1110 *Organometallics* **1995,** *14,* 1110−1114

Articles

Preparation and X-ray Crystal and Molecular Structure of *cis*-$[(dppp)Pd(H_2O)(OSO_2CF_3)]^+(OSO_2CF_3)^-$ and *cis*-$[(dppp)Pd(H_2O)_2]^{2+}(OSO_2CF_3)^-{}_2$. Coordinated Water−Triflate Hydrogen Bonds[†]

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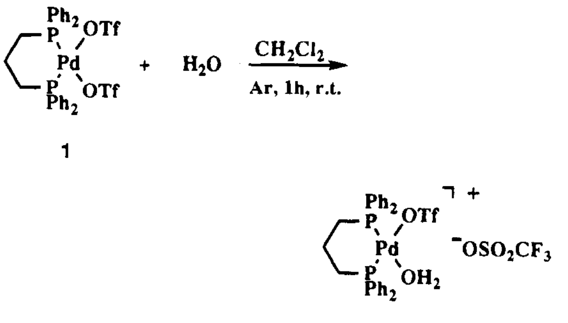
Reaction of 1 and 2 equiv of water, respectively, with *cis*-(1,3-bis(diphenylphosphino)-propane)palladium(II) triflate yields the corresponding monoaquo and diaquo cationic Pd complexes **2** and **3** in 86% and 99% yield respectively, as yellow, air-stable, microcrystalline solids. The molecular structures of $[(dppp)Pd(OH_2)(OSO_2CF_3)_2]$, (**2**) and $[(dppp)Pd(OH_2)_2(OSO_2CF_3)_2]$, (**3**) have been determined by single-crystal X-ray crystallography. Complex **2** crystallizes in the monoclinic space group $P2_1/n$ with $Z = 4$, $a = 13.857(5)$ Å, $b = 13.335(5)$ Å, $c = 19.054(8)$ Å, $\beta = 102.98(2)°$, $R = 0.0461$, and $R_w = 0.0614$ at 298 K. Complex **3** crystallizes in the triclinic space group $P\bar{1}$ with $Z = 2$, $a = 11.440(1)$ Å, $b = 11.800(1)$ Å, $c = 14.269(1)$ Å, $\alpha = 95.66(1)°$, $\beta = 94.49(1)°$, $\gamma = 109.15(1)°$, $R = 0.0301$, and $R_w = 0.0467$ at 298 K.

There is considerable current interest in transition-metal solvent complexes in general and water complexes in particular.[1,2] Although several monoaquo cationic transition-metal complexes are known,[2] there is much less information on diaquo complexes and the molecular structure of aquo complexes in general. Moreover, whereas a number of platinum aquo complexes are known, there have been very few palladium aquo complexes reported. Therefore, in this paper we wish to report the ready, high-yield preparation and the X-ray crystal molecular structures of both the monoaquo and diaquo palladium(II) cationic complexes **2** and **3**.

Results and Discussion

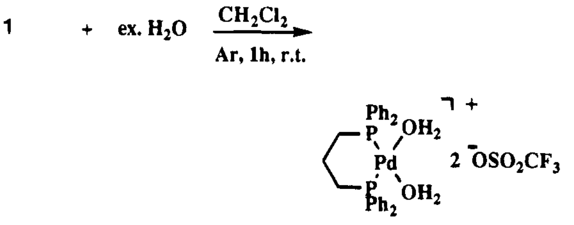
Reaction of exactly 1 equiv of water with anhydrous $[(dppp)Pd(OSO_2CF_3)_2]$ (**1**)[3] in CH_2Cl_2 at room temperature under an argon atmosphere results in an 86% yield of the monoaquo complex **2** (eq 1). Likewise, interaction of **1** with 2 equiv or more of water yields the diaquo complex **3** in 99% isolated yield (eq 2). Complexes **2** and **3** are respectively light yellow and yellow, air-stable, microcrystalline solids.



