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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G T O T H E P A P E R

Synthesis and Characterization of *N*-Heterocyclic Carbene Phospha-Palladacycles and their Properties in Heck-Catalysis

by

Guido D. Frey, Jan Schütz, Eberhardt Herdtweck, and **Wolfgang A. Herrmann**

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Table S1 - Crystal Data and Details of the Structure Determination for: **Compound 6**

Crystal Data

Formula			C43 H38 N3 O2 P Pd
Formula Weight			766.15
Crystal System			Triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	10.4761(1)	12.1957(1)	16.3896(1)
alpha, beta, gamma [deg]	109.4464(4)	92.8248(4)	112.4486(3)
V [Ang**3]			1787.13(3)
Z			2
D(calc) [g/cm**3]			1.424
Mu(MoKa) [/mm]			0.606
F(000)			788
Crystal Size [mm]		0.20 x 0.30 x 0.84	

Data Collection

Temperature (K)			123
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			1.9, 25.3
Dataset		-12: 12 ; -14: 14 ; -19: 19	
Tot., Uniq. Data, R(int)		40884, 6532, 0.036	
Observed data [I > 2.0 sigma(I)]			5888

Refinement

Nref, Npar			6532, 603
R, wR2, S		0.0250, 0.0583, 1.05	
Max. and Av. Shift/Error			0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]			-0.40, 0.77

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound 6**

Atom	x	y	z	U(eq) [Ang^2]
Pd	0.08244(1)	0.70225(1)	0.23541(1)	0.0191(1)
P	0.03744(5)	0.64585(5)	0.35459(3)	0.0182(2)
O1	0.14228(15)	0.89807(13)	0.30758(9)	0.0267(5)
O2	0.34802(16)	0.96833(15)	0.26528(10)	0.0353(5)
N1	0.08324(17)	0.79832(15)	0.08546(10)	0.0198(5)
N2	0.22768(17)	0.71409(15)	0.07779(10)	0.0202(5)
N3	0.15317(17)	0.82373(16)	0.01994(10)	0.0220(5)
C1	0.12810(19)	0.73540(18)	0.12356(12)	0.0182(5)
C2	0.2422(2)	0.77203(19)	0.01692(12)	0.0207(6)
C3	0.2563(2)	0.9847(2)	0.30576(13)	0.0250(6)
C4	0.2753(3)	1.1196(2)	0.3594(2)	0.0447(10)
C11	-0.0162(2)	0.85134(19)	0.10958(12)	0.0210(6)
C12	-0.1238(2)	0.7963(2)	0.14876(14)	0.0255(6)
C13	-0.2176(2)	0.8506(2)	0.17114(14)	0.0291(7)
C14	-0.2056(2)	0.9566(2)	0.15443(14)	0.0283(7)
C15	-0.0984(3)	1.0110(2)	0.11453(15)	0.0319(7)
C16	-0.0021(2)	0.9587(2)	0.09283(14)	0.0280(7)
C21	0.3038(2)	0.6445(2)	0.09420(13)	0.0221(6)
C22	0.2874(2)	0.5306(2)	0.02943(15)	0.0299(7)
C23	0.3574(3)	0.4629(2)	0.04777(16)	0.0352(8)
C24	0.4412(2)	0.5081(2)	0.13004(16)	0.0349(8)
C25	0.4564(2)	0.6224(2)	0.19417(15)	0.0314(7)
C26	0.3889(2)	0.6925(2)	0.17649(14)	0.0265(7)
C31	0.3470(2)	0.78640(19)	-0.03999(13)	0.0228(6)

Table S2 (cont.) - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound 6**

Atom	x	y	z	U(eq) [Ang^2]
C32	0.3114(2)	0.7933(2)	-0.12076(14)	0.0264(7)
C33	0.4131(3)	0.8236(2)	-0.17018(15)	0.0321(7)
C34	0.5501(3)	0.8460(2)	-0.14055(15)	0.0352(8)
C35	0.5844(3)	0.8356(3)	-0.06202(16)	0.0399(8)
C36	0.4838(2)	0.8064(2)	-0.01129(15)	0.0326(7)
C41	0.0769(2)	0.50704(18)	0.32142(13)	0.0201(6)
C42	0.1266(2)	0.4626(2)	0.37819(14)	0.0242(6)
C43	0.1729(2)	0.3676(2)	0.34499(15)	0.0291(7)
C44	0.1679(2)	0.3169(2)	0.25515(16)	0.0325(7)
C45	0.1156(2)	0.3589(2)	0.19779(15)	0.0284(7)
C46	0.0695(2)	0.45500(18)	0.23010(13)	0.0213(6)
C47	0.0142(2)	0.50709(19)	0.17237(13)	0.0220(6)
C51	0.1477(2)	0.75111(18)	0.46428(12)	0.0206(6)
C52	0.0859(2)	0.7769(2)	0.53743(14)	0.0281(7)
C53	0.1671(3)	0.8581(2)	0.62117(15)	0.0364(8)
C54	0.3122(3)	0.9140(2)	0.63214(15)	0.0347(7)
C55	0.3748(2)	0.8878(2)	0.56009(14)	0.0294(7)
C56	0.2958(2)	0.80743(19)	0.47562(13)	0.0228(6)
C57	0.3691(2)	0.7817(2)	0.39964(16)	0.0286(7)
C61	-0.1426(2)	0.5914(2)	0.37375(12)	0.0222(6)
C62	-0.2122(2)	0.4670(2)	0.37174(14)	0.0291(7)
C63	-0.3492(2)	0.4217(3)	0.38542(16)	0.0388(8)
C64	-0.4177(3)	0.5007(3)	0.40038(16)	0.0426(8)
C65	-0.3508(3)	0.6239(3)	0.40222(15)	0.0374(8)
C66	-0.2124(2)	0.6723(2)	0.38914(13)	0.0285(7)
C67	-0.1433(3)	0.8075(3)	0.3939(2)	0.0408(9)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 6**

Atom	x	y	z	U(iso) [Ang^2]
H41	0.192(4)	1.126(3)	0.354(2)	0.091(13)
H42	0.298(4)	1.135(3)	0.419(2)	0.082(12)
H43	0.347(4)	1.182(3)	0.347(2)	0.070(10)
H121	-0.129(2)	0.724(2)	0.1604(14)	0.028(6)
H131	-0.287(3)	0.817(2)	0.2003(16)	0.035(6)
H141	-0.273(2)	0.990(2)	0.1662(15)	0.032(6)
H151	-0.094(2)	1.081(2)	0.1006(16)	0.037(7)
H161	0.074(3)	0.997(2)	0.0689(15)	0.032(6)
H221	0.231(2)	0.502(2)	-0.0248(16)	0.032(6)
H231	0.346(2)	0.387(2)	0.0061(16)	0.034(6)
H241	0.488(3)	0.459(2)	0.1419(16)	0.038(7)
H251	0.510(2)	0.650(2)	0.2512(16)	0.033(6)
H261	0.397(2)	0.768(2)	0.2163(15)	0.023(6)
H321	0.217(2)	0.7785(19)	-0.1397(13)	0.017(5)
H331	0.391(3)	0.831(2)	-0.2213(17)	0.038(7)
H341	0.619(3)	0.868(2)	-0.1741(16)	0.036(6)
H351	0.676(3)	0.847(2)	-0.0415(17)	0.045(7)
H361	0.511(2)	0.802(2)	0.0456(16)	0.035(6)
H421	0.133(2)	0.499(2)	0.4380(15)	0.020(5)
H431	0.211(2)	0.340(2)	0.3836(15)	0.030(6)
H441	0.201(2)	0.257(2)	0.2343(15)	0.034(6)
H451	0.115(2)	0.323(2)	0.1364(16)	0.027(6)
H471	0.039(2)	0.484(2)	0.1159(15)	0.027(6)

Table S3 (cont.) - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 6**

Atom	x	y	z	U(iso) [Ang^2]
H472	-0.086(2)	0.475(2)	0.1630(14)	0.026(6)
H521	-0.014(2)	0.737(2)	0.5304(14)	0.024(6)
H531	0.122(3)	0.875(2)	0.6700(17)	0.045(7)
H541	0.368(3)	0.967(2)	0.6856(17)	0.038(7)
H551	0.474(3)	0.926(2)	0.5680(14)	0.030(6)
H571	0.338(3)	0.802(3)	0.3534(19)	0.056(8)
H572	0.469(3)	0.830(2)	0.4190(15)	0.033(6)
H573	0.349(3)	0.693(3)	0.3742(17)	0.045(7)
H621	-0.166(2)	0.414(2)	0.3608(15)	0.029(6)
H631	-0.397(3)	0.332(3)	0.3837(17)	0.046(7)
H641	-0.509(3)	0.471(2)	0.4094(16)	0.043(7)
H651	-0.391(3)	0.681(2)	0.4135(16)	0.037(7)
H671	-0.087(3)	0.822(3)	0.359(2)	0.064(10)
H672	-0.213(3)	0.838(3)	0.3895(19)	0.062(9)
H673	-0.083(4)	0.867(4)	0.450(3)	0.092(13)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters for: **Compound 6**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Pd	0.0214(1)	0.0214(1)	0.0174(1)	0.0108(1)	0.0065(1)	0.0088(1)
P	0.0196(3)	0.0207(3)	0.0169(2)	0.0099(2)	0.0063(2)	0.0084(2)
O1	0.0322(8)	0.0230(8)	0.0264(8)	0.0109(6)	0.0098(6)	0.0114(7)
O2	0.0293(8)	0.0310(9)	0.0402(9)	0.0111(7)	0.0107(7)	0.0090(7)
N1	0.0217(8)	0.0235(9)	0.0183(8)	0.0120(7)	0.0058(7)	0.0100(7)
N2	0.0218(8)	0.0231(9)	0.0172(8)	0.0094(7)	0.0058(7)	0.0092(7)
N3	0.0256(9)	0.0252(9)	0.0181(8)	0.0119(7)	0.0083(7)	0.0101(7)
C1	0.0157(9)	0.0200(10)	0.0142(9)	0.0044(8)	0.0021(7)	0.0047(8)
C2	0.0223(10)	0.0229(10)	0.0149(9)	0.0085(8)	0.0029(8)	0.0064(8)
C3	0.0289(11)	0.0239(11)	0.0235(11)	0.0111(9)	0.0006(9)	0.0114(9)
C4	0.0483(17)	0.0253(13)	0.0577(19)	0.0133(13)	0.0142(14)	0.0146(12)
C11	0.0212(10)	0.0235(10)	0.0163(10)	0.0065(8)	0.0005(8)	0.0087(8)
C12	0.0250(11)	0.0285(11)	0.0275(11)	0.0140(9)	0.0066(9)	0.0129(9)
C13	0.0267(11)	0.0363(13)	0.0277(11)	0.0143(10)	0.0103(9)	0.0144(10)
C14	0.0270(11)	0.0340(12)	0.0257(11)	0.0060(9)	0.0045(9)	0.0195(10)
C15	0.0437(14)	0.0322(12)	0.0304(12)	0.0158(10)	0.0095(10)	0.0233(11)
C16	0.0325(12)	0.0297(12)	0.0266(11)	0.0155(10)	0.0097(10)	0.0136(10)
C21	0.0203(10)	0.0297(11)	0.0226(10)	0.0160(9)	0.0094(8)	0.0113(9)
C22	0.0327(12)	0.0357(13)	0.0247(12)	0.0108(10)	0.0066(10)	0.0183(10)
C23	0.0392(14)	0.0375(14)	0.0357(13)	0.0115(11)	0.0123(11)	0.0246(11)
C24	0.0339(13)	0.0459(14)	0.0428(14)	0.0257(12)	0.0163(11)	0.0266(12)
C25	0.0265(11)	0.0486(14)	0.0295(12)	0.0229(11)	0.0080(10)	0.0193(11)
C26	0.0258(11)	0.0337(12)	0.0251(11)	0.0142(10)	0.0108(9)	0.0146(10)
C31	0.0271(11)	0.0219(10)	0.0198(10)	0.0091(8)	0.0079(8)	0.0093(9)
C32	0.0320(12)	0.0301(12)	0.0229(11)	0.0126(9)	0.0091(9)	0.0163(10)
C33	0.0472(14)	0.0377(13)	0.0229(11)	0.0172(10)	0.0156(10)	0.0238(11)
C34	0.0387(14)	0.0403(14)	0.0307(12)	0.0186(11)	0.0203(11)	0.0148(11)
C35	0.0254(12)	0.0582(17)	0.0355(13)	0.0219(12)	0.0106(10)	0.0130(12)
C36	0.0272(12)	0.0458(14)	0.0244(12)	0.0172(10)	0.0070(9)	0.0114(10)
C41	0.0171(9)	0.0190(10)	0.0246(10)	0.0107(8)	0.0069(8)	0.0058(8)
C42	0.0242(11)	0.0248(11)	0.0238(11)	0.0136(9)	0.0060(9)	0.0067(9)
C43	0.0280(12)	0.0289(12)	0.0386(13)	0.0204(10)	0.0074(10)	0.0138(10)

