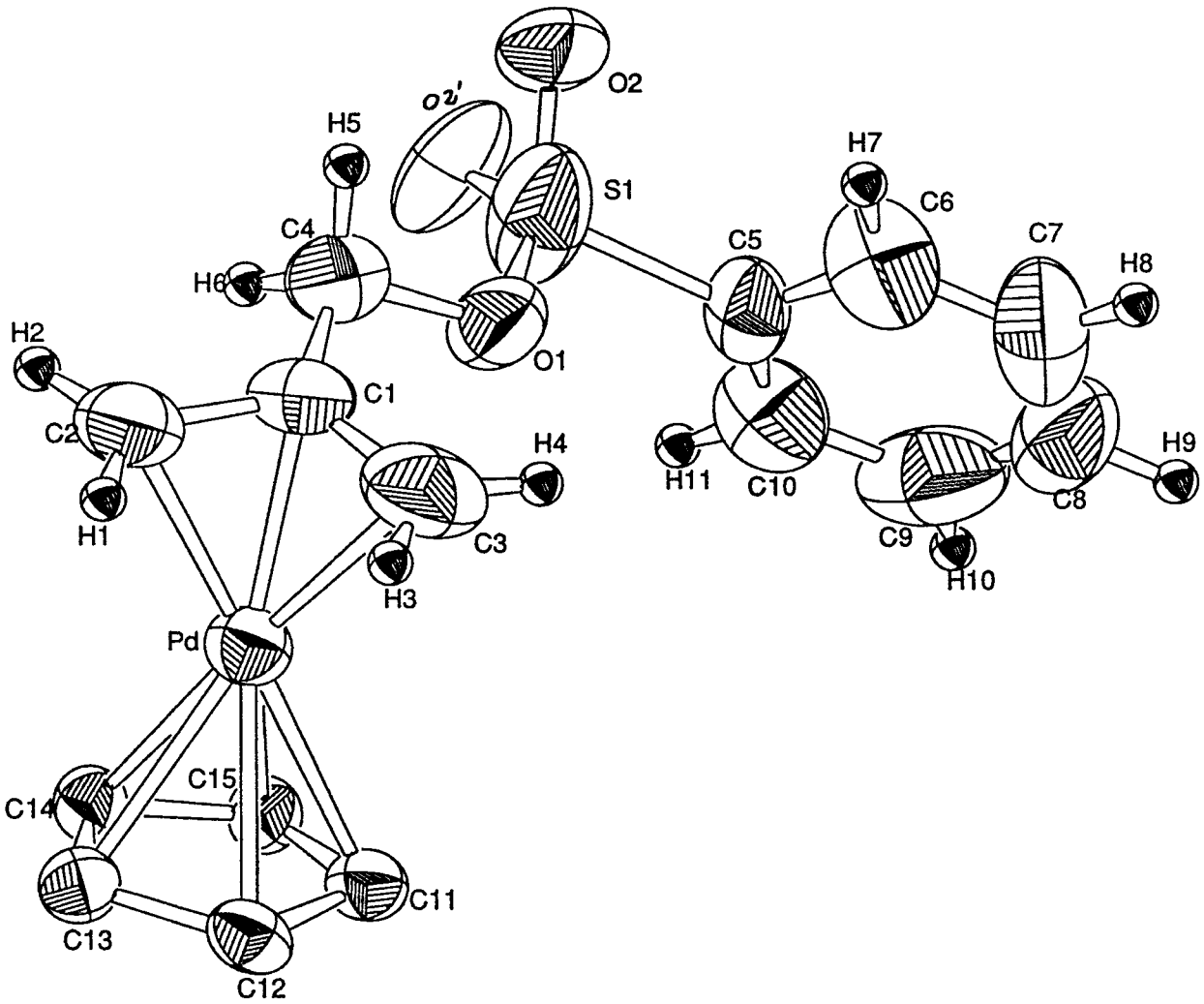
ORGANOMETALLICS
Organometallics, 1998, 17(3), 479-482, DOI:10.1021/om9708135


