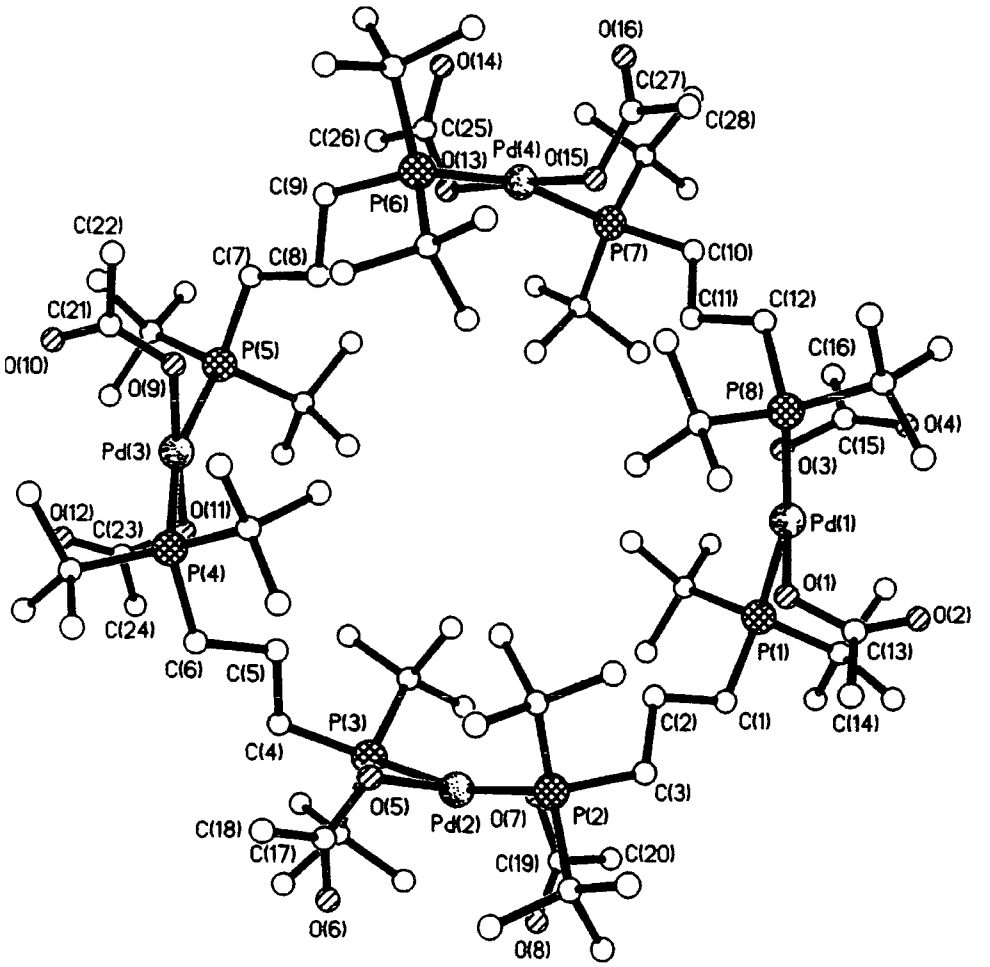


Table 26B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (52). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	4635.04(16)	6141.8(3)	847.9(3)	17.90(13)
Pd(2)	5363.52(16)	9766.5(3)	1538.4(3)	18.87(14)
Pd(3)	7212.10(16)	8265.7(3)	1921.7(3)	21.09(14)
Pd(4)	6472.98(16)	4604.8(3)	1225.9(3)	20.27(14)
P(1)	4580.5(6)	7131.0(11)	149.5(10)	21.4(5)
P(2)	4913.7(6)	9194.4(11)	2146.9(10)	19.7(5)
P(3)	5862.6(5)	10066.3(10)	900.9(11)	19.5(4)
P(4)	6887.3(6)	8927.9(11)	2704.9(11)	22.4(5)
P(5)	7377.5(6)	7469.2(11)	1077.6(10)	21.1(5)
P(6)	6775.3(6)	4951.1(11)	2200.9(11)	21.9(5)
P(7)	6111.8(6)	4525.8(11)	267.8(10)	20.2(5)
P(8)	4822.8(5)	5250.9(10)	1596.3(10)	17.5(4)
C(1)	4501(2)	7921(4)	628(4)	21.7(18)
C(2)	4776(2)	8150(4)	1138(4)	17.8(16)
C(3)	4620(2)	8722(4)	1581(4)	22.4(17)
C(4)	6253(2)	10106(4)	1415(4)	22.7(19)
C(5)	6373(2)	9448(4)	1776(4)	23.3(19)
C(6)	6645(2)	9639(4)	2293(4)	22.3(18)
C(7)	7388(2)	6563(4)	1379(4)	21.7(18)
C(8)	7053(2)	6231(4)	1637(4)	22.5(18)
C(9)	7138(2)	5533(4)	1980(4)	22.2(18)
C(10)	5657(2)	4382(4)	505(4)	22.3(18)
C(11)	5471.3(19)	4939(4)	917(4)	18.3(17)
C(12)	5134(2)	4643(4)	1194(4)	21.6(17)
O(1)	4424.3(14)	6700(3)	1590(3)	21.0(12)
O(2)	3892.4(16)	6341(3)	1319(3)	35.1(15)
C(13)	4094(2)	6682(4)	1650(4)	25.7(19)
C(14)	3952(3)	7129(5)	2199(5)	40(2)
O(3)	4869.1(15)	5626(3)	96(3)	22.4(13)
O(4)	4424.0(17)	4889(3)	8(3)	33.5(15)
C(15)	4706(2)	5108(4)	-168(4)	21.9(19)
C(16)	4893(3)	4798(5)	-734(4)	38(2)
O(5)	5638.0(15)	9871(3)	2388(3)	23.2(13)
O(6)	5544.2(19)	11014(3)	2390(3)	39.6(17)
C(17)	5658(2)	10489(5)	2648(5)	31(2)
C(18)	5834(3)	10537(5)	3292(4)	37(2)
O(7)	5094.9(15)	9599(3)	692(3)	25.3(13)
O(8)	4799.5(17)	10594(3)	845(3)	38.1(15)
C(19)	4860(2)	10062(5)	542(4)	26(2)
C(20)	4685(3)	9922(5)	-112(5)	40(2)
O(9)	7288.1(16)	7488(3)	2592(3)	27.9(14)
O(10)	7838.0(17)	7829(3)	2718(3)	38.4(16)
C(21)	7595(2)	7430(4)	2835(4)	24.8(19)
C(22)	7643(3)	6810(5)	3281(5)	38(2)
O(11)	7125.0(15)	9000(3)	1235(3)	28.7(13)
O(12)	7598.3(17)	9605(3)	1549(4)	42.2(17)
C(23)	7352(2)	9520(5)	1199(5)	37(2)
C(24)	7275(3)	10014(5)	627(5)	50(3)
O(13)	6862.6(15)	5003(3)	662(3)	25.0(13)
O(14)	7154.2(19)	3997(4)	739(4)	57(2)
C(25)	7120(2)	4596(5)	524(4)	31(2)

Table 26C. Bond lengths (Å) and angles (°) for (52).

Pd(1)-O(1)	2.024(5)	Pd(1)-O(3)	2.035(5)
Pd(1)-P(1)	2.382(2)	Pd(1)-P(8)	2.403(2)
Pd(2)-O(7)	2.037(5)	Pd(2)-O(5)	2.039(6)
Pd(2)-P(3)	2.391(2)	Pd(2)-P(2)	2.397(2)
Pd(3)-O(11)	2.015(6)	Pd(3)-O(9)	2.044(6)
Pd(3)-P(5)	2.388(2)	Pd(3)-P(4)	2.394(2)
Pd(4)-O(15)	2.038(5)	Pd(4)-O(13)	2.039(5)
Pd(4)-P(6)	2.397(2)	Pd(4)-P(7)	2.402(2)
P(1)-C(1)	1.829(8)	P(1)-C(29)	1.879(8)
P(1)-C(33)	1.902(9)	P(2)-C(3)	1.854(8)
P(2)-C(41)	1.893(9)	P(2)-C(37)	1.907(9)
P(3)-C(4)	1.833(8)	P(3)-C(49)	1.895(8)
P(3)-C(45)	1.897(8)	P(4)-C(6)	1.856(8)
P(4)-C(53)	1.893(9)	P(4)-C(57)	1.897(9)
P(5)-C(7)	1.845(8)	P(5)-C(65)	1.888(8)
P(5)-C(61)	1.890(9)	P(6)-C(9)	1.844(8)
P(6)-C(73)	1.868(9)	P(6)-C(69)	1.895(9)
P(7)-C(10)	1.840(8)	P(7)-C(77)	1.877(9)
P(7)-C(81)	1.900(8)	P(8)-C(12)	1.863(8)
P(8)-C(89)	1.885(8)	P(8)-C(85)	1.891(8)
C(1)-C(2)	1.545(10)	C(2)-C(3)	1.543(10)
C(4)-C(5)	1.534(11)	C(5)-C(6)	1.531(11)
C(7)-C(8)	1.534(11)	C(8)-C(9)	1.547(10)
C(10)-C(11)	1.535(11)	C(11)-C(12)	1.527(10)
O(1)-C(13)	1.278(10)	O(2)-C(13)	1.220(10)
C(13)-C(14)	1.514(12)	O(3)-C(15)	1.293(9)
O(4)-C(15)	1.221(10)	C(15)-C(16)	1.484(12)
O(5)-C(17)	1.300(10)	O(6)-C(17)	1.217(11)
C(17)-C(18)	1.482(13)	O(7)-C(19)	1.305(10)
O(8)-C(19)	1.216(10)	C(19)-C(20)	1.518(13)
O(9)-C(21)	1.288(10)	O(10)-C(21)	1.232(10)
C(21)-C(22)	1.509(12)	O(11)-C(23)	1.330(11)
O(12)-C(23)	1.198(11)	C(23)-C(24)	1.531(14)
O(13)-C(25)	1.294(11)	O(14)-C(25)	1.238(11)
C(25)-C(26)	1.518(13)	O(15)-C(27)	1.311(9)
O(16)-C(27)	1.201(11)	C(27)-C(28)	1.519(13)
C(29)-C(31)	1.520(14)	C(29)-C(32)	1.542(12)
C(29)-C(30)	1.556(12)	C(33)-C(34)	1.522(12)
C(33)-C(36)	1.534(12)	C(33)-C(35)	1.544(11)
C(37)-C(38)	1.539(12)	C(37)-C(39)	1.550(11)
C(37)-C(40)	1.554(11)	C(41)-C(44)	1.531(12)
C(41)-C(43)	1.540(12)	C(41)-C(42)	1.567(12)
C(45)-C(48)	1.537(12)	C(45)-C(47)	1.545(11)
C(45)-C(46)	1.564(12)	C(49)-C(51)	1.531(12)
C(49)-C(50)	1.531(13)	C(49)-C(52)	1.551(13)
C(53)-C(56)	1.523(12)	C(53)-C(54)	1.531(12)
C(53)-C(55)	1.542(11)	C(57)-C(58)	1.520(12)
C(57)-C(60)	1.540(13)	C(57)-C(59)	1.549(13)
C(61)-C(64)	1.527(12)	C(61)-C(62)	1.531(12)
C(61)-C(63)	1.538(12)	C(65)-C(67)	1.516(12)
C(65)-C(66)	1.531(11)	C(65)-C(68)	1.577(11)
C(69)-C(71)	1.501(13)	C(69)-C(72)	1.543(13)
C(69)-C(70)	1.558(13)	C(73)-C(74)	1.548(11)
C(73)-C(75)	1.551(12)	C(73)-C(76)	1.560(12)
C(77)-C(80)	1.523(13)	C(77)-C(79)	1.555(12)
C(77)-C(78)	1.561(13)	C(81)-C(82)	1.525(12)
C(81)-C(84)	1.538(12)	C(81)-C(83)	1.556(11)
C(85)-C(87)	1.529(12)	C(85)-C(86)	1.529(11)

C(85)-C(88)	1.563(11)	C(89)-C(91)	1.524(11)
C(89)-C(92)	1.540(11)	C(89)-C(90)	1.544(11)
C(93)-Cl(2)	1.732(9)	C(93)-Cl(1)	1.751(9)
C(94)-Cl(3)	1.738(9)	C(94)-Cl(4)	1.743(9)
C(95)-Cl(6)	1.732(10)	C(95)-Cl(5)	1.735(10)
C(96)-Cl(8)	1.725(10)	C(96)-Cl(7)	1.738(10)
C(97)-Cl(10)	1.760(10)	C(97)-Cl(9)	1.772(12)
C(98)-Cl(12)	1.733(10)	C(98)-Cl(11)	1.742(10)
C(99)-Cl(14)	1.722(10)	C(99)-Cl(13)	1.725(10)
C(100)-Cl(15)	1.764(12)	C(100)-Cl(16)	1.772(11)
C(101)-Cl(18)	1.735(13)	C(101)-Cl(17)	1.763(14)
C(102)-Cl(20)	1.753(13)	C(102)-Cl(19)	1.753(13)
C(103)-Cl(22)	1.731(15)	C(103)-Cl(21)	1.764(15)