Table S4 (cont.) - (An)isotropic Displacement Parameters for: **Compound 6**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C44	0.0329(12)	0.0293(12)	0.0445(14)	0.0162(11)	0.0142(11)	0.0199(10)
C45	0.0301(12)	0.0249(11)	0.0284(12)	0.0090(10)	0.0094(9)	0.0104(9)
C46	0.0173(10)	0.0199(10)	0.0235(10)	0.0094(8)	0.0056(8)	0.0036(8)
C47	0.0233(11)	0.0234(11)	0.0176(10)	0.0087(8)	0.0037(8)	0.0075(9)
C51	0.0242(10)	0.0202(10)	0.0181(10)	0.0098(8)	0.0036(8)	0.0079(8)
C52	0.0267(12)	0.0303(12)	0.0234(11)	0.0105(9)	0.0068(9)	0.0078(10)
C53	0.0399(14)	0.0398(14)	0.0200(11)	0.0085(10)	0.0079(10)	0.0096(11)
C54	0.0391(14)	0.0317(12)	0.0188(11)	0.0063(10)	-0.0026(10)	0.0042(11)
C55	0.0263(12)	0.0262(11)	0.0312(12)	0.0131(10)	-0.0002(10)	0.0055(10)
C56	0.0253(11)	0.0217(10)	0.0245(11)	0.0122(9)	0.0043(8)	0.0102(9)
C57	0.0208(12)	0.0337(13)	0.0320(12)	0.0143(11)	0.0071(9)	0.0104(10)
C61	0.0194(10)	0.0314(11)	0.0146(9)	0.0098(8)	0.0037(8)	0.0087(9)
C62	0.0249(11)	0.0335(12)	0.0245(11)	0.0108(10)	0.0069(9)	0.0078(10)
C63	0.0253(12)	0.0407(14)	0.0361(13)	0.0121(11)	0.0089(10)	0.0014(11)
C64	0.0194(12)	0.0629(18)	0.0320(13)	0.0130(12)	0.0082(10)	0.0078(12)
C65	0.0321(13)	0.0624(17)	0.0254(12)	0.0157(12)	0.0094(10)	0.0282(13)
C66	0.0282(11)	0.0447(13)	0.0198(10)	0.0151(10)	0.0069(9)	0.0201(10)
C67	0.0480(16)	0.0522(17)	0.0476(16)	0.0298(14)	0.0259(14)	0.0357(14)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom) for: **Compound 6**

Pd	-P	2.2910(5)	C55	-C56	1.388(3)
Pd	-O1	2.0972(15)	C56	-C57	1.502(3)
Pd	-C1	2.0457(19)	C61	-C62	1.398(3)
Pd	-C47	2.058(2)	C61	-C66	1.405(3)
P	-C41	1.810(2)	C62	-C63	1.387(4)
P	-C51	1.828(2)	C63	-C64	1.375(5)
P	-C61	1.827(2)	C64	-C65	1.383(5)
O1	-C3	1.267(3)	C65	-C66	1.399(4)
O2	-C3	1.235(3)	C66	-C67	1.499(4)
N1	-N3	1.383(2)	C4	-H41	0.91(4)
N1	-C1	1.329(3)	C4	-H42	0.93(3)
N1	-C11	1.430(3)	C4	-H43	0.93(4)
N2	-C1	1.369(3)	C12	-H121	0.95(2)
N2	-C2	1.386(3)	C13	-H131	0.93(3)
N2	-C21	1.441(3)	C14	-H141	0.94(2)
N3	-C2	1.305(3)	C15	-H151	0.94(2)
C2	-C31	1.473(3)	C16	-H161	0.94(3)
C3	-C4	1.513(4)	C22	-H221	0.92(2)
C11	-C12	1.383(3)	C23	-H231	0.91(2)
C11	-C16	1.381(3)	C24	-H241	0.96(3)
C12	-C13	1.382(3)	C25	-H251	0.95(2)
C13	-C14	1.370(3)	C26	-H261	0.90(2)
C14	-C15	1.386(4)	C32	-H321	0.95(2)
C15	-C16	1.388(4)	C33	-H331	0.90(3)
C21	-C22	1.380(3)	C34	-H341	0.94(3)
C21	-C26	1.383(3)	C35	-H351	0.94(3)
C22	-C23	1.384(4)	C36	-H361	0.99(2)
C23	-C24	1.383(4)	C42	-H421	0.92(2)
C24	-C25	1.383(3)	C43	-H431	0.94(2)
C25	-C26	1.386(3)	C44	-H441	0.90(2)

Table S5 (cont.) - Bond Distances (Angstrom) for: **Compound 6**

C31	-C32	1.396(3)	C45	-H451	0.95(2)
C31	-C36	1.387(3)	C47	-H471	0.95(2)
C32	-C33	1.383(4)	C47	-H472	0.95(2)
C33	-C34	1.383(5)	C52	-H521	0.95(2)
C34	-C35	1.378(4)	C53	-H531	0.95(3)
C35	-C36	1.388(4)	C54	-H541	0.90(3)
C41	-C42	1.391(3)	C55	-H551	0.94(3)
C41	-C46	1.403(3)	C57	-H571	0.95(3)
C42	-C43	1.382(3)	C57	-H572	0.96(3)
C43	-C44	1.384(3)	C57	-H573	0.95(3)
C44	-C45	1.389(3)	C62	-H621	0.92(2)
C45	-C46	1.390(3)	C63	-H631	1.00(4)
C46	-C47	1.504(3)	C64	-H641	0.92(3)
C51	-C52	1.392(3)	C65	-H651	0.92(3)
C51	-C56	1.409(3)	C67	-H671	0.85(3)
C52	-C53	1.387(3)	C67	-H672	0.95(3)
C53	-C54	1.381(4)	C67	-H673	0.96(5)
C54	-C55	1.383(3)			

Table S6 - Bond Angles (Degrees) for: **Compound 6**

P	-Pd	-O1	94.16(4)	C41	-C42	-C43	119.9(2)
P	-Pd	-C1	173.58(6)	C42	-C43	-C44	119.4(2)
P	-Pd	-C47	81.51(6)	C43	-C44	-C45	121.1(2)
O1	-Pd	-C1	91.45(7)	C44	-C45	-C46	120.3(2)
O1	-Pd	-C47	175.25(7)	C41	-C46	-C45	118.1(2)
C1	-Pd	-C47	92.98(8)	C41	-C46	-C47	118.50(19)
Pd	-P	-C41	98.82(7)	C45	-C46	-C47	123.37(19)
Pd	-P	-C51	120.51(7)	Pd	-C47	-C46	110.18(14)
Pd	-P	-C61	119.12(7)	P	-C51	-C52	120.18(17)
C41	-P	-C51	105.59(10)	P	-C51	-C56	120.46(15)
C41	-P	-C61	106.53(11)	C52	-C51	-C56	119.36(18)
C51	-P	-C61	104.51(9)	C51	-C52	-C53	121.3(2)
Pd	-O1	-C3	122.66(14)	C52	-C53	-C54	119.3(2)
N3	-N1	-C1	113.81(18)	C53	-C54	-C55	119.9(2)
N3	-N1	-C11	117.86(17)	C54	-C55	-C56	121.9(2)
C1	-N1	-C11	128.04(17)	C51	-C56	-C55	118.26(19)
C1	-N2	-C2	108.58(18)	C51	-C56	-C57	121.98(18)
C1	-N2	-C21	123.73(17)	C55	-C56	-C57	119.8(2)
C2	-N2	-C21	127.69(18)	P	-C61	-C62	119.42(17)
N1	-N3	-C2	104.05(17)	P	-C61	-C66	120.83(18)
Pd	-C1	-N1	128.37(15)	C62	-C61	-C66	119.7(2)
Pd	-C1	-N2	127.64(15)	C61	-C62	-C63	121.2(2)
N1	-C1	-N2	103.40(17)	C62	-C63	-C64	119.1(3)
N2	-C2	-N3	110.08(18)	C63	-C64	-C65	120.5(3)
N2	-C2	-C31	127.9(2)	C64	-C65	-C66	121.6(3)
N3	-C2	-C31	121.85(19)	C61	-C66	-C65	117.8(2)
O1	-C3	-O2	126.6(2)	C61	-C66	-C67	122.6(2)
O1	-C3	-C4	113.8(2)	C65	-C66	-C67	119.6(3)
O2	-C3	-C4	119.6(2)	C3	-C4	-H41	111(2)
N1	-C11	-C12	120.7(2)	C3	-C4	-H42	108(2)
N1	-C11	-C16	118.37(19)	C3	-C4	-H43	113(2)
C12	-C11	-C16	120.9(2)	H41	-C4	-H42	104(3)
C11	-C12	-C13	118.9(2)	H41	-C4	-H43	113(3)
C12	-C13	-C14	120.9(2)	H42	-C4	-H43	108(3)
C13	-C14	-C15	120.1(2)	C11	-C12	-H121	118.6(14)
C14	-C15	-C16	119.7(2)	C13	-C12	-H121	122.5(14)
C11	-C16	-C15	119.5(2)	C12	-C13	-H131	119.4(18)
N2	-C21	-C22	119.93(18)	C14	-C13	-H131	119.7(18)
N2	-C21	-C26	118.51(19)	C13	-C14	-H141	120.7(15)
C22	-C21	-C26	121.5(2)	C15	-C14	-H141	119.0(15)
C21	-C22	-C23	119.0(2)	C14	-C15	-H151	119.4(15)

