SUPPORTING INFORMATION

The First Structurally Characterized Example of a η^5-Coordinate Mesitylato Palladium Complex

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Supplementary Figures (Figures S1 – S2 = 2 pages)

Figure S1 View along the b axis in [(COD)Pd(OMes)](SbF$_6$) in the crystal.

Figure S2 View upon one layer of molecules [(COD)Pd(OMes)](SbF$_6$) in the b-c plane.

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Table S2 Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (Å^2 x 10^3) for [(COD)Pd(OMes)](SbF$_6$). U(eq) is defined as one Third of the Trace of the Orthogonalized U_{ij} Tensor.

Table S3 Bond lengths [Å] and angles [°] for [(COD)Pd(OMes)](SbF$_6$).

Table S4 Anisotropic Displacement Parameters (Å^2 x 10^3) for [(COD)Pd(OMes)](SbF$_6$). The Anisotropic Displacement Factor Exponent takes the Form: $-2\pi^2 \cdot [h^2 \cdot a^{*2} \cdot U11 + ... + 2 \cdot h \cdot k \cdot a^* \cdot b^* \cdot U12]$

Table S5 Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters (Å^2 x 10^3) for [(COD)Pd(OMes)](SbF$_6$).

Figure S1

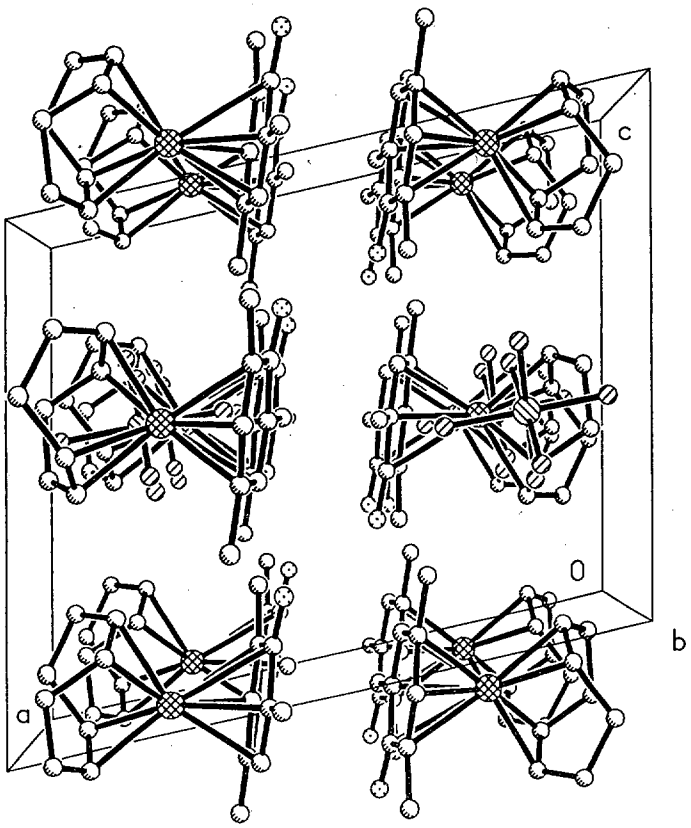

Figure S2

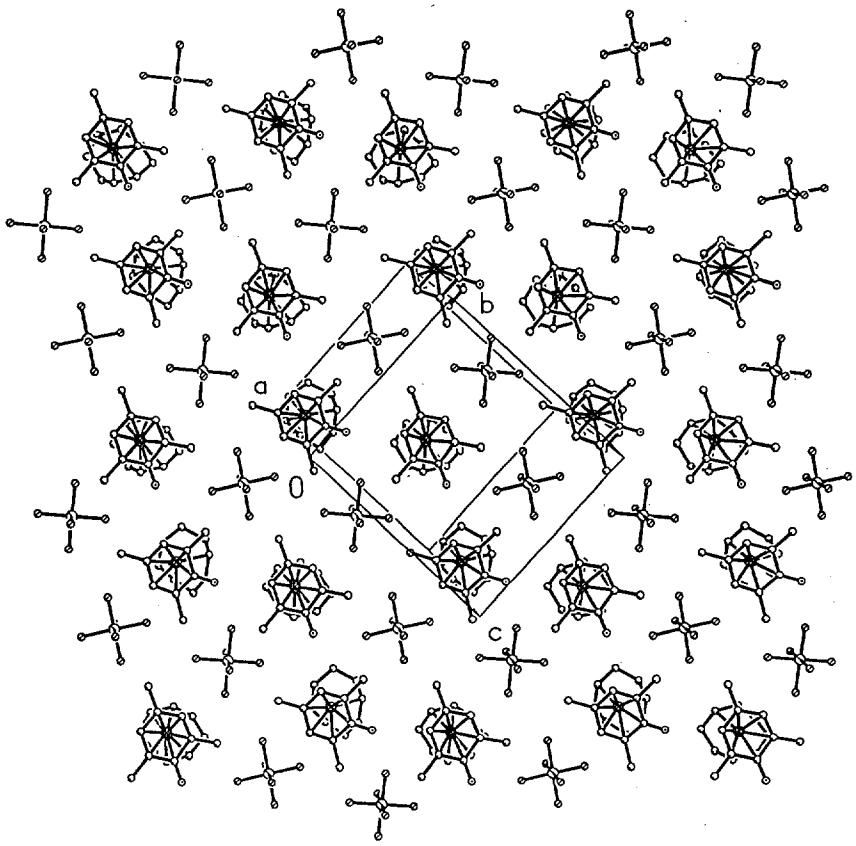

Table S1. Crystal data and structure refinement for [(COD)Pd(OMes)](SbF$_6$).

Identification code	akb01a
Empirical formula	$C_{17}H_{23}O_1Pd_1Sb_1F_6$
Formula weight	585.5
Temperature	183(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P2(1)/c
Unit cell dimensions	
a: =	14.710(5) Å alpha = 90°
b: =	11.018(3) Å beta = 102.5(3)°
c: =	12.064(3) Å gamma = 90°
Volume, Z	1908.8(10) Å^3, 4
Density (calculated)	2.037 g · cm^{-1}
Absorption coefficient	2.416 mm^{-1}