O(1)-Pd(1)-O(3)	176.5(2)	O(1)-Pd(1)-P(1)	89.34(16)
O(3)-Pd(1)-P(1)	88.71(16)	O(1)-Pd(1)-P(8)	91.37(16)
O(3)-Pd(1)-P(8)	89.87(16)	P(1)-Pd(1)-P(8)	166.66(8)
O(7)-Pd(2)-O(5)	176.5(2)	O(7)-Pd(2)-P(3)	89.23(17)
O(5)-Pd(2)-P(3)	91.17(17)	O(7)-Pd(2)-P(2)	89.90(17)
O(5)-Pd(2)-P(2)	88.91(17)	P(3)-Pd(2)-P(2)	166.58(7)
O(11)-Pd(3)-O(9)	177.3(2)	O(11)-Pd(3)-P(5)	89.53(18)
O(9)-Pd(3)-P(5)	88.60(16)	O(11)-Pd(3)-P(4)	90.27(18)
O(9)-Pd(3)-P(4)	90.98(17)	P(5)-Pd(3)-P(4)	163.71(8)
O(15)-Pd(4)-O(13)	177.5(2)	O(15)-Pd(4)-P(6)	89.39(17)
O(13)-Pd(4)-P(6)	90.34(17)	O(15)-Pd(4)-P(7)	90.17(17)
O(13)-Pd(4)-P(7)	89.52(17)	P(6)-Pd(4)-P(7)	166.55(8)
C(1)-P(1)-C(29)	102.3(4)	C(1)-P(1)-C(33)	105.7(4)
C(29)-P(1)-C(33)	111.3(4)	C(1)-P(1)-Pd(1)	110.9(3)
C(29)-P(1)-Pd(1)	116.0(3)	C(33)-P(1)-Pd(1)	110.0(3)
C(3)-P(2)-C(41)	101.9(4)	C(3)-P(2)-C(37)	104.9(3)
C(41)-P(2)-C(37)	110.5(4)	C(3)-P(2)-Pd(2)	110.2(3)
C(41)-P(2)-Pd(2)	118.2(3)	C(37)-P(2)-Pd(2)	110.1(3)
C(4)-P(3)-C(49)	101.8(4)	C(4)-P(3)-C(45)	105.1(4)
C(49)-P(3)-C(45)	110.7(4)	C(4)-P(3)-Pd(2)	111.0(3)
C(49)-P(3)-Pd(2)	117.4(3)	C(45)-P(3)-Pd(2)	109.8(3)
C(6)-P(4)-C(53)	105.7(4)	C(6)-P(4)-C(57)	101.7(4)
C(53)-P(4)-C(57)	110.7(4)	C(6)-P(4)-Pd(3)	110.7(3)
C(53)-P(4)-Pd(3)	108.9(3)	C(57)-P(4)-Pd(3)	118.3(3)
C(7)-P(5)-C(65)	105.4(4)	C(7)-P(5)-C(61)	101.3(4)
C(65)-P(5)-C(61)	111.8(4)	C(7)-P(5)-Pd(3)	111.7(3)
C(65)-P(5)-Pd(3)	108.8(3)	C(61)-P(5)-Pd(3)	117.0(3)
C(9)-P(6)-C(73)	105.9(4)	C(9)-P(6)-C(69)	101.7(4)
C(73)-P(6)-C(69)	110.1(4)	C(9)-P(6)-Pd(4)	109.5(3)
C(73)-P(6)-Pd(4)	111.0(3)	C(69)-P(6)-Pd(4)	117.6(3)
C(10)-P(7)-C(77)	101.8(4)	C(10)-P(7)-C(81)	105.4(4)
C(77)-P(7)-C(81)	110.1(4)	C(10)-P(7)-Pd(4)	110.4(3)
C(77)-P(7)-Pd(4)	118.2(3)	C(81)-P(7)-Pd(4)	110.0(3)
C(12)-P(8)-C(89)	104.6(4)	C(12)-P(8)-C(85)	102.5(4)
C(89)-P(8)-C(85)	110.7(4)	C(12)-P(8)-Pd(1)	111.1(3)
C(89)-P(8)-Pd(1)	107.7(3)	C(85)-P(8)-Pd(1)	119.1(3)
C(2)-C(1)-P(1)	118.7(6)	C(3)-C(2)-C(1)	109.2(6)
C(2)-C(3)-P(2)	118.3(6)	C(5)-C(4)-P(3)	119.2(5)
C(6)-C(5)-C(4)	109.8(6)	C(5)-C(6)-P(4)	118.6(5)
C(8)-C(7)-P(5)	119.2(5)	C(7)-C(8)-C(9)	109.7(6)
C(8)-C(9)-P(6)	118.3(5)	C(11)-C(10)-P(7)	118.9(5)
C(12)-C(11)-C(10)	109.9(6)	C(11)-C(12)-P(8)	118.5(5)
C(13)-O(1)-Pd(1)	117.2(5)	O(2)-C(13)-O(1)	126.6(8)
O(2)-C(13)-C(14)	118.8(8)	O(1)-C(13)-C(14)	114.6(8)
C(15)-O(3)-Pd(1)	118.3(5)	O(4)-C(15)-O(3)	125.0(8)
O(4)-C(15)-C(16)	121.6(7)	O(3)-C(15)-C(16)	113.4(8)
C(17)-O(5)-Pd(2)	117.8(5)	O(6)-C(17)-O(5)	123.9(9)
O(6)-C(17)-C(18)	119.7(9)	O(5)-C(17)-C(18)	116.4(8)

C(19)-O(7)-Pd(2)	116.3(5)	O(8)-C(19)-O(7)	125.9(8)
O(8)-C(19)-C(20)	120.6(8)	O(7)-C(19)-C(20)	113.2(8)
C(21)-O(9)-Pd(3)	116.9(6)	O(10)-C(21)-O(9)	124.7(8)
O(10)-C(21)-C(22)	120.9(8)	O(9)-C(21)-C(22)	114.4(8)
C(23)-O(11)-Pd(3)	117.0(6)	O(12)-C(23)-O(11)	126.2(9)
O(12)-C(23)-C(24)	121.6(9)	O(11)-C(23)-C(24)	112.2(9)
C(25)-O(13)-Pd(4)	117.5(6)	O(14)-C(25)-O(13)	124.4(8)
O(14)-C(25)-C(26)	121.0(9)	O(13)-C(25)-C(26)	114.6(8)
C(27)-O(15)-Pd(4)	114.4(5)	O(16)-C(27)-O(15)	125.7(8)
O(16)-C(27)-C(28)	120.9(8)	O(15)-C(27)-C(28)	113.3(8)
C(31)-C(29)-C(32)	108.9(8)	C(31)-C(29)-C(30)	107.3(8)
C(32)-C(29)-C(30)	108.2(7)	C(31)-C(29)-P(1)	109.1(6)
C(32)-C(29)-P(1)	113.8(6)	C(30)-C(29)-P(1)	109.3(6)
C(34)-C(33)-C(36)	107.7(7)	C(34)-C(33)-C(35)	109.3(7)
C(36)-C(33)-C(35)	107.5(7)	C(34)-C(33)-P(1)	108.1(6)
C(36)-C(33)-P(1)	112.6(6)	C(35)-C(33)-P(1)	111.4(6)
C(38)-C(37)-C(39)	110.5(7)	C(38)-C(37)-C(40)	108.9(7)
C(39)-C(37)-C(40)	107.1(7)	C(38)-C(37)-P(2)	112.5(6)
C(39)-C(37)-P(2)	106.6(5)	C(40)-C(37)-P(2)	111.1(5)
C(44)-C(41)-C(43)	108.5(8)	C(44)-C(41)-C(42)	109.5(7)
C(43)-C(41)-C(42)	106.9(7)	C(44)-C(41)-P(2)	114.8(6)
C(43)-C(41)-P(2)	107.5(6)	C(42)-C(41)-P(2)	109.3(6)
C(48)-C(45)-C(47)	109.7(7)	C(48)-C(45)-C(46)	109.0(7)
C(47)-C(45)-C(46)	107.2(7)	C(48)-C(45)-P(3)	113.2(6)
C(47)-C(45)-P(3)	106.3(5)	C(46)-C(45)-P(3)	111.2(6)
C(51)-C(49)-C(50)	107.8(8)	C(51)-C(49)-C(52)	107.3(8)
C(50)-C(49)-C(52)	109.7(8)	C(51)-C(49)-P(3)	108.3(6)
C(50)-C(49)-P(3)	111.7(6)	C(52)-C(49)-P(3)	111.9(6)
C(56)-C(53)-C(54)	108.6(7)	C(56)-C(53)-C(55)	108.2(7)
C(54)-C(53)-C(55)	108.3(7)	C(56)-C(53)-P(4)	112.8(6)
C(54)-C(53)-P(4)	106.3(6)	C(55)-C(53)-P(4)	112.5(6)
C(58)-C(57)-C(60)	108.8(8)	C(58)-C(57)-C(59)	108.9(8)
C(60)-C(57)-C(59)	108.5(8)	C(58)-C(57)-P(4)	110.0(6)
C(60)-C(57)-P(4)	113.8(6)	C(59)-C(57)-P(4)	106.6(6)
C(64)-C(61)-C(62)	107.9(7)	C(64)-C(61)-C(63)	107.7(7)
C(62)-C(61)-C(63)	110.4(7)	C(64)-C(61)-P(5)	108.1(6)
C(62)-C(61)-P(5)	109.2(6)	C(63)-C(61)-P(5)	113.4(6)
C(67)-C(65)-C(66)	107.6(7)	C(67)-C(65)-C(68)	108.5(7)
C(66)-C(65)-C(68)	108.7(7)	C(67)-C(65)-P(5)	107.8(6)
C(66)-C(65)-P(5)	112.4(6)	C(68)-C(65)-P(5)	111.6(6)
C(71)-C(69)-C(72)	109.0(8)	C(71)-C(69)-C(70)	107.4(8)
C(72)-C(69)-C(70)	108.9(8)	C(71)-C(69)-P(6)	108.0(6)
C(72)-C(69)-P(6)	113.8(6)	C(70)-C(69)-P(6)	109.4(6)
C(74)-C(73)-C(75)	106.4(7)	C(74)-C(73)-C(76)	107.9(7)
C(75)-C(73)-C(76)	107.7(7)	C(74)-C(73)-P(6)	113.6(6)
C(75)-C(73)-P(6)	106.3(6)	C(76)-C(73)-P(6)	114.5(6)
C(80)-C(77)-C(79)	107.1(7)	C(80)-C(77)-C(78)	108.1(7)
C(79)-C(77)-C(78)	108.0(8)	C(80)-C(77)-P(7)	110.2(6)
C(79)-C(77)-P(7)	108.2(6)	C(78)-C(77)-P(7)	114.9(6)
C(82)-C(81)-C(84)	108.8(7)	C(82)-C(81)-C(83)	109.2(7)
C(84)-C(81)-C(83)	108.4(7)	C(82)-C(81)-P(7)	113.0(6)
C(84)-C(81)-P(7)	111.4(6)	C(83)-C(81)-P(7)	105.9(5)
C(87)-C(85)-C(86)	107.9(7)	C(87)-C(85)-C(88)	107.7(7)
C(86)-C(85)-C(88)	109.1(7)	C(87)-C(85)-P(8)	107.8(6)
C(86)-C(85)-P(8)	111.0(6)	C(88)-C(85)-P(8)	113.1(6)
C(91)-C(89)-C(92)	107.6(7)	C(91)-C(89)-C(90)	108.7(7)
C(92)-C(89)-C(90)	109.3(6)	C(91)-C(89)-P(8)	107.2(5)
C(92)-C(89)-P(8)	110.5(6)	C(90)-C(89)-P(8)	113.3(5)
Cl(2)-C(93)-Cl(1)	111.3(6)	Cl(3)-C(94)-Cl(4)	113.1(5)
Cl(6)-C(95)-Cl(5)	113.6(6)	Cl(8)-C(96)-Cl(7)	112.8(7)
Cl(10)-C(97)-Cl(9)	108.9(6)	Cl(12)-C(98)-Cl(11)	113.0(6)
Cl(14)-C(99)-Cl(13)	111.5(6)	Cl(15)-C(100)-Cl(16)	107.3(8)

Cl(18)-C(101)-Cl(17)	109.8(12)	Cl(20)-C(102)-Cl(19)	107.3(10)
Cl(22)-C(103)-Cl(21)	101.3(15)		

Table 26D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (52).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	24.1(3)	12.5(3)	17.0(3)	0.1(2)	-0.3(3)	-2.5(3)
Pd(2)	26.7(3)	10.9(3)	19.0(3)	-0.2(2)	-1.6(3)	1.2(3)
Pd(3)	23.2(3)	17.6(3)	22.4(3)	2.1(3)	-1.5(3)	0.4(3)
Pd(4)	23.1(3)	14.9(3)	22.8(3)	3.4(3)	3.1(3)	2.0(3)
P(1)	30.5(13)	15.2(11)	18.4(11)	1.6(8)	-3.6(9)	-4.4(9)
P(2)	25.7(12)	15.1(11)	18.3(10)	-2.7(8)	-0.3(9)	0.8(9)
P(3)	24.7(11)	11.6(10)	22.1(11)	3.5(9)	-2.9(9)	-1.6(8)
P(4)	26.5(12)	18.9(12)	21.8(11)	-1.1(9)	-3.4(9)	2.1(9)
P(5)	21.1(11)	19.8(11)	22.4(12)	3.0(8)	1.7(8)	-0.7(9)
P(6)	23.7(12)	20.1(12)	22.0(11)	6.4(9)	1.6(9)	0.6(9)
P(7)	26.0(12)	14.6(11)	20.1(11)	1.4(8)	5.3(9)	0.1(9)
P(8)	22.7(10)	10.6(9)	19.3(10)	1.9(8)	1.6(9)	-1.9(8)
C(1)	36(5)	12(4)	17(4)	4(3)	-10(4)	-1(4)
C(2)	23(4)	13(4)	17(4)	-2(3)	-5(3)	3(3)
C(3)	34(5)	13(4)	20(4)	-3(3)	-1(4)	-4(3)
C(4)	28(4)	12(4)	29(5)	5(3)	-2(4)	-7(3)
C(5)	37(5)	16(4)	17(4)	-6(3)	2(3)	4(4)
C(6)	31(5)	18(4)	18(4)	-4(3)	-2(4)	-1(4)
C(7)	22(4)	18(4)	25(5)	4(3)	-3(3)	2(3)
C(8)	20(4)	16(4)	31(5)	5(4)	-5(4)	2(3)
C(9)	23(4)	10(4)	33(5)	1(4)	1(4)	-4(3)
C(10)	28(5)	10(4)	29(5)	-5(3)	2(4)	-3(3)
C(11)	19(4)	11(4)	25(4)	-1(3)	7(3)	-5(3)
C(12)	27(4)	16(4)	22(4)	1(4)	2(4)	-3(3)
O(1)	23(3)	18(3)	23(3)	0(2)	2(3)	-2(2)
O(2)	29(4)	36(4)	40(4)	9(3)	-3(3)	0(3)
C(13)	33(5)	16(4)	28(5)	10(4)	1(4)	2(4)
C(14)	43(6)	33(6)	42(6)	0(5)	11(5)	11(5)
O(3)	33(3)	19(3)	15(3)	-1(2)	0(2)	-9(3)
O(4)	37(4)	27(4)	36(4)	-9(3)	1(3)	-15(3)
C(15)	35(5)	13(4)	18(4)	-8(3)	-13(4)	-1(4)
C(16)	51(6)	41(6)	24(5)	-21(4)	9(4)	-9(5)
O(5)	41(4)	8(3)	21(3)	-4(2)	2(3)	1(2)
O(6)	54(5)	17(3)	48(4)	-7(3)	-9(3)	6(3)
C(17)	25(5)	27(5)	41(6)	-4(4)	1(4)	4(4)
C(18)	48(6)	33(6)	30(5)	-20(4)	-3(5)	-2(5)
O(7)	28(3)	23(3)	25(3)	2(2)	-4(3)	-2(3)
O(8)	42(4)	34(4)	38(4)	-1(3)	-3(3)	15(3)
C(19)	28(5)	20(5)	31(5)	8(4)	-6(4)	-1(4)
C(20)	47(6)	43(6)	29(5)	1(4)	-10(4)	14(5)
O(9)	33(4)	29(4)	21(3)	3(3)	2(3)	6(3)
O(10)	35(4)	27(4)	53(5)	4(3)	-8(3)	3(3)
C(21)	22(5)	26(5)	27(5)	-7(4)	-12(4)	11(4)
C(22)	51(6)	32(6)	31(5)	8(4)	-14(5)	0(5)
O(11)	33(3)	22(3)	31(3)	5(3)	-3(3)	-8(3)
O(12)	42(4)	36(4)	49(4)	0(3)	-19(4)	-10(3)
C(23)	39(5)	28(5)	43(6)	-6(5)	1(5)	0(4)
C(24)	69(8)	29(6)	52(7)	17(5)	-8(6)	4(5)
O(13)	24(3)	23(3)	28(3)	-1(2)	10(2)	2(3)
O(14)	53(5)	40(4)	77(6)	17(4)	15(4)	29(4)
C(25)	31(5)	38(6)	25(5)	-1(4)	3(4)	1(4)