Table S6 (cont.) - Bond Angles (Degrees) for: **Compound 6**

C22	-C23	-C24	120.5(2)	C16	-C15	-H151	120.9(14)
C23	-C24	-C25	119.8(2)	C11	-C16	-H161	119.6(17)
C24	-C25	-C26	120.5(2)	C15	-C16	-H161	120.8(17)
C21	-C26	-C25	118.7(2)	C21	-C22	-H221	119.3(15)
C2	-C31	-C32	118.7(2)	C23	-C22	-H221	121.8(15)
C2	-C31	-C36	121.51(19)	C22	-C23	-H231	119.8(15)
C32	-C31	-C36	119.4(2)	C24	-C23	-H231	119.7(15)
C31	-C32	-C33	120.0(2)	C23	-C24	-H241	119.3(15)
C32	-C33	-C34	120.4(2)	C25	-C24	-H241	120.9(15)
C33	-C34	-C35	119.6(3)	C24	-C25	-H251	118.9(15)
C34	-C35	-C36	120.6(3)	C26	-C25	-H251	120.5(15)
C31	-C36	-C35	119.9(2)	C21	-C26	-H261	118.0(15)
P	-C41	-C42	125.74(16)	C25	-C26	-H261	123.2(15)
P	-C41	-C46	112.61(16)	C31	-C32	-H321	118.3(13)
C42	-C41	-C46	121.2(2)	C33	-C32	-H321	121.7(13)
C32	-C33	-H331	120(2)	C53	-C54	-H541	122(2)
C34	-C33	-H331	119(2)	C55	-C54	-H541	119(2)
C33	-C34	-H341	119.9(17)	C54	-C55	-H551	119.5(13)
C35	-C34	-H341	120.5(18)	C56	-C55	-H551	118.6(13)
C34	-C35	-H351	121.3(16)	C56	-C57	-H571	112(2)
C36	-C35	-H351	118.1(16)	C56	-C57	-H572	110.6(14)
C31	-C36	-H361	120.6(14)	C56	-C57	-H573	110.5(19)
C35	-C36	-H361	119.5(14)	H571	-C57	-H572	109(3)
C41	-C42	-H421	120.2(15)	H571	-C57	-H573	106(3)
C43	-C42	-H421	119.8(15)	H572	-C57	-H573	109(3)
C42	-C43	-H431	120.2(14)	C61	-C62	-H621	119.2(15)
C44	-C43	-H431	120.4(14)	C63	-C62	-H621	119.6(15)
C43	-C44	-H441	118.8(15)	C62	-C63	-H631	120(2)
C45	-C44	-H441	120.1(15)	C64	-C63	-H631	121(2)
C44	-C45	-H451	119.0(14)	C63	-C64	-H641	119.5(17)
C46	-C45	-H451	120.6(15)	C65	-C64	-H641	120.0(17)
Pd	-C47	-H471	112.5(15)	C64	-C65	-H651	123.8(18)
Pd	-C47	-H472	103.7(14)	C66	-C65	-H651	114.6(18)
C46	-C47	-H471	111.0(14)	C66	-C67	-H671	117(2)
C46	-C47	-H472	111.6(14)	C66	-C67	-H672	109(2)
H471	-C47	-H472	107.6(19)	C66	-C67	-H673	113(3)
C51	-C52	-H521	119.7(13)	H671	-C67	-H672	112(3)
C53	-C52	-H521	119.0(13)	H671	-C67	-H673	101(4)
C52	-C53	-H531	119.6(18)	H672	-C67	-H673	103(3)
C54	-C53	-H531	121.1(18)				

Table S7 - Crystal Data and Details of the Structure Determination for: **Compound 13•($C_6H_{12}O_2$)**

Crystal Data

Formula	C51 H68 N4 P Pd, C6 H12 O2, C2 H3 O2		
Formula Weight			1049.68
Crystal System			Monoclinic
Space group		P21/n	(No. 14)
a, b, c [Angstrom]	10.6600(1)	13.4585(2)	38.2426(9)
alpha, beta, gamma [deg]	90	94.103(1)	90
V [Ang**3]			5472.51(16)
Z			4
D(calc) [g/cm**3]			1.274
Mu(MoKa) [/mm]			0.417
F(000)			2232
Crystal Size [mm]		0.20 x 0.23 x 0.30	

Table S7 (cont.) - Crystal Data and Details of the Structure Determination for: **Compound 13•($C_6H_{12}O_2$)**

Data Collection

Temperature (K)	123
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.6, 25.3
Dataset	-12: 12 ; -16: 16 ; -46: 46
Tot., Uniq. Data, R(int)	83297, 9981, 0.039
Observed data [I > 2.0 sigma(I)]	7779

Refinement

Nref, Npar	9981, 630
R, wR2, S	0.0350, 0.0813, 1.02
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.42, 0.65

Table S8 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound 13•($C_6H_{12}O_2$)**

Atom	x	y	z	U(eq) [Ang^2]
Pd	0.43521(2)	0.03153(1)	0.13855(1)	0.0173(1)
P	0.33127(6)	0.12322(4)	0.17917(2)	0.0184(2)
N1	0.57343(18)	-0.16594(13)	0.13841(5)	0.0226(6)
N2	0.61943(18)	-0.08076(14)	0.09359(5)	0.0219(7)
N3	0.21029(18)	-0.05439(13)	0.08875(5)	0.0193(6)
N4	0.24894(18)	0.09603(13)	0.07558(5)	0.0191(6)
C1	0.5476(2)	-0.07890(16)	0.12124(6)	0.0191(8)
C2	0.6599(2)	-0.22065(18)	0.12113(7)	0.0287(9)
C3	0.6896(2)	-0.16814(17)	0.09333(7)	0.0281(9)
C4	0.2888(2)	0.02217(16)	0.09804(6)	0.0182(7)
C5	0.1238(2)	-0.02849(17)	0.06135(6)	0.0215(8)
C6	0.1486(2)	0.06598(17)	0.05300(6)	0.0215(8)
C11	0.5344(2)	-0.19225(17)	0.17357(7)	0.0250(8)
C12	0.6506(2)	-0.20105(19)	0.19958(7)	0.0314(9)
C13	0.6137(3)	-0.2288(2)	0.23632(7)	0.0407(10)
C14	0.5358(3)	-0.3239(2)	0.23530(7)	0.0377(10)
C15	0.4207(3)	-0.3135(2)	0.20992(8)	0.0379(10)
C16	0.4582(2)	-0.28806(18)	0.17311(7)	0.0311(9)
C21	0.6433(2)	0.00608(17)	0.07164(6)	0.0222(8)
C22	0.6462(2)	-0.02282(18)	0.03318(6)	0.0270(8)
C23	0.6788(2)	0.0668(2)	0.01091(7)	0.0299(9)
C24	0.8042(3)	0.1113(2)	0.02428(7)	0.0357(10)
C25	0.8004(3)	0.1427(2)	0.06251(7)	0.0340(9)
C26	0.7665(2)	0.05499(18)	0.08525(7)	0.0266(8)
C31	0.2200(2)	-0.15593(16)	0.10295(6)	0.0210(8)
C32	0.2613(2)	-0.22594(17)	0.07442(7)	0.0261(8)
C33	0.2694(3)	-0.33409(17)	0.08686(7)	0.0300(9)
C34	0.1493(3)	-0.36695(17)	0.10269(7)	0.0307(9)
C35	0.1083(2)	-0.29592(17)	0.13072(7)	0.0279(8)
C36	0.0966(2)	-0.18981(17)	0.11654(7)	0.0249(8)
C41	0.3094(2)	0.19364(16)	0.07266(6)	0.0223(8)
C42	0.3705(2)	0.20008(17)	0.03789(7)	0.0243(8)
C43	0.4363(2)	0.30018(18)	0.03444(7)	0.0330(9)
C44	0.3415(3)	0.38429(18)	0.03667(7)	0.0312(9)
C45	0.2784(3)	0.37969(18)	0.07092(7)	0.0356(10)
C46	0.2166(2)	0.27857(16)	0.07617(7)	0.0282(9)
C51	0.4449(2)	0.12164(16)	0.21714(6)	0.0190(8)
C52	0.4202(2)	0.15631(17)	0.25027(6)	0.0248(8)

Table S8 (cont.) - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **Compound 13•($C_6H_{12}O_2$)**

Atom	x	y	z	U(eq) [Ang^2]
C53	0.5084(2)	0.14348(18)	0.27821(7)	0.0293(9)
C54	0.6215(2)	0.09604(18)	0.27289(7)	0.0301(9)
C55	0.6477(2)	0.06570(18)	0.23977(7)	0.0279(9)
C56	0.5607(2)	0.07958(16)	0.21099(6)	0.0219(8)
C57	0.5900(2)	0.05589(17)	0.17415(6)	0.0222(8)
C61	0.1985(2)	0.04893(16)	0.19308(6)	0.0202(8)
C62	0.2185(2)	-0.01356(16)	0.22217(7)	0.0237(8)
C63	0.1248(2)	-0.07511(18)	0.23281(7)	0.0289(9)
C64	0.0083(2)	-0.07568(18)	0.21447(7)	0.0308(9)
C65	-0.0126(2)	-0.01485(18)	0.18551(7)	0.0269(8)
C66	0.0807(2)	0.04702(16)	0.17404(6)	0.0217(8)
C67	0.0497(2)	0.10791(18)	0.14130(6)	0.0273(8)
C71	0.2788(2)	0.25349(16)	0.17908(6)	0.0209(8)
C72	0.1647(2)	0.28003(17)	0.19218(7)	0.0256(8)
C73	0.1265(2)	0.37898(18)	0.19286(7)	0.0289(9)
C74	0.2024(3)	0.45167(18)	0.18027(7)	0.0297(9)
C75	0.3164(3)	0.42678(18)	0.16787(7)	0.0285(9)
C76	0.3582(2)	0.32794(17)	0.16752(6)	0.0230(8)
C77	0.4884(2)	0.30675(18)	0.15646(7)	0.0286(8)
O1	0.53684(19)	0.52033(14)	0.10926(6)	0.0469(8)
O2	0.83919(17)	0.57864(13)	0.11168(5)	0.0389(7)
C81	0.5780(3)	0.5998(2)	0.05549(8)	0.0459(11)
C82	0.6026(3)	0.5251(2)	0.08408(8)	0.0357(10)
C83	0.7093(3)	0.4553(2)	0.08030(8)	0.0426(11)
C84	0.8197(3)	0.47417(18)	0.10779(8)	0.0350(10)
C85	0.9369(3)	0.4237(2)	0.09582(9)	0.0493(11)
C86	0.7924(3)	0.4374(2)	0.14383(8)	0.0473(11)
O3	0.92440(18)	0.80865(13)	0.02079(5)	0.0424(7)
O4	0.86380(19)	0.68073(15)	0.05134(6)	0.0479(8)
C91	0.9241(2)	0.71999(19)	0.02795(7)	0.0288(9)
C92	1.0029(3)	0.6497(2)	0.00709(8)	0.0414(10)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S9 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 13•($C_6H_{12}O_2$)**