O2
O2'
H5
S1
H7
C6
C4
C5
C7
H8
H6
O1
H2
C1
C2
H4
H9
H11
C10
C8
H1
C3
C9
H10
H3
Pd
C15
C14
C11
C13
C12

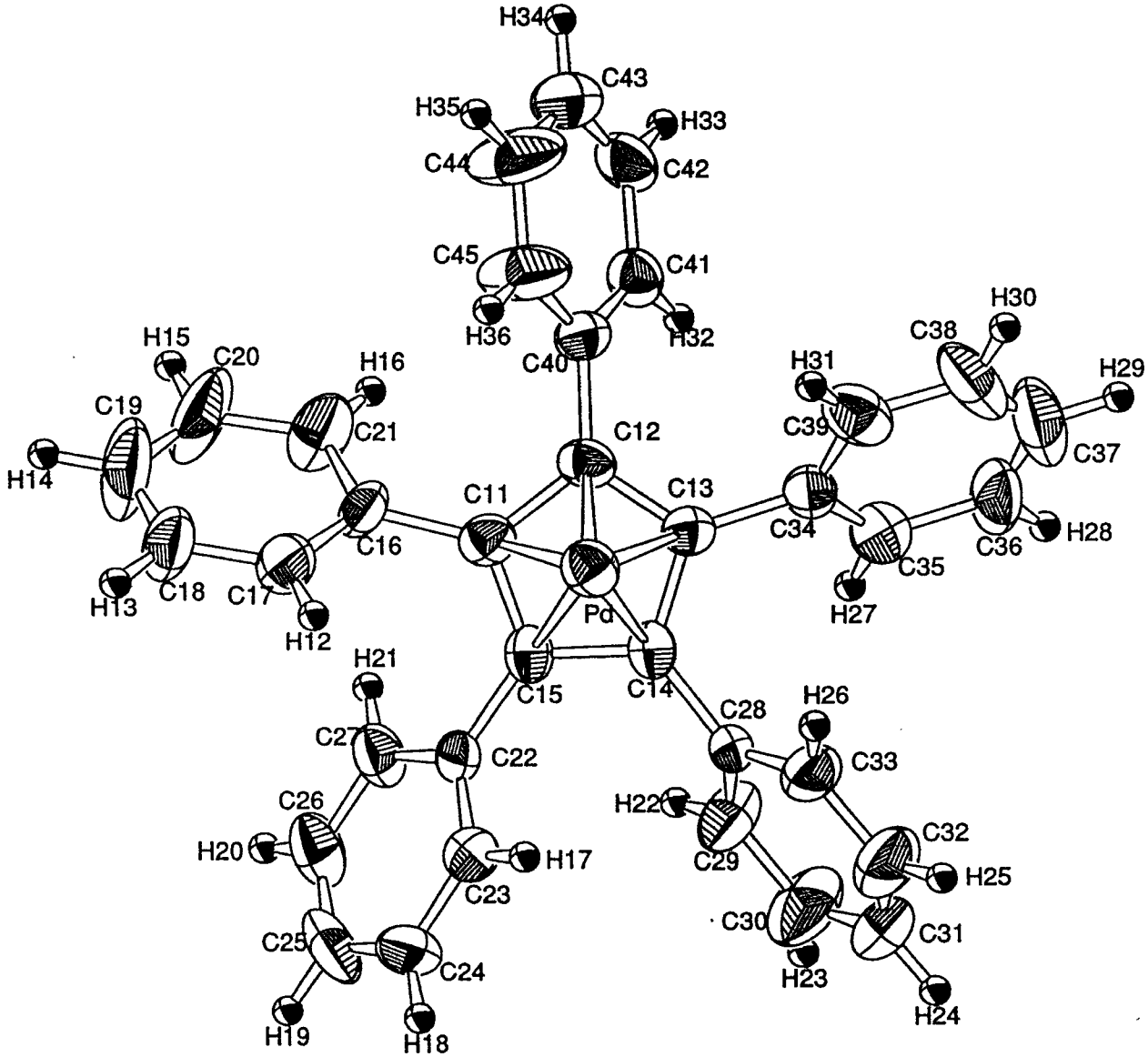

H34
C43
H35
H33
C44
C42
C45
C41
H36
H32
C40
H30
C38
H15
C20
H16
H31
H29
C19
C21
C12
C39
C37
H14
C11
C13
C34
H28
C16
C36
C18
C17
C35
H13
H27
Pd
H12
H21
C15
C14
C28
H26
C27
C22
C33
C26
H22
C32
H20
H17
C29
H25
C23
C30
C31
C25
C24
H23
H19
H18
H24