C(26)	34(6)	43(6)	59(7)	8(5)	23(5)	3(5)
O(15)	30(3)	18(3)	28(3)	8(2)	1(3)	-8(2)
O(16)	71(5)	10(3)	63(5)	7(3)	14(4)	8(3)
C(27)	42(5)	12(4)	28(5)	12(4)	-5(4)	-7(4)
C(28)	58(7)	40(6)	37(6)	14(5)	-1(5)	-13(5)
C(29)	40(6)	19(5)	22(5)	1(3)	-23(4)	-6(4)
C(30)	52(6)	25(5)	36(6)	-3(4)	-29(5)	-12(5)
C(31)	41(6)	37(6)	40(6)	1(5)	-17(5)	-3(5)
C(32)	74(8)	24(5)	36(6)	4(4)	-25(5)	-11(5)
C(33)	46(6)	11(4)	24(5)	4(3)	8(4)	3(4)
C(34)	32(5)	18(5)	32(5)	3(4)	8(4)	1(4)
C(35)	54(7)	16(5)	34(5)	5(4)	3(5)	-10(4)
C(36)	51(6)	17(5)	27(5)	0(4)	7(4)	-10(4)
C(37)	27(5)	15(4)	21(4)	-7(3)	-1(4)	-7(3)
C(38)	32(5)	39(6)	22(5)	4(4)	-1(4)	-3(4)
C(39)	27(5)	13(4)	26(4)	2(3)	0(3)	4(3)
C(40)	42(6)	25(5)	24(5)	4(4)	-3(4)	-1(4)
C(41)	27(5)	22(4)	26(5)	-9(4)	2(4)	-8(4)
C(42)	54(7)	19(5)	42(6)	-17(4)	7(5)	-2(5)
C(43)	41(6)	33(6)	41(6)	-11(4)	-4(5)	23(4)
C(44)	48(7)	42(6)	37(6)	-5(5)	17(5)	-3(5)
C(45)	29(5)	16(4)	21(4)	3(3)	-4(4)	3(4)
C(46)	47(6)	25(5)	27(5)	1(4)	2(4)	-5(4)
C(47)	32(5)	14(4)	28(5)	-3(3)	1(4)	-2(4)
C(48)	37(5)	25(5)	25(5)	1(4)	0(4)	-7(4)
C(49)	46(6)	8(4)	31(5)	4(4)	-2(4)	0(4)
C(50)	51(6)	21(5)	41(6)	15(4)	-14(5)	10(4)
C(51)	55(7)	19(5)	41(6)	4(4)	-2(5)	-2(4)
C(52)	61(7)	23(5)	46(6)	18(4)	9(5)	-9(5)
C(53)	28(5)	30(5)	20(4)	2(4)	-5(4)	-1(4)
C(54)	23(5)	26(5)	36(5)	-6(4)	4(4)	-1(4)
C(55)	42(6)	26(5)	22(5)	8(4)	1(4)	10(4)
C(56)	32(5)	31(5)	24(5)	1(4)	6(4)	13(4)
C(57)	28(5)	27(5)	25(5)	-8(4)	-9(4)	2(4)
C(58)	40(6)	36(6)	36(6)	1(4)	-16(5)	6(4)
C(59)	37(6)	31(6)	48(6)	-5(5)	-11(5)	-9(4)
C(60)	39(6)	46(7)	45(6)	-18(5)	-12(5)	5(5)
C(61)	24(5)	31(5)	28(5)	-1(4)	0(4)	-10(4)
C(62)	29(5)	18(5)	46(6)	7(4)	6(4)	-1(4)
C(63)	33(5)	36(6)	34(5)	10(4)	9(4)	8(4)
C(64)	18(4)	39(5)	44(6)	9(5)	7(4)	1(4)
C(65)	32(5)	11(4)	27(5)	4(3)	-4(4)	-6(4)
C(66)	39(6)	28(5)	25(5)	8(4)	-3(4)	-5(4)
C(67)	26(5)	23(5)	28(5)	7(4)	-4(4)	-6(4)
C(68)	41(5)	21(5)	26(5)	-8(4)	2(4)	-8(4)
C(69)	29(5)	18(5)	44(6)	15(4)	-7(4)	-5(4)
C(70)	48(7)	23(5)	87(9)	36(6)	-3(6)	1(5)
C(71)	43(6)	29(5)	45(6)	12(5)	0(5)	16(4)
C(72)	50(7)	44(6)	42(6)	14(5)	-14(5)	3(5)
C(73)	28(5)	25(5)	21(4)	2(3)	-1(4)	-6(4)
C(74)	27(5)	38(5)	23(5)	7(4)	1(4)	-8(4)
C(75)	29(5)	25(5)	27(5)	1(4)	7(4)	1(4)
C(76)	47(6)	40(6)	23(5)	3(4)	-10(4)	-1(5)
C(77)	35(5)	15(4)	31(5)	1(4)	8(4)	7(4)
C(78)	49(6)	34(6)	29(5)	-15(4)	8(4)	-7(5)
C(79)	68(8)	18(5)	37(6)	3(4)	15(5)	0(5)
C(80)	43(6)	31(6)	36(6)	-7(4)	10(5)	13(4)
C(81)	42(6)	16(4)	18(4)	4(3)	0(4)	-2(4)
C(82)	44(6)	17(5)	28(5)	2(4)	-2(4)	-1(4)
C(83)	33(5)	10(4)	34(5)	-4(3)	5(4)	0(4)
C(84)	38(6)	32(5)	30(5)	8(4)	10(4)	-3(4)
C(85)	23(4)	25(5)	24(4)	12(4)	-1(4)	-7(3)

C(86)	26(5)	17(4)	46(6)	3(4)	14(4)	-1(4)
C(87)	33(5)	27(5)	38(6)	2(4)	5(4)	-6(4)
C(88)	28(5)	26(5)	31(5)	10(4)	1(4)	3(4)
C(89)	30(5)	20(4)	15(4)	-1(3)	-4(3)	1(4)
C(90)	26(4)	17(4)	20(4)	0(3)	3(4)	1(3)
C(91)	25(4)	17(4)	32(5)	0(4)	-4(4)	-12(3)
C(92)	41(6)	21(5)	21(4)	-1(4)	6(4)	-4(4)
C(93)	54(8)	56(8)	65(8)	3(6)	-1(6)	-4(6)
Cl(1)	105(3)	108(3)	87(3)	-8(2)	37(3)	.17(3)
Cl(2)	47.2(18)	95(3)	97(3)	0(2)	0.1(19)	12.8(17)
C(94)	46(7)	36(6)	56(7)	11(5)	1(5)	0(5)
Cl(3)	91(3)	54(2)	76(2)	-16.5(17)	2.8(19)	-26.1(18)
Cl(4)	99(3)	70(2)	73(2)	-1.9(18)	24(2)	-8(2)
C(95)	39(7)	106(12)	111(12)	-44(10)	-22(7)	-27(7)
Cl(5)	57(2)	144(4)	120(4)	9(3)	-23(2)	4(2)
Cl(6)	124(4)	96(3)	163(5)	-9(3)	2(4)	-62(3)
C(96)	39(7)	87(10)	71(9)	-13(7)	-2(6)	9(6)
Cl(7)	81(3)	77(3)	161(4)	23(3)	17(3)	23(2)
Cl(8)	80(3)	154(4)	75(3)	5(3)	-19(2)	30(3)
C(97)	210(2)	38(8)	55(9)	5(6)	-40(11)	-27(10)
Cl(9)	230(7)	81(3)	115(4)	14(3)	93(4)	65(4)
Cl(10)	85(2)	58(2)	62(2)	12.1(16)	7.2(17)	-11.0(18)
C(98)	140(14)	45(7)	59(8)	0(6)	19(9)	31(8)
Cl(11)	222(6)	54(2)	71(3)	11.2(19)	9(3)	53(3)
Cl(12)	104(3)	46.9(18)	103(3)	-11(2)	9(2)	29.2(18)
C(99)	117(13)	88(11)	58(9)	-10(8)	-1(8)	57(9)
Cl(13)	120(4)	104(3)	67(2)	4(2)	22(2)	-8(3)
Cl(14)	66(2)	104(3)	87(3)	24(2)	-13(2)	-3.2(19)
C(100)	148(18)	74(12)	220(2)	-76(15)	17(17)	20(11)
Cl(15)	251(9)	169(7)	249(9)	70(7)	-79(8)	-5(6)
Cl(16)	143(5)	87(4)	239(7)	-35(4)	-32(5)	4(3)
C(101)	330(5)	140(3)	610(9)	-130(4)	120(6)	-150(3)
Cl(17)	210(14)	670(3)	470(3)	170(3)	70(15)	65(17)
Cl(18)	260(11)	170(8)	434(17)	37(10)	-102(12)	-83(7)
C(102)	160(2)	84(15)	320(4)	-40(19)	60(2)	35(14)
Cl(19)	334(14)	222(10)	213(10)	-29(8)	47(9)	-36(9)
Cl(20)	202(7)	93(4)	249(8)	-21(4)	119(6)	-8(4)

Table 26E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (52).

	x	y	z	U
H(1A)	4470	8310	315	26
H(1B)	4278	7859	863	26
H(2A)	4846	7746	1408	21
H(2B)	4984	8332	910	21
H(3A)	4434	8506	1848	27
H(3B)	4507	9071	1293	27
H(4A)	6447	10263	1133	27
H(4B)	6215	10473	1749	27
H(5A)	6172	9221	1990	28
H(5B)	6474	9115	1458	28
H(6A)	6527	9915	2638	27
H(6B)	6816	9951	2082	27
H(7A)	7474	6266	1016	26
H(7B)	7562	6539	1735	26
H(8A)	6890	6149	1269	27
H(8B)	6939	6551	1953	27
H(9A)	7267	5640	2387	27
H(9B)	7297	5269	1690	27
H(10A)	5521	4317	97	27
H(10B)	5646	3938	751	27
H(11A)	5624	5089	1281	22
H(11B)	5420	5350	641	22
H(12A)	5196	4279	1518	26
H(12B)	5010	4408	830	26
H(14A)	3848	7552	2014	59
H(14B)	4140	7258	2498	59
H(14C)	3775	6868	2441	59
H(16A)	5023	4388	-587	58
H(16B)	5055	5142	-916	58
H(16C)	4726	4661	-1071	58
H(18A)	6027	10869	3262	56
H(18B)	5924	10077	3416	56
H(18C)	5669	10696	3625	56
H(20A)	4620	10366	-316	60
H(20B)	4477	9639	-42	60
H(20C)	4846	9672	-401	60
H(22A)	7855	6872	3543	57
H(22B)	7664	6386	3017	57
H(22C)	7443	6770	3575	57
H(24A)	7195	10462	799	75
H(24B)	7094	9810	348	75
H(24C)	7486	10084	368	75
H(26A)	7482	5333	248	68
H(26B)	7273	5017	-361	68
H(26C)	7573	4570	-17	68
H(28A)	5550	3482	2154	67
H(28B)	5822	3506	2747	67
H(28C)	5778	2809	2324	67
H(30A)	4155	6035	-440	56
H(30B)	4392	6318	-1026	56
H(30C)	3979	6390	-1068	56
H(31A)	3855	7702	116	59

H(31B)	3867	6901	332	59
H(31C)	3669	7124	-326	59
H(32A)	4012	7666	-1241	68
H(32B)	4426	7606	-1243	68
H(32C)	4238	8148	-763	68
H(34A)	5294	6602	253	41
H(34B)	5280	7367	563	41
H(34C)	5524	7214	-56	41
H(35A)	5032	8358	-127	52
H(35B)	4850	8180	-812	52
H(35C)	5262	8124	-743	52
H(36A)	5268	6917	-1122	48
H(36B)	4857	6964	-1235	48
H(36C)	5017	6346	-803	48
H(38A)	4968	7530	3089	47
H(38B)	4763	7706	2426	47
H(38C)	4656	8081	3098	47
H(39A)	5606	8573	2294	33
H(39B)	5364	8050	1889	33
H(39C)	5528	7810	2574	33
H(40A)	5038	8950	3617	46
H(40B)	5387	9203	3266	46
H(40C)	5369	8447	3596	46
H(42A)	4645	10557	3326	58
H(42B)	4924	10625	2746	58
H(42C)	4979	10059	3313	58
H(43A)	4201	9857	1943	57
H(43B)	4529	10337	1778	57
H(43C)	4267	10557	2351	57
H(44A)	4168	9657	3234	64
H(44B)	4483	9166	3456	64
H(44C)	4250	8957	2836	64
H(46A)	5763	9053	-647	50
H(46B)	5778	9882	-565	50
H(46C)	5476	9445	-217	50
H(47A)	5605	8684	740	37
H(47B)	5995	8584	995	37
H(47C)	5882	8278	296	37
H(48A)	6365	8966	-274	43
H(48B)	6481	9205	446	43
H(48C)	6407	9777	-108	43
H(50A)	5338	11154	492	56
H(50B)	5463	10740	-147	56
H(50C)	5539	11556	-80	56
H(51A)	6167	11485	1177	57
H(51B)	5770	11416	1398	57
H(51C)	5878	11969	846	57
H(52A)	6204	11517	-111	65
H(52B)	6107	10771	-410	65
H(52C)	6380	10828	180	65
H(54A)	6229	7573	2705	42
H(54B)	6616	7540	2422	42
H(54C)	6352	8122	2162	42
H(55A)	6536	7512	3743	45
H(55B)	6710	8194	4053	45
H(55C)	6922	7728	3540	45
H(56A)	6115	8975	2971	44
H(56B)	6311	9106	3653	44
H(56C)	6073	8430	3560	44
H(58A)	7544	9224	3986	56
H(58B)	7564	8781	3321	56
H(58C)	7297	8563	3886	56