1

(1)

2



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(2)

3

Single-Crystal Molecular Structure Determination. Suitable single crystals for X-ray structure determination of **2** and **3**, were obtained by careful layering of diethyl ether over a CH_2Cl_2 solution of **2** and **3**, respectively, at room temperature. Both compounds crystallize as hexagonal platelets. Crystallographic data are summarized in Table 1, and the final atomic coordinates of the heavy atoms are given in Tables 2 and 3. Relevant bond distances and bond angles are reported in Table 4. ORTEP diagrams are displayed in Figures 1 and 2, respectively.

[†] Dedicated to Professor William M. Jones on the occasion of his 65th birthday.

[⊗] Abstract published in *Advance ACS Abstracts,* February 15, 1995.

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0276-7333/95/2314-1110$09.00/0

Table 1. Crystal and Data Collection Parameters for Compounds 2 and 3

	2	3
molecular formula	$PdS_2P_2F_6O_7C_{29}H_{28}$	$PdS_2P_2F_6O_8C_{29}H_{30}$
fw	835.009	853.024
space group	$P2_1/n$	$P\bar{1}$
space group no.	14	2
cryst syst	monoclinic	triclinic
cell constants		
a (Å)	13.857(5)	11.440(1)
b (Å)	13.335(5)	11.800(1)
c (Å)	19.054(8)	14.269(1)
α (deg)		95.66(1)
β (deg)	102.98(2)	94.49(1)
γ (deg)		109.15(1)
V (Å^3)	3431.08	1798.15
Z	4	2
D_{calc} (g cm^{-3})	1.618	1.575
cryst dimens (mm)	0.33 × 0.30 × 0.27	0.29 × 0.32 × 0.37
abs coeff (cm^{-1})	8.158	7.809
radiation	Mo (0.710 73 Å)	Mo (0.710 73 Å)
no. of unique rflns	5337	6310
2θ range (deg)	2.00–50.00	2.00–50.00
scan technique	$\theta/2\theta$	$\theta/2\theta$
scan speed (deg min^{-1})	variable	4.5
scan width (deg)	0.8000 + 0.3400 (tan θ)	K −1.2 to K +1.2
no of rflns between stds	1 X-ray h	98
abs cor	empirical	empirical
min transmissn (%)	84.8748	90.03
max transmissn (%)	99.9052	99.99
highest peak, final diff Fourier (e Å^{-3})	1.151 (about 1.050 Å from Pd)	0.698
weighting scheme	non-Poisson contribn	non-Poisson contribn
ignorance factor, P	0.04	0.05
data rejected if I	$<3.00\sigma(I)$	$<3.00\sigma(I)$
data rejected if (sin θ)/λ	<0.0500	<0.0500
no. of observs	4198	5566
no. of variables	509	554
data to param ratio	8.248	10.047
shift to error ratio	0.018	0.016
error in an observn of unit wt (GOF)	2.2949	1.3400
R (R_w)	0.0461 (0.0614)	0.0301 (0.0467)

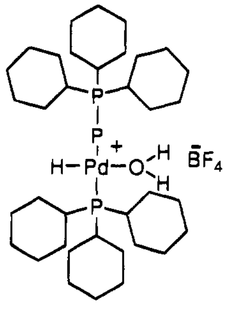
Table 2. Positional Parameters and Estimated Standard Deviations for Compound 2