F(000)	1136
Crystal size	0.3 x 0.2 x 0.2 mm
θ range for data collection	2.33 to 27.49°
Limiting indices	-19 < h: < 18, -14 < k: < 1, -15 < l: < 15
Reflections collected	5044
Independent reflections	4123 (R_{int} = 0.0633)
Completeness to θ = 27.49°	94.3 %
Absorption correction	XABS 2
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4123 / 0 / 260
Goodness-of-fit on F^2	0.988
Final R indices [I>2σ(I)]	R1 = 0.0511, wR2 = 0.0876
R indices (all data)	R1 = 0.1127, wR2 = 0.1058
Largest diff. peak and hole	0.897 and –0.693 e·Å^{-3}

Table S2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for [(COD)Pd(OMes)](SbF_6). U(eq) is defined as one Third of the Trace of the Orthogonalized U_{ij} Tensor.

	x	y	z	U(eq)
Pd	2547(1)	-877(1)	9411(1)	22(1)
Sb	2031(1)	1106(1)	4331(1)	27(1)
F(1)	770(4)	1079(7)	4278(6)	98(3)
F(2)	1888(6)	2452(5)	3381(5)	87(3)
F(3)	1840(4)	85(4)	3057(4)	45(1)
F(4)	3303(4)	1155(5)	4393(5)	65(2)
F(5)	2216(5)	-261(4)	5269(4)	60(2)
F(6)	2202(4)	2120(4)	5596(4)	54(2)
O	4257(4)	-1728(5)	7903(5)	42(2)
C(1)	4088(5)	-1246(7)	8756(7)	26(2)
C(2)	4043(5)	-1940(7)	9780(7)	28(2)
C(3)	3899(5)	-1368(6)	10759(6)	24(2)
C(4)	3681(6)	-105(7)	10739(7)	28(2)
C(5)	3734(5)	594(7)	9764(6)	22(2)
C(6)	3860(5)	79(7)	8767(7)	27(2)
C(7)	4239(7)	-3291(7)	9771(9)	42(2)
C(8)	3548(6)	514(8)	11811(7)	34(2)
C(9)	3839(7)	797(8)	7723(7)	42(2)
C(12)	768(6)	-2508(7)	8668(7)	31(2)
C(13)	1632(6)	-2166(7)	8242(7)	28(2)
C(14)	1749(5)	-1127(7)	7647(6)	29(2)
C(15)	1073(6)	-56(7)	7437(6)	31(2)
C(16)	603(6)	221(7)	8424(7)	31(2)
C(17)	1249(5)	83(7)	9601(6)	23(2)
C(18)	1341(5)	-943(7)	10261(6)	26(2)
C(19)	860(6)	-2142(7)	9925(7)	34(2)