H(59A)	7484	10255	3310	58
H(59B)	7142	10387	2883	58
H(59C)	7436	9870	2619	58
H(60A)	6802	9331	4162	66
H(60B)	6715	9995	3717	66
H(60C)	7042	10010	4202	66
H(62A)	8137	8387	418	47
H(62B)	7877	8604	994	47
H(62C)	7735	8505	262	47
H(63A)	7751	7309	-251	51
H(63B)	7824	6640	197	51
H(63C)	8137	7141	-9	51
H(64A)	8325	7405	1096	51
H(64B)	8055	6824	1335	51
H(64C)	8049	7584	1658	51
H(66A)	6902	8074	-399	46
H(66B)	7313	8022	-296	46
H(66C)	7087	8523	163	46
H(67A)	6696	8001	1021	38
H(67B)	6630	7177	1007	38
H(67C)	6508	7650	403	38
H(68A)	6972	6391	322	44
H(68B)	7254	6690	-180	44
H(68C)	6849	6799	-322	44
H(70A)	6685	3417	2404	79
H(70B)	6542	3814	3040	79
H(70C)	6864	3290	3103	79
H(71A)	7423	3610	2516	58
H(71B)	7455	4348	2155	58
H(71C)	7200	3764	1869	58
H(72A)	7295	4131	3544	68
H(72B)	6966	4631	3641	68
H(72C)	7304	4911	3268	68
H(74A)	6392	4749	3500	44
H(74B)	6115	4697	2916	44
H(74C)	6090	5319	3437	44
H(75A)	6092	5577	2057	41
H(75B)	6383	6167	1989	41
H(75C)	6102	6212	2566	41
H(76A)	6514	6258	3466	55
H(76B)	6818	6318	2935	55
H(76C)	6839	5740	3499	55
H(78A)	6039	3434	-1252	55
H(78B)	6087	4261	-1226	55
H(78C)	5748	3909	-915	55
H(79A)	6147	2701	-238	61
H(79B)	5810	3096	34	61
H(79C)	6158	3077	463	61
H(80A)	6696	3591	-41	55
H(80B)	6668	4143	-628	55
H(80C)	6612	3331	-770	55
H(82A)	5798	5967	-803	45
H(82B)	5583	5487	-304	45
H(82C)	5767	5147	-931	45
H(83A)	6146	6422	132	39
H(83B)	6362	5899	588	39
H(83C)	5948	5930	643	39
H(84A)	6403	5120	-1018	50
H(84B)	6642	5325	-405	50
H(84C)	6449	5920	-817	50
H(86A)	4068	5293	1827	45
H(86B)	4237	5362	2542	45

H(86C)	3999	4705	2369	45
H(87A)	4145	3950	1522	49
H(87B)	4542	3754	1382	49
H(87C)	4364	4388	998	49
H(88A)	4706	4497	2897	43
H(88B)	4838	3924	2385	43
H(88C)	4456	3867	2690	43
H(90A)	5510	5017	2256	32
H(90B)	5229	4803	2796	32
H(90C)	5481	5452	2924	32
H(91A)	5432	6504	2277	37
H(91B)	5108	6641	1801	37
H(91C)	5412	6124	1579	37
H(92A)	4976	6270	3101	42
H(92B)	4730	5601	3035	42
H(92C)	4662	6271	2587	42
H(93A)	6891	9789	-2587	70
H(93B)	6991	8995	-2436	70
H(94A)	6183	7806	-2268	55
H(94B)	6561	7729	-1954	55
H(95A)	3875	5117	86	102
H(95B)	3684	5062	780	102
H(96A)	8017	4081	1794	79
H(96B)	8427	4209	1760	79
H(97A)	5733	7103	4908	121
H(97B)	5611	6313	4795	121
H(98A)	4824	8291	-3021	98
H(98B)	5185	8439	-3382	98
H(99A)	5992	8895	6006	105
H(99B)	5624	8636	5737	105
H(10C)	7101	12693	1354	177
H(10D)	6689	12559	1325	177
H(10G)	2561	6778	499	435
H(10H)	2949	6487	414	435
H(10G)	6876	10337	6101	224
H(10H)	6849	11078	5738	224
H(10E)	7009	11050	-1369	310
H(10F)	6977	11628	-797	310

Table 27A. Crystal data, structure solution and refinement for (53).

Identification code	exti8
Chemical formula	$C_{24}H_{44}Cl_2P_2Pd$
Formula weight	571.83
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.1581(10) Å $\alpha = 90^\circ$
	b = 19.656(2) Å $\beta = 101.694(3)^\circ$
	c = 15.180(2) Å $\gamma = 90^\circ$
Volume	2675.8(5) $Å^3$
Z	4
Density (calculated)	1.419 g/cm^3
Absorption coefficient μ	1.022 mm^{-1}
F(000)	1192
Reflections for cell refinement	10708 (θ range 1.71 to 26.29°)
Crystal colour	yellow
Crystal size	0.42 × 0.28 × 0.08 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.72 to 26.42°
Index ranges	$-11 \le h \le 10$, $-24 \le k \le 23$, $-15 \le \ell \le 18$
Intensity decay	0%
Reflections collected	15154
Independent reflections	5351 (R_{int} = 0.0620)
Reflections with I>2σ(I)	4795
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.845 and 0.678
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0031, 7.2638
Data / restraints / parameters	5348 / 0 / 275
Final R indices [I>2σ(I)]	R1 = 0.0453, wR2 = 0.0923
R indices (all data)	R1 = 0.0556, wR2 = 0.0975
Goodness-of-fit on F^2	1.309
Extinction coefficient	0.00011(13)
Largest and mean shift/esd	0.000 and 0.000
Largest diff. peak and hole	0.503 and -1.042 $eÅ^{-3}$

The Crystal Structure of [o-$C_6H_4(CH_2PBu'_2)_2Pd(Cl)_2$] (53)

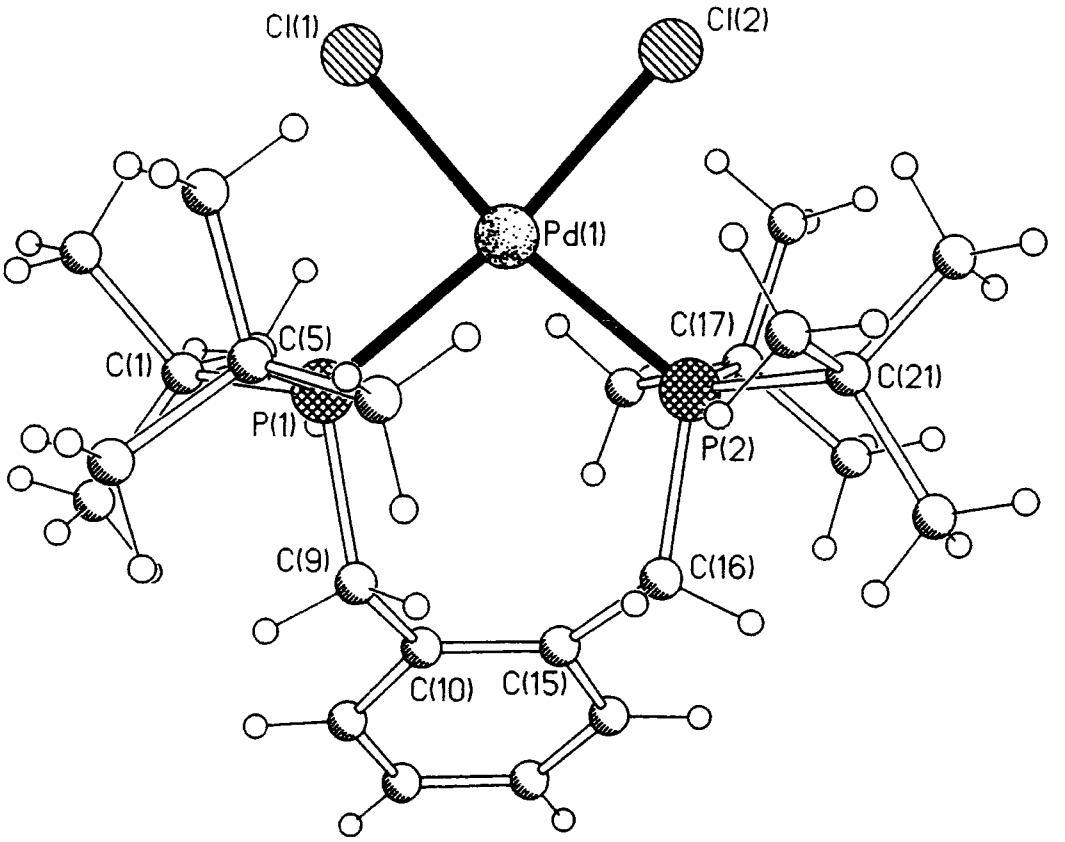


Table 27B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (53). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2989.9(3)	2651.68(15)	9834.3(2)	13.99(10)
Cl(1)	3683.1(11)	1989.6(5)	11150.9(6)	22.1(2)
Cl(2)	3893.3(12)	3562.7(5)	10804.7(7)	25.2(2)
P(1)	2875.1(11)	1672.3(5)	8961.9(7)	15.1(2)
P(2)	1829.1(11)	3439.2(5)	8796.7(7)	14.9(2)
C(1)	1948(5)	904(2)	9381(3)	24.1(9)
C(2)	562(5)	1178(3)	9700(4)	36.6(12)
C(3)	1418(6)	370(2)	8638(3)	37.6(12)
C(4)	2940(5)	512(2)	10153(3)	29.6(10)
C(5)	4881(4)	1482(2)	8890(3)	19.7(8)
C(6)	5906(5)	1405(3)	9822(3)	29.0(10)
C(7)	5027(5)	838(2)	8332(3)	29.1(10)
C(8)	5458(5)	2094(2)	8433(3)	31.0(10)
C(9)	2036(4)	1714(2)	7748(3)	18.0(8)
C(10)	416(4)	1921(2)	7432(3)	17.7(8)
C(11)	-662(5)	1439(2)	7089(3)	23.4(9)
C(12)	-2124(5)	1613(2)	6722(3)	25.2(9)
C(13)	-2526(5)	2287(2)	6656(3)	26.5(9)
C(14)	-1458(5)	2780(2)	6958(3)	25.3(9)
C(15)	9(4)	2608(2)	7362(3)	18.8(8)
C(16)	1136(4)	3176(2)	7619(3)	18.6(8)
C(17)	98(4)	3718(2)	9202(3)	20.5(8)
C(18)	-814(5)	3075(2)	9290(3)	27.7(10)
C(19)	-836(5)	4222(2)	8543(3)	27.7(10)
C(20)	429(5)	4044(2)	10141(3)	27.1(9)
C(21)	3027(4)	4200(2)	8577(3)	19.2(8)
C(22)	4623(5)	3930(2)	8632(3)	29.6(10)
C(23)	2503(5)	4514(2)	7637(3)	28.7(10)
C(24)	3070(5)	4784(2)	9256(3)	27.1(10)

Table 27C. Bond lengths (Å) and angles (°) for (53).

Pd(1)-P(2)	2.3084(10)	Pd(1)-P(1)	2.3269(10)
Pd(1)-Cl(2)	2.3594(10)	Pd(1)-Cl(1)	2.3615(10)
P(1)-C(9)	1.849(4)	P(1)-C(5)	1.899(4)
P(1)-C(1)	1.905(4)	P(2)-C(16)	1.846(4)
P(2)-C(17)	1.894(4)	P(2)-C(21)	1.924(4)
C(1)-C(4)	1.536(6)	C(1)-C(3)	1.544(6)
C(1)-C(2)	1.545(6)	C(5)-C(8)	1.535(6)
C(5)-C(6)	1.538(6)	C(5)-C(7)	1.544(6)
C(9)-C(10)	1.520(5)	C(10)-C(11)	1.390(6)
C(10)-C(15)	1.399(6)	C(11)-C(12)	1.384(6)
C(12)-C(13)	1.373(6)	C(13)-C(14)	1.387(6)
C(14)-C(15)	1.400(6)	C(15)-C(16)	1.517(5)
C(17)-C(20)	1.536(6)	C(17)-C(18)	1.536(6)
C(17)-C(19)	1.539(6)	C(21)-C(24)	1.538(6)
C(21)-C(23)	1.539(6)	C(21)-C(22)	1.541(5)
P(2)-Pd(1)-P(1)	101.83(4)	P(2)-Pd(1)-Cl(2)	88.38(4)
P(1)-Pd(1)-Cl(2)	162.34(4)	P(2)-Pd(1)-Cl(1)	162.69(4)
P(1)-Pd(1)-Cl(1)	89.95(4)	Cl(2)-Pd(1)-Cl(1)	83.67(4)
C(9)-P(1)-C(5)	99.4(2)	C(9)-P(1)-C(1)	104.1(2)
C(5)-P(1)-C(1)	111.4(2)	C(9)-P(1)-Pd(1)	119.52(13)
C(5)-P(1)-Pd(1)	105.24(13)	C(1)-P(1)-Pd(1)	115.99(14)
C(16)-P(2)-C(17)	104.5(2)	C(16)-P(2)-C(21)	98.4(2)
C(17)-P(2)-C(21)	112.1(2)	C(16)-P(2)-Pd(1)	119.58(13)
C(17)-P(2)-Pd(1)	105.83(13)	C(21)-P(2)-Pd(1)	116.09(13)
C(4)-C(1)-C(3)	105.4(4)	C(4)-C(1)-C(2)	109.4(4)
C(3)-C(1)-C(2)	108.0(4)	C(4)-C(1)-P(1)	114.7(3)
C(3)-C(1)-P(1)	113.0(3)	C(2)-C(1)-P(1)	106.1(3)
C(8)-C(5)-C(6)	106.9(4)	C(8)-C(5)-C(7)	108.6(4)
C(6)-C(5)-C(7)	108.6(3)	C(8)-C(5)-P(1)	107.3(3)
C(6)-C(5)-P(1)	112.6(3)	C(7)-C(5)-P(1)	112.7(3)
C(10)-C(9)-P(1)	120.6(3)	C(11)-C(10)-C(15)	118.1(4)
C(11)-C(10)-C(9)	120.6(4)	C(15)-C(10)-C(9)	120.7(3)
C(12)-C(11)-C(10)	122.5(4)	C(13)-C(12)-C(11)	119.4(4)
C(12)-C(13)-C(14)	119.3(4)	C(13)-C(14)-C(15)	121.7(4)
C(10)-C(15)-C(14)	118.9(4)	C(10)-C(15)-C(16)	122.3(3)
C(14)-C(15)-C(16)	118.5(4)	C(15)-C(16)-P(2)	122.5(3)
C(20)-C(17)-C(18)	105.7(3)	C(20)-C(17)-C(19)	108.3(3)
C(18)-C(17)-C(19)	110.2(3)	C(20)-C(17)-P(2)	113.7(3)
C(18)-C(17)-P(2)	107.2(3)	C(19)-C(17)-P(2)	111.6(3)
C(24)-C(21)-C(23)	106.5(3)	C(24)-C(21)-C(22)	109.0(3)
C(23)-C(21)-C(22)	107.6(3)	C(24)-C(21)-P(2)	113.7(3)
C(23)-C(21)-P(2)	113.0(3)	C(22)-C(21)-P(2)	106.9(3)