Atom	x	y	z	U(iso) [Ang^2]
H21	0.6923	-0.2841	0.1279	0.034
H31	0.7471	-0.1866	0.0766	0.034
H51	0.0597	-0.0696	0.0506	0.026
H61	0.1058	0.1047	0.0351	0.026
H111	0.4804	-0.1373	0.1817	0.030
H121	0.7078	-0.2524	0.1912	0.038
H122	0.6963	-0.1370	0.2007	0.038
H131	0.6906	-0.2382	0.2521	0.049
H132	0.5645	-0.1739	0.2458	0.049
H141	0.5878	-0.3801	0.2280	0.045
H142	0.5091	-0.3385	0.2590	0.045
H151	0.3656	-0.2605	0.2182	0.045
H152	0.3727	-0.3765	0.2091	0.045
H161	0.5087	-0.3430	0.1642	0.037
H162	0.3816	-0.2804	0.1571	0.037

Table S9 (cont.) - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 13•($C_6H_{12}O_2$)**

Atom	x	y	z	U(iso) [Ang^2]
H211	0.5735	0.0549	0.0738	0.027
H221	0.5630	-0.0494	0.0246	0.032
H222	0.7095	-0.0758	0.0308	0.032
H231	0.6831	0.0458	-0.0138	0.036
H232	0.6120	0.1177	0.0118	0.036
H241	0.8231	0.1698	0.0098	0.043
H242	0.8718	0.0617	0.0221	0.043
H251	0.8835	0.1692	0.0711	0.041
H252	0.7374	0.1962	0.0643	0.041
H261	0.7588	0.0783	0.1096	0.032
H262	0.8350	0.0052	0.0857	0.032
H311	0.2861	-0.1565	0.1229	0.025
H321	0.3445	-0.2047	0.0672	0.031
H322	0.2005	-0.2213	0.0536	0.031
H331	0.2851	-0.3776	0.0668	0.036
H332	0.3412	-0.3413	0.1046	0.036
H341	0.1625	-0.4338	0.1131	0.037
H342	0.0811	-0.3722	0.0838	0.037
H351	0.1706	-0.2975	0.1512	0.033
H352	0.0262	-0.3177	0.1386	0.033
H361	0.0293	-0.1870	0.0973	0.030
H362	0.0732	-0.1445	0.1354	0.030
H411	0.3770	0.1996	0.0921	0.027
H421	0.3055	0.1918	0.0183	0.029
H422	0.4325	0.1457	0.0365	0.029
H431	0.5038	0.3074	0.0534	0.040
H432	0.4751	0.3034	0.0117	0.040
H441	0.3849	0.4489	0.0349	0.037
H442	0.2769	0.3793	0.0168	0.037
H451	0.2137	0.4324	0.0711	0.043
H452	0.3417	0.3924	0.0906	0.043
H461	0.1838	0.2762	0.0997	0.034
H462	0.1447	0.2702	0.0586	0.034
H521	0.3429	0.1887	0.2537	0.030
H531	0.4920	0.1669	0.3009	0.035
H541	0.6808	0.0845	0.2922	0.036
H551	0.7262	0.0349	0.2364	0.033
H571	0.6437	-0.0042	0.1747	0.027
H572	0.6399	0.1114	0.1653	0.027
H621	0.2983	-0.0137	0.2349	0.028
H631	0.1404	-0.1169	0.2527	0.035
H641	-0.0569	-0.1175	0.2217	0.037
H651	-0.0930	-0.0153	0.1731	0.032
H671	0.0210	0.0638	0.1220	0.041
H672	0.1250	0.1438	0.1351	0.041
H673	-0.0169	0.1556	0.1456	0.041
H721	0.1123	0.2299	0.2008	0.031
H731	0.0488	0.3962	0.2019	0.035
H741	0.1760	0.5191	0.1801	0.036
H751	0.3680	0.4777	0.1594	0.034
H771	0.5186	0.3641	0.1437	0.043
H772	0.4860	0.2481	0.1412	0.043
H773	0.5453	0.2943	0.1773	0.043
H2	0.855(3)	0.6100(10)	0.0871(7)	0.047
H811	0.5092	0.6437	0.0613	0.069
H812	0.5547	0.5655	0.0334	0.069
H813	0.6541	0.6394	0.0530	0.069

Table S9 (cont.) - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 13•($C_6H_{12}O_2$)**

Atom	x	y	z	U(iso) [Ang^2]
H831	0.7395	0.4625	0.0565	0.051
H832	0.6792	0.3862	0.0827	0.051
H851	1.0069	0.4334	0.1136	0.074
H852	0.9586	0.4528	0.0735	0.074
H853	0.9208	0.3525	0.0927	0.074
H861	0.8658	0.4492	0.1602	0.071
H862	0.7742	0.3660	0.1428	0.071
H863	0.7196	0.4730	0.1519	0.071
H921	1.0304	0.6843	-0.0136	0.062
H922	0.9522	0.5917	-0.0004	0.062
H923	1.0767	0.6279	0.0219	0.062

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S10 - (An)isotropic Displacement Parameters for: **Compound 13•($C_6H_{12}O_2$)**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Pd	0.0197(1)	0.0152(1)	0.0172(1)	-0.0011(1)	0.0021(1)	0.0011(1)
P	0.0207(3)	0.0164(3)	0.0183(4)	-0.0008(3)	0.0031(3)	0.0014(3)
N1	0.0254(11)	0.0185(10)	0.0240(12)	-0.0003(9)	0.0032(9)	0.0032(9)
N2	0.0248(12)	0.0200(10)	0.0215(12)	-0.0014(9)	0.0050(9)	0.0024(9)
N3	0.0213(11)	0.0171(10)	0.0192(12)	0.0001(8)	-0.0002(9)	-0.0002(8)
N4	0.0231(11)	0.0149(10)	0.0191(12)	0.0008(8)	0.0009(9)	0.0007(8)
C1	0.0189(13)	0.0183(12)	0.0200(14)	-0.0012(10)	0.0000(11)	-0.0018(10)
C2	0.0332(16)	0.0199(13)	0.0336(17)	-0.0020(12)	0.0069(13)	0.0076(11)
C3	0.0280(15)	0.0227(13)	0.0346(17)	-0.0047(12)	0.0090(12)	0.0081(11)
C4	0.0223(13)	0.0175(12)	0.0153(13)	-0.0017(10)	0.0054(10)	0.0023(10)
C5	0.0235(13)	0.0215(12)	0.0193(14)	-0.0034(11)	-0.0004(11)	0.0006(11)
C6	0.0246(14)	0.0213(12)	0.0180(14)	-0.0010(10)	-0.0033(11)	0.0027(10)
C11	0.0287(14)	0.0206(12)	0.0262(15)	0.0041(11)	0.0061(12)	0.0026(11)
C12	0.0358(16)	0.0270(14)	0.0305(17)	0.0032(12)	-0.0041(13)	-0.0019(12)
C13	0.055(2)	0.0402(16)	0.0263(17)	0.0033(13)	-0.0023(14)	0.0059(14)
C14	0.0483(18)	0.0364(16)	0.0300(17)	0.0121(13)	0.0135(14)	0.0101(14)
C15	0.0371(17)	0.0332(15)	0.0448(19)	0.0132(14)	0.0133(14)	0.0027(13)
C16	0.0297(15)	0.0278(14)	0.0354(18)	0.0062(12)	-0.0004(13)	-0.0017(12)
C21	0.0246(14)	0.0210(12)	0.0215(15)	0.0013(10)	0.0044(11)	0.0007(10)
C22	0.0239(14)	0.0343(15)	0.0226(15)	-0.0042(12)	0.0009(11)	-0.0014(12)
C23	0.0268(15)	0.0420(15)	0.0213(15)	0.0024(12)	0.0043(12)	0.0000(12)
C24	0.0327(16)	0.0444(17)	0.0300(17)	0.0082(13)	0.0028(13)	-0.0082(13)
C25	0.0363(16)	0.0340(15)	0.0314(17)	0.0032(12)	-0.0004(13)	-0.0084(13)
C26	0.0304(15)	0.0305(14)	0.0187(15)	-0.0020(11)	0.0007(11)	-0.0039(11)
C31	0.0256(14)	0.0167(12)	0.0207(14)	0.0033(10)	0.0012(11)	0.0003(10)
C32	0.0299(15)	0.0229(13)	0.0263(16)	0.0032(11)	0.0076(12)	0.0020(11)
C33	0.0427(17)	0.0199(13)	0.0275(16)	-0.0015(11)	0.0042(13)	0.0044(12)
C34	0.0474(18)	0.0175(12)	0.0272(16)	0.0033(11)	0.0030(13)	-0.0018(12)
C35	0.0343(15)	0.0245(13)	0.0253(16)	0.0024(11)	0.0048(12)	-0.0074(11)
C36	0.0314(15)	0.0198(12)	0.0240(15)	-0.0016(11)	0.0060(12)	-0.0005(11)
C41	0.0267(14)	0.0156(12)	0.0240(15)	-0.0003(10)	-0.0016(11)	-0.0014(10)
C42	0.0236(14)	0.0238(13)	0.0257(15)	0.0005(11)	0.0024(11)	0.0023(11)
C43	0.0326(16)	0.0325(15)	0.0339(17)	0.0103(13)	0.0026(13)	-0.0077(12)
C44	0.0436(17)	0.0197(13)	0.0294(16)	0.0050(11)	-0.0028(13)	-0.0072(12)