atom	x	y	z
Pd	0.21098(2)	0.16094(3)	0.47998(2)
S1	0.3985(1)	0.1034(1)	0.61921(7)
S2	0.1414(1)	−0.2548(1)	0.48825(7)
P1	0.19812(8)	0.32802(9)	0.48256(6)
P2	0.12216(8)	0.15671(9)	0.36697(6)
F1	0.4719(3)	0.1155(3)	0.5051(2)
F2	0.5124(3)	0.2364(3)	0.5796(3)
F3	0.5802(3)	0.0934(3)	0.6037(3)
F4	0.3092(3)	−0.3188(5)	0.5632(4)
F5	0.2537(5)	−0.1942(4)	0.6078(3)
F6	0.1927(4)	−0.3369(4)	0.6139(3)
O1	0.2331(3)	0.0046(3)	0.4843(2)
O2	0.3142(3)	0.1655(3)	0.5833(2)
O3	0.4377(4)	0.1298(4)	0.6917(2)
O4	0.3855(3)	−0.0010(3)	0.6041(2)
O5	0.1231(3)	−0.3515(3)	0.4565(3)
O6	0.0573(3)	−0.2150(4)	0.5111(2)
O7	0.1862(3)	−0.1844(4)	0.4490(2)
C1	0.0853(3)	0.3862(4)	0.4326(3)
C2	0.0624(4)	0.3601(4)	0.3525(3)
C3	0.0280(3)	0.2521(3)	0.3375(2)
C4	0.2981(3)	0.3837(3)	0.4496(2)
C5	0.3060(4)	0.4861(5)	0.4440(4)
C6	0.3838(5)	0.5252(5)	0.4170(4)
C7	0.4516(4)	0.4687(5)	0.3981(3)
C8	0.4457(4)	0.3667(5)	0.4034(3)
C9	0.3689(4)	0.3237(4)	0.4278(3)
C10	0.2095(3)	0.3691(4)	0.5741(2)
C11	0.3029(4)	0.3895(4)	0.6185(3)
C12	0.3101(4)	0.4196(5)	0.6877(3)
C13	0.2298(5)	0.4302(5)	0.7166(3)
C14	0.1391(4)	0.4076(5)	0.6752(3)
C15	0.1277(4)	0.3776(4)	0.6040(3)
C16	0.0536(3)	0.0401(3)	0.3513(2)
C17	0.0661(4)	−0.0268(4)	0.2991(3)
C18	0.0065(5)	−0.1112(4)	0.2860(3)
C19	−0.0652(5)	−0.1273(4)	0.3236(3)
C20	−0.0775(4)	−0.0619(4)	0.3757(3)
C21	−0.0178(4)	0.0215(4)	0.3906(3)
C22	0.2077(3)	0.1591(4)	0.3075(2)
C23	0.1919(4)	0.2193(4)	0.2462(3)
C24	0.2589(4)	0.2175(5)	0.2031(3)
C25	0.3399(4)	0.1576(5)	0.2187(3)
C26	0.3564(4)	0.0982(5)	0.2779(3)
C27	0.2911(4)	0.0989(5)	0.3228(3)
C28	0.4960(4)	0.1390(5)	0.5743(4)
C29	0.2277(5)	−0.2760(5)	0.5703(5)

Perusal of the data in Table 4 reveals a number of unusual and interesting aspects about the molecular structures of complexes **2** and **3**. In both complexes the Pd(II) atom has a distorted-square-planar coordination: the two cis sites are occupied by the dppp ligand, while the remaining two sites are taken up by the coordinated water and a covalently bound triflate in **2** and two coordinated water molecules in **3**.

The bond angles around the palladium atom are close to the expected values of 90°, ranging in values from 86.1 to 93.2° for **2** and 87.66 to 93.38° for **3**. The P–Pd–P chelation angle is just over 90° in both **2** and **3**, whereas the O_1–Pd–O_2 angles are 86.1 and 87.66° for **2** and **3**, respectively. The palladium–phosphorus bond distances of 2.226–2.237 Å are in the normal range for cis-chelated phosphorus. The Pd–OH_2 distance in **2** is 2.159 Å, whereas in **3** these distances are 2.127 and 2.135 Å. These values compare favorably with the corresponding bond angles and bond distances in the related Pd–OH_2 complex *trans*-$[(Cy_3P)_2Pd(H)(OH_2)]^+BF_4^-$ (**4**), recently reported by Leoni and coworkers.[2b]