Table S3. Bond lengths [Å] and angles [°] for [(COD)Pd(OMes)](SbF$_6$).

bond lenghts (Å)	
Pd-C(14)	2.213(7)
Pd-C(4)	2.219(8)
Pd-C(13)	2.234(7)
Pd-C(18)	2.234(7)
Pd-C(17)	2.238(7)
Pd-C(3)	2.345(8)
Pd-C(5)	2.353(7)
Pd-C(2)	2.447(8)
Pd-C(6)	2.468(8)
Pd-C(1)	2.588(8)
Sb-F(1)	1.842(6)
Sb-F(4)	1.858(6)
Sb-F(2)	1.858(5)
Sb-F(6)	1.864(5)
Sb-F(5)	1.868(5)
Sb-F(3)	1.876(5)
O-C(1)	1.230(9)
C(1)-C(2)	1.467(10)
C(1)-C(6)	1.499(10)
C(2)-C(3)	1.394(10)
C(2)-C(7)	1.517(10)
C(3)-C(4)	1.428(10)
C(4)-C(5)	1.422(10)
C(4)-C(8)	1.511(10)
C(5)-C(6)	1.378(10)
C(6)-C(9)	1.482(10)
C(12)-C(13)	1.517(11)
C(12)-C(19)	1.547(11)
C(13)-C(14)	1.382(10)
C(14)-C(15)	1.529(10)
C(15)-C(16)	1.531(10)
C(16)-C(17)	1.535(10)
C(17)-C(18)	1.373(10)
C(18)-C(19)	1.512(10)

angles (°)	
C(14)-Pd-C(4)	154.4(3)
C(14)-Pd-C(13)	36.2(3)
C(4)-Pd-C(13)	162.9(3)
C(14)-Pd-C(18)	97.4(3)
C(4)-Pd-C(18)	103.2(3)
C(13)-Pd-C(18)	80.8(3)
C(14)-Pd-C(17)	82.6(3)
C(4)-Pd-C(17)	105.6(3)
C(13)-Pd-C(17)	87.4(3)
C(18)-Pd-C(17)	35.8(3)
C(14)-Pd-C(3)	146.3(3)
C(4)-Pd-C(3)	36.3(3)
C(13)-Pd-C(3)	126.6(3)
C(18)-Pd-C(3)	108.2(3)
C(17)-Pd-C(3)	130.7(3)
C(14)-Pd-C(5)	118.5(3)
C(4)-Pd-C(5)	36.1(3)
C(13)-Pd-C(5)	150.9(3)
C(18)-Pd-C(5)	124.8(3)
C(17)-Pd-C(5)	105.8(3)
C(3)-Pd-C(5)	63.1(3)