Table S10 (cont.) - (An)isotropic Displacement Parameters for: **Compound 13•($C_6H_{12}O_2$)**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
C45	0.0545(19)	0.0173(13)	0.0351(18)	-0.0003(12)	0.0042(14)	0.0003(12)
C46	0.0405(16)	0.0178(12)	0.0274(16)	0.0005(11)	0.0093(13)	0.0032(11)
C51	0.0238(14)	0.0150(11)	0.0185(14)	0.0001(10)	0.0028(11)	-0.0028(10)
C52	0.0297(15)	0.0214(13)	0.0240(15)	-0.0022(11)	0.0061(12)	-0.0039(11)
C53	0.0383(17)	0.0307(14)	0.0190(15)	-0.0040(11)	0.0036(13)	-0.0113(12)
C54	0.0330(16)	0.0320(14)	0.0237(16)	0.0005(12)	-0.0083(12)	-0.0060(12)
C55	0.0262(14)	0.0263(13)	0.0307(17)	-0.0010(12)	-0.0018(12)	-0.0011(11)
C56	0.0263(14)	0.0154(12)	0.0236(15)	-0.0029(10)	-0.0011(11)	-0.0054(10)
C57	0.0200(13)	0.0198(12)	0.0266(15)	-0.0040(10)	0.0013(11)	-0.0003(10)
C61	0.0223(13)	0.0176(12)	0.0215(14)	-0.0047(10)	0.0070(11)	0.0015(10)
C62	0.0272(14)	0.0203(12)	0.0232(15)	-0.0010(11)	-0.0003(11)	-0.0003(11)
C63	0.0368(16)	0.0221(13)	0.0280(16)	0.0030(11)	0.0029(13)	-0.0051(12)
C64	0.0325(16)	0.0258(13)	0.0352(17)	-0.0017(12)	0.0098(13)	-0.0088(12)
C65	0.0227(14)	0.0292(14)	0.0290(16)	-0.0077(12)	0.0040(12)	-0.0035(11)
C66	0.0252(14)	0.0208(12)	0.0192(14)	-0.0066(10)	0.0025(11)	0.0037(10)
C67	0.0265(14)	0.0299(14)	0.0253(15)	-0.0016(12)	0.0008(12)	0.0012(11)
C71	0.0259(14)	0.0182(12)	0.0183(14)	0.0010(10)	-0.0001(11)	0.0028(10)
C72	0.0305(15)	0.0212(13)	0.0253(15)	0.0006(11)	0.0029(12)	0.0011(11)
C73	0.0325(15)	0.0270(14)	0.0275(16)	-0.0018(12)	0.0033(12)	0.0090(12)
C74	0.0440(17)	0.0190(13)	0.0261(16)	0.0008(11)	0.0015(13)	0.0088(12)
C75	0.0431(17)	0.0194(12)	0.0230(15)	0.0033(11)	0.0025(13)	-0.0017(12)
C76	0.0320(15)	0.0209(12)	0.0163(14)	-0.0001(10)	0.0023(11)	-0.0011(11)
C77	0.0320(15)	0.0222(13)	0.0319(16)	0.0017(12)	0.0045(13)	-0.0050(11)
O1	0.0423(12)	0.0480(13)	0.0513(15)	0.0149(11)	0.0098(11)	0.0011(10)
O2	0.0415(12)	0.0276(10)	0.0480(13)	-0.0048(9)	0.0063(10)	-0.0034(9)
C81	0.0447(19)	0.0474(18)	0.046(2)	0.0088(15)	0.0052(15)	-0.0050(15)
C82	0.0376(17)	0.0339(16)	0.0357(18)	-0.0006(13)	0.0025(14)	-0.0096(13)
C83	0.0415(18)	0.0388(17)	0.047(2)	-0.0072(14)	0.0003(15)	-0.0026(14)
C84	0.0354(16)	0.0248(14)	0.0445(19)	-0.0004(13)	0.0008(14)	-0.0055(12)
C85	0.0467(19)	0.0314(16)	0.070(2)	-0.0085(16)	0.0051(17)	0.0013(14)
C86	0.0429(19)	0.0462(18)	0.052(2)	0.0074(16)	-0.0026(16)	-0.0058(15)
O3	0.0462(12)	0.0273(10)	0.0516(14)	0.0017(9)	-0.0117(10)	0.0015(9)
O4	0.0457(13)	0.0507(13)	0.0498(14)	0.0074(11)	0.0199(11)	-0.0029(10)
C91	0.0284(15)	0.0313(15)	0.0260(16)	-0.0026(12)	-0.0026(12)	-0.0060(12)
C92	0.0425(18)	0.0455(17)	0.0360(19)	-0.0105(14)	0.0015(14)	0.0023(14)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S11 - Bond Distances (Angstrom) for: **Compound 13•($C_6H_{12}O_2$)**

Pd	-P	2.3259(7)	C56	-C57	1.499(3)
Pd	-C1	2.048(2)	C61	-C62	1.399(3)
Pd	-C4	2.123(2)	C61	-C66	1.406(3)
Pd	-C57	2.089(2)	C62	-C63	1.381(3)
P	-C51	1.823(2)	C63	-C64	1.382(3)
P	-C61	1.842(2)	C64	-C65	1.382(4)
P	-C71	1.840(2)	C65	-C66	1.392(3)
O1	-C82	1.233(4)	C66	-C67	1.513(3)
O2	-C84	1.427(3)	C71	-C76	1.403(3)

Table S11 (cont.) - Bond Distances (Angstrom) for: **Compound 13•($C_6H_{12}O_2$)**

O2	-H2	1.05	C71	-C72	1.395(3)
O3	-C91	1.224(3)	C72	-C73	1.393(3)
O4	-C91	1.255(3)	C73	-C74	1.378(4)
N1	-C2	1.384(3)	C74	-C75	1.377(4)
N1	-C11	1.479(3)	C75	-C76	1.403(3)
N1	-C1	1.361(3)	C76	-C77	1.507(3)
N2	-C21	1.472(3)	C2	-H21	0.95
N2	-C3	1.394(3)	C3	-H31	0.95
N2	-C1	1.349(3)	C5	-H51	0.95
N3	-C31	1.471(3)	C6	-H61	0.95
N3	-C5	1.390(3)	C11	-H111	1.00
N3	-C4	1.359(3)	C12	-H121	0.99
N4	-C6	1.386(3)	C12	-H122	0.99
N4	-C41	1.471(3)	C13	-H131	0.99
N4	-C4	1.362(3)	C13	-H132	0.99
C2	-C3	1.333(4)	C14	-H142	0.99
C5	-C6	1.342(3)	C14	-H141	0.99
C11	-C12	1.537(3)	C15	-H152	0.99
C11	-C16	1.523(3)	C15	-H151	0.99
C12	-C13	1.532(4)	C16	-H162	0.99
C13	-C14	1.525(4)	C16	-H161	0.99
C14	-C15	1.515(4)	C21	-H211	1.00
C15	-C16	1.529(4)	C22	-H222	0.99
C21	-C22	1.524(3)	C22	-H221	0.99
C21	-C26	1.527(3)	C23	-H232	0.99
C22	-C23	1.531(4)	C23	-H231	0.99
C23	-C24	1.520(4)	C24	-H242	0.99
C24	-C25	1.525(4)	C24	-H241	0.99
C25	-C26	1.525(4)	C25	-H251	0.99
C31	-C36	1.519(3)	C25	-H252	0.99
C31	-C32	1.530(3)	C26	-H262	0.99
C32	-C33	1.532(3)	C26	-H261	0.99
C33	-C34	1.521(4)	C31	-H311	1.00
C34	-C35	1.523(4)	C32	-H321	0.99
C35	-C36	1.529(3)	C32	-H322	0.99
C41	-C42	1.524(3)	C33	-H331	0.99
C41	-C46	1.524(3)	C33	-H332	0.99
C42	-C43	1.529(3)	C34	-H342	0.99
C43	-C44	1.524(4)	C34	-H341	0.99
C44	-C45	1.516(4)	C35	-H351	0.99
C45	-C46	1.531(3)	C35	-H352	0.99
C51	-C56	1.393(3)	C36	-H362	0.99
C51	-C52	1.393(3)	C36	-H361	0.99
C52	-C53	1.383(3)	C41	-H411	1.00
C53	-C54	1.392(3)	C42	-H421	0.99
C54	-C55	1.378(4)	C42	-H422	0.99
C55	-C56	1.400(3)	C43	-H432	0.99
C55	-C56	1.400(3)	C43	-H432	0.99
C43	-H431	0.99	C77	-H773	0.98
C44	-H442	0.99	C77	-H772	0.98
C44	-H441	0.99	C77	-H771	0.98
C45	-H452	0.99	C81	-C82	1.495(4)
C45	-H451	0.99	C82	-C83	1.490(4)
C46	-H462	0.99	C83	-C84	1.542(4)
C46	-H461	0.99	C84	-C86	1.512(4)
C52	-H521	0.95	C84	-C85	1.521(4)
C53	-H531	0.95	C81	-H811	0.98
C54	-H541	0.95	C81	-H812	0.98
C55	-H551	0.95	C81	-H813	0.98
C57	-H571	0.99	C83	-H831	0.99
C57	-H572	0.99	C83	-H832	0.99
C62	-H621	0.95	C85	-H852	0.98

Table S11 (cont.) - Bond Distances (Angstrom) for: **Compound 13•($C_6H_{12}O_2$)**

C63	-H631	0.95	C85	-H853	0.98
C64	-H641	0.95	C85	-H851	0.98
C65	-H651	0.95	C86	-H863	0.98
C67	-H671	0.98	C86	-H861	0.98
C67	-H672	0.98	C86	-H862	0.98
C67	-H673	0.98	C91	-C92	1.527(4)
C72	-H721	0.95	C92	-H921	0.98
C73	-H731	0.95	C92	-H922	0.98
C74	-H741	0.95	C92	-H923	0.98
C75	-H751	0.95			

Table S12 - Bond Angles (Degrees) for: **Compound 13•($C_6H_{12}O_2$)**

P	-Pd	-C1	156.69(7)	C33	-C34	-C35	112.9(2)
P	-Pd	-C4	99.11(6)	C34	-C35	-C36	110.9(2)
P	-Pd	-C57	82.72(6)	C31	-C36	-C35	110.55(18)
C1	-Pd	-C4	97.91(9)	N4	-C41	-C42	109.50(18)
C1	-Pd	-C57	82.62(9)	N4	-C41	-C46	111.87(17)
C4	-Pd	-C57	172.05(9)	C42	-C41	-C46	110.78(19)
Pd	-P	-C51	101.81(7)	C41	-C42	-C43	110.7(2)
Pd	-P	-C61	108.51(7)	C42	-C43	-C44	109.85(19)
Pd	-P	-C71	131.57(8)	C43	-C44	-C45	110.8(2)
C51	-P	-C61	104.13(10)	C44	-C45	-C46	111.8(2)
C51	-P	-C71	101.37(10)	C41	-C46	-C45	111.53(19)
C61	-P	-C71	106.14(10)	P	-C51	-C52	124.23(17)
C84	-O2	-H2	109.42	P	-C51	-C56	114.61(17)
C1	-N1	-C2	110.25(19)	C52	-C51	-C56	121.1(2)
C2	-N1	-C11	123.17(19)	C51	-C52	-C53	119.9(2)
C1	-N1	-C11	125.75(18)	C52	-C53	-C54	119.5(2)
C1	-N2	-C21	124.28(19)	C53	-C54	-C55	120.3(2)
C3	-N2	-C21	123.44(19)	C54	-C55	-C56	121.1(2)
C1	-N2	-C3	110.86(19)	C51	-C56	-C55	117.8(2)
C4	-N3	-C31	125.60(19)	C51	-C56	-C57	119.5(2)
C5	-N3	-C31	122.45(18)	C55	-C56	-C57	122.7(2)
C4	-N3	-C5	111.71(18)	Pd	-C57	-C56	115.98(15)
C4	-N4	-C6	111.84(18)	P	-C61	-C62	118.65(16)
C6	-N4	-C41	122.42(18)	C62	-C61	-C66	118.7(2)
C4	-N4	-C41	125.53(19)	P	-C61	-C66	122.45(17)
Pd	-C1	-N1	124.84(16)	C61	-C62	-C63	121.5(2)
N1	-C1	-N2	104.80(18)	C62	-C63	-C64	119.8(2)
Pd	-C1	-N2	130.13(16)	C63	-C64	-C65	119.4(2)
N1	-C2	-C3	107.6(2)	C64	-C65	-C66	121.9(2)
N2	-C3	-C2	106.5(2)	C61	-C66	-C65	118.7(2)
Pd	-C4	-N4	126.66(15)	C65	-C66	-C67	117.8(2)
N3	-C4	-N4	103.30(18)	C61	-C66	-C67	123.56(19)
Pd	-C4	-N3	130.01(16)	P	-C71	-C72	121.07(17)
N3	-C5	-C6	106.60(19)	C72	-C71	-C76	119.4(2)
N4	-C6	-C5	106.54(19)	P	-C71	-C76	119.39(16)
N1	-C11	-C16	112.1(2)	C71	-C72	-C73	121.0(2)
C12	-C11	-C16	110.3(2)	C72	-C73	-C74	119.5(2)
N1	-C11	-C12	109.93(18)	C73	-C74	-C75	120.1(2)
C11	-C12	-C13	111.4(2)	C74	-C75	-C76	121.5(2)
C12	-C13	-C14	110.9(2)	C71	-C76	-C75	118.3(2)
C13	-C14	-C15	110.7(2)	C75	-C76	-C77	118.8(2)
C14	-C15	-C16	110.9(2)	C71	-C76	-C77	122.8(2)
C11	-C16	-C15	110.7(2)	C3	-C2	-H21	126.24
N2	-C21	-C22	111.35(19)	N1	-C2	-H21	126.13
N2	-C21	-C26	109.12(19)	N2	-C3	-H31	126.70
C22	-C21	-C26	111.27(19)	C2	-C3	-H31	126.85
C21	-C22	-C23	110.9(2)	N3	-C5	-H51	126.75
C22	-C23	-C24	110.6(2)	C6	-C5	-H51	126.65