Particularly noteworthy are the hydrogen-bonding patterns in complexes **2** and **3**. In the monoaquo complex **2**, the hydrogens of the complexed water molecule are hydrogen-bonded intramolecularly to the coordinated triflate and intermolecularly to the anionic triflate counterion with an O–H- - -O distance of approximately 2.0 Å. A comparable hydrogen-bonding pattern was observed in the chelated Pt–OH_2 complex $[Pt(NH(CH_3)C_2H_4NH(CH_3))(H_2O)(SO_4)]{\cdot}H_2O$ (**5**), reported by Rochon and Melanson.[5] In complex **3**, however, both coordinated water molecules are doubly hydrogen-bonded to the two triflate counterions. Interestingly, the two water molecules are each hydrogen-bonded to different triflates rather than the same one, as seen in the ORTEP representation. Similarly, both hydrogens in the aquo complex **4** are hydrogen-bonded to the fluorines of the BF_4^- anion.[2b] The role of



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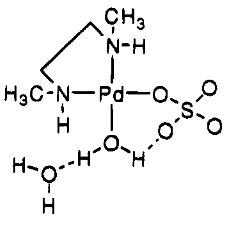

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Table 3. Positional Parameters and Estimated Standard Deviations for Compound 3

atom	*x*	*y*	*z*
Pd	0.17963(1)	0.12857(1)	0.29772(1)
S1	−0.04504(6)	−0.22004(7)	0.41900(5)
S2	0.29620(6)	−0.12651(7)	0.13519(5)
P1	0.07386(5)	0.23363(5)	0.23057(4)
P2	0.34196(5)	0.29797(5)	0.34223(4)
F1	−0.0166(3)	−0.4258(2)	0.4330(3)
F2	−0.1936(3)	−0.4389(3)	0.3622(3)
F3	−0.0309(3)	−0.3856(3)	0.2918(2)
F4	0.2059(3)	−0.3318(2)	0.0261(2)
F5	0.3438(2)	−0.3277(2)	0.1361(2)
F6	0.1648(3)	−0.3390(2)	0.1707(2)
O1	0.0388(2)	−0.0347(2)	0.2339(1)
O2	0.2649(2)	0.0199(2)	0.3691(1)
O3	−0.1023(2)	−0.2306(2)	0.5033(2)
O4	−0.1055(2)	−0.1800(2)	0.3439(2)
O5	0.0880(2)	−0.1652(3)	0.4332(2)
O6	0.1820(2)	−0.1067(2)	0.1130(2)
O7	0.3448(2)	−0.0991(2)	0.2347(2)
O8	0.3866(2)	−0.0920(3)	0.0708(2)
C1	0.0917(2)	0.3787(2)	0.2969(2)
C2	0.2224(2)	0.4681(2)	0.3200(2)
C3	0.3058(2)	0.4287(2)	0.3888(2)
C4	−0.0898(2)	0.1501(2)	0.2288(2)
C5	−0.1306(2)	0.1123(3)	0.3123(2)
C6	−0.2557(3)	0.0527(4)	0.3155(3)
C7	−0.3381(3)	0.0284(3)	0.2356(3)
C8	−0.2980(3)	0.0648(4)	0.1538(3)
C9	−0.1739(3)	0.1249(3)	0.1472(2)
C10	0.1057(2)	0.2546(2)	0.1105(2)
C11	0.1023(3)	0.3554(3)	0.0707(2)
C12	0.1264(4)	0.3661(3)	−0.0213(2)
C13	0.1534(3)	0.2773(3)	−0.0746(2)
C14	0.1563(3)	0.1769(3)	−0.0363(2)
C15	0.1328(3)	0.1642(3)	0.0557(2)
C16	0.4478(2)	0.2746(2)	0.4338(2)
C17	0.5652(3)	0.2760(3)	0.4162(2)
C18	0.6421(3)	0.2528(3)	0.4872(3)
C19	0.6047(3)	0.2310(3)	0.5722(3)
C20	0.4887(4)	0.2301(3)	0.5904(2)
C21	0.4086(3)	0.2519(3)	0.5212(2)
C22	0.4281(2)	0.3391(2)	0.2433(2)
C23	0.4306(3)	0.2497(3)	0.1738(2)
C24	0.4973(4)	0.2791(5)	0.0984(3)
C25	0.5562(4)	0.3974(5)	0.0899(3)
C26	0.5562(4)	0.4874(4)	0.1566(3)
C27	0.4908(3)	0.4580(3)	0.2344(3)
C28	−0.0735(4)	−0.3772(4)	0.3725(3)
C29	0.2512(4)	−0.2893(3)	0.1166(3)