Table S3 continued

C(14)-Pd-C(2)	112.6(3)
C(4)-Pd-C(2)	63.0(3)
C(13)-Pd-C(2)	101.9(3)
C(18)-Pd-C(2)	132.3(3)
C(17)-Pd-C(2)	164.0(3)
C(3)-Pd-C(2)	33.7(2)
C(5)-Pd-C(2)	72.2(3)
C(14)-Pd-C(6)	92.2(3)
C(4)-Pd-C(6)	63.0(3)
C(13)-Pd-C(6)	118.6(3)
C(18)-Pd-C(6)	155.7(3)
C(17)-Pd-C(6)	125.0(3)
C(3)-Pd-C(6)	73.3(3)
C(5)-Pd-C(6)	33.1(2)
C(2)-Pd-C(6)	61.8(2)
C(14)-Pd-C(1)	90.2(3)
C(4)-Pd-C(1)	73.1(3)
C(13)-Pd-C(1)	98.9(3)
C(18)-Pd-C(1)	165.8(3)
C(17)-Pd-C(1)	158.2(3)
C(3)-Pd-C(1)	60.5(3)
C(5)-Pd-C(1)	59.9(2)
C(2)-Pd-C(1)	33.7(2)
C(6)-Pd-C(1)	34.4(2)
F(1)-Sb-F(4)	179.2(3)
F(1)-Sb-F(2)	90.8(4)
F(4)-Sb-F(2)	88.8(3)
F(1)-Sb-F(6)	89.7(3)
F(4)-Sb-F(6)	89.6(3)
F(2)-Sb-F(6)	90.2(2)
F(1)-Sb-F(5)	91.3(3)
F(4)-Sb-F(5)	89.2(3)
F(2)-Sb-F(5)	177.8(3)
F(6)-Sb-F(5)	90.7(2)
F(1)-Sb-F(3)	89.5(3)
F(4)-Sb-F(3)	91.2(2)
F(2)-Sb-F(3)	89.8(2)
F(6)-Sb-F(3)	179.2(3)
F(5)-Sb-F(3)	89.4(2)
O-C(1)-C(2)	122.3(7)
O-C(1)-C(6)	120.9(7)
C(2)-C(1)-C(6)	116.7(7)
O-C(1)-Pd	132.2(6)
C(2)-C(1)-Pd	67.8(4)
C(6)-C(1)-Pd	68.4(4)
C(3)-C(2)-C(1)	121.4(7)
C(3)-C(2)-C(7)	120.9(7)
C(1)-C(2)-C(7)	117.5(8)
C(3)-C(2)-Pd	69.1(4)
C(1)-C(2)-Pd	78.4(4)
C(7)-C(2)-Pd	129.3(6)
C(2)-C(3)-C(4)	120.1(7)
C(2)-C(3)-Pd	77.2(5)
C(4)-C(3)-Pd	67.0(4)
C(5)-C(4)-C(3)	119.3(7)
C(5)-C(4)-C(8)	120.2(7)
C(3)-C(4)-C(8)	119.7(7)
C(5)-C(4)-Pd	77.1(5)

Table S3 continued

C(3)-C(4)-Pd	76.6(5)
C(8)-C(4)-Pd	125.1(6)
C(6)-C(5)-C(4)	122.7(7)
C(6)-C(5)-Pd	78.0(5)
C(4)-C(5)-Pd	66.8(4)
C(5)-C(6)-C(9)	122.7(7)
C(5)-C(6)-C(1)	118.8(7)
C(9)-C(6)-C(1)	118.4(7)
C(5)-C(6)-Pd	68.9(4)
C(9)-C(6)-Pd	128.5(6)
C(1)-C(6)-Pd	77.2(4)
C(13)-C(12)-C(19)	111.4(6)
C(14)-C(13)-C(12)	126.1(8)
C(14)-C(13)-Pd	71.1(4)
C(12)-C(13)-Pd	112.3(5)
C(13)-C(14)-C(15)	125.1(7)
C(13)-C(14)-Pd	72.7(4)
C(15)-C(14)-Pd	104.7(5)
C(14)-C(15)-C(16)	114.3(6)
C(15)-C(16)-C(17)	114.0(6)
C(18)-C(17)-C(16)	125.6(7)
C(18)-C(17)-Pd	72.0(4)
C(16)-C(17)-Pd	108.8(5)
C(17)-C(18)-C(19)	125.6(7)
C(17)-C(18)-Pd	72.3(4)
C(19)-C(18)-Pd	106.1(5)
C(18)-C(19)-C(12)	115.3(6)