Table S12 (cont.) - Bond Angles (Degrees) for: **Compound 13•($C_6H_{12}O_2$)**

C23	-C24	-C25	110.4(2)	C5	-C6	-H61	126.74
C24	-C25	-C26	110.8(2)	N4	-C6	-H61	126.72
C21	-C26	-C25	111.9(2)	N1	-C11	-H111	108.13
N3	-C31	-C36	111.43(18)	C12	-C11	-H111	108.12
C32	-C31	-C36	111.08(18)	C16	-C11	-H111	108.13
N3	-C31	-C32	108.97(18)	C11	-C12	-H121	109.32
C31	-C32	-C33	112.1(2)	C11	-C12	-H122	109.42
C32	-C33	-C34	111.7(2)	C13	-C12	-H122	109.30
H121	-C12	-H122	108.02	H321	-C32	-H322	107.76
C13	-C12	-H121	109.34	C33	-C32	-H322	109.16
C12	-C13	-H132	109.36	C32	-C33	-H331	109.31
C14	-C13	-H131	109.50	C32	-C33	-H332	109.23
C12	-C13	-H131	109.52	C34	-C33	-H332	109.28
H131	-C13	-H132	108.02	H331	-C33	-H332	107.94
C14	-C13	-H132	109.52	C34	-C33	-H331	109.31
C13	-C14	-H141	109.50	C33	-C34	-H342	109.00
C15	-C14	-H141	109.52	C35	-C34	-H341	109.09
C15	-C14	-H142	109.41	C35	-C34	-H342	109.00
H141	-C14	-H142	108.08	H341	-C34	-H342	107.72
C13	-C14	-H142	109.59	C33	-C34	-H341	108.96
C14	-C15	-H152	109.53	C34	-C35	-H351	109.46
C16	-C15	-H151	109.46	C36	-C35	-H351	109.48
C14	-C15	-H151	109.47	C36	-C35	-H352	109.44
H151	-C15	-H152	108.07	C34	-C35	-H352	109.43
C16	-C15	-H152	109.34	H351	-C35	-H352	108.08
C11	-C16	-H162	109.54	C31	-C36	-H362	109.51
C15	-C16	-H161	109.52	C35	-C36	-H361	109.59
C11	-C16	-H161	109.50	C31	-C36	-H361	109.47
H161	-C16	-H162	108.04	H361	-C36	-H362	108.10
C15	-C16	-H162	109.52	C35	-C36	-H362	109.59
N2	-C21	-H211	108.33	N4	-C41	-H411	108.14
C26	-C21	-H211	108.38	C46	-C41	-H411	108.17
C22	-C21	-H211	108.29	C42	-C41	-H411	108.27
C21	-C22	-H221	109.42	C41	-C42	-H422	109.47
C21	-C22	-H222	109.48	C43	-C42	-H421	109.55
C23	-C22	-H222	109.44	C41	-C42	-H421	109.52
H221	-C22	-H222	108.03	H421	-C42	-H422	108.06
C23	-C22	-H221	109.51	C43	-C42	-H422	109.55
C22	-C23	-H232	109.48	C42	-C43	-H431	109.72
C24	-C23	-H231	109.50	C44	-C43	-H431	109.67
C24	-C23	-H232	109.46	C44	-C43	-H432	109.69
H231	-C23	-H232	108.22	H431	-C43	-H432	108.17
C22	-C23	-H231	109.50	C42	-C43	-H432	109.72
C23	-C24	-H242	109.51	C43	-C44	-H442	109.52
C25	-C24	-H241	109.62	C45	-C44	-H441	109.48
C23	-C24	-H241	109.51	C43	-C44	-H441	109.50
H241	-C24	-H242	108.07	H441	-C44	-H442	108.05
C25	-C24	-H242	109.69	C45	-C44	-H442	109.45
C24	-C25	-H251	109.49	C44	-C45	-H452	109.25
C26	-C25	-H251	109.45	C46	-C45	-H451	109.24
C26	-C25	-H252	109.50	C46	-C45	-H452	109.29
H251	-C25	-H252	108.09	H451	-C45	-H452	107.97
C24	-C25	-H252	109.41	C44	-C45	-H451	109.22
C21	-C26	-H262	109.23	C41	-C46	-H462	109.34
C25	-C26	-H261	109.24	C45	-C46	-H461	109.35
C21	-C26	-H261	109.24	C41	-C46	-H461	109.27
H261	-C26	-H262	107.95	H461	-C46	-H462	107.90
C25	-C26	-H262	109.22	C45	-C46	-H462	109.38
C32	-C31	-H311	108.43	C51	-C52	-H521	120.12
C36	-C31	-H311	108.46	C53	-C52	-H521	119.96
N3	-C31	-H311	108.39	C54	-C53	-H531	120.20

Table S12 (cont.) - Bond Angles (Degrees) for: **Compound 13•($C_6H_{12}O_2$)**

C31	-C32	-H322	109.20	C52	-C53	-H531	120.29
C33	-C32	-H321	109.23	C53	-C54	-H541	119.77
C31	-C32	-H321	109.29	C55	-C54	-H541	119.91
C31	-C32	-H321	109.29	C55	-C54	-H541	119.91
C56	-C55	-H551	119.44	O2	-C84	-C85	110.8(2)
C54	-C55	-H551	119.46	O2	-C84	-C86	105.3(2)
Pd	-C57	-H571	108.31	O2	-C84	-C83	109.4(2)
Pd	-C57	-H572	108.31	C83	-C84	-C86	112.3(3)
C56	-C57	-H572	108.29	C85	-C84	-C86	110.1(2)
H571	-C57	-H572	107.42	C83	-C84	-C85	108.9(2)
C56	-C57	-H571	108.23	C82	-C81	-H811	109.56
C63	-C62	-H621	119.21	C82	-C81	-H812	109.54
C61	-C62	-H621	119.28	C82	-C81	-H813	109.48
C62	-C63	-H631	120.10	H811	-C81	-H812	109.41
C64	-C63	-H631	120.13	H811	-C81	-H813	109.40
C65	-C64	-H641	120.29	H812	-C81	-H813	109.45
C63	-C64	-H641	120.32	C82	-C83	-H831	109.12
C64	-C65	-H651	118.99	C82	-C83	-H832	109.17
C66	-C65	-H651	119.08	C84	-C83	-H831	109.12
C66	-C67	-H672	109.44	C84	-C83	-H832	109.15
C66	-C67	-H673	109.51	H831	-C83	-H832	107.79
H671	-C67	-H672	109.48	C84	-C85	-H851	109.40
H671	-C67	-H673	109.43	C84	-C85	-H852	109.46
H672	-C67	-H673	109.48	C84	-C85	-H853	109.46
C66	-C67	-H671	109.48	H851	-C85	-H852	109.54
C71	-C72	-H721	119.50	H851	-C85	-H853	109.42
C73	-C72	-H721	119.50	H852	-C85	-H853	109.55
C74	-C73	-H731	120.23	C84	-C86	-H861	109.42
C72	-C73	-H731	120.28	C84	-C86	-H862	109.54
C73	-C74	-H741	119.96	C84	-C86	-H863	109.59
C75	-C74	-H741	119.89	H861	-C86	-H862	109.35
C76	-C75	-H751	119.25	H861	-C86	-H863	109.49
C74	-C75	-H751	119.25	H862	-C86	-H863	109.44
C76	-C77	-H771	109.44	O3	-C91	-O4	125.4(2)
C76	-C77	-H773	109.44	O3	-C91	-C92	118.5(2)
H771	-C77	-H772	109.46	O4	-C91	-C92	116.1(2)
H771	-C77	-H773	109.46	C91	-C92	-H921	109.55
H772	-C77	-H773	109.53	C91	-C92	-H922	109.48
C76	-C77	-H772	109.51	C91	-C92	-H923	109.39
O1	-C82	-C83	121.6(3)	H921	-C92	-H922	109.43
C81	-C82	-C83	116.6(3)	H921	-C92	-H923	109.52
O1	-C82	-C81	121.8(3)	H922	-C92	-H923	109.46
C82	-C83	-C84	112.4(2)				

Table S13 - Crystal Data and Details of the Structure Determination for: **Compound 16**

Crystal Data

Formula	C35 H38 N3 O2 P Pd		
Formula Weight	670.07		
Crystal System	Orthorhombic		
Space group	Pbca		(No. 61)
a, b, c [Angstrom]	12.6248(1)	17.9528(1)	27.0927(2)
V [Ang**3]	6140.57(7)		
Z	8		
D(calc) [g/cm**3]	1.450		
Mu(MoKa) [/mm]	0.693		
F(000)	2768		
Crystal Size [mm]	0.08 x	0.10 x	0.43

Table S13 (cont.) - Crystal Data and Details of the Structure Determination for: **Compound 16**

Data Collection

Temperature (K)	173
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	4.1, 25.4
Dataset	-15: 15 ; -21: 21 ; -32: 32
Tot., Uniq. Data, R(int)	136328, 5611, 0.058
Observed data [I > 2.0 sigma(I)]	4793

Refinement

Nref, Npar	5611, 531
R, wR2, S	0.0291, 0.0717, 1.03
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.51, 0.64

