Supporting Information

Highly Active NHC-Pd (II) Complexes for Cross Coupling of Aryl Chlorides and Arylboronic Acids: An Investigation of the Remote Bulky Group Effect

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Content:

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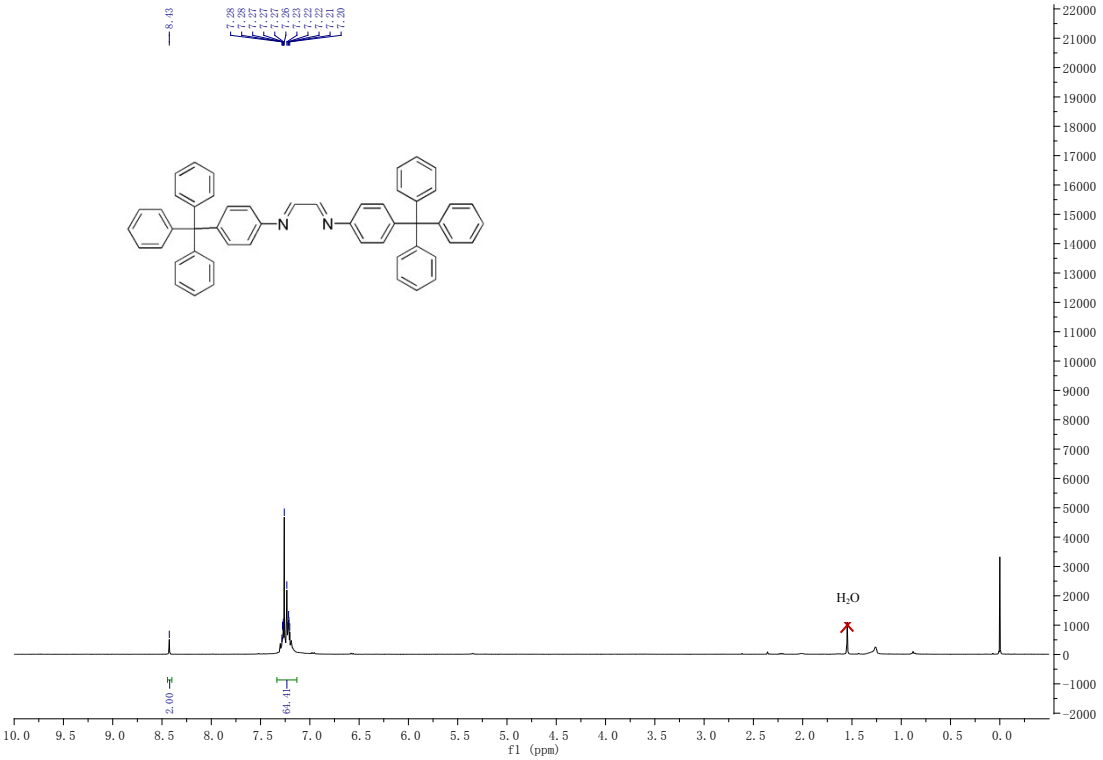