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [(COD)Pd(OMes)](SbF$_6$). The Anisotropic Displacement Factor Exponent takes the Form:

$-2\pi^2 \cdot [h^2 \cdot a^{*2} \cdot U11 + ... + 2 \cdot h \cdot k \cdot a^* \cdot b^* \cdot U12]$

	U11	U22	U33	U23	U13	U12
Pd	18(1)	25(1)	22(1)	-3(1)	3(1)	-1(1)
Sb	29(1)	24(1)	28(1)	-3(1)	5(1)	1(1)
F(1)	29(3)	157(7)	108(6)	-73(5)	12(4)	-3(4)
F(2)	159(8)	38(3)	56(4)	13(3)	3(4)	27(4)
F(3)	62(4)	44(3)	32(3)	-12(2)	14(3)	-14(3)
F(4)	40(3)	77(4)	82(5)	-21(4)	23(3)	-15(3)
F(5)	102(5)	35(3)	44(3)	10(2)	20(3)	-2(3)
F(6)	81(5)	39(3)	39(3)	-15(3)	10(3)	0(3)
O	40(4)	53(4)	36(3)	-11(3)	18(3)	-4(3)
C(1)	12(4)	36(4)	29(4)	-6(4)	3(3)	-1(4)
C(2)	21(4)	27(4)	33(5)	5(4)	-1(4)	-1(3)
C(3)	24(4)	28(4)	20(4)	2(3)	5(3)	2(3)
C(4)	21(4)	30(4)	31(4)	-3(4)	2(4)	1(3)
C(5)	11(3)	27(4)	28(4)	3(3)	2(3)	2(3)
C(6)	15(4)	36(4)	26(4)	11(4)	-1(3)	5(3)
C(7)	42(6)	22(4)	64(7)	-8(4)	15(5)	-2(4)
C(8)	29(5)	46(5)	29(4)	-10(4)	9(4)	-5(4)
C(9)	49(6)	54(6)	22(4)	14(4)	4(4)	-1(5)
C(12)	24(5)	26(4)	40(5)	-3(4)	1(4)	-8(3)
C(13)	24(4)	26(4)	30(4)	-11(4)	1(4)	-3(3)
C(14)	28(4)	37(4)	20(4)	-10(4)	4(3)	1(4)
C(15)	30(5)	38(4)	23(4)	-1(4)	-1(4)	-8(4)
C(16)	25(4)	28(4)	39(5)	8(4)	4(4)	6(4)
C(17)	19(4)	30(4)	24(4)	-11(3)	9(3)	4(3)
C(18)	23(4)	36(4)	21(4)	0(4)	10(3)	1(4)
C(19)	25(5)	37(5)	42(5)	4(4)	13(4)	-11(4)

Table S5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for [(COD)Pd(OMes)](SbF$_6$).

	x	y	z	U(eq)
H(3A)	3851	-1867	11437	30(20)
H(5A)	3548	1468	9751	16(18)
H(7A)	4901	-3421	9785	100(40)
H(7B)	3861	-3655	9082	40(30)
H(7C)	4082	-3670	10441	80(40)
H(8A)	4155	765	12264	90(40)
H(8B)	3253	-51	12252	70(40)
H(8C)	3151	1230	11611	30(20)
H(9A)	4474	884	7602	18(19)
H(9B)	3579	1603	7806	100(50)
H(9C)	3452	381	7071	100(40)
H(12A)	668	-3395	8588	30(20)
H(12B)	219	-2098	8196	60(30)
H(13A)	1975	-2883	8031	130(50)
H(14A)	2137	-1231	7067	11(17)
H(15A)	585	-226	6751	37
H(15B)	1416	676	7281	70(30)
H(16A)	65	-331	8375	40(20)
H(16B)	362	1062	8343	60(30)
H(17A)	1364	856	10043	50(30)
H(18A)	1505	-788	11097	50(30)
H(19A)	228	-2105	10085	50(30)
H(19B)	1207	-2787	10410	50(30)