Table 4. Relevant Bond Distances (Å) and Angles (deg) for Compounds 2 and 3[a]

Compound 2			
Pd−O1	2.106(4)	P2−C3	1.819(5)
Pd−O2	2.159(3)	P2−C16	1.812(5)
Pd−P1	2.237(1)	P2−C22	1.815(5)
Pd−P2	2.228(1)	S1−O2	1.469(4)
P1−C1	1.812(5)	S1−O3	1.411(5)
P1−C4	1.805(5)	S1−O4	1.425(5)
P1−C10	1.801(5)	S2−O5	1.424(4)
O1−H1	0.71(6)	S2−O6	1.435(5)
O1−H2	0.74(6)	S2−O7	1.426(5)
O4- - -H2	2.04(6)	S1−C28	1.817(8)
O7- - -H1	2.00(7)	S2−C29	1.76(1)
P1−Pd−P2	90.98(4)	P2−Pd−O2	172.3(1)
O1−Pd−O2	86.1(2)	P1−Pd−O1	175.5(1)
P1−Pd−O2	89.5(1)	H1−O1−H2	107(7)
P2−Pd−O1	93.2(1)	O1−H1−O7	153(7)
		O1−H2−O4	157(7)
Compound 3			
Pd−O1	2.127(2)	P2−C3	1.804(3)
Pd−O2	2.135(2)	P2−C16	1.815(3)
Pd−P1	2.2264(7)	P2−C22	1.799(3)
Pd−P2	2.2309(7)	S1−O3	1.411(2)
P1−C1	1.814(3)	S1−O4	1.431(3)
P1−C4	1.804(3)	S1−O5	1.434(3)
P1−C10	1.803(3)	S2−O6	1.419(2)
O1−H1	0.72(4)	S2−O7	1.448(3)
O1−H2	0.76(4)	S2−O8	1.423(3)
O2−H3	0.74(3)	S1−C28	1.820(6)
O2−H4	0.83(4)	S2−C29	1.804(5)
O4- - -H2	1.93(5)		
O5- - -H3	2.00(3)		
O6- - -H1	2.03(4)		
O7- - -H4	1.83(4)		
P1−Pd−P2	90.33(2)	P2−Pd−O1	170.37(9)
P1−Pd−O1	89.42(6)	P1−Pd−O2	174.23(8)
P2−Pd−O2	93.38(6)	H1−O1−H2	114(5)
O1−Pd−O2	87.66(8)	H3−O2−H4	109(4)
O1−H1−O6	163(4)		
O1−H2−O4	172(4)		
O2−H3−O5	172(4)		
O2−H4−O7	173(4)		

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

hydrogen bonding in the formation of aquo transition-metal complexes has long been recognized[5−7] and is important in stabilizing the solid-state structure of these molecules.[8−10] In both of our complexes **2** and **3** and complex **5** the S−O bond distance of the coordinated oxygen is significantly longer than the remaining non-coordinated S−O bonds. Finally, reaction of the mono-aquo complex **2** with additional water readily forms the diaquo complex **3**.

Experimental Section

General Methods. All reactions were conducted under a dry nitrogen atmosphere using Schlenk techniques, unless otherwise noted. IR spectra were recorded on a Mattson Polaris FT-IR spectrophotometer. NMR spectra were recorded on a Varian XL-300 spectrometer. ^{1}H NMR spectra were recorded at 300 MHz, and all chemical shifts (δ) are reported in ppm relative to the proton resonance resulting from incomplete deuteration of the NMR solvent CD_2Cl_2 (5.32 ppm). ^{13}C NMR spectra were recorded at 75 MHz, and all chemical shifts (δ) are reported in ppm relative to the carbon resonance of the deuterated NMR solvent CD_2Cl_2 (53.8 ppm). ^{31}P NMR spectra were recorded at 121 MHz, and all chemical shifts (δ) are reported in ppm relative to external 85% H_3PO_4 at 0.00 ppm. ^{19}F NMR spectra were recorded at 282 MHz, and all chemical shifts are reported upfield relative to external $CFCl_3$ at 0.00 ppm. Microanalyses were performed by Atlantic Microlab Inc., Norcross, GA. Melting points were obtained with a Mel-Temp capillary melting point apparatus and were not corrected.