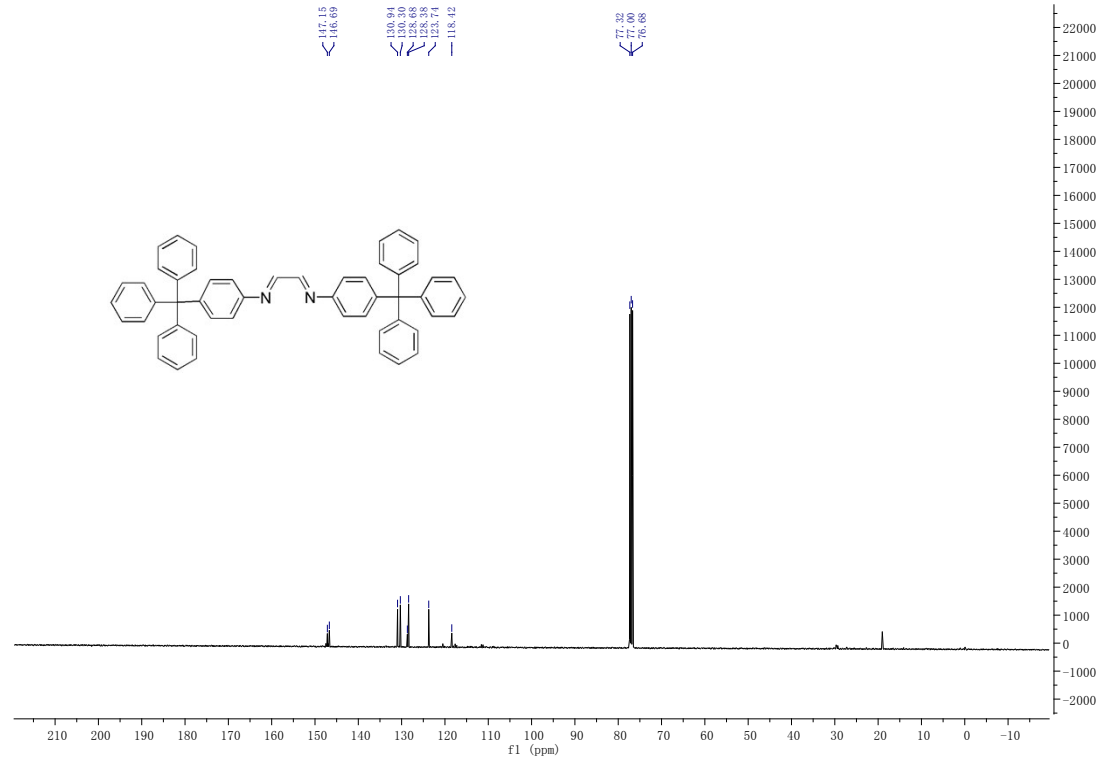

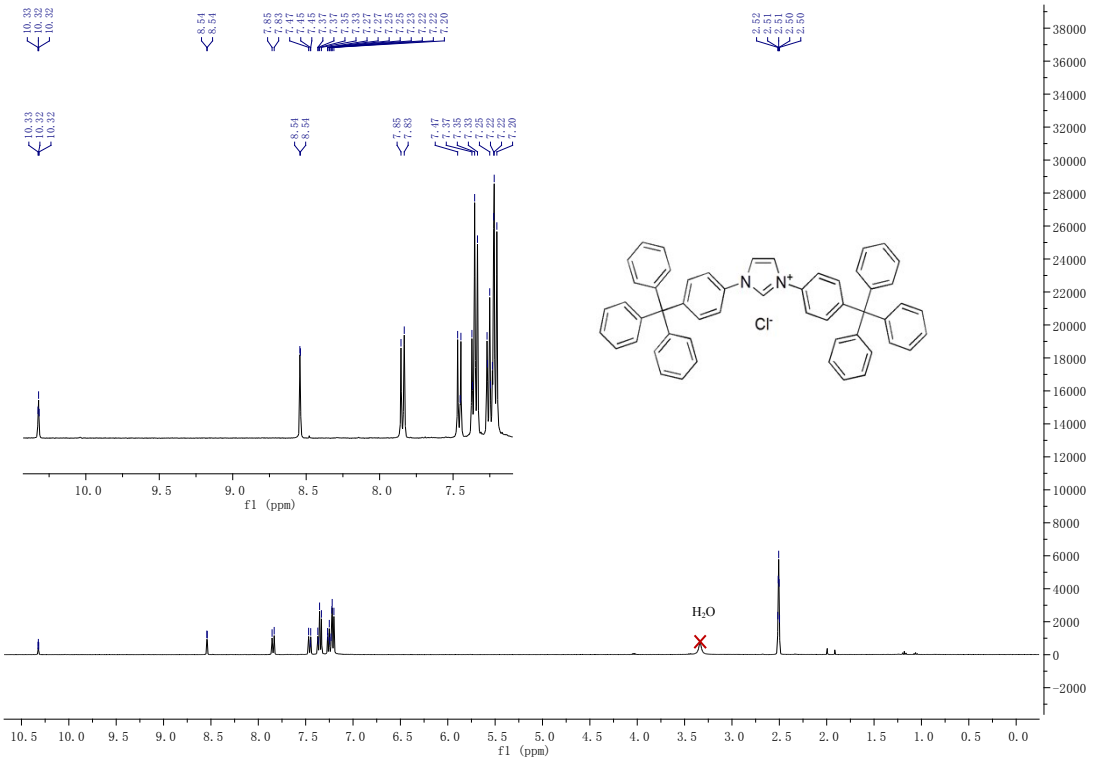
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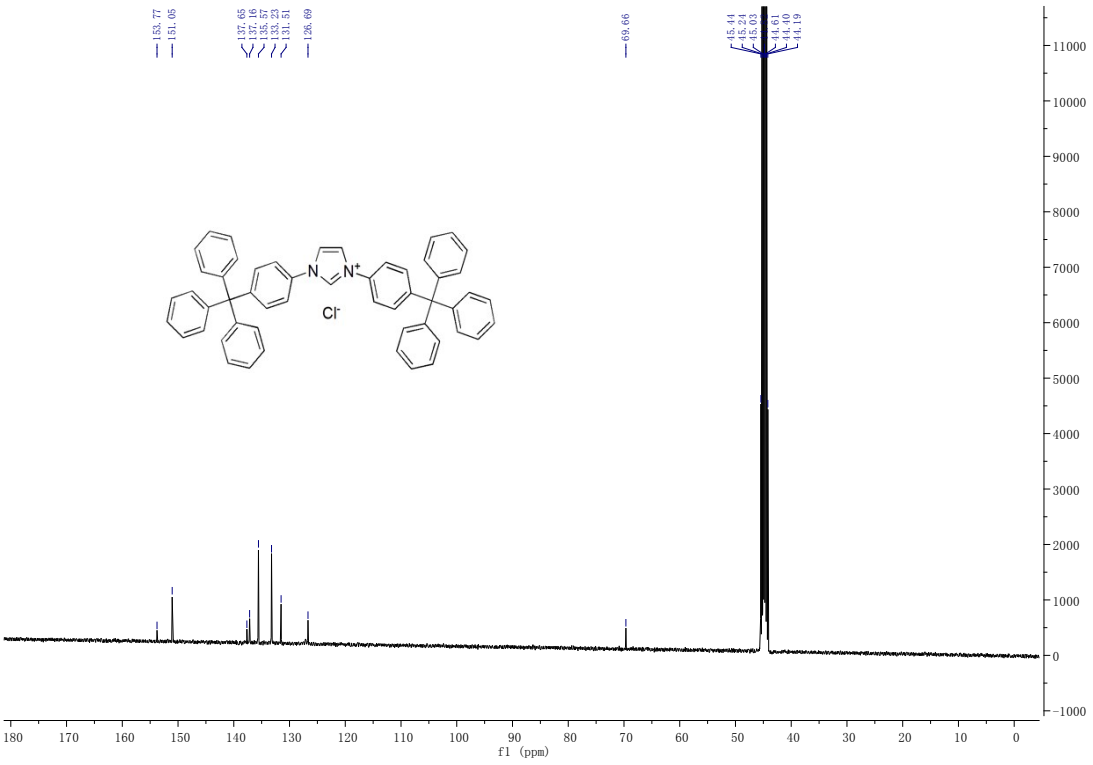
7.33
7.27
7.25
7.23
7.22
7.20
2.52
2.51
2.51
2.50
2.50
Cl-
H2O