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

atom	x	y	z	B_{eq}	occ
Pd	0.19298(7)	0.27104(5)	0.05975(8)	3.67(2)	1.0000
S(1)	-0.0570(5)	0.0522(2)	-0.2298(4)	8.3(1)	1.0000
O(1)	-0.0331(7)	0.1338(4)	-0.1243(7)	5.9(2)	1.0000
O(2)	-0.141(1)	-0.0006(7)	-0.204(1)	6.1(4)	0.64(2)
O(2')	0.002(3)	-0.007(1)	-0.247(2)	7.2(9)	0.31(2)
C(1)	0.0392(10)	0.2022(6)	0.099(1)	4.4(3)	1.0000
C(2)	0.129(1)	0.2075(7)	0.213(1)	6.2(3)	1.0000
C(3)	-0.006(1)	0.2719(8)	0.071(1)	6.8(4)	1.0000
C(4)	0.008(1)	0.1238(7)	0.013(1)	5.9(3)	1.0000
C(5)	-0.118(1)	0.1018(6)	-0.3673(10)	4.8(3)	1.0000
C(6)	-0.237(1)	0.1271(8)	-0.372(1)	7.2(4)	1.0000
C(7)	-0.282(1)	0.1606(9)	-0.480(2)	8.4(5)	1.0000
C(8)	-0.213(2)	0.1653(9)	-0.581(2)	8.4(5)	1.0000
C(9)	-0.098(2)	0.1379(9)	-0.578(2)	8.5(5)	1.0000
C(10)	-0.048(1)	0.1063(7)	-0.470(1)	6.3(4)	1.0000
C(11)	0.2711(8)	0.3355(5)	-0.1058(9)	3.3(2)	1.0000
C(12)	0.3172(8)	0.3792(5)	0.0275(9)	3.3(2)	1.0000
C(13)	0.3953(8)	0.3310(5)	0.0974(9)	3.1(2)	1.0000
C(14)	0.4001(8)	0.2569(5)	0.0056(8)	3.1(2)	1.0000
C(15)	0.3306(7)	0.2624(5)	-0.1216(8)	3.1(2)	1.0000
C(16)	0.1899(8)	0.3625(5)	-0.2177(9)	3.8(2)	1.0000
C(17)	0.0880(9)	0.3143(5)	-0.287(1)	4.4(3)	1.0000
C(18)	0.019(1)	0.3353(7)	-0.397(1)	6.5(3)	1.0000
C(19)	0.049(1)	0.4051(9)	-0.441(1)	9.7(5)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(20)	0.148(1)	0.4534(7)	-0.377(2)	9.7(5)	1.0000
C(21)	0.2182(10)	0.4340(6)	-0.263(1)	6.5(3)	1.0000
C(22)	0.3259(7)	0.2049(5)	-0.2486(8)	3.0(2)	1.0000
C(23)	0.2991(8)	0.1251(5)	-0.2519(9)	3.7(2)	1.0000
C(24)	0.3020(9)	0.0724(6)	-0.370(1)	4.8(3)	1.0000
C(25)	0.329(1)	0.1005(8)	-0.484(1)	5.7(3)	1.0000
C(26)	0.3558(10)	0.1790(7)	-0.4827(9)	5.1(3)	1.0000
C(27)	0.3538(9)	0.2313(5)	-0.3666(9)	4.1(2)	1.0000
C(28)	0.4774(8)	0.1908(5)	0.0355(8)	2.9(2)	1.0000
C(29)	0.5731(9)	0.1693(6)	-0.040(1)	5.1(3)	1.0000
C(30)	0.647(1)	0.1094(8)	-0.011(1)	7.2(4)	1.0000
C(31)	0.624(1)	0.0697(7)	0.094(1)	6.1(3)	1.0000
C(32)	0.531(1)	0.0898(7)	0.171(1)	6.0(3)	1.0000
C(33)	0.4576(9)	0.1501(6)	0.1421(9)	4.3(3)	1.0000
C(34)	0.4700(9)	0.3511(5)	0.2330(9)	3.7(2)	1.0000
C(35)	0.5988(10)	0.3419(6)	0.244(1)	4.9(3)	1.0000
C(36)	0.670(1)	0.3606(7)	0.369(1)	6.4(3)	1.0000
C(37)	0.617(2)	0.3887(8)	0.478(1)	7.5(4)	1.0000
C(38)	0.492(2)	0.3981(7)	0.470(1)	6.7(4)	1.0000
C(39)	0.4161(10)	0.3792(6)	0.348(1)	4.9(3)	1.0000
C(40)	0.2935(8)	0.4630(5)	0.0789(9)	3.6(2)	1.0000
C(41)	0.3922(8)	0.5199(6)	0.1175(9)	3.7(2)	1.0000
C(42)	0.372(1)	0.5977(6)	0.1563(9)	4.6(3)	1.0000
C(43)	0.253(1)	0.6213(6)	0.161(1)	6.1(3)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(44)	0.154(1)	0.5661(8)	0.127(2)	8.7(4)	1.0000
C(45)	0.1738(10)	0.4879(6)	0.086(1)	7.2(4)	1.0000
H(1)	0.1499	0.2569	0.2693	7.4310	1.0000
H(2)	0.1676	0.1616	0.2338	7.4310	1.0000
H(3)	0.0184	0.3196	0.1314	8.0555	1.0000
H(4)	-0.0620	0.2727	-0.0082	8.0555	1.0000
H(5)	-0.0578	0.0959	0.0483	7.0469	1.0000
H(6)	0.0806	0.0944	0.0138	7.0469	1.0000
H(7)	-0.2878	0.1213	-0.3007	8.5205	1.0000
H(8)	-0.3634	0.1809	-0.4834	9.9685	1.0000
H(9)	-0.2449	0.1883	-0.6566	9.9898	1.0000
H(10)	-0.0500	0.1405	-0.6526	10.1155	1.0000
H(11)	0.0347	0.0878	-0.4666	7.5485	1.0000
H(12)	0.0655	0.2656	-0.2568	5.2751	1.0000
H(13)	-0.0492	0.3010	-0.4434	7.7146	1.0000
H(14)	0.0000	0.4199	-0.5162	11.5871	1.0000
H(15)	0.1702	0.5010	-0.4106	11.5798	1.0000
H(16)	0.2852	0.4696	-0.2160	7.8190	1.0000
H(17)	0.2781	0.1057	-0.1719	4.4177	1.0000
H(18)	0.2851	0.0171	-0.3702	5.7296	1.0000
H(19)	0.3299	0.0649	-0.5660	6.8178	1.0000
H(20)	0.3759	0.1979	-0.5632	6.0379	1.0000
H(21)	0.3717	0.2863	-0.3672	4.8900	1.0000
H(22)	0.5889	0.1961	-0.1143	6.1366	1.0000