Preparation of [(dppp)Pd(OH$_2$)(OSO$_2$CF$_3$)]$^+$(OSO$_2$CF$_3$)$^-$ (2). A 25 mL Schlenk flask flame-dried under argon and equipped with a stirbar and rubber septum was charged with (dppp)Pd(OTf)$_2$ (0.100 g, 0.122 mmol) and 15 mL of CH_2Cl_2. To the homogeneous yellow mixture was added via syringe deionized water (2.0 mL, 0.11 mmol). The reaction mixture was stirred for 1 h at ambient temperature, followed by reduction of the solvent to 4 mL under vacuum. Via syringe 20 mL of dry *n*-pentane was added immediately, yielding a yellow precipitate. The solvent was decanted via syringe, and the residue was dried under vacuum to afford **2**, as a light

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(4) The H atoms were located by X-ray, and since they are based on X-ray-derived H-atom positions with considerable uncertainties, all H-atom structural parameters need to be interpreted with caution.

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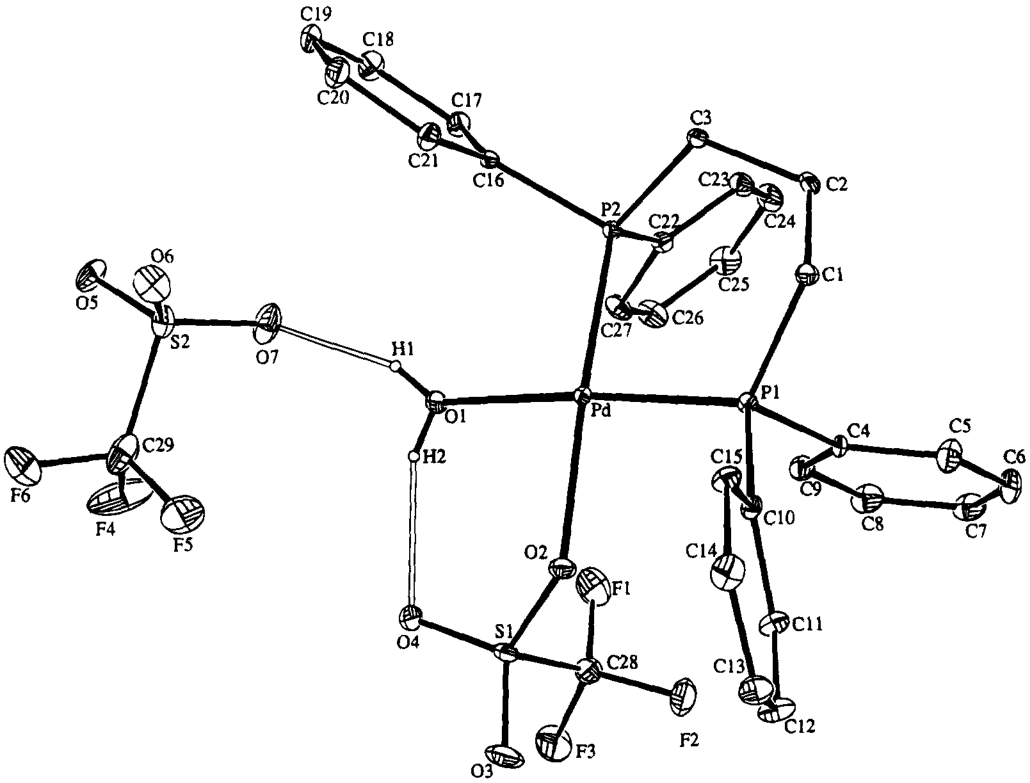

Figure 1. ORTEP plot of [(dppp)Pd(OH_2)(OSO_2CF_3)$_2$] (**2**).