f1 (ppm)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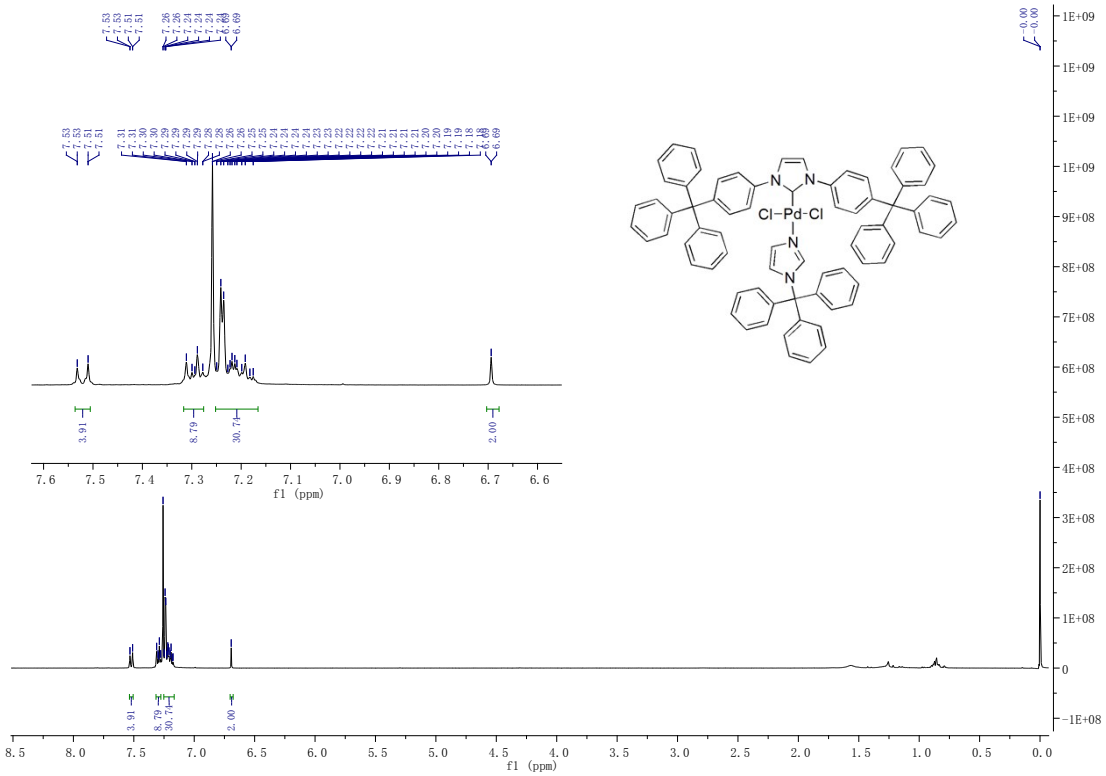
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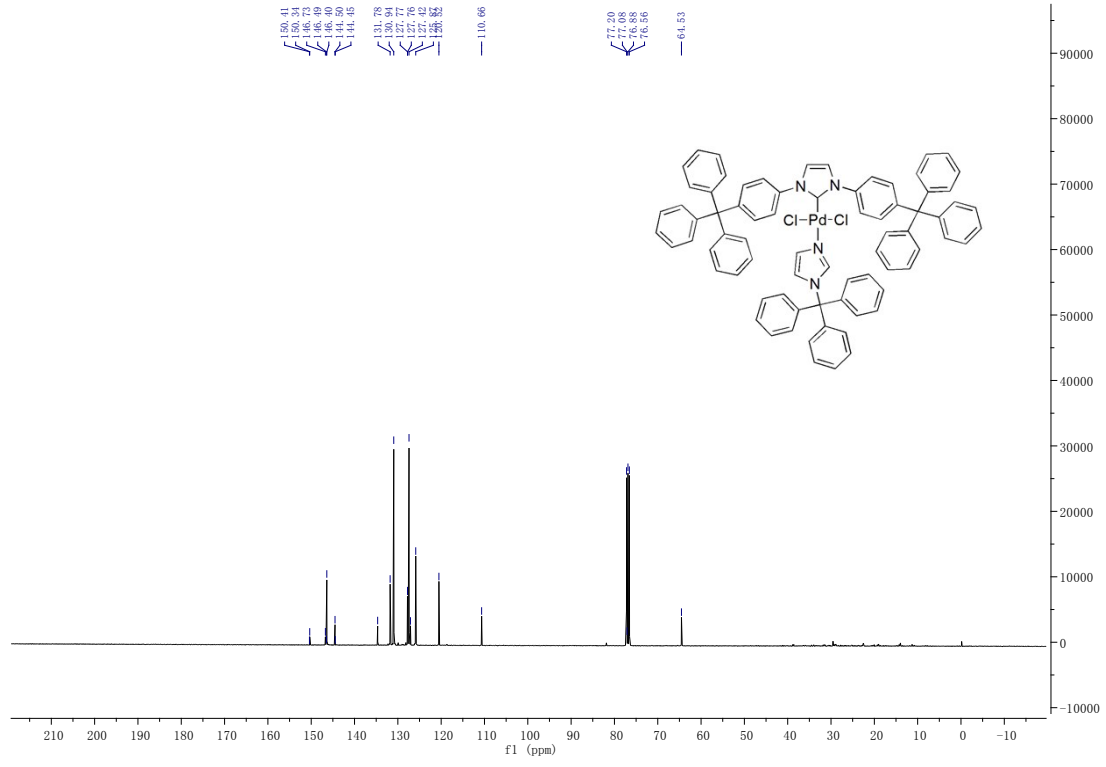
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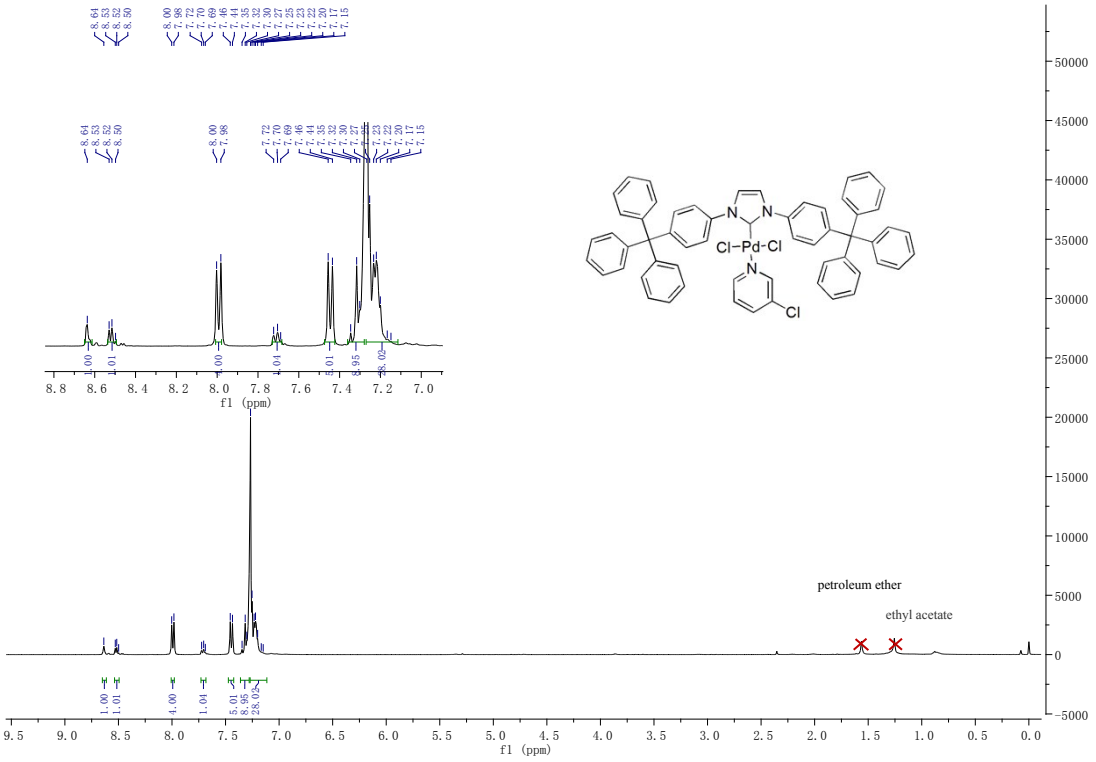