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

atom	x	y	z	B_{eq}	occ
H(23)	0.7137	0.0954	-0.0633	8.5976	1.0000
H(24)	0.6741	0.0278	0.1137	7.3223	1.0000
H(25)	0.5153	0.0623	0.2440	7.2506	1.0000
H(26)	0.3921	0.1642	0.1969	5.1244	1.0000
H(27)	0.6382	0.3229	0.1653	5.9113	1.0000
H(28)	0.7576	0.3532	0.3760	7.6356	1.0000
H(29)	0.6670	0.4020	0.5629	8.9662	1.0000
H(30)	0.4555	0.4184	0.5492	8.0617	1.0000
H(31)	0.3277	0.3854	0.3443	5.8116	1.0000
H(32)	0.4766	0.5046	0.1170	4.3973	1.0000
H(33)	0.4426	0.6356	0.1803	5.4952	1.0000
H(34)	0.2396	0.6754	0.1874	7.3404	1.0000
H(35)	0.0702	0.5817	0.1307	10.4106	1.0000
H(36)	0.1032	0.4503	0.0623	8.5504	1.0000

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd	0.0461(4)	0.0446(5)	0.0474(5)	-0.0024(3)	0.0038(3)	0.0052(3)
S(1)	0.156(4)	0.071(3)	0.075(2)	0.015(3)	-0.038(2)	0.000(2)
O(1)	0.101(6)	0.060(5)	0.057(5)	-0.018(4)	-0.015(4)	0.018(4)
O(2)	0.10(1)	0.041(8)	0.089(10)	-0.020(7)	-0.009(8)	0.013(6)
O(2')	0.15(3)	0.05(2)	0.09(2)	0.05(2)	0.02(2)	0.02(1)
C(1)	0.061(7)	0.051(7)	0.054(6)	-0.014(5)	0.013(5)	0.004(5)
C(2)	0.079(8)	0.087(9)	0.066(8)	-0.033(7)	-0.007(7)	0.022(7)
C(3)	0.055(7)	0.09(1)	0.12(1)	-0.006(7)	0.024(7)	0.019(8)
C(4)	0.078(8)	0.072(8)	0.073(8)	-0.015(6)	-0.003(6)	0.025(7)
C(5)	0.075(8)	0.053(7)	0.045(6)	0.005(6)	-0.016(6)	-0.006(5)
C(6)	0.079(9)	0.11(1)	0.076(9)	0.015(8)	0.007(8)	-0.001(8)
C(7)	0.10(1)	0.12(1)	0.09(1)	0.029(9)	-0.030(10)	0.01(1)
C(8)	0.15(2)	0.070(10)	0.08(1)	-0.02(1)	-0.05(1)	0.019(8)
C(9)	0.15(2)	0.09(1)	0.07(1)	-0.04(1)	0.02(1)	0.008(8)
C(10)	0.076(9)	0.088(10)	0.071(9)	0.003(7)	0.009(7)	-0.002(8)
C(11)	0.039(5)	0.034(5)	0.052(6)	-0.001(4)	0.003(4)	0.007(4)
C(12)	0.036(5)	0.034(5)	0.051(6)	-0.003(4)	0.002(4)	-0.002(4)
C(13)	0.042(5)	0.034(5)	0.043(5)	0.003(4)	0.003(4)	0.005(4)
C(14)	0.036(5)	0.048(6)	0.033(5)	0.000(4)	0.002(4)	0.010(4)
C(15)	0.037(5)	0.050(6)	0.033(5)	0.001(4)	0.004(4)	0.011(4)
C(16)	0.042(6)	0.041(6)	0.060(6)	0.010(4)	-0.011(5)	0.015(5)