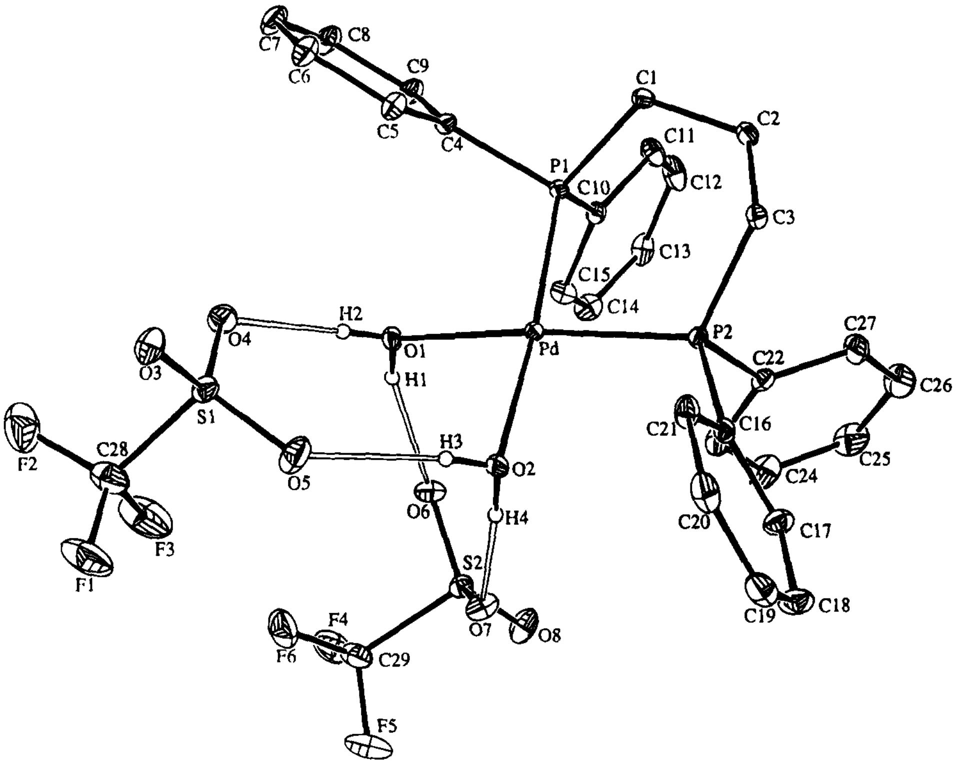

Figure 2. ORTEP plot of [(dppp)Pd(OH_2)$_2$(OSO_2CF_3)$_2$] (**3**).

yellow microcrystalline solid: yield 87.4 mg (86%); mp 206–209 °C dec; IR (KBr, cm^{-1}) 3222 (m, OH), 2919 (w), 1229 (m), 1168 (m), 1098 (w), 1020 (m); ^{1}H NMR (CD_2Cl_2) 7.3–7.7 (m, 20H, C_6H_5), 5.1 (s, 2H, H_2O), 2.7–2.9 (m, 4H, CH_2), 2.1–2.4 (m, 2H, CH_2); ^{31}P NMR (CD_2Cl_2) 20.4 (s); ^{19}F NMR (CD_2Cl_2) −76. Anal. Calcd for $C_{29}H_{26}PdP_2S_2O_6F_6{\cdot}H_2O$: C, 41.71; H, 3.38; S 7.68. Found: C, 41.61; H, 3.49; S, 7.48.

X-ray-quality crystals were grown by careful layering with a CH_2Cl_2/diethyl ether mixture at ambient temperature.