Table S14 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atomsfor: **Compound 16**

Atom	x	y	z	U(eq) [Ang^2]
Pd	0.43280(1)	0.39573(1)	0.12002(1)	0.0231(1)
P	0.26908(5)	0.39506(3)	0.08569(2)	0.0212(2)
O1	0.40302(15)	0.48851(10)	0.16652(7)	0.0366(6)
O2	0.41377(15)	0.43453(10)	0.23993(7)	0.0395(6)
N1	0.67457(16)	0.39840(12)	0.15509(8)	0.0334(7)
N2	0.58727(15)	0.29980(12)	0.17352(7)	0.0295(7)
N16	0.53055(19)	0.17794(12)	0.16249(8)	0.0391(8)
C1	0.57702(18)	0.36759(14)	0.15120(9)	0.0280(7)
C2	0.7430(2)	0.35057(18)	0.17994(10)	0.0443(10)
C3	0.6894(2)	0.28914(18)	0.19094(10)	0.0412(9)
C4	0.40674(19)	0.48808(14)	0.21239(10)	0.0304(8)
C5	0.4035(3)	0.56616(17)	0.23608(13)	0.0502(11)
C6	0.7065(2)	0.47357(17)	0.13564(10)	0.0414(9)
C7	0.6616(4)	0.5329(2)	0.16925(18)	0.0687(16)
C8	0.8268(3)	0.4784(3)	0.13480(17)	0.0637(15)
C9	0.6655(4)	0.4818(3)	0.08331(15)	0.0677(16)
C11	0.50447(19)	0.24583(13)	0.17739(8)	0.0281(7)
C12	0.4055(2)	0.26659(14)	0.19403(9)	0.0288(8)
C13	0.3262(2)	0.21330(14)	0.19296(10)	0.0333(8)
C14	0.3498(2)	0.14270(16)	0.17612(11)	0.0427(10)
C15	0.4516(3)	0.12720(16)	0.16231(12)	0.0445(10)
C21	0.17192(17)	0.33915(12)	0.12004(8)	0.0210(6)
C22	0.1473(2)	0.26742(13)	0.10345(9)	0.0269(8)
C23	0.0788(2)	0.22182(15)	0.12913(10)	0.0336(8)
C24	0.0315(2)	0.24763(15)	0.17182(10)	0.0333(8)
C25	0.05543(19)	0.31788(14)	0.18923(10)	0.0292(8)
C26	0.12722(18)	0.36406(13)	0.16470(8)	0.0243(7)
C27	0.1533(3)	0.43756(15)	0.18792(11)	0.0335(9)
C31	0.19860(19)	0.47967(13)	0.06683(8)	0.0258(7)
C32	0.0885(2)	0.48101(15)	0.06718(10)	0.0334(8)
C33	0.0329(3)	0.54245(16)	0.05042(11)	0.0430(10)
C34	0.0880(3)	0.60367(16)	0.03364(12)	0.0458(10)
C35	0.1968(3)	0.60310(15)	0.03277(10)	0.0406(10)
C36	0.2555(2)	0.54166(13)	0.04908(9)	0.0304(8)
C37	0.3740(2)	0.54339(18)	0.04626(13)	0.0408(10)
C41	0.28830(19)	0.34676(12)	0.02772(8)	0.0237(7)
C42	0.2134(2)	0.34085(14)	-0.00993(9)	0.0301(8)
C43	0.2383(2)	0.30541(15)	-0.05361(9)	0.0351(8)

Table S14 (cont.) - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atomsfor: **Compound 16**

Atom	x	y	z	U(eq) [Ang^2]
C44	0.3401(2)	0.27729(15)	-0.05976(10)	0.0365(9)
C45	0.4144(2)	0.28311(14)	-0.02242(9)	0.0306(8)
C46	0.38965(19)	0.31717(13)	0.02245(8)	0.0247(7)
C47	0.4663(2)	0.32031(16)	0.06498(9)	0.0298(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S15 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **Compound 16**

Atom	x	y	z	U(iso) [Ang^2]
H21	0.815(3)	0.3624(17)	0.1872(11)	0.054(9)
H31	0.706(2)	0.2451(16)	0.2063(10)	0.037(7)
H51	0.385(3)	0.604(2)	0.2110(15)	0.077(12)
H52	0.350(4)	0.566(3)	0.264(2)	0.134(19)
H53	0.478(5)	0.584(3)	0.249(2)	0.15(2)
H71	0.687(3)	0.582(2)	0.1594(15)	0.085(12)
H72	0.585(3)	0.533(2)	0.1688(14)	0.077(12)
H73	0.687(3)	0.5247(18)	0.2036(14)	0.062(11)
H81	0.843(3)	0.526(2)	0.1211(13)	0.071(12)
H82	0.856(3)	0.478(2)	0.1696(16)	0.087(13)
H83	0.851(3)	0.443(2)	0.1105(13)	0.059(10)
H91	0.681(3)	0.529(2)	0.0717(13)	0.063(10)
H92	0.691(4)	0.440(3)	0.0635(19)	0.12(2)
H93	0.586(3)	0.482(2)	0.0824(14)	0.074(11)
H121	0.392(2)	0.3127(14)	0.2063(9)	0.028(7)
H131	0.255(2)	0.2263(14)	0.2046(10)	0.037(7)
H141	0.291(3)	0.1052(16)	0.1744(11)	0.048(8)
H151	0.470(2)	0.0766(19)	0.1517(12)	0.055(9)
H221	0.1797(19)	0.2503(13)	0.0751(9)	0.023(6)
H231	0.063(2)	0.1761(18)	0.1181(10)	0.042(8)
H241	-0.016(2)	0.2195(15)	0.1897(10)	0.039(8)
H251	0.0263(19)	0.3353(13)	0.2175(10)	0.023(6)
H271	0.092(3)	0.459(2)	0.1998(14)	0.068(11)
H272	0.194(3)	0.4273(19)	0.2146(14)	0.065(11)
H273	0.186(2)	0.4684(16)	0.1660(11)	0.038(8)
H321	0.049(2)	0.4392(15)	0.0786(10)	0.033(7)
H331	-0.042(3)	0.5404(16)	0.0512(11	0.046(8)
H341	0.051(3)	0.644(2)	0.0219(13)	0.067(10)
H351	0.236(2)	0.6422(16)	0.0212(11	0.044(8)
H371	0.401(2)	0.5032(17)	0.0267(11)	0.043(8)
H372	0.398(3)	0.5887(19)	0.0292(12)	0.056(9)
H373	0.402(3)	0.5399(17)	0.0781(14)	0.057(10)
H421	0.148(2)	0.3630(14)	-0.0052(9)	0.029(7)
H431	0.192(2)	0.3018(14)	-0.0791(10)	0.031(7)
H441	0.359(2)	0.2544(15)	-0.0889(11)	0.038(7)
H451	0.482(2)	0.2634(14)	-0.0264(9)	0.034(7)
H471	0.472(2)	0.2749(17)	0.0796(11)	0.045(8)
H472	0.536(3)	0.3320(16)	0.0519(11)	0.052(9)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S16 - (An)isotropic Displacement Parameters for: **Compound 16**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Pd	0.0199(1)	0.0282(1)	0.0212(1)	0.0008(1)	-0.0018(1)	-0.0020(1)
P	0.0205(3)	0.0230(3)	0.0201(3)	0.0003(2)	-0.0007(2)	0.0004(2)
O1	0.0391(10)	0.0392(10)	0.0314(11)	-0.0031(8)	-0.0052(8)	-0.0052(8)
O2	0.0482(12)	0.0347(10)	0.0355(11)	0.0014(9)	-0.0024(9)	0.0025(8)
N1	0.0227(11)	0.0520(14)	0.0255(11)	0.0019(10)	-0.0031(9)	-0.0076(10)
N2	0.0238(11)	0.0392(12)	0.0255(11)	0.0023(9)	-0.0038(8)	0.0021(9)
N16	0.0410(13)	0.0372(13)	0.0392(13)	0.0033(10)	0.0042(11)	0.0091(11)
C1	0.0242(12)	0.0400(14)	0.0197(12)	0.0003(10)	-0.0009(10)	-0.0018(10)
C2	0.0237(14)	0.071(2)	0.0382(16)	0.0022(15)	-0.0088(12)	-0.0014(14)
C3	0.0300(15)	0.0582(19)	0.0355(15)	0.0068(14)	-0.0078(12)	0.0065(14)
C4	0.0196(12)	0.0357(14)	0.0359(15)	0.0063(12)	-0.0008(10)	-0.0027(10)
C5	0.074(2)	0.0361(17)	0.0405(18)	-0.0028(14)	-0.0020(17)	-0.0054(16)
C6	0.0318(15)	0.0570(18)	0.0355(15)	0.0042(13)	0.0000(12)	-0.0172(13)
C7	0.067(3)	0.057(2)	0.082(3)	-0.005(2)	0.029(2)	-0.0218(19)
C8	0.0370(18)	0.089(3)	0.065(3)	0.004(2)	0.0060(17)	-0.0257(19)
C9	0.064(3)	0.083(3)	0.056(2)	0.031(2)	-0.0173(19)	-0.040(2)
C11	0.0302(13)	0.0317(13)	0.0223(12)	0.0041(10)	-0.0033(10)	0.0022(11)
C12	0.0353(14)	0.0286(13)	0.0226(12)	0.0003(10)	-0.0017(10)	0.0039(11)
C13	0.0332(15)	0.0334(14)	0.0332(14)	0.0040(11)	0.0029(11)	0.0011(11)
C14	0.0450(17)	0.0344(15)	0.0487(18)	0.0001(13)	-0.0008(14)	-0.0029(13)
C15	0.0540(19)	0.0322(15)	0.0474(18)	0.0030(13)	0.0055(15)	0.0060(14)
C21	0.0189(11)	0.0228(11)	0.0214(11)	0.0032(9)	-0.0028(9)	0.0020(9)
C22	0.0297(13)	0.0268(13)	0.0243(13)	-0.0020(10)	-0.0006(11)	0.0003(10)
C23	0.0366(15)	0.0274(13)	0.0367(15)	-0.0009(11)	-0.0048(12)	-0.0060(11)
C24	0.0273(14)	0.0352(14)	0.0374(15)	0.0080(12)	-0.0003(11)	-0.0061(11)
C25	0.0263(13)	0.0340(13)	0.0272(13)	0.0033(11)	0.0043(11)	0.0037(11)
C26	0.0221(12)	0.0250(12)	0.0258(12)	0.0010(10)	-0.0034(10)	0.0043(10)
C27	0.0387(16)	0.0308(14)	0.0309(15)	-0.0013(12)	0.0063(13)	0.0001(12)
C31	0.0323(13)	0.0247(12)	0.0205(12)	0.0009(10)	-0.0013(10)	0.0028(10)
C32	0.0321(14)	0.0336(14)	0.0344(15)	0.0075(12)	0.0027(11)	0.0066(11)
C33	0.0394(17)	0.0451(17)	0.0446(17)	0.0131(13)	0.0041(14)	0.0160(13)
C34	0.057(2)	0.0349(16)	0.0455(18)	0.0100(13)	-0.0007(14)	0.0150(14)
C35	0.060(2)	0.0253(14)	0.0366(16)	0.0075(12)	-0.0030(14)	-0.0027(13)
C36	0.0378(14)	0.0290(13)	0.0244(12)	0.0010(10)	-0.0031(11)	-0.0015(11)
C37	0.0435(17)	0.0412(17)	0.0378(17)	0.0116(14)	-0.0057(14)	-0.0120(14)
C41	0.0244(12)	0.0250(12)	0.0217(12)	0.0016(9)	0.0017(10)	-0.0018(9)
C42	0.0275(13)	0.0354(14)	0.0274(13)	0.0020(11)	-0.0018(11)	0.0011(11)
C43	0.0388(15)	0.0429(15)	0.0236(13)	-0.0006(11)	-0.0067(12)	-0.0047(12)
C44	0.0459(17)	0.0411(15)	0.0226(13)	-0.0055(11)	0.0042(12)	-0.0006(12)
C45	0.0303(14)	0.0316(13)	0.0299(14)	0.0011(11)	0.0057(11)	0.0020(11)
C46	0.0272(12)	0.0251(12)	0.0217(12)	0.0026(9)	0.0019(10)	-0.0015(10)
C47	0.0267(13)	0.0368(15)	0.0258(13)	-0.0025(11)	-0.0009(11)	0.0066(11)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S17 - Bond Distances (Angstrom) for: **Compound 16**