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ethyl acetate
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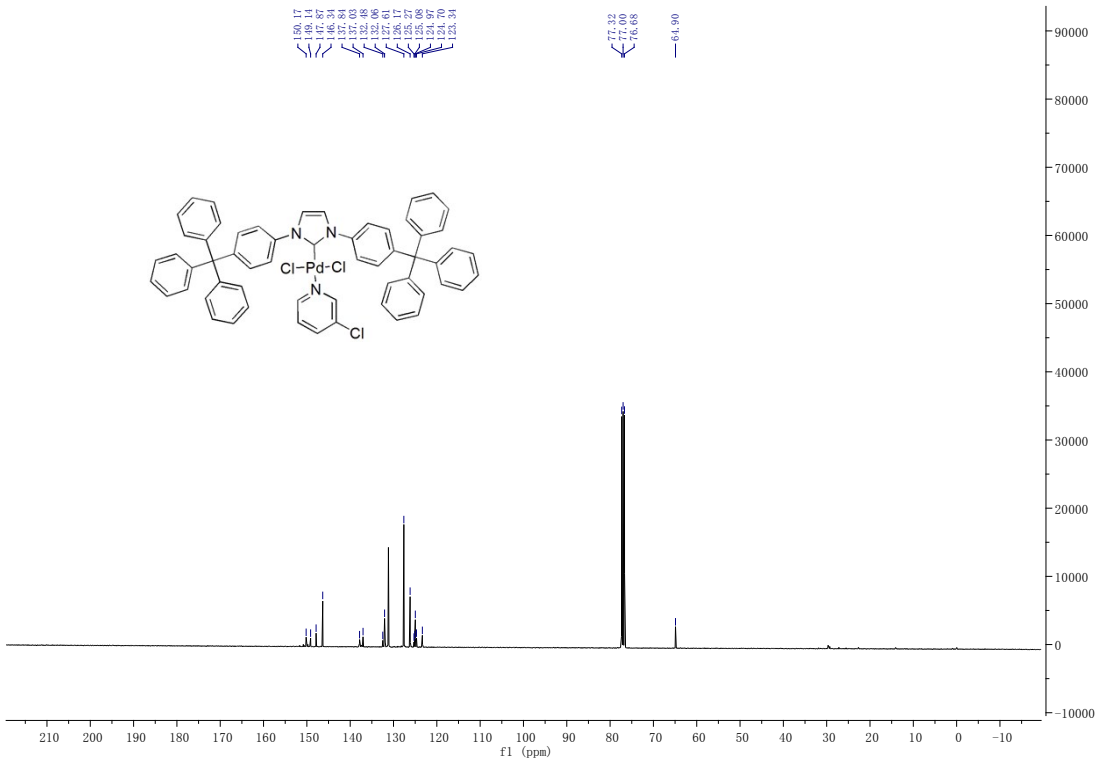
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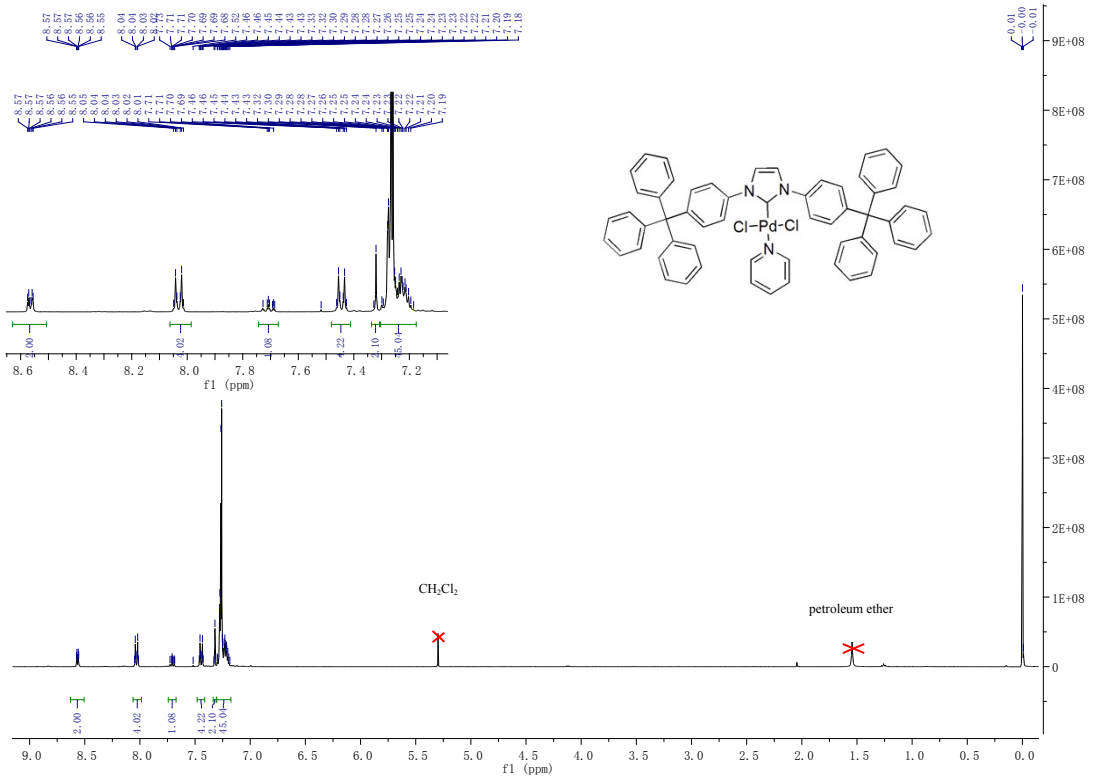