Table 27D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (53).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	12.91(14)	12.73(15)	16.6(2)	0.01(12)	3.71(10)	0.98(11)
Cl(1)	25.8(5)	20.9(5)	19.6(5)	3.6(4)	4.3(4)	-0.1(4)
Cl(2)	28.1(5)	18.7(5)	25.8(5)	-4.8(4)	-1.3(4)	0.8(4)
P(1)	13.9(5)	12.3(5)	19.1(5)	-0.1(4)	3.4(4)	0.7(4)
P(2)	13.5(5)	11.9(5)	19.8(5)	0.9(4)	4.6(4)	1.3(4)
C(1)	29(2)	15(2)	27(2)	4(2)	3(2)	-5(2)
C(2)	24(2)	33(3)	56(3)	9(2)	16(2)	-8(2)
C(3)	50(3)	19(2)	37(3)	3(2)	-6(2)	-14(2)
C(4)	37(3)	21(2)	31(2)	4(2)	6(2)	1(2)
C(5)	18(2)	18(2)	23(2)	0(2)	3(2)	7(2)
C(6)	19(2)	38(3)	28(2)	-1(2)	1(2)	6(2)
C(7)	29(2)	29(2)	30(2)	-5(2)	8(2)	12(2)
C(8)	20(2)	32(2)	44(3)	5(2)	12(2)	1(2)
C(9)	15(2)	17(2)	21(2)	-2(2)	5(2)	4(2)
C(10)	17(2)	19(2)	17(2)	-1(2)	2.3(15)	1(2)
C(11)	24(2)	19(2)	26(2)	1(2)	4(2)	2(2)
C(12)	21(2)	27(2)	27(2)	-3(2)	2(2)	-4(2)
C(13)	15(2)	35(2)	27(2)	-2(2)	-2(2)	2(2)
C(14)	22(2)	24(2)	28(2)	1(2)	0(2)	5(2)
C(15)	17(2)	21(2)	18(2)	0(2)	2.3(15)	-1(2)
C(16)	19(2)	19(2)	18(2)	0(2)	5(2)	-1(2)
C(17)	18(2)	17(2)	29(2)	0(2)	10(2)	1(2)
C(18)	24(2)	27(2)	36(3)	-1(2)	16(2)	-2(2)
C(19)	21(2)	25(2)	37(3)	1(2)	6(2)	9(2)
C(20)	24(2)	28(2)	32(2)	-5(2)	13(2)	3(2)
C(21)	16(2)	12(2)	30(2)	2(2)	6(2)	-0.1(15)
C(22)	21(2)	24(2)	47(3)	2(2)	14(2)	-1(2)
C(23)	37(3)	18(2)	33(2)	7(2)	10(2)	-6(2)
C(24)	26(2)	16(2)	38(3)	-2(2)	4(2)	-4(2)

Table 27E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (53).

	x	y	z	U
H(2A)	879(5)	1487(14)	10209(16)	55
H(2B)	4(22)	797(3)	9887(23)	55
H(2C)	-77(20)	1424(16)	9206(8)	55
H(3A)	2235(13)	265(14)	8331(16)	56
H(3B)	570(26)	553(7)	8202(13)	56
H(3C)	1113(38)	-45(7)	8909(4)	56
H(4A)	2336(9)	177(11)	10397(14)	44
H(4B)	3384(28)	831(3)	10628(10)	44
H(4C)	3733(22)	277(13)	9925(6)	44
H(6A)	5558(22)	1025(11)	10143(9)	44
H(6B)	5885(28)	1825(6)	10166(9)	44
H(6C)	6928(8)	1316(17)	9749(3)	44
H(7A)	4636(32)	445(4)	8607(12)	44
H(7B)	6080(6)	761(9)	8319(18)	44
H(7C)	4460(29)	899(7)	7717(6)	44
H(8A)	4887(24)	2137(10)	7816(8)	46
H(8B)	6515(11)	2027(8)	8422(20)	46
H(8C)	5341(33)	2509(3)	8769(13)	46
H(9A)	2647(4)	2033(2)	7471(3)	22
H(9B)	2154(4)	1258(2)	7492(3)	22
H(11)	-384(5)	973(2)	7107(3)	28
H(12)	-2841(5)	1269(2)	6518(3)	30
H(13)	-3525(5)	2414(2)	6406(3)	32
H(14)	-1729(5)	3246(2)	6889(3)	30
H(16A)	703(4)	3587(2)	7288(3)	22
H(16B)	2022(4)	3051(2)	7373(3)	22
H(18A)	-1075(30)	2847(9)	8704(6)	42
H(18B)	-1728(17)	3201(3)	9492(20)	42
H(18C)	-222(14)	2766(7)	9729(16)	42
H(19A)	-1070(29)	4020(7)	7940(5)	42
H(19B)	-269(14)	4643(6)	8525(16)	42
H(19C)	-1765(16)	4325(12)	8743(12)	42
H(20A)	1037(30)	4453(9)	10131(6)	41
H(20B)	972(31)	3719(6)	10577(5)	41
H(20C)	-511(5)	4168(15)	10314(9)	41
H(22A)	4611(7)	3573(12)	8180(15)	44
H(22B)	5001(14)	3742(15)	9233(8)	44
H(22C)	5270(9)	4303(4)	8519(22)	44
H(23A)	2634(34)	4183(6)	7177(3)	43
H(23B)	3094(25)	4922(10)	7582(8)	43
H(23C)	1447(11)	4638(15)	7554(9)	43
H(24A)	3365(34)	4605(3)	9869(3)	41
H(24B)	2080(10)	4991(10)	9179(14)	41
H(24C)	3793(26)	5127(8)	9153(14)	41

Table 28A. Crystal data, structure solution and refinement for (54).

Identification code	exti4
Chemical formula	$C_{44}H_{63}ClO_2P_2Pd$
Formula weight	827.73
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 10.2985(7) Å α = 90.228(2)°
	b = 11.3708(7) Å β = 96.288(2)°
	c = 19.5555(13) Å γ = 115.134(2)°
Volume	2057.4(2) Å^3
Z	2
Density (calculated)	1.336 g/cm^3
Absorption coefficient μ	0.629 mm^{-1}
F(000)	872
Reflections for cell refinement	8238 (θ range 1.98 to 26.35°)
Crystal colour	yellow
Crystal size	0.31 × 0.22 × 0.14 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.98 to 26.38°
Index ranges	$-9 \le h \le 12$, $-13 \le k \le 14$, $-24 \le \ell \le 23$
Reflections collected	11286
Independent reflections	7934 (R_{int} = 0.0333)
Reflections with I>2σ(I)	7144
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.875 and 0.583
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0334, 4.7085
Data / restraints / parameters	7931 / 0 / 465
Final R indices [I>2σ(I)]	R1 = 0.0437, wR2 = 0.0997
R indices (all data)	R1 = 0.0517, wR2 = 0.1093
Goodness-of-fit on F^2	1.164
Extinction coefficient	0.0024(4)
Largest and mean shift/esd	-0.001 and 0.000
Largest diff. peak and hole	0.922 and -1.057 eÅ^{-3}

The Crystal Structure of [o-$C_6H_4(CH_2PBu^t_2)_2Pd(COC_2H_5)(Cl)$].dba (54)

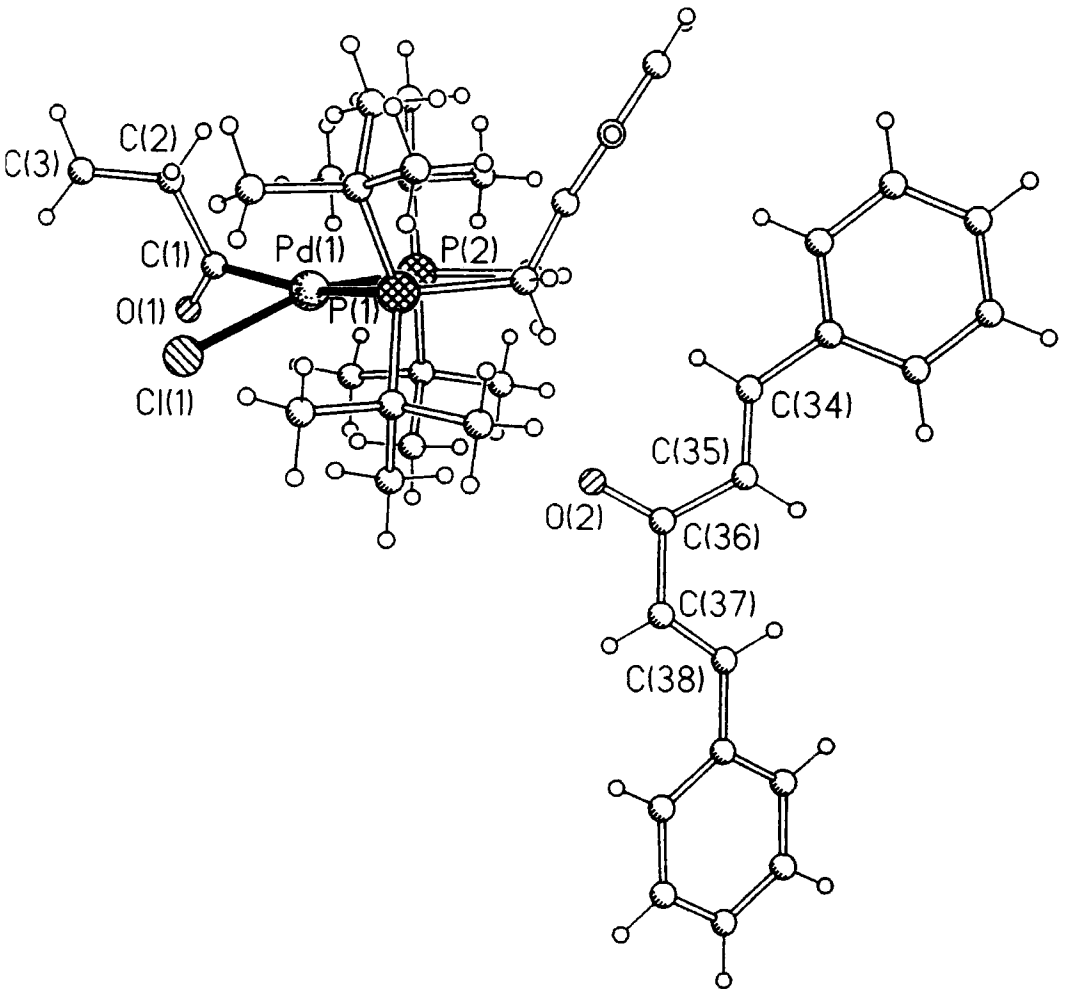


Table 28B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (54). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	-162.1(3)	-2136.6(2)	6651.87(13)	19.13(9)
Cl(1)	-2579.0(9)	-3057.2(9)	6974.5(5)	35.2(2)
C(1)	-1329(4)	-3305(3)	5822(2)	27.4(8)
C(2)	-1934(4)	-2547(4)	5340(2)	37.5(9)
C(3)	-3284(7)	-3360(6)	4892(4)	88(2)
O(1)	-1692(3)	-4453(3)	5723(2)	38.8(7)
P(1)	606.7(9)	-366.5(8)	7562.2(4)	18.7(2)
P(2)	2011.7(9)	-2058.4(8)	6387.4(4)	17.6(2)
C(4)	-33(4)	-884(3)	8439(2)	25.2(7)
C(5)	40(4)	-2200(3)	8536(2)	28.1(8)
C(6)	919(4)	52(4)	9050(2)	33.6(9)
C(7)	-1585(4)	-1067(4)	8472(2)	33.7(9)
C(8)	-31(4)	862(3)	7199(2)	25.1(7)
C(9)	-1683(4)	288(4)	7015(2)	34.6(9)
C(10)	467(4)	2094(4)	7675(2)	31.5(8)
C(11)	613(4)	1238(4)	6512(2)	30.6(8)
C(12)	2561(3)	616(3)	7859(2)	21.6(7)
C(13)	3611(3)	1275(3)	7347(2)	20.6(7)
C(14)	4203(4)	2634(3)	7351(2)	26.3(7)
C(15)	5256(4)	3336(3)	6941(2)	28.7(8)
C(16)	5776(4)	2674(4)	6527(2)	28.1(8)
C(17)	5229(4)	1339(3)	6540(2)	23.9(7)
C(18)	4115(3)	600(3)	6928(2)	18.7(6)
C(19)	3635(3)	-854(3)	6941(2)	20.3(7)
C(20)	2481(4)	-1742(3)	5477(2)	23.5(7)
C(21)	3983(4)	-1640(4)	5390(2)	32.3(8)
C(22)	2371(4)	-468(4)	5307(2)	28.8(8)
C(23)	1404(5)	-2801(4)	4946(2)	37.1(9)
C(24)	2131(4)	-3607(3)	6683(2)	23.3(7)
C(25)	1510(6)	-3876(5)	7362(2)	49.1(12)
C(26)	3663(5)	-3522(5)	6800(3)	48.0(12)
C(27)	1233(6)	-4762(4)	6178(3)	56.9(14)
C(28)	7550(4)	2761(4)	8308(2)	31.7(8)
C(29)	8665(4)	3985(4)	8307(2)	34.9(9)
C(30)	9744(4)	4438(4)	8856(2)	38.0(9)
C(31)	9719(5)	3653(4)	9403(2)	38.2(9)
C(32)	8594(4)	2429(4)	9405(2)	32.9(8)
C(33)	7483(4)	1963(4)	8857(2)	28.1(8)
C(34)	6235(4)	703(4)	8842(2)	29.6(8)
C(35)	5970(4)	-195(4)	9301(2)	27.0(7)
C(36)	4612(4)	-1392(4)	9231(2)	29.6(8)
O(2)	3617(3)	-1559(3)	8776(2)	48.5(8)
C(37)	4414(4)	-2404(4)	9729(2)	28.0(8)
C(38)	5476(4)	-2570(3)	10104(2)	26.5(7)
C(39)	5303(4)	-3600(3)	10580(2)	25.2(7)
C(40)	6498(4)	-3845(4)	10812(2)	31.3(8)
C(41)	6371(5)	-4811(4)	11260(2)	36.7(9)
C(42)	5055(5)	-5548(4)	11489(2)	37.2(9)
C(43)	3872(4)	-5309(4)	11269(2)	35.0(9)
C(44)	3984(4)	-4358(4)	10815(2)	29.5(8)

Table 28C. Bond lengths (Å) and angles (°) for (54).