Pd	-P	2.2666(6)	C43	-C44	1.391(4)
Pd	-O1	2.1220(18)	C44	-C45	1.384(4)
Pd	-C1	2.070(2)	C45	-C46	1.396(3)
Pd	-C47	2.058(3)	C46	-C47	1.506(3)
P	-C21	1.838(2)	C2	-H21	0.95(4)

Table S17 (cont.) - Bond Distances (Angstrom) for: **Compound 16**

P	-C31	1.833(2)	C3	-H31	0.92(3)
P	-C41	1.810(2)	C5	-H51	0.99(4)
O1	-C4	1.244(3)	C5	-H52	1.01(5)
O2	-C4	1.220(3)	C5	-H53	1.05(6)
N1	-C1	1.354(3)	C7	-H71	0.98(4)
N1	-C2	1.392(4)	C7	-H72	0.97(4)
N1	-C6	1.504(4)	C7	-H73	1.00(4)
N2	-C1	1.365(3)	C8	-H81	0.95(4)
N2	-C3	1.386(3)	C8	-H82	1.01(4)
N2	-C11	1.429(3)	C8	-H83	0.96(4)
N16	-C11	1.325(3)	C9	-H91	0.92(4)
N16	-C15	1.350(4)	C9	-H92	0.98(5)
C2	-C3	1.328(4)	C9	-H93	1.00(4)
C4	-C5	1.542(4)	C12	-H121	0.91(3)
C6	-C7	1.512(5)	C13	-H131	0.98(3)
C6	-C8	1.521(5)	C14	-H141	1.00(3)
C6	-C9	1.517(5)	C15	-H151	0.98(3)
C11	-C12	1.380(3)	C22	-H221	0.92(2)
C12	-C13	1.385(4)	C23	-H231	0.90(3)
C13	-C14	1.380(4)	C24	-H241	0.92(3)
C14	-C15	1.367(5)	C25	-H251	0.91(3)
C21	-C22	1.399(3)	C27	-H271	0.92(4)
C21	-C26	1.408(3)	C27	-H272	0.91(4)
C22	-C23	1.379(4)	C27	-H273	0.91(3)
C23	-C24	1.382(4)	C32	-H321	0.95(3)
C24	-C25	1.380(4)	C33	-H331	0.95(4)
C25	-C26	1.397(3)	C34	-H341	0.92(4)
C26	-C27	1.498(4)	C35	-H351	0.91(3)
C31	-C32	1.390(3)	C37	-H371	0.96(3)
C31	-C36	1.409(3)	C37	-H372	0.98(3)
C32	-C33	1.384(4)	C37	-H373	0.93(4)
C33	-C34	1.378(4)	C42	-H421	0.93(3)
C34	-C35	1.374(5)	C43	-H431	0.91(3)
C35	-C36	1.400(4)	C44	-H441	0.92(3)
C36	-C37	1.498(4)	C45	-H451	0.93(3)
C41	-C42	1.395(3)	C47	-H471	0.91(3)
C41	-C46	1.393(3)	C47	-H472	0.97(4)
C42	-C43	1.380(4)			

Table S18 - Bond Angles (Degrees) for: **Compound 16**

P	-Pd	-O1	94.95(5)	C33	-C34	-C35	120.3(3)
P	-Pd	-C1	165.55(7)	C34	-C35	-C36	122.0(3)
P	-Pd	-C47	83.49(7)	C31	-C36	-C35	117.4(2)
O1	-Pd	-C1	96.04(9)	C31	-C36	-C37	122.9(2)
O1	-Pd	-C47	169.41(9)	C35	-C36	-C37	119.7(3)
C1	-Pd	-C47	87.38(10)	P	-C41	-C42	125.45(18)
Pd	-P	-C21	113.81(7)	P	-C41	-C46	113.25(17)
Pd	-P	-C31	123.55(8)	C42	-C41	-C46	121.3(2)
Pd	-P	-C41	103.67(8)	C41	-C42	-C43	120.5(2)
C21	-P	-C31	105.65(10)	C42	-C43	-C44	118.7(2)
C21	-P	-C41	105.49(10)	C43	-C44	-C45	120.8(2)
C31	-P	-C41	102.72(10)	C44	-C45	-C46	121.2(2)
Pd	-O1	-C4	125.57(17)	C41	-C46	-C45	117.5(2)
C1	-N1	-C2	110.5(2)	C41	-C46	-C47	119.8(2)
C1	-N1	-C6	125.7(2)	C45	-C46	-C47	122.6(2)
C2	-N1	-C6	123.8(2)	Pd	-C47	-C46	116.55(17)
C1	-N2	-C3	111.2(2)	N1	-C2	-H21	123.6(18)
C1	-N2	-C11	124.58(19)	C3	-C2	-H21	128.6(18)
C3	-N2	-C11	124.2(2)	N2	-C3	-H31	119.1(16)
C11	-N16	-C15	116.0(2)	C2	-C3	-H31	134.5(16)

Table S18 (cont.) - Bond Angles (Degrees) for: **Compound 16**

Pd	-C1	-N1	137.06(19)	C4	-C5	-H51	110(2)
Pd	-C1	-N2	118.80(16)	C4	-C5	-H52	109(3)
N1	-C1	-N2	104.1(2)	C4	-C5	-H53	113(3)
N1	-C2	-C3	107.7(2)	H51	-C5	-H52	111(4)
N2	-C3	-C2	106.4(3)	H51	-C5	-H53	103(4)
O1	-C4	-O2	128.2(2)	H52	-C5	-H53	110(4)
O1	-C4	-C5	114.2(2)	C6	-C7	-H71	110(2)
O2	-C4	-C5	117.6(2)	C6	-C7	-H72	112(2)
N1	-C6	-C7	108.7(2)	C6	-C7	-H73	110(2)
N1	-C6	-C8	108.9(3)	H71	-C7	-H72	109(3)
N1	-C6	-C9	108.9(3)	H71	-C7	-H73	106(3)
C7	-C6	-C8	110.1(3)	H72	-C7	-H73	110(3)
C7	-C6	-C9	111.5(3)	C6	-C8	-H81	106(2)
C8	-C6	-C9	108.7(3)	C6	-C8	-H82	110(2)
N2	-C11	-N16	114.8(2)	C6	-C8	-H83	107(2)
N2	-C11	-C12	120.2(2)	H81	-C8	-H82	107(3)
N16	-C11	-C12	125.0(2)	H81	-C8	-H83	105(3)
C11	-C12	-C13	117.5(2)	H82	-C8	-H83	121(3)
C12	-C13	-C14	119.0(2)	C6	-C9	-H91	110(2)
C13	-C14	-C15	118.7(3)	C6	-C9	-H92	109(3)
N16	-C15	-C14	123.8(3)	C6	-C9	-H93	111(2)
P	-C21	-C22	119.23(17)	H91	-C9	-H92	117(4)
P	-C21	-C26	121.95(17)	H91	-C9	-H93	102(3)
C22	-C21	-C26	118.6(2)	H92	-C9	-H93	109(4)
C21	-C22	-C23	121.6(2)	C11	-C12	-H121	122.4(16)
C22	-C23	-C24	119.6(2)	C13	-C12	-H121	120.1(16)
C23	-C24	-C25	119.9(2)	C12	-C13	-H131	119.4(15)
C24	-C25	-C26	121.5(2)	C14	-C13	-H131	121.5(15)
C21	-C26	-C25	118.7(2)	C13	-C14	-H141	118.2(19)
C21	-C26	-C27	123.5(2)	C15	-C14	-H141	123.1(19)
C25	-C26	-C27	117.7(2)	N16	-C15	-H151	116.8(16)
P	-C31	-C32	119.85(19)	C14	-C15	-H151	119.4(16)
P	-C31	-C36	120.14(18)	C21	-C22	-H221	118.4(15)
C32	-C31	-C36	119.9(2)	C23	-C22	-H221	120.0(15)
C31	-C32	-C33	121.2(3)	C22	-C23	-H231	121.0(17)
C32	-C33	-C34	119.2(3)	C24	-C23	-H231	119.4(17)
C23	-C24	-H241	122.5(17)	C36	-C37	-H372	110(2)
C25	-C24	-H241	117.6(17)	C36	-C37	-H373	109(2)
C24	-C25	-H251	121.1(15)	H371	-C37	-H372	105(3)
C26	-C25	-H251	117.5(15)	H371	-C37	-H373	109(3)
C26	-C27	-H271	109(2)	H372	-C37	-H373	112(3)
C26	-C27	-H272	106(2)	C41	-C42	-H421	118.1(15)
C26	-C27	-H273	111.2(19)	C43	-C42	-H421	121.3(15)
H271	-C27	-H272	106(3)	C42	-C43	-H431	122.6(17)
H271	-C27	-H273	111(3)	C44	-C43	-H431	118.6(17)
H272	-C27	-H273	113(3)	C43	-C44	-H441	120.3(16)
C31	-C32	-H321	120.8(16)	C45	-C44	-H441	119.0(16)
C33	-C32	-H321	118.0(16)	C44	-C45	-H451	120.6(15)
C32	-C33	-H331	117.9(18)	C46	-C45	-H451	118.2(15)
C34	-C33	-H331	122.9(18)	Pd	-C47	-H471	106.9(19)
C33	-C34	-H341	119(2)	Pd	-C47	-H472	108.0(17)
C35	-C34	-H341	121(2)	C46	-C47	-H471	110.5(18)
C34	-C35	-H351	122.8(17)	C46	-C47	-H472	108.1(18)
C36	-C35	-H351	115.2(17)	H471	-C47	-H472	106(2)
C36	-C37	-H371	111.6(16)				