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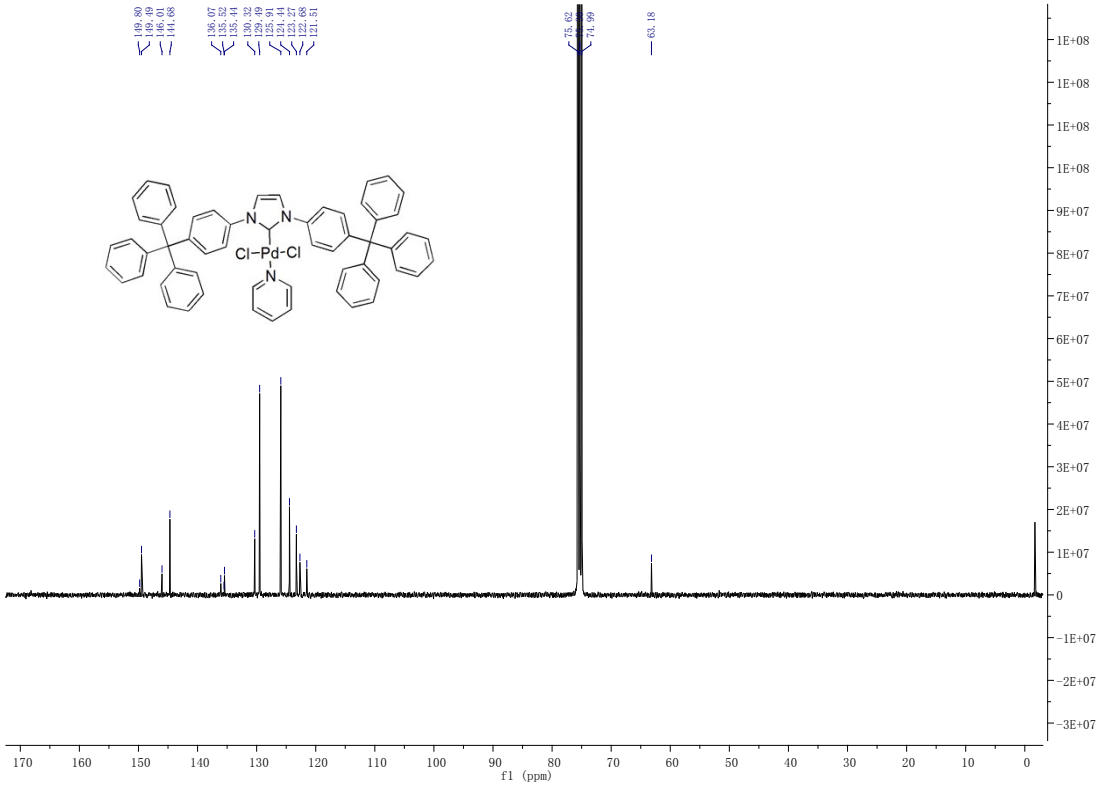
f1 (ppm)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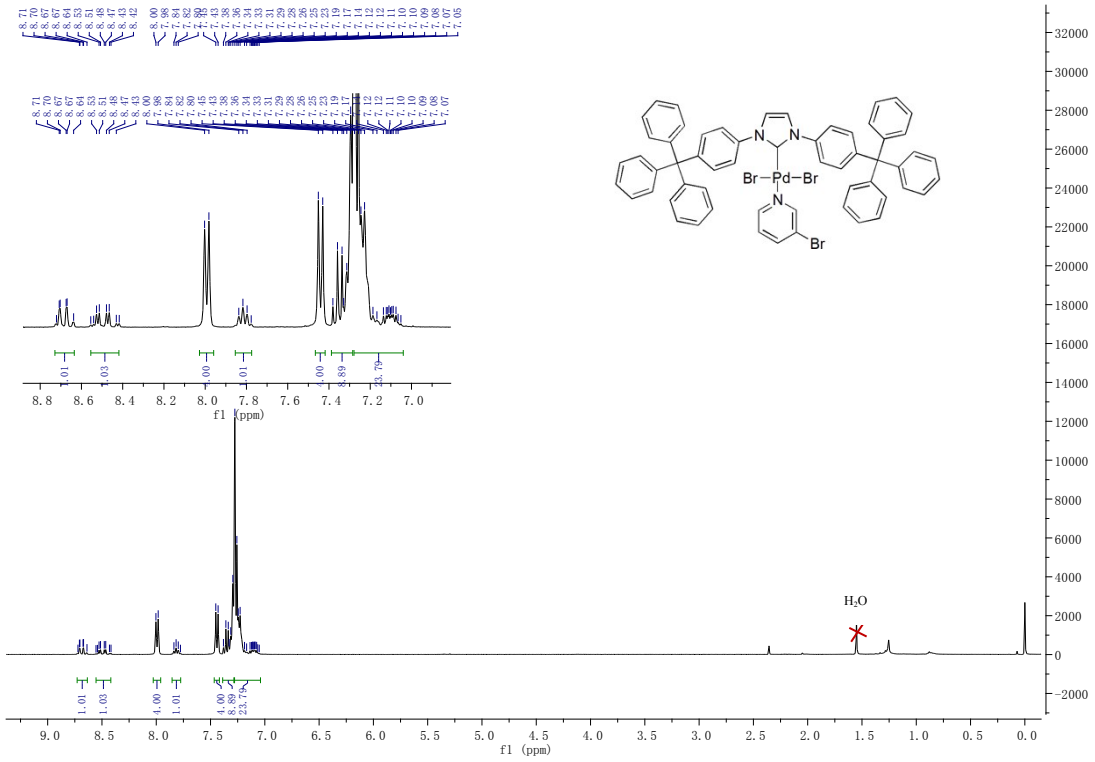
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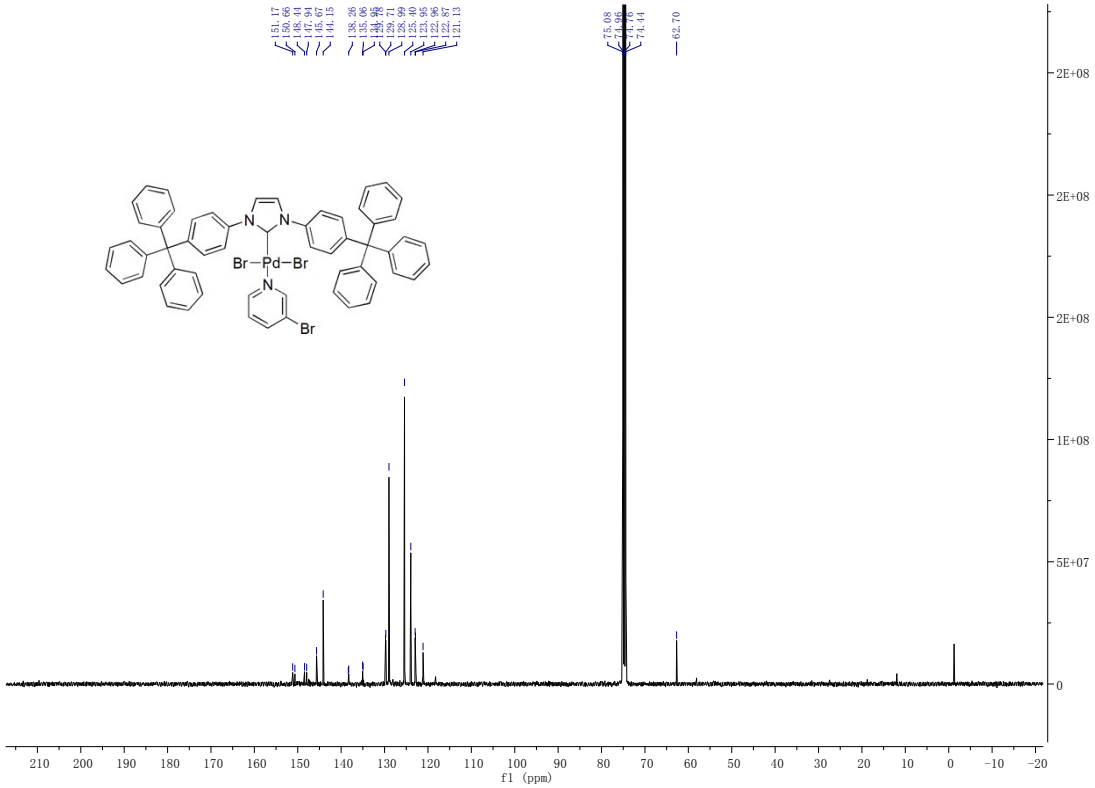
f1 (ppm)