C(17)	0.048(6)	0.044(6)	0.071(7)	-0.001(5)	-0.013(5)	0.008(5)
C(18)	0.085(9)	0.054(8)	0.096(9)	-0.008(6)	-0.055(7)	0.022(7)
C(19)	0.12(1)	0.10(1)	0.13(1)	-0.025(9)	-0.092(10)	0.049(10)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(20)	0.14(1)	0.070(9)	0.15(1)	-0.014(8)	-0.08(1)	0.071(9)
C(21)	0.073(8)	0.046(7)	0.12(1)	-0.023(6)	-0.041(7)	0.035(7)
C(22)	0.033(5)	0.043(6)	0.036(5)	0.007(4)	-0.005(4)	0.004(4)
C(23)	0.055(6)	0.041(6)	0.044(6)	0.005(5)	0.002(5)	0.010(5)
C(24)	0.067(7)	0.042(6)	0.066(7)	0.005(5)	-0.004(6)	-0.010(5)
C(25)	0.069(8)	0.10(1)	0.035(6)	0.001(7)	-0.006(5)	-0.019(6)
C(26)	0.077(8)	0.080(9)	0.033(6)	-0.007(7)	0.000(5)	0.009(6)
C(27)	0.065(7)	0.055(6)	0.034(5)	-0.007(5)	-0.001(5)	0.008(5)
C(28)	0.042(5)	0.033(5)	0.034(5)	0.003(4)	-0.007(4)	0.002(4)
C(29)	0.059(7)	0.079(8)	0.066(7)	0.030(6)	0.013(6)	0.031(6)
C(30)	0.079(9)	0.12(1)	0.090(9)	0.064(8)	0.024(7)	0.032(8)
C(31)	0.091(9)	0.069(8)	0.073(8)	0.040(7)	-0.012(7)	0.012(7)
C(32)	0.100(10)	0.070(9)	0.068(8)	0.026(7)	0.004(7)	0.034(7)
C(33)	0.069(7)	0.048(6)	0.050(6)	0.016(5)	0.008(5)	0.016(5)
C(34)	0.062(7)	0.028(5)	0.047(6)	-0.007(4)	-0.009(5)	0.008(4)
C(35)	0.064(7)	0.055(7)	0.063(7)	0.005(5)	-0.011(6)	0.001(5)
C(36)	0.084(9)	0.063(8)	0.083(9)	-0.012(6)	-0.051(8)	0.012(7)
C(37)	0.14(1)	0.09(1)	0.048(8)	-0.028(10)	-0.036(9)	0.020(7)
C(38)	0.15(1)	0.063(8)	0.033(6)	-0.037(9)	-0.006(8)	0.002(5)
C(39)	0.083(8)	0.049(7)	0.050(6)	-0.012(6)	0.011(6)	0.003(5)
C(40)	0.047(6)	0.035(5)	0.054(6)	0.006(4)	-0.002(5)	0.004(4)
C(41)	0.046(6)	0.045(6)	0.046(6)	-0.005(5)	-0.001(4)	0.007(5)
C(42)	0.075(8)	0.040(6)	0.052(6)	-0.013(5)	-0.007(5)	0.001(5)
C(43)	0.084(9)	0.050(7)	0.092(9)	0.016(7)	-0.013(7)	-0.005(6)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(44)	0.056(8)	0.061(9)	0.20(2)	0.028(7)	-0.016(9)	-0.017(9)
C(45)	0.046(7)	0.050(7)	0.16(1)	0.007(6)	-0.007(7)	-0.020(7)

The general temperature factor expression:

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

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Pd	C(1)	2.068(9)	Pd	C(2)	2.15(1)
Pd	C(3)	2.14(1)	Pd	C(11)	2.315(8)
Pd	C(12)	2.294(8)	Pd	C(13)	2.309(8)
Pd	C(14)	2.346(8)	Pd	C(15)	2.443(8)
S(1)	O(1)	1.619(7)	S(1)	O(2)	1.31(1)
S(1)	O(2')	1.22(2)	S(1)	C(5)	1.81(1)
O(1)	C(4)	1.44(1)	C(1)	C(2)	1.40(1)
C(1)	C(3)	1.37(1)	C(1)	C(4)	1.49(1)
C(2)	H(1)	0.95	C(2)	H(2)	0.95
C(3)	H(3)	0.95	C(3)	H(4)	0.95
C(4)	H(5)	0.95	C(4)	H(6)	0.95
C(5)	C(6)	1.37(1)	C(5)	C(10)	1.34(1)
C(6)	C(7)	1.36(2)	C(6)	H(7)	0.95
C(7)	C(8)	1.32(2)	C(7)	H(8)	0.95
C(8)	C(9)	1.34(2)	C(8)	H(9)	0.95
C(9)	C(10)	1.36(2)	C(9)	H(10)	0.95
C(10)	H(11)	0.95	C(11)	C(12)	1.46(1)
C(11)	C(15)	1.43(1)	C(11)	C(16)	1.49(1)
C(12)	C(13)	1.41(1)	C(12)	C(40)	1.50(1)
C(13)	C(14)	1.46(1)	C(13)	C(34)	1.49(1)
C(14)	C(15)	1.43(1)	C(14)	C(28)	1.49(1)
C(15)	C(22)	1.49(1)	C(16)	C(17)	1.39(1)
C(16)	C(21)	1.39(1)	C(17)	C(18)	1.37(1)
C(17)	H(12)	0.95	C(18)	C(19)	1.36(2)

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

atom	atom	distance	atom	atom	distance
C(18)	H(13)	0.95	C(19)	C(20)	1.35(2)
C(19)	H(14)	0.95	C(20)	C(21)	1.40(1)
C(20)	H(15)	0.95	C(21)	H(16)	0.95
C(22)	C(23)	1.38(1)	C(22)	C(27)	1.38(1)
C(23)	C(24)	1.38(1)	C(23)	H(17)	0.95
C(24)	C(25)	1.36(1)	C(24)	H(18)	0.95
C(25)	C(26)	1.35(1)	C(25)	H(19)	0.95
C(26)	C(27)	1.37(1)	C(26)	H(20)	0.95
C(27)	H(21)	0.95	C(28)	C(29)	1.37(1)
C(28)	C(33)	1.38(1)	C(29)	C(30)	1.38(1)
C(29)	H(22)	0.95	C(30)	C(31)	1.37(1)
C(30)	H(23)	0.95	C(31)	C(32)	1.34(1)
C(31)	H(24)	0.95	C(32)	C(33)	1.37(1)
C(32)	H(25)	0.95	C(33)	H(26)	0.95
C(34)	C(35)	1.39(1)	C(34)	C(39)	1.38(1)
C(35)	C(36)	1.38(1)	C(35)	H(27)	0.95
C(36)	C(37)	1.33(2)	C(36)	H(28)	0.95
C(37)	C(38)	1.34(2)	C(37)	H(29)	0.95
C(38)	C(39)	1.38(1)	C(38)	H(30)	0.95
C(39)	H(31)	0.95	C(40)	C(41)	1.38(1)
C(40)	C(45)	1.38(1)	C(41)	C(42)	1.37(1)
C(41)	H(32)	0.95	C(42)	C(43)	1.36(1)
C(42)	H(33)	0.95	C(43)	C(44)	1.36(1)
C(43)	H(34)	0.95	C(44)	C(45)	1.38(1)