Preparation of [(dppp)Pd(OH_2)$_2$]$^+$(OSO_2CF_3)$^-{}_2$, (3). A 25 mL Schlenk flask flame-dried under argon and equipped with a stirbar and rubber septum was charged with (dppp)-Pd(OTf)$_2$ (137 mg, 0.168 mmol) and 20 mL of CH_2Cl_2. To the homogeneous yellow mixture was added via syringe an excess of deionized water (10 mL, 0.55 mmol). The reaction mixture was stirred for 1 h at ambient temperature, followed by reduction of the solvent to 4 mL under vacuum. Via syringe 20 mL of dry n-pentane was added immediately, yielding a yellow precipitate. The solvent was decanted via syringe, and the residue was dried under vacuum to afford **3**, as a light yellow microcrystalline solid: yield 137 mg (99%); mp 232–238 °C dec; IR (KBr, cm^{-1}) 3285 (s, OH), 2917 (m), 1252 (m), 1167 (s), 1099 (m), 1031 (m); ^{1}H NMR (CD_2Cl_2) 7.3–7.7 (m, 20H, C_6H_5), 4.1 (s, 4H, H_2O), 2.7–2.9 (m, 4H, CH_2), 2.2–2.5 (m, 2H, CH_2); ^{31}P NMR (CD_2Cl_2) 20.4 (s); ^{19}F NMR (CD_2Cl_2) −76. Anal. Calcd for $C_{29}H_{26}PdP_2S_2O_6F_6 \cdot 2H_2O$: C, 40.83; H, 3.54; S, 7.52. Found: C, 40.57; H, 3.56; S, 7.55.

X-ray-quality crystals were grown by careful layering with a CH_2Cl_2/diethyl ether mixture at ambient temperature.

X-ray Crystallographic Analysis of 2. A light yellow crystal, 0.33 mm × 0.30 mm × 0.27 mm, was glued onto a glass fiber and mounted for data collection on a CAD4 diffractometer. The unit cell parameters were obtained by a least-squares refinement of 25 centered reflections in the range $20 < 2\theta < 30°$. The space group was determined from systematic absences ($h0l$, $h + l = 2n + 1$, $0k0$, $k = 2n+1$) and subsequent least-squares refinement. The data were collected by the $\theta - 2\theta$ scan technique, with variable scanning rate, using monochromatic Mo radiation. A total of 5337 unique reflections were measured in the range of $2.0 < 2\theta < 50°$, of which 4198 were considered observed; i.e., $I > 3\sigma(I)$. Standard reflections showed no decay during data collection. Lorentz and polarization corrections, and an empirical absorption correction based upon a series of ψ scans, were applied to the data. Intensities of equivalent reflections were averaged.

The structure was solved by the standard heavy-atom techniques with the Molen/VAX package. Non-hydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atoms were located and refined with fixed isotropic thermal parameter. Scattering factors, and $\Delta f'$ and $\Delta f''$ values, were taken from the literature.

X-ray Crystallographic Analysis of 3. A yellow crystal, 0.29 mm × 0.32 mm × 0.37 mm, was glued onto a glass fiber and mounted for data collection on a Syntex P1 diffractometer. The unit cell parameters were obtained by a least-squares refinement of 30 centered reflections in the range $10 < 2\theta < 20°$. The space group was determined from subsequent least-squares refinement. The data were collected by the $\theta - 2\theta$ scan technique, with fixed rate, using monochromatic Mo radiation. A total of 6310 unique reflections were measured in the range of $2.0 < 2\theta < 50°$, of which 5566 were considered observed; i.e., $I > 3\sigma(I)$. Standard reflections showed no decay during data collection. Lorentz and polarization corrections, and an empirical absorption correction based upon a series of ψ scans, were applied to the data. Intensities of equivalent reflections were averaged.

The structure was solved by the standard heavy-atom techniques with the Molen/VAX package. Non-hydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atoms were located and refined isotropically. Scattering factors, and $\Delta f'$ and $\Delta f''$ values, were taken from the literature.

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Supplementary Material Available: Crystal structure data for compounds **2** and **3**, including tables of calculated positional parameters for the hydrogen atoms and anisotropic displacement parameters and extended lists of bond lengths, bond angles, and torsion angles (22 pages). Ordering information is given on any current masthead page.

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