Pd(1)-C(1)	2.010(4)	Pd(1)-P(2)	2.3177(8)
Pd(1)-Cl(1)	2.4135(9)	Pd(1)-P(1)	2.4812(9)
C(1)-O(1)	1.203(4)	C(1)-C(2)	1.535(5)
C(2)-C(3)	1.480(6)	P(1)-C(12)	1.861(3)
P(1)-C(8)	1.890(4)	P(1)-C(4)	1.910(3)
P(2)-C(19)	1.867(3)	P(2)-C(20)	1.892(3)
P(2)-C(24)	1.904(3)	C(4)-C(7)	1.530(5)
C(4)-C(6)	1.539(5)	C(4)-C(5)	1.541(5)
C(8)-C(10)	1.537(5)	C(8)-C(9)	1.540(5)
C(8)-C(11)	1.546(5)	C(12)-C(13)	1.512(4)
C(13)-C(14)	1.399(5)	C(13)-C(18)	1.400(5)
C(14)-C(15)	1.385(5)	C(15)-C(16)	1.392(5)
C(16)-C(17)	1.378(5)	C(17)-C(18)	1.404(4)
C(18)-C(19)	1.513(4)	C(20)-C(21)	1.530(5)
C(20)-C(22)	1.535(5)	C(20)-C(23)	1.536(5)
C(24)-C(25)	1.514(5)	C(24)-C(27)	1.520(5)
C(24)-C(26)	1.531(5)	C(28)-C(29)	1.378(6)
C(28)-C(33)	1.397(5)	C(29)-C(30)	1.380(6)
C(30)-C(31)	1.391(6)	C(31)-C(32)	1.382(6)
C(32)-C(33)	1.397(6)	C(33)-C(34)	1.460(5)
C(34)-C(35)	1.322(5)	C(35)-C(36)	1.472(5)
C(36)-O(2)	1.230(5)	C(36)-C(37)	1.473(5)
C(37)-C(38)	1.331(5)	C(38)-C(39)	1.461(5)
C(39)-C(44)	1.394(5)	C(39)-C(40)	1.403(5)
C(40)-C(41)	1.380(6)	C(41)-C(42)	1.382(6)
C(42)-C(43)	1.382(6)	C(43)-C(44)	1.377(5)
C(1)-Pd(1)-P(2)	94.10(10)	C(1)-Pd(1)-Cl(1)	77.42(10)
P(2)-Pd(1)-Cl(1)	158.37(3)	C(1)-Pd(1)-P(1)	158.56(11)
P(2)-Pd(1)-P(1)	103.08(3)	Cl(1)-Pd(1)-P(1)	90.40(3)
O(1)-C(1)-C(2)	121.8(4)	O(1)-C(1)-Pd(1)	129.0(3)
C(2)-C(1)-Pd(1)	108.6(3)	C(3)-C(2)-C(1)	114.9(4)
C(12)-P(1)-C(8)	104.1(2)	C(12)-P(1)-C(4)	98.3(2)
C(8)-P(1)-C(4)	111.4(2)	C(12)-P(1)-Pd(1)	120.22(11)
C(8)-P(1)-Pd(1)	106.16(12)	C(4)-P(1)-Pd(1)	116.01(11)
C(19)-P(2)-C(20)	104.53(15)	C(19)-P(2)-C(24)	98.4(2)
C(20)-P(2)-C(24)	110.8(2)	C(19)-P(2)-Pd(1)	114.16(10)
C(20)-P(2)-Pd(1)	119.20(12)	C(24)-P(2)-Pd(1)	107.84(11)
C(7)-C(4)-C(6)	107.3(3)	C(7)-C(4)-C(5)	109.1(3)
C(6)-C(4)-C(5)	107.8(3)	C(7)-C(4)-P(1)	112.8(3)
C(6)-C(4)-P(1)	114.5(2)	C(5)-C(4)-P(1)	105.1(2)
C(10)-C(8)-C(9)	109.0(3)	C(10)-C(8)-C(11)	109.3(3)
C(9)-C(8)-C(11)	106.1(3)	C(10)-C(8)-P(1)	113.3(3)
C(9)-C(8)-P(1)	112.9(2)	C(11)-C(8)-P(1)	106.0(2)
C(13)-C(12)-P(1)	120.6(2)	C(14)-C(13)-C(18)	119.2(3)
C(14)-C(13)-C(12)	117.5(3)	C(18)-C(13)-C(12)	122.9(3)
C(15)-C(14)-C(13)	122.1(3)	C(14)-C(15)-C(16)	119.0(3)
C(17)-C(16)-C(15)	119.0(3)	C(16)-C(17)-C(18)	123.0(3)
C(13)-C(18)-C(17)	117.6(3)	C(13)-C(18)-C(19)	122.6(3)
C(17)-C(18)-C(19)	119.4(3)	C(18)-C(19)-P(2)	123.1(2)
C(21)-C(20)-C(22)	111.0(3)	C(21)-C(20)-C(23)	106.8(3)
C(22)-C(20)-C(23)	107.3(3)	C(21)-C(20)-P(2)	113.2(3)
C(22)-C(20)-P(2)	105.6(2)	C(23)-C(20)-P(2)	112.8(2)
C(25)-C(24)-C(27)	108.3(4)	C(25)-C(24)-C(26)	108.0(4)
C(27)-C(24)-C(26)	107.5(4)	C(25)-C(24)-P(2)	106.1(2)
C(27)-C(24)-P(2)	111.8(3)	C(26)-C(24)-P(2)	115.0(3)
C(29)-C(28)-C(33)	121.4(4)	C(28)-C(29)-C(30)	119.7(4)
C(29)-C(30)-C(31)	120.1(4)	C(32)-C(31)-C(30)	120.1(4)

C(31)-C(32)-C(33)	120.5(4)	C(32)-C(33)-C(28)	118.2(4)
C(32)-C(33)-C(34)	123.1(3)	C(28)-C(33)-C(34)	118.6(4)
C(35)-C(34)-C(33)	128.2(4)	C(34)-C(35)-C(36)	121.7(3)
O(2)-C(36)-C(35)	121.8(4)	O(2)-C(36)-C(37)	118.7(3)
C(35)-C(36)-C(37)	119.5(3)	C(38)-C(37)-C(36)	125.2(3)
C(37)-C(38)-C(39)	126.0(3)	C(44)-C(39)-C(40)	118.2(3)
C(44)-C(39)-C(38)	122.4(3)	C(40)-C(39)-C(38)	119.4(3)
C(41)-C(40)-C(39)	120.8(4)	C(40)-C(41)-C(42)	119.9(4)
C(43)-C(42)-C(41)	119.8(4)	C(44)-C(43)-C(42)	120.6(4)
C(43)-C(44)-C(39)	120.5(4)		

Table 28D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (54).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	15.41(13)	18.66(14)	21.75(15)	-0.54(9)	1.43(9)	5.99(10)
Cl(1)	18.1(4)	33.8(5)	47.8(6)	-2.9(4)	9.6(4)	4.1(4)
C(1)	20(2)	27(2)	33(2)	-3.9(15)	3.1(14)	7.4(14)
C(2)	36(2)	44(2)	32(2)	-2(2)	-6(2)	19(2)
C(3)	68(4)	69(4)	103(5)	-10(4)	-56(4)	22(3)
O(1)	33.4(15)	29.5(15)	50(2)	-8.8(13)	1.7(13)	10.7(12)
P(1)	16.9(4)	19.0(4)	20.2(4)	0.2(3)	3.6(3)	7.4(3)
P(2)	16.9(4)	18.0(4)	17.6(4)	0.1(3)	3.2(3)	7.0(3)
C(4)	24(2)	29(2)	22(2)	2.8(14)	8.1(14)	10.1(15)
C(5)	29(2)	29(2)	29(2)	9.8(15)	11(2)	13(2)
C(6)	37(2)	33(2)	23(2)	-1(2)	10(2)	7(2)
C(7)	27(2)	36(2)	42(2)	6(2)	16(2)	14(2)
C(8)	25(2)	27(2)	28(2)	2.6(14)	3.9(14)	15.0(15)
C(9)	26(2)	31(2)	51(3)	9(2)	5(2)	17(2)
C(10)	35(2)	23(2)	41(2)	-1(2)	6(2)	16(2)
C(11)	32(2)	32(2)	30(2)	9(2)	5(2)	16(2)
C(12)	19(2)	23(2)	21(2)	-1.8(13)	2.9(13)	7.3(13)
C(13)	16.0(15)	23(2)	20(2)	-0.7(13)	0.0(13)	6.3(13)
C(14)	26(2)	20(2)	30(2)	-1.0(14)	1.7(15)	8.5(14)
C(15)	26(2)	19(2)	34(2)	4.9(14)	1(2)	3.4(14)
C(16)	22(2)	30(2)	24(2)	5.2(14)	3.8(14)	2.2(15)
C(17)	18(2)	28(2)	21(2)	-0.5(14)	1.9(13)	5.8(14)
C(18)	15.0(14)	23(2)	16(2)	0.1(12)	-2.6(12)	7.1(13)
C(19)	20(2)	20(2)	21(2)	-0.2(13)	3.1(13)	7.8(13)
C(20)	26(2)	23(2)	18(2)	0.7(13)	4.7(13)	7.4(14)
C(21)	36(2)	37(2)	27(2)	5(2)	15(2)	17(2)
C(22)	33(2)	31(2)	21(2)	5.0(14)	3.6(15)	12(2)
C(23)	43(2)	33(2)	22(2)	-6(2)	4(2)	4(2)
C(24)	27(2)	19(2)	26(2)	2.1(13)	2.7(14)	12.1(14)
C(25)	75(3)	42(2)	49(3)	24(2)	36(3)	36(2)
C(26)	39(2)	47(3)	72(3)	27(2)	17(2)	29(2)
C(27)	76(4)	25(2)	61(3)	-10(2)	-29(3)	22(2)
C(28)	30(2)	38(2)	33(2)	7(2)	11(2)	19(2)
C(29)	34(2)	38(2)	39(2)	14(2)	18(2)	18(2)
C(30)	31(2)	29(2)	53(3)	2(2)	17(2)	9(2)
C(31)	33(2)	38(2)	40(2)	-4(2)	2(2)	13(2)
C(32)	36(2)	33(2)	32(2)	3(2)	5(2)	16(2)
C(33)	27(2)	31(2)	30(2)	2.3(15)	8.3(15)	14(2)
C(34)	26(2)	37(2)	27(2)	2(2)	0.7(15)	15(2)
C(35)	22(2)	33(2)	28(2)	0.8(15)	2.3(14)	12.6(15)
C(36)	26(2)	34(2)	33(2)	2(2)	4(2)	16(2)
O(2)	30(2)	50(2)	55(2)	16(2)	-9.1(14)	10.3(14)
C(37)	22(2)	28(2)	32(2)	2.4(15)	5.9(15)	9.0(15)
C(38)	25(2)	27(2)	26(2)	-0.9(14)	6.6(14)	9.8(15)
C(39)	26(2)	25(2)	23(2)	-3.1(14)	1.5(14)	9.2(14)
C(40)	26(2)	30(2)	36(2)	-5(2)	0(2)	11(2)
C(41)	43(2)	34(2)	36(2)	-5(2)	-7(2)	23(2)
C(42)	50(3)	27(2)	31(2)	2(2)	-1(2)	15(2)
C(43)	36(2)	31(2)	35(2)	3(2)	9(2)	10(2)
C(44)	26(2)	31(2)	33(2)	3(2)	5(2)	13(2)

Table 28E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (54).