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

atom	atom	distance	atom	atom	distance
C(44)	H(35)	0.95	C(45)	H(36)	0.95

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Pd	C(2)	38.8(4)	C(1)	Pd	C(3)	37.9(4)
C(1)	Pd	C(11)	142.7(4)	C(1)	Pd	C(12)	160.9(4)
C(1)	Pd	C(13)	156.5(4)	C(1)	Pd	C(14)	139.4(4)
C(1)	Pd	C(15)	134.1(3)	C(2)	Pd	C(3)	66.5(5)
C(2)	Pd	C(11)	177.1(4)	C(2)	Pd	C(12)	143.1(4)
C(2)	Pd	C(13)	117.7(4)	C(2)	Pd	C(14)	118.0(4)
C(2)	Pd	C(15)	142.3(4)	C(3)	Pd	C(11)	116.1(4)
C(3)	Pd	C(12)	123.6(4)	C(3)	Pd	C(13)	152.2(4)
C(3)	Pd	C(14)	169.1(4)	C(3)	Pd	C(15)	135.7(4)
C(11)	Pd	C(12)	36.9(3)	C(11)	Pd	C(13)	60.6(3)
C(11)	Pd	C(14)	59.1(3)	C(11)	Pd	C(15)	34.9(3)
C(12)	Pd	C(13)	35.7(3)	C(12)	Pd	C(14)	59.7(3)
C(12)	Pd	C(15)	59.1(3)	C(13)	Pd	C(14)	36.6(3)
C(13)	Pd	C(15)	59.4(3)	C(14)	Pd	C(15)	34.7(3)
O(1)	S(1)	O(2)	117.0(7)	O(1)	S(1)	O(2')	132(1)
O(1)	S(1)	C(5)	92.9(4)	O(2)	S(1)	O(2')	80(1)
O(2)	S(1)	C(5)	110.9(7)	O(2')	S(1)	C(5)	123(1)
S(1)	O(1)	C(4)	114.6(6)	Pd	C(1)	C(2)	73.8(6)
Pd	C(1)	C(3)	73.9(6)	Pd	C(1)	C(4)	118.0(7)
C(2)	C(1)	C(3)	116(1)	C(2)	C(1)	C(4)	118(1)
C(3)	C(1)	C(4)	125(1)	Pd	C(2)	C(1)	67.4(6)
Pd	C(2)	H(1)	82.8	Pd	C(2)	H(2)	120.5
C(1)	C(2)	H(1)	120.0	C(1)	C(2)	H(2)	119.9
H(1)	C(2)	H(2)	120.1	Pd	C(3)	C(1)	68.2(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Pd	C(3)	H(3)	82.5	Pd	C(3)	H(4)	120.2
C(1)	C(3)	H(3)	119.9	C(1)	C(3)	H(4)	120.1
H(3)	C(3)	H(4)	120.0	O(1)	C(4)	C(1)	110.5(9)
O(1)	C(4)	H(5)	109.2	O(1)	C(4)	H(6)	109.1
C(1)	C(4)	H(5)	109.3	C(1)	C(4)	H(6)	109.3
H(5)	C(4)	H(6)	109.5	S(1)	C(5)	C(6)	120(1)
S(1)	C(5)	C(10)	118(1)	C(6)	C(5)	C(10)	121(1)
C(5)	C(6)	C(7)	119(1)	C(5)	C(6)	H(7)	120.4
C(7)	C(6)	H(7)	120.6	C(6)	C(7)	C(8)	119(1)
C(6)	C(7)	H(8)	120.2	C(8)	C(7)	H(8)	119.9
C(7)	C(8)	C(9)	120(1)	C(7)	C(8)	H(9)	119.8
C(9)	C(8)	H(9)	119.3	C(8)	C(9)	C(10)	120(1)
C(8)	C(9)	H(10)	119.7	C(10)	C(9)	H(10)	119.5
C(5)	C(10)	C(9)	118(1)	C(5)	C(10)	H(11)	120.8
C(9)	C(10)	H(11)	121.0	Pd	C(11)	C(12)	70.7(5)
Pd	C(11)	C(15)	77.4(5)	Pd	C(11)	C(16)	123.8(6)
C(12)	C(11)	C(15)	108.0(7)	C(12)	C(11)	C(16)	128.5(8)
C(15)	C(11)	C(16)	123.0(8)	Pd	C(12)	C(11)	72.3(5)
Pd	C(12)	C(13)	72.7(5)	Pd	C(12)	C(40)	124.0(6)
C(11)	C(12)	C(13)	108.6(7)	C(11)	C(12)	C(40)	126.1(8)
C(13)	C(12)	C(40)	125.2(8)	Pd	C(13)	C(12)	71.5(5)
Pd	C(13)	C(14)	73.0(5)	Pd	C(13)	C(34)	124.7(6)
C(12)	C(13)	C(14)	106.7(7)	C(12)	C(13)	C(34)	128.6(8)
C(14)	C(13)	C(34)	124.5(8)	Pd	C(14)	C(13)	70.3(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Pd	C(14)	C(15)	76.4(5)	Pd	C(14)	C(28)	124.9(6)
C(13)	C(14)	C(15)	109.2(7)	C(13)	C(14)	C(28)	124.9(7)