Br—Pd—Br
Br
f1 (ppm)

2. X-Ray Crystal Structure of Complexes 4-7

Table S1. Crystal data and structure refinement for Complex **4**

Empirical formula	**4**
Formula weight	1362.40
Temperature/K	173(2)
Crystal system	Triclinic
Space group	P -1
a/Å	11.0025(8)
b/Å	17.0704(12)
c/Å	18.8271(13)
α/°	67.6860(10)
β/°	87.6640(10)
γ/°	87.070(2)
Volume/Å^3	2073.17(7)
Z	2
ρ_{calc}g/cm^3	1.385
μ/mm^{-1}	0.577
F(000)	1400
Crystal size/mm^3	0.18 × 0.14 × 0.13
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	1.375 to 28.361
Index ranges	-12 ≤ h ≤ 14, -19 ≤ k ≤ 22, -25 ≤ l ≤ 23
Reflections collected	24592
Independent reflections	16228 [R_{int} = 0.0334]
Data/restraints/parameters	16228 / 6 / 793
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.0968
Final R indexes [all data]	R_1 = 0.0716, wR_2 = 0.1081
Largest diff. peak/hole / e Å^{-3}	0.79/-0.83

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **4**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	Y	z	U(eq)
Pd1	-356(1)	2827(1)	1886(1)	11(1)
Cl1	-1526(1	1979(1)	1510(1)	19(1)
Cl2	771(1)	3748(1)	2219(1)	20(1)
Cl3	1927(1)	5894(1)	2167(1)	59(1)
Cl4	74(1)	6893(1)	2624(1)	105(1)
Cl5	4735(1)	3439(1)	917(1)	44(1)
Cl6	4349(1)	4995(1)	1201(1)	37(1)
N3	235(2)	1782(1)	2829(1)	14(1)
N4	1480(2)	879(1)	3671(1)	14(1)
N1	-1763(2)	4371(1)	866(1)	11(1)
N2	-561(2)	3837(1)	223(1)	13(1)
C23	1301(3)	1682(2)	3157(2)	15(1)
C2	-300(3)	1010(2)	3152(2)	16(1)
C3	455(3)	449(2)	3674(2)	14(1)
C4	2550(2)	575(2)	4192(2)	13(1)
C5	2295(3)	817(2)	4899(2)	15(1)
C6	1365(3)	1377(2)	4929(2)	16(1)
C7	1152(3)	1559(2)	5590(2)	21(1)
C8	1875(3)	1182(2)	6222(2)	25(1)
C9	2820(3)	619(2)	6192(2)	25(1)
C10	3033(3)	435(2)	5542(2)	22(1)
C11	3672(3)	1002(2)	3713(2)	15(1)
C12	4519(3)	1394(2)	3983(2)	21(1)
C13	5555(3)	1732(2)	3540(2)	28(1)

C14	5752(3)	1694(2)	2831(2)	30(1)
C15	4894(3)	1325(2)	2542(2)	27(1)
C16	3870(3)	992(2)	2970(2)	21(1)
C17	2661(3)	-404(2)	4463(2)	14(1)
C18	1848(3)	-897(2)	5031(2)	17(1)
C19	1874(3)	-1773(2)	5268(2)	20(1)
C20	2708(3)	-2177(2)	4944(2)	24(1)
C21	3547(3)	-1704(2)	4399(2)	25(1)
C22	3522(3)	-822(2)	4160(2)	19(1)
C1	-907(2)	3751(2)	946(2)	12(1)
C24	-1969(3)	4840(2)	92(2)	16(1)
C25	-1223(3)	4508(2)	-311(2)	17(1)
C26	322(2)	3273(2)	69(2)	13(1)
C27	1387(2)	3062(2)	485(2)	13(1)
C28	2184(2)	2446(2)	411(2)	14(1)
C29	1927(2)	2010(2)	-67(2)	14(1)
C30	901(3)	2273(2)	-515(2)	16(1)
C31	87(3)	2900(2)	-445(2)	16(1)
C32	2818(2)	1264(2)	-36(2)	13(1)
C33	2543(3)	900(2)	-648(2)	15(1)
C34	1446(3)	498(2)	-594(2)	22(1)
C35	1181(3)	118(2)	-1097(2)	28(1)
C36	2026(3)	115(2)	-1668(2)	26(1)
C37	3109(3)	488(2)	-1719(2)	23(1)
C38	3374(3)	885(2)	-1215(2)	17(1)
C39	2669(2)	522(2)	754(2)	14(1)
C40	1928(3)	561(2)	1357(2)	17(1)
C41	1827(3)	-138(2)	2045(2)	24(1)
C42	2442(3)	-899(2)	2140(2)	26(1)

C43	3169(3)	-956(2)	1540(2)	27(1)
C44	3284(3)	-258(2)	862(2)	21(1)
C45	4097(3)	1632(2)	-157(2)	14(1)
C46	5018(3)	1321(2)	375(2)	18(1)
C47	6120(3)	1727(2)	259(2)	26(1)
C48	6317(3)	2449(2)	-389(2)	30(1)
C49	5412(3)	2760(2)	-927(2)	25(1)
C50	4317(3)	2356(2)	-811(2)	19(1)
C51	-2353(2)	4528(2)	1498(2)	12(1)
C52	-2774(3)	3853(2)	2121(2)	16(1)
C53	-3250(3)	3992(2)	2754(2)	16(1)
C54	-3330(2)	4810(2)	2775(2)	13(1)
C55	-2957(2)	5478(2)	2124(2)	14(1)
C56	-2455(3)	5348(2)	1482(2)	14(1)
C57	-3756(2)	4902(2)	3534(2)	13(1)
C58	-4104(3)	5841(2)	3386(1)	14(1)
C59	-5308(3)	6150(2)	3344(2)	19(1)
C60	-5582(3)	7013(2)	3148(2)	27(1)
C61	-4658(3)	7581(2)	2988(2)	26(1)
C62	-3457(3)	7285(2)	3039(2)	24(1)
C63	-3187(3)	6422(2)	3249(2)	20(1)
C64	-2684(3)	4619(2)	4097(2)	15(1)
C65	-2789(3)	4747(2)	4794(2)	20(1)
C66	-1863(3)	4489(2)	5318(2)	27(1)
C67	-798(3)	4115(2)	5168(2)	31(1)
C68	-655(3)	4007(2)	4476(2)	26(1)
C69	-1592(3)	4257(2)	3946(2)	19(1)
C70	-4871(3)	4341(2)	3848(2)	13(1)
C71	-5782(3)	4379(2)	3335(2)	18(1)

C72	-6810(3)	3896(2)	3572(2)	23(1)
C73	-6949(3)	3357(2)	4333(2)	24(1)
C74	-6064(3)	3311(2)	4847(2)	24(1)
C75	-5039(3)	3796(2)	4608(2)	18(1)
C76	472(5)	5898(4)	2548(3)	73(2)
C77	4145(3)	3886(2)	1571(2)	36(1)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Pd1	13(1)	11(1)	9(1)	-3(1)	-1(1)	0(1)
Cl1	24(1)	17(1)	16(1)	-5(1)	-5(1)	-7(1)
Cl2	25(1)	16(1)	19(1)	-5(1)	-9(1)	-4(1)
Cl3	44(1)	60(1)	54(1)	4(1)	-21(1)	-8(1)
Cl4	63(1)	192(2)	52(1)	-40(1)	7(1)	10(1)
Cl5	60(1)	39(1)	39(1)	-20(1)	-2(1)	-10(1)
Cl6	39(1)	39(1)	37(1)	-18(1)	-14(1)	4(1)
N3	17(1)	13(1)	10(1)	-2(1)	-1(1)	0(1)
N4	16(1)	13(1)	12(1)	-3(1)	-1(1)	-1(1)
N1	13(1)	9(1)	10(1)	-2(1)	0(1)	0(1)
N2	13(1)	15(1)	11(1)	-5(1)	0(1)	2(1)
C2	18(1)	11(1)	12(1)	-2(1)	-2(1)	-2(1)
C2	16(1)	17(1)	14(1)	-4(1)	0(1)	-5(1)
C3	16(1)	14(1)	10(1)	-2(1)	1(1)	-3(1)
C4	13(1)	12(1)	13(1)	-3(1)	-3(1)	0(1)
C5	20(2)	13(1)	12(1)	-4(1)	0(1)	-4(1)
C6	19(2)	14(1)	16(1)	-5(1)	-1(1)	-1(1)
C7	23(2)	15(1)	25(2)	-9(1)	6(1)	-4(1)