	x	y	z	U
H(2A)	-2116(4)	-1922(4)	5624(2)	45
H(2B)	-1190(4)	-2038(4)	5045(2)	45
H(3A)	-3584(32)	-2801(8)	4598(20)	131
H(3B)	-4045(17)	-3840(40)	5178(4)	131
H(3C)	-3118(16)	-3976(35)	4603(19)	131
H(5A)	1035(7)	-2085(6)	8525(14)	42
H(5B)	-596(23)	-2827(8)	8165(8)	42
H(5C)	-274(28)	-2524(13)	8981(6)	42
H(6A)	1898(9)	101(22)	9081(9)	50
H(6B)	508(18)	-268(15)	9478(3)	50
H(6C)	959(25)	919(8)	8981(7)	50
H(7A)	-2214(7)	-1622(23)	8075(8)	51
H(7B)	-1616(7)	-218(5)	8464(15)	51
H(7C)	-1917(12)	-1478(26)	8898(7)	51
H(9A)	-2016(6)	-524(15)	6733(13)	52
H(9B)	-1940(5)	912(12)	6756(13)	52
H(9C)	-2146(4)	112(27)	7439(2)	52
H(10A)	44(25)	1860(5)	8108(6)	47
H(10B)	152(27)	2712(12)	7448(6)	47
H(10C)	1524(5)	2493(16)	7773(12)	47
H(11A)	269(24)	459(6)	6202(6)	46
H(11B)	1670(4)	1621(25)	6600(3)	46
H(11C)	307(25)	1872(21)	6298(7)	46
H(12A)	2632(3)	1303(3)	8194(2)	26
H(12B)	2913(3)	40(3)	8117(2)	26
H(14)	3872(4)	3089(3)	7644(2)	32
H(15)	5619(4)	4257(3)	6941(2)	34
H(16)	6496(4)	3135(4)	6241(2)	34
H(17)	5623(4)	898(3)	6274(2)	29
H(19A)	3490(3)	-1084(3)	7423(2)	24
H(19B)	4465(3)	-1019(3)	6837(2)	24
H(21A)	3991(10)	-2494(7)	5445(15)	48
H(21B)	4699(6)	-1011(21)	5740(9)	48
H(21C)	4222(13)	-1350(27)	4930(6)	48
H(22A)	1388(9)	-571(9)	5346(14)	43
H(22B)	2595(29)	-255(14)	4836(5)	43
H(22C)	3060(21)	235(7)	5632(9)	43
H(23A)	417(5)	-2945(21)	5008(10)	56
H(23B)	1508(23)	-3612(9)	5013(10)	56
H(23C)	1600(22)	-2523(13)	4480(2)	56
H(25A)	2099(23)	-3156(17)	7700(6)	74
H(25B)	1512(37)	-4686(19)	7530(10)	74
H(25C)	516(14)	-3961(34)	7297(4)	74
H(26A)	4231(12)	-2872(25)	7175(12)	72
H(26B)	4121(14)	-3268(33)	6377(6)	72
H(26C)	3619(5)	-4372(10)	6923(18)	72
H(27A)	1687(23)	-4653(19)	5754(8)	85
H(27B)	258(13)	-4813(22)	6072(15)	85
H(27C)	1176(36)	-5564(6)	6385(8)	85
H(28)	6812(4)	2454(4)	7927(2)	38
H(29)	8691(4)	4514(4)	7929(2)	42
H(30)	10505(4)	5288(4)	8861(2)	46

H(31)	10476(5)	3958(4)	9775(2)	46
H(32)	8576(4)	1901(4)	9782(2)	40
H(34)	5523(4)	503(4)	8453(2)	36
H(35)	6675(4)	-65(4)	9685(2)	32
H(37)	3450(4)	-2985(4)	9788(2)	34
H(38)	6437(4)	-1963(3)	10059(2)	32
H(40)	7406(4)	-3340(4)	10658(2)	38
H(41)	7188(5)	-4969(4)	11412(2)	44
H(42)	4963(5)	-6217(4)	11796(2)	45
H(43)	2972(4)	-5806(4)	11433(2)	42
H(44)	3157(4)	-4216(4)	10661(2)	35

Table 29A. Crystal data, structure solution and refinement for (55).

Identification code	exti15
Chemical formula	$C_{25}H_{46}Cl_4P_2Pd$
Formula weight	656.76
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/c$
Unit cell dimensions	a = 7.4876(5) Å α = 90°
	b = 21.9249(14) Å β = 95.225(2)°
	c = 18.3797(12) Å γ = 90°
Volume	3004.8(3) Å^3
Z	4
Density (calculated)	1.452 g/cm^3
Absorption coefficient μ	1.093 mm^{-1}
F(000)	1360
Reflections for cell refinement	13126 (θ range 2.16 to 28.57°)
Crystal colour	yellow
Crystal size	0.48 × 0.36 × 0.24 mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	1.86 to 28.61°
Index ranges	$-9 \le h \le 8$, $-27 \le k \le 26$, $-24 \le \ell \le 23$
Intensity decay	0%
Reflections collected	18660
Independent reflections	6925 (R_{int} = 0.0261)
Reflections with I>2σ(I)	6150
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.878 and 0.715
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0272, 8.1756
Data / restraints / parameters	6925 / 0 / 302
Final R indices [I>2σ(I)]	R1 = 0.0426, wR2 = 0.0936
R indices (all data)	R1 = 0.0495, wR2 = 0.0988
Goodness-of-fit on F^2	1.052
Extinction coefficient	0.00066(13)
Largest and mean shift/esd	0.031 and 0.000
Largest diff. peak and hole	1.263 and -1.182 eÅ^{-3}

The Crystal Structure of [o-$C_6H_4(CH_2PBu^t_2)_2Pd(Cl)_2$].$CH_2Cl_2$ (55)

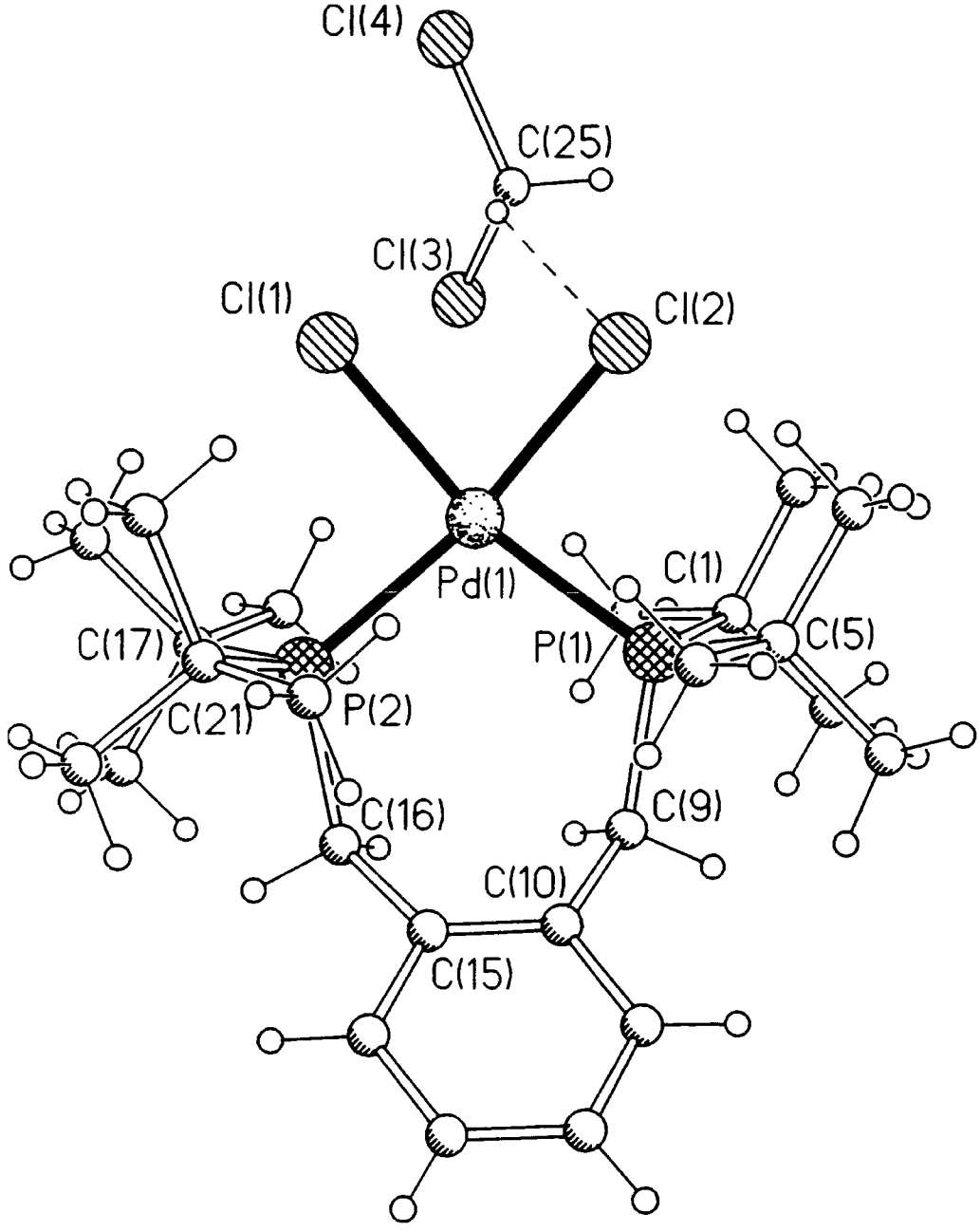


Table 29B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (55). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	542.4(3)	3539.13(12)	7376.68(12)	29.32(8)
Cl(1)	-1788.2(14)	3040.2(6)	6669.0(5)	63.1(3)
Cl(2)	-1513(2)	4332.5(9)	7242.0(11)	107.2(6)
P(1)	2525.8(14)	4243.0(4)	7907.6(5)	37.9(2)
P(2)	2172.8(10)	2636.8(4)	7490.3(4)	24.1(2)
C(1)	2987(7)	4835(2)	7188(2)	56.4(11)
C(2)	3426(10)	4486(3)	6513(3)	91(2)
C(3)	4544(9)	5245(3)	7425(3)	87(2)
C(4)	1416(12)	5249(4)	6979(6)	190(6)
C(5)	1750(7)	4603(2)	8766(2)	63.9(14)
C(6)	165(13)	5018(4)	8630(3)	173(5)
C(7)	3243(11)	4975(3)	9182(3)	113(3)
C(8)	1278(10)	4084(3)	9261(3)	94(2)
C(9)	4860(5)	3998(2)	8166(2)	41.9(8)
C(10)	5359(4)	3524(2)	8743(2)	33.8(7)
C(11)	6216(6)	3706(2)	9417(2)	52.6(11)
C(12)	6824(5)	3291(2)	9948(2)	48.5(10)
C(13)	6623(5)	2681(2)	9813(2)	40.6(8)
C(14)	5835(4)	2492(2)	9141(2)	33.3(7)
C(15)	5185(4)	2905.8(14)	8601(2)	25.5(6)
C(16)	4552(4)	2666.5(14)	7853(2)	25.0(6)
C(17)	2508(4)	2274(2)	6565(2)	33.2(7)
C(18)	4183(5)	1864(2)	6579(2)	44.4(9)
C(19)	2761(5)	2802(2)	6040(2)	41.0(8)
C(20)	896(6)	1888(2)	6262(2)	58.0(12)
C(21)	1104(4)	2096(2)	8125(2)	35.5(7)
C(22)	1087(5)	2424(2)	8864(2)	44.9(9)
C(23)	2145(5)	1497(2)	8224(2)	46.8(9)
C(24)	-865(5)	1951(2)	7873(2)	48.9(10)
C(25)	7434(8)	706(3)	10341(3)	77(2)
Cl(3)	9353(3)	947.5(8)	9947.8(8)	97.5(5)
Cl(4)	5435(2)	886.6(6)	9794.3(7)	77.7(4)

Table 29C. Bond lengths (Å) and angles (°) for (55).

Pd(1)-P(1)	2.2968(10)	Pd(1)-Cl(2)	2.3210(13)
Pd(1)-P(2)	2.3240(8)	Pd(1)-Cl(1)	2.3496(10)
P(1)-C(9)	1.849(4)	P(1)-C(5)	1.901(4)
P(1)-C(1)	1.907(4)	P(2)-C(16)	1.845(3)
P(2)-C(21)	1.890(3)	P(2)-C(17)	1.914(3)
C(1)-C(3)	1.506(7)	C(1)-C(4)	1.508(8)
C(1)-C(2)	1.518(7)	C(5)-C(6)	1.499(7)
C(5)-C(8)	1.519(8)	C(5)-C(7)	1.532(8)
C(9)-C(10)	1.507(5)	C(10)-C(15)	1.384(4)
C(10)-C(11)	1.400(5)	C(11)-C(12)	1.382(6)
C(12)-C(13)	1.366(6)	C(13)-C(14)	1.384(5)
C(14)-C(15)	1.398(4)	C(15)-C(16)	1.508(4)
C(17)-C(19)	1.529(5)	C(17)-C(20)	1.537(5)
C(17)-C(18)	1.542(5)	C(21)-C(23)	1.530(5)
C(21)-C(24)	1.537(5)	C(21)-C(22)	1.539(5)
C(25)-Cl(3)	1.748(6)	C(25)-Cl(4)	1.770(6)
P(1)-Pd(1)-Cl(2)	86.48(5)	P(1)-Pd(1)-P(2)	102.69(3)
Cl(2)-Pd(1)-P(2)	170.19(6)	P(1)-Pd(1)-Cl(1)	165.23(4)
Cl(2)-Pd(1)-Cl(1)	80.68(6)	P(2)-Pd(1)-Cl(1)	90.63(4)
C(9)-P(1)-C(5)	105.1(2)	C(9)-P(1)-C(1)	98.6(2)
C(5)-P(1)-C(1)	112.4(2)	C(9)-P(1)-Pd(1)	118.27(12)
C(5)-P(1)-Pd(1)	113.4(2)	C(1)-P(1)-Pd(1)	108.24(14)
C(16)-P(2)-C(21)	104.39(14)	C(16)-P(2)-C(17)	97.76(14)
C(21)-P(2)-C(17)	112.6(2)	C(16)-P(2)-Pd(1)	118.97(10)
C(21)-P(2)-Pd(1)	109.92(11)	C(17)-P(2)-Pd(1)	112.57(11)
C(3)-C(1)-C(4)	106.2(6)	C(3)-C(1)-C(2)	108.5(5)
C(4)-C(1)-C(2)	108.5(6)	C(3)-C(1)-P(1)	112.9(3)
C(4)-C(1)-P(1)	113.6(4)	C(2)-C(1)-P(1)	106.9(3)
C(6)-C(5)-C(8)	109.3(6)	C(6)-C(5)-C(7)	106.9(5)
C(8)-C(5)-C(7)	107.4(5)	C(6)-C(5)-P(1)	114.3(3)
C(8)-C(5)-P(1)	106.9(3)	C(7)-C(5)-P(1)	111.8(4)
C(10)-C(9)-P(1)	123.3(3)	C(15)-C(10)-C(11)	118.3(3)
C(15)-C(10)-C(9)	121.9(3)	C(11)-C(10)-C(9)	119.3(3)
C(12)-C(11)-C(10)	122.1(4)	C(13)-C(12)-C(11)	119.6(3)
C(12)-C(13)-C(14)	119.1(3)	C(13)-C(14)-C(15)	122.2(3)
C(10)-C(15)-C(14)	118.7(3)	C(10)-C(15)-C(16)	122.0(3)
C(14)-C(15)-C(16)	118.8(3)	C(15)-C(16)-P(2)	123.7(2)
C(19)-C(17)-C(20)	109.1(3)	C(19)-C(17)-C(18)	107.6(3)
C(20)-C(17)-C(18)	107.2(3)	C(19)-C(17)-P(2)	106.3(2)
C(20)-C(17)-P(2)	112.9(2)	C(18)-C(17)-P(2)	113.6(2)
C(23)-C(21)-C(24)	108.8(3)	C(23)-C(21)-C(22)	109.9(3)
C(24)-C(21)-C(22)	106.1(3)	C(23)-C(21)-P(2)	111.9(2)
C(24)-C(21)-P(2)	113.1(2)	C(22)-C(21)-P(2)	106.8(2)
Cl(3)-C(25)-Cl(4)	112.5(3)		