C(15)	C(14)	C(28)	125.6(8)	Pd	C(15)	C(11)	67.7(4)
Pd	C(15)	C(14)	69.0(4)	Pd	C(15)	C(22)	130.6(6)
C(11)	C(15)	C(14)	107.0(7)	C(11)	C(15)	C(22)	126.4(7)
C(14)	C(15)	C(22)	126.6(8)	C(11)	C(16)	C(17)	120.7(8)
C(11)	C(16)	C(21)	121.5(8)	C(17)	C(16)	C(21)	117.6(9)
C(16)	C(17)	C(18)	121.4(9)	C(16)	C(17)	H(12)	119.3
C(18)	C(17)	H(12)	119.3	C(17)	C(18)	C(19)	120(1)
C(17)	C(18)	H(13)	119.8	C(19)	C(18)	H(13)	119.8
C(18)	C(19)	C(20)	120(1)	C(18)	C(19)	H(14)	119.9
C(20)	C(19)	H(14)	120.0	C(19)	C(20)	C(21)	120(1)
C(19)	C(20)	H(15)	119.7	C(21)	C(20)	H(15)	119.6
C(16)	C(21)	C(20)	119.8(9)	C(16)	C(21)	H(16)	120.1
C(20)	C(21)	H(16)	120.1	C(15)	C(22)	C(23)	122.2(8)
C(15)	C(22)	C(27)	119.6(8)	C(23)	C(22)	C(27)	118.1(8)
C(22)	C(23)	C(24)	121.1(8)	C(22)	C(23)	H(17)	119.4
C(24)	C(23)	H(17)	119.5	C(23)	C(24)	C(25)	119.2(9)
C(23)	C(24)	H(18)	120.4	C(25)	C(24)	H(18)	120.4
C(24)	C(25)	C(26)	120.4(9)	C(24)	C(25)	H(19)	119.9
C(26)	C(25)	H(19)	119.8	C(25)	C(26)	C(27)	120.7(9)
C(25)	C(26)	H(20)	119.6	C(27)	C(26)	H(20)	119.6
C(22)	C(27)	C(26)	120.5(9)	C(22)	C(27)	H(21)	119.8
C(26)	C(27)	H(21)	119.8	C(14)	C(28)	C(29)	120.8(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(28)	C(33)	121.5(8)	C(29)	C(28)	C(33)	117.6(8)
C(28)	C(29)	C(30)	120.9(9)	C(28)	C(29)	H(22)	119.5
C(30)	C(29)	H(22)	119.5	C(29)	C(30)	C(31)	119.9(10)
C(29)	C(30)	H(23)	120.0	C(31)	C(30)	H(23)	120.1
C(30)	C(31)	C(32)	120(1)	C(30)	C(31)	H(24)	119.7
C(32)	C(31)	H(24)	119.9	C(31)	C(32)	C(33)	119(1)
C(31)	C(32)	H(25)	120.1	C(33)	C(32)	H(25)	120.1
C(28)	C(33)	C(32)	121.3(9)	C(28)	C(33)	H(26)	119.3
C(32)	C(33)	H(26)	119.4	C(13)	C(34)	C(35)	118.9(9)
C(13)	C(34)	C(39)	122.5(9)	C(35)	C(34)	C(39)	118.6(9)
C(34)	C(35)	C(36)	119(1)	C(34)	C(35)	H(27)	120.2
C(36)	C(35)	H(27)	120.3	C(35)	C(36)	C(37)	121(1)
C(35)	C(36)	H(28)	119.4	C(37)	C(36)	H(28)	119.6
C(36)	C(37)	C(38)	120(1)	C(36)	C(37)	H(29)	119.8
C(38)	C(37)	H(29)	120.1	C(37)	C(38)	C(39)	121(1)
C(37)	C(38)	H(30)	119.2	C(39)	C(38)	H(30)	119.3
C(34)	C(39)	C(38)	119(1)	C(34)	C(39)	H(31)	120.4
C(38)	C(39)	H(31)	120.5	C(12)	C(40)	C(41)	120.9(8)
C(12)	C(40)	C(45)	122.4(8)	C(41)	C(40)	C(45)	116.6(9)
C(40)	C(41)	C(42)	121.8(9)	C(40)	C(41)	H(32)	119.0
C(42)	C(41)	H(32)	119.1	C(41)	C(42)	C(43)	120.6(9)
C(41)	C(42)	H(33)	119.6	C(43)	C(42)	H(33)	119.8
C(42)	C(43)	C(44)	118(1)	C(42)	C(43)	H(34)	120.5
C(44)	C(43)	H(34)	120.6	C(43)	C(44)	C(45)	120(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(43)	C(44)	H(35)	119.7	C(45)	C(44)	H(35)	119.7
C(40)	C(45)	C(44)	121.5(10)	C(40)	C(45)	H(36)	119.2
C(44)	C(45)	H(36)	119.3				