C8	37(2)	25(2)	16(2)	-12(1)	1(1)	-7(2)
C9	35(2)	26(2)	15(2)	-7(1)	-8(1)	-2(1)
C10	28(2)	21(2)	17(2)	-7(1)	-7(1)	3(1)
C11	14(1)	12(1)	16(1)	-1(1)	-2(1)	2(1)
C12	20(2)	15(1)	25(2)	-4(1)	-4(1)	0(1)
C13	17(2)	17(2)	41(2)	-1(2)	-6(2)	-3(1)
C14	19(2)	17(2)	42(2)	3(2)	11(2)	-5(1)
C15	27(2)	21(2)	27(2)	-4(1)	12(1)	0(1)
C16	21(2)	20(2)	20(2)	-4(1)	0(1)	-2(1)
C17	15(1)	14(1)	12(1)	-4(1)	-3(1)	0(1)
C18	17(1)	16(1)	15(1)	-4(1)	-1(1)	4(1)
C19	18(2)	15(1)	21(2)	0(1)	-1(1)	-2(1)
C20	29(2)	9(1)	28(2)	-2(1)	-4(1)	2(1)
C21	31(2)	20(2)	24(2)	-11(1)	4(1)	6(1)
C22	21(2)	16(1)	15(1)	-1(1)	2(1)	2(1)
C11	12(1)	13(1)	12(1)	-5(1)	-1(1)	-1(1)
C24	22(2)	12(1)	11(1)	-2(1)	-5(1)	4(1)
C25	20(2)	18(1)	9(1)	-2(1)	-5(1)	5(1)
C26	14(1)	12(1)	10(1)	-3(1)	3(1)	0(1)
C27	14(1)	15(1)	10(1)	-6(1)	1(1)	-1(1)
C28	12(1)	16(1)	13(1)	-6(1)	-2(1)	0(1)
C29	11(1)	17(1)	13(1)	-7(1)	3(1)	-1(1)
C30	17(1)	24(2)	13(1)	-12(1)	-1(1)	0(1)
C31	13(1)	22(2)	14(1)	-7(1)	-3(1)	4(1)
C32	14(1)	15(1)	13(1)	-7(1)	2(1)	0(1)
C33	21(2)	11(1)	13(1)	-6(1)	-2(1)	1(1)
C34	24(2)	27(2)	20(2)	-13(1)	6(1)	-9(1)
C35	32(2)	32(2)	25(2)	-14(2)	-1(1)	-15(2)
C36	49(2)	18(2)	16(2)	-10(1)	-5(1)	-6(2)

C37	36(2)	23(2)	13(1)	-10(1)	1(1)	3(1)
C38	23(2)	14(1)	14(1)	-6(1)	2(1)	-1(1)
C39	11(1)	20(2)	14(1)	-8(1)	-3(1)	1(1)
C40	18(2)	19(2)	16(1)	-8(1)	-2(1)	1(1)
C41	26(2)	28(2)	17(2)	-10(1)	5(1)	0(1)
C42	31(2)	23(2)	18(2)	-2(1)	1(1)	-2(1)
C43	31(2)	18(2)	27(2)	-5(1)	-3(1)	7(1)
C44	22(2)	23(2)	19(2)	-9(1)	3(1)	1(1)
C45	14(1)	16(1)	16(1)	-10(1)	1(1)	1(1)
C46	16(2)	23(2)	18(1)	-10(1)	-2(1)	0(1)
C47	17(2)	34(2)	32(2)	-18(2)	-5(1)	-2(1)
C48	16(2)	33(2)	47(2)	-22(2)	4(2)	-8(1)
C49	24(2)	21(2)	30(2)	-10(1)	6(1)	-5(1)
C50	17(2)	19(2)	23(2)	-9(1)	1(1)	-2(1)
C51	12(1)	15(1)	11(1)	-6(1)	1(1)	1(1)
C52	18(2)	11(1)	20(1)	-7(1)	0(1)	1(1)
C53	17(1)	13(1)	16(1)	-4(1)	5(1)	-5(1)
C54	10(1)	15(1)	15(1)	-6(1)	-1(1)	1(1)
C55	15(1)	10(1)	14(1)	-3(1)	0(1)	1(1)
C56	16(1)	12(1)	12(1)	0(1)	1(1)	1(1)
C57	14(1)	11(1)	12(1)	-2(1)	2(1)	-2(1)
C58	23(2)	12(1)	7(1)	-5(1)	1(1)	1(1)
C59	22(2)	17(2)	16(1)	-5(1)	4(1)	3(1)
C60	29(2)	21(2)	25(2)	-5(1)	2(1)	11(1)
C61	45(2)	12(2)	17(2)	-5(1)	4(1)	9(1)
C62	40(2)	14(2)	19(2)	-7(1)	2(1)	-7(1)
C63	27(2)	18(2)	18(1)	-9(1)	-2(1)	0(1)
C64	15(1)	13(1)	17(1)	-4(1)	-1(1)	-3(1)
C65	20(2)	21(2)	19(2)	-8(1)	-1(1)	-3(1)

C66	28(2)	34(2)	20(2)	-10(2)	-4(1)	-6(2)
C67	25(2)	34(2)	31(2)	-7(2)	-12(2)	-3(2)
C68	17(2)	26(2)	32(2)	-6(2)	-4(1)	0(1)
C69	18(2)	15(1)	24(2)	-8(1)	1(1)	-2(1)
C70	16(1)	12(1)	15(1)	-8(1)	4(1)	1(1)
C71	18(2)	21(2)	15(1)	-8(1)	1(1)	0(1)
C72	21(2)	23(2)	26(2)	-12(1)	-3(1)	0(1)
C73	20(2)	17(2)	34(2)	-8(1)	9(1)	-6(1)
C74	28(2)	17(2)	22(2)	-3(1)	8(1)	-2(1)
C75	21(2)	17(1)	15(1)	-6(1)	0(1)	3(1)
C76	62(3)	105(5)	37(2)	-7(3)	8(2)	-42(3)
C77	30(2)	47(2)	31(2)	-14(2)	-2(2)	-10(2)