Table 29D. Anisotropic displacement parameters ($Å^2$ x 10^3) for (55).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Pd(1)	22.93(12)	43.43(15)	21.06(12)	1.26(10)	-0.97(8)	6.83(10)
Cl(1)	41.5(5)	102.7(9)	41.6(5)	18.7(5)	-15.2(4)	-30.0(6)
Cl(2)	74.7(9)	118.3(13)	122.3(13)	-23.0(11)	-24.4(9)	62.0(10)
P(1)	53.5(5)	29.2(4)	28.1(4)	-2.9(3)	-11.9(4)	8.5(4)
P(2)	20.9(3)	30.5(4)	20.6(3)	-0.3(3)	-0.1(3)	-2.3(3)
C(1)	76(3)	35(2)	54(2)	14(2)	-16(2)	2(2)
C(2)	165(6)	68(3)	40(2)	11(2)	5(3)	-42(4)
C(3)	122(5)	59(3)	78(4)	4(3)	0(3)	-32(3)
C(4)	133(7)	192(10)	249(12)	181(10)	41(7)	78(7)
C(5)	97(4)	56(3)	34(2)	-19(2)	-17(2)	33(2)
C(6)	235(10)	212(9)	61(4)	-63(5)	-41(5)	186(8)
C(7)	186(8)	87(4)	61(3)	-41(3)	-21(4)	-14(5)
C(8)	143(6)	93(4)	51(3)	-26(3)	39(3)	3(4)
C(9)	48(2)	29(2)	44(2)	2.7(14)	-18(2)	-7.4(15)
C(10)	34(2)	35(2)	30(2)	-1.8(13)	-9.9(13)	0.3(13)
C(11)	62(3)	43(2)	48(2)	-11(2)	-27(2)	5(2)
C(12)	47(2)	66(3)	29(2)	-10(2)	-17(2)	10(2)
C(13)	32(2)	62(2)	26(2)	11(2)	-4.5(13)	8(2)
C(14)	30(2)	37(2)	32(2)	7.2(13)	-2.0(12)	2.2(13)
C(15)	18.6(13)	36(2)	21.7(13)	-0.7(11)	0.5(10)	1.9(11)
C(16)	20.8(13)	31.4(15)	22.6(13)	-2.0(11)	-0.2(10)	1.7(11)
C(17)	36(2)	38(2)	25.2(14)	-7.9(13)	0.5(12)	-5.4(14)
C(18)	58(2)	42(2)	35(2)	-10.6(15)	9(2)	6(2)
C(19)	49(2)	52(2)	22.3(15)	-1.1(14)	5.3(14)	1(2)
C(20)	61(3)	68(3)	43(2)	-22(2)	-4(2)	-25(2)
C(21)	30(2)	44(2)	33(2)	9.1(14)	4.8(13)	-7.2(14)
C(22)	41(2)	63(2)	33(2)	11(2)	11.7(15)	-5(2)
C(23)	45(2)	41(2)	53(2)	15(2)	3(2)	-5(2)
C(24)	30(2)	65(3)	51(2)	19(2)	3(2)	-14(2)
C(25)	110(4)	75(3)	45(2)	12(2)	-5(3)	-36(3)
Cl(3)	127.6(14)	100.8(12)	66.7(8)	-8.2(8)	22.4(9)	-45.1(10)
Cl(4)	121.7(12)	50.5(6)	59.7(7)	10.6(5)	1.2(7)	-0.8(7)

Table 29E. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (55).

	x	y	z	U
H(2A)	4366(39)	4186(13)	6649(5)	109
H(2B)	3848(54)	4772(4)	6156(9)	109
H(2C)	2348(16)	4277(15)	6298(13)	109
H(3A)	5670(9)	5023(6)	7396(20)	104
H(3B)	4454(29)	5378(14)	7930(8)	104
H(3C)	4521(31)	5603(9)	7105(14)	104
H(4A)	360(32)	5003(5)	6819(43)	228
H(4B)	1704(45)	5518(27)	6580(32)	228
H(4C)	1162(70)	5495(27)	7402(15)	228
H(6A)	-743(42)	4823(14)	8289(32)	207
H(6B)	546(21)	5403(13)	8420(38)	207
H(6C)	-345(64)	5101(28)	9093(7)	207
H(7A)	3811(45)	5239(17)	8839(5)	136
H(7B)	4141(35)	4698(3)	9421(22)	136
H(7C)	2733(15)	5226(17)	9552(18)	136
H(8A)	2319(19)	3816(11)	9357(18)	112
H(8B)	273(36)	3851(12)	9022(10)	112
H(8C)	937(56)	4251(3)	9723(9)	112
H(9A)	5340(5)	3852(2)	7713(2)	50
H(9B)	5543(5)	4371(2)	8317(2)	50
H(11)	6386(6)	4129(2)	9512(2)	63
H(12)	7379(5)	3428(2)	10404(2)	58
H(13)	7019(5)	2390(2)	10176(2)	49
H(14)	5731(4)	2068(2)	9043(2)	40
H(16A)	5016(4)	2244.9(14)	7829(2)	30
H(16B)	5179(4)	2909.2(14)	7499(2)	30
H(18A)	4131(18)	1552(7)	6958(10)	53
H(18B)	5262(6)	2113(3)	6684(14)	53
H(18C)	4221(19)	1667(9)	6102(5)	53
H(19A)	3762(21)	3058(6)	6238(7)	49
H(19B)	1663(12)	3046(7)	5980(10)	49
H(19C)	3021(33)	2639(2)	5564(4)	49
H(20A)	845(24)	1513(7)	6551(10)	70
H(20B)	1025(21)	1783(12)	5752(5)	70
H(20C)	-212(7)	2121(5)	6292(15)	70
H(22A)	392(29)	2802(6)	8799(3)	54
H(22B)	2319(6)	2521(11)	9055(7)	54
H(22C)	538(32)	2159(5)	9210(5)	54
H(23A)	3397(10)	1584(2)	8395(14)	56
H(23B)	2096(30)	1281(6)	7757(4)	56
H(23C)	1608(22)	1243(5)	8585(11)	56
H(24A)	-1547(9)	2332(2)	7812(14)	59
H(24B)	-1374(12)	1696(11)	8241(7)	59
H(24C)	-929(6)	1733(11)	7407(8)	59
H(25A)	7405(8)	901(3)	10826(3)	93
H(25B)	7497(8)	259(3)	10416(3)	93

C(26)	7386(3)	4906(5)	57(6)	46(3)
O(15)	6074.6(15)	4250(3)	1792(3)	25.7(13)
O(16)	6245(2)	3162(3)	1566(4)	47.9(19)
C(27)	6057(2)	3569(4)	1839(4)	27(2)
C(28)	5777(3)	3320(5)	2308(5)	45(3)
C(29)	4202(2)	7123(4)	-431(4)	27(2)
C(30)	4180(3)	6399(5)	-773(5)	38(2)
C(31)	3869(3)	7221(5)	-43(5)	40(2)
C(32)	4221(3)	7687(5)	-969(5)	45(3)
C(33)	5005(2)	7289(4)	-304(4)	27(2)
C(34)	5302(2)	7102(4)	155(4)	27(2)
C(35)	5041(3)	8058(4)	-516(5)	35(2)
C(36)	5040(3)	6838(4)	-922(4)	32(2)
C(37)	5108(2)	8490(4)	2695(4)	21.0(18)
C(38)	4850(2)	7898(5)	2840(4)	31(2)
C(39)	5431(2)	8204(4)	2329(4)	21.8(18)
C(40)	5238(2)	8801(5)	3354(4)	30(2)
C(41)	4598(2)	9752(4)	2629(4)	25.3(19)
C(42)	4806(3)	10300(5)	3042(5)	38(2)
C(43)	4379(3)	10163(5)	2130(5)	38(2)
C(44)	4353(3)	9346(5)	3079(5)	43(3)
C(45)	5954(2)	9356(4)	278(4)	22.3(18)
C(46)	5721(3)	9442(5)	-346(4)	33(2)
C(47)	5849(2)	8662(4)	607(4)	24.5(19)
C(48)	6336(2)	9323(5)	66(4)	29(2)
C(49)	5867(2)	10954(4)	495(4)	28(2)
C(50)	5520(3)	11116(5)	160(5)	38(2)
C(51)	5926(3)	11506(5)	1027(4)	38(2)
C(52)	6167(3)	11024(5)	-8(5)	43(3)
C(53)	6546(2)	8346(5)	3088(4)	26(2)
C(54)	6425(2)	7851(4)	2546(4)	28(2)
C(55)	6692(2)	7905(5)	3658(4)	30(2)
C(56)	6234(2)	8750(5)	3340(4)	29(2)
C(57)	7134(2)	9424(4)	3361(4)	27(2)
C(58)	7409(3)	8957(5)	3666(5)	38(2)
C(59)	7316(3)	10041(5)	3011(5)	39(2)
C(60)	6902(3)	9716(5)	3910(5)	44(3)
C(61)	7830(2)	7564(5)	730(4)	28(2)
C(62)	7901(2)	8334(4)	588(5)	31(2)
C(63)	7891(2)	7123(5)	110(5)	34(2)
C(64)	8088(2)	7323(5)	1251(5)	34(2)
C(65)	7036(2)	7481(4)	413(4)	23.2(19)
C(66)	7089(2)	8079(5)	-74(4)	31(2)
C(67)	6687(2)	7586(4)	740(4)	25.2(19)
C(68)	7027(2)	6773(4)	21(4)	29(2)
C(69)	7006(2)	4248(4)	2686(5)	30(2)
C(70)	6751(3)	3636(5)	2821(6)	53(3)
C(71)	7296(3)	3968(5)	2271(5)	39(2)
C(72)	7157(3)	4504(6)	3345(5)	45(3)
C(73)	6487(2)	5470(4)	2753(4)	24.5(19)
C(74)	6249(2)	5017(5)	3192(4)	29(2)
C(75)	6244(2)	5896(4)	2299(4)	27(2)
C(76)	6683(3)	5995(5)	3205(4)	37(2)
C(77)	6189(2)	3786(4)	-317(4)	27(2)
C(78)	5998(3)	3854(5)	-990(4)	37(2)
C(79)	6064(3)	3102(4)	16(5)	41(3)
C(80)	6575(3)	3706(5)	-451(5)	37(2)
C(81)	6115(2)	5387(4)	-192(4)	25.4(19)
C(82)	5786(2)	5508(4)	-593(4)	30(2)
C(83)	6145(2)	5963(4)	342(4)	26(2)
C(84)	6431(2)	5443(5)	-650(5)	33(2)
C(85)	4490(2)	4637(4)	1958(4)	23.8(18)

C(86)	4170(2)	5035(4)	2195(5)	30(2)
C(87)	4375(2)	4137(4)	1416(4)	33(2)
C(88)	4636(2)	4189(4)	2537(4)	29(2)
C(89)	5083(2)	5684(4)	2265(4)	21.7(18)
C(90)	5350(2)	5194(4)	2590(4)	21.0(17)
C(91)	5276(2)	6293(4)	1953(4)	24.6(19)
C(92)	4841(2)	5984(4)	2795(4)	28(2)
C(93)	6796(3)	9331(6)	-2457(4)	58(3)
Cl(1)	6602.6(12)	9399(2)	-1683(2)	99.8(14)
Cl(2)	6499.8(8)	9056(2)	-3042(2)	79.8(10)
C(94)	6326(3)	7522(4)	-1966(4)	46(3)
Cl(3)	6354.8(10)	6679.3(17)	-2272.8(17)	73.6(10)
Cl(4)	6145.8(11)	7558.7(19)	-1182.4(18)	80.9(11)
C(95)	3656(3)	4982(5)	304(8)	85(5)
Cl(5)	3324.3(10)	5512(3)	16(2)	107.1(15)
Cl(6)	3583.2(14)	4103(2)	171(3)	127.5(19)
C(96)	8211(3)	4353(5)	1985(5)	66(4)
Cl(7)	8138.8(11)	5233(2)	1838(3)	106.3(15)
Cl(8)	8244.7(11)	4160(3)	2809(2)	102.8(15)
C(97)	5592(3)	6794(7)	4626(5)	101(6)
Cl(9)	5152.3(18)	7065(2)	4640(3)	142(2)
Cl(10)	5744.8(9)	6830.1(17)	3812.5(16)	68.2(9)
C(98)	5043(4)	8074(6)	-3167(5)	81(5)
Cl(11)	5266.5(15)	7765(2)	-2482(2)	116.0(19)
Cl(12)	4950.5(10)	7426.6(16)	-3733(2)	84.6(11)
C(99)	5874(4)	8521(6)	5757(5)	87(5)
Cl(13)	6040.2(12)	8489(2)	4971.5(19)	97.3(13)
Cl(14)	5927.9(9)	7740(2)	6159.5(19)	85.6(11)
C(100)	6920(5)	12337(7)	1275(6)	148(9)
Cl(15)	6965(2)	11643(4)	1835(5)	223(4)
Cl(16)	6964.5(17)	11984(3)	476(4)	156(3)
C(101)	2808(10)	6916(12)	458(10)	360(3)
Cl(17)	2863(4)	7442(12)	-243(8)	450(13)
Cl(18)	2936(3)	7370(5)	1153(6)	288(6)
C(102)	6714(4)	10707(10)	5958(9)	186(13)
Cl(19)	6403(3)	10365(5)	5418(5)	256(5)
Cl(20)	6490.4(18)	11048(3)	6634(4)	182(3)
C(103)	6959(6)	11550(3)	-1280(3)	260(3)
Cl(21)	7238(7)	12103(19)	-1719(18)	430(2)
Cl(22)	6558(3)	11793(6)	-1576(6)	139(4)