Table S4. Bond Lengths for Complex **4.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	C1	1.965(3)	C35	H35	0.9500
Pd1	N3	2.080(2)	C36	C37	1.362(5)
Pd1	Cl1	2.3012(7)	C36	H36	0.9500
Pd1	Cl2	2.3272(7)	C37	C38	1.405(4)
Cl3	C76	1.729(5)	C37	H37	0.9500
Cl4	C76	1.789(6)	C38	H38	0.9500
Cl5	C77	1.766(4)	C39	C40	1.391(4)
Cl6	C77	1.774(4)	C39	C44	1.409(4)
N3	C23	1.321(3)	C40	C41	1.393(4)
N3	C2	1.376(4)	C40	H40	0.9500
N4	C23	1.354(3)	C41	C42	1.385(4)
N4	C3	1.376(4)	C41	H41	0.9500
N4	C4	1.504(3)	C42	C43	1.388(4)

N1	C1	1.348(3)	C42	H42	0.9500
N1	C24	1.393(3)	C43	C44	1.384(4)
N1	C51	1.439(3)	C43	H43	0.9500
N2	C1	1.353(3)	C44	H44	0.9500
N2	C25	1.397(3)	C45	C46	1.392(4)
N2	C26	1.432(3)	C45	C50	1.398(4)
C23	H23	0.9500	C46	C47	1.395(4)
C2	C3	1.358(4)	C46	H46	0.9500
C2	H2	0.9500	C47	C48	1.385(5)
C3	H3	0.9500	C47	H47	0.9500
C4	C11	1.539(4)	C48	C49	1.386(5)
C4	C5	1.548(4)	C48	H48	0.9500
C4	C17	1.552(4)	C49	C50	1.387(4)
C5	C6	1.379(4)	C49	H49	0.9500
C5	C10	1.405(4)	C50	H50	0.9500
C6	C7	1.400(4)	C51	C52	1.380(4)
C6	H6	0.9500	C51	C56	1.386(4)
C7	C8	1.380(4)	C52	C53	1.380(4)
C7	H7	0.9500	C52	H52	0.9500
C8	C9	1.394(4)	C53	C54	1.408(4)
C8	H8	0.9500	C53	H53	0.9500
C9	C10	1.384(4)	C54	C55	1.385(4)
C9	H9	0.9500	C54	C57	1.548(4)
C10	H10	0.9500	C55	C56	1.397(4)
C11	C12	1.390(4)	C55	H55	0.9500
C11	C16	1.413(4)	C56	H56	0.9500
C12	C13	1.397(4)	C57	C58	1.549(4)
C12	H12	0.9500	C57	C64	1.551(4)
C13	C14	1.369(5)	C57	C70	1.551(4)

C13	H13	0.9500	C58	C59	1.395(4)
C14	C15	1.395(5)	C58	C63	1.398(4)
C14	H14	0.9500	C59	C60	1.396(4)
C15	C16	1.373(4)	C59	H59	0.9500
C15	H15	0.9500	C60	C61	1.384(5)
C16	H16	0.9500	C60	H60	0.9500
C17	C22	1.388(4)	C61	C62	1.385(5)
C17	C18	1.403(4)	C61	H61	0.9500
C18	C19	1.388(4)	C62	C63	1.393(4)
C18	H18	0.9500	C62	H62	0.9500
C19	C20	1.379(4)	C63	H63	0.9500
C19	H19	0.9500	C64	C69	1.391(4)
C20	C21	1.388(5)	C64	C65	1.408(4)
C20	H20	0.9500	C65	C66	1.383(4)
C21	C22	1.397(4)	C65	H65	0.9500
C21	H21	0.9500	C66	C67	1.377(5)
C22	H22	0.9500	C66	H66	0.9500
C24	C25	1.341(4)	C67	C68	1.386(5)
C24	H24	0.9500	C67	H67	0.9500
C25	H25	0.9500	C68	C69	1.399(4)
C26	C31	1.383(4)	C68	H68	0.9500
C26	C27	1.390(4)	C69	H69	0.9500
C27	C28	1.378(4)	C70	C75	1.390(4)
C27	H27	0.9500	C70	C71	1.403(4)
C28	C29	1.412(3)	C71	C72	1.390(4)
C28	H28	0.9500	C71	H71	0.9500
C29	C30	1.388(4)	C72	C73	1.385(4)
C29	C32	1.552(4)	C72	H72	0.9500
C30	C31	1.401(4)	C73	C74	1.379(4)

C30	H30	0.9500	C73	H73	0.9500
C31	H31	0.9500	C74	C75	1.390(4)
C32	C45	1.543(4)	C74	H74	0.9500
C32	C33	1.547(3)	C75	H75	0.9500
C32	C39	1.554(4)	C76	H76A	0.9900
C33	C38	1.385(4)	C76	H76B	0.9900
C33	C34	1.399(4)	C77	H77A	0.9900
C34	C35	1.383(4)	C77	H77B	0.9900

Table S5. Bond Angles for Complex **4**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Pd1	N3	175.17(9)	C36	C37	C38	121.0(3)
C1	Pd1	Cl1	85.55(8)	C36	C37	H37	119.5
N3	Pd1	Cl1	90.64(7)	C38	C37	H37	119.5
C1	Pd1	Cl2	91.41(8)	C33	C38	C37	120.7(3)
N3	Pd1	Cl2	92.43(7)	C33	C38	H38	119.6
Cl1	Pd1	Cl2	176.85(3)	C37	C38	H38	119.6
C23	N3	C2	105.9(2)	C40	C39	C44	117.2(3)
C23	N3	Pd1	126.10(19)	C40	C39	C32	124.5(2)
C2	N3	Pd1	127.18(19)	C44	C39	C32	118.2(2)
C23	N4	C3	106.9(2)	C39	C40	C41	121.0(3)
C23	N4	C4	124.7(2)	C39	C40	H40	119.5
C3	N4	C4	128.0(2)	C41	C40	H40	119.5
C1	N1	C24	110.4(2)	C42	C41	C40	120.8(3)
C1	N1	C51	124.2(2)	C42	C41	H41	119.6
C24	N1	C51	125.4(2)	C40	C41	H41	119.6
C1	N2	C25	110.2(2)	C41	C42	C43	119.1(3)
C1	N2	C26	122.4(2)	C41	C42	H42	120.5
C25	N2	C26	127.4(2)	C43	C42	H42	120.5

N3	C23	N4	111.2(2)	C44	C43	C42	120.1(3)
N3	C23	H23	124.4	C44	C43	H43	120.0
N4	C23	H23	124.4	C42	C43	H43	120.0
C3	C2	N3	109.6(3)	C43	C44	C39	121.7(3)
C3	C2	H2	125.2	C43	C44	H44	119.1
N3	C2	H2	125.2	C39	C44	H44	119.1
C2	C3	N4	106.3(2)	C46	C45	C50	117.9(3)
C2	C3	H3	126.8	C46	C45	C32	123.7(3)
N4	C3	H3	126.8	C50	C45	C32	118.3(2)
N4	C4	C11	106.5(2)	C45	C46	C47	120.7(3)
N4	C4	C5	108.4(2)	C45	C46	H46	119.6
C11	C4	C5	112.9(2)	C47	C46	H46	119.6
N4	C4	C17	107.8(2)	C48	C47	C46	120.6(3)
C11	C4	C17	112.0(2)	C48	C47	H47	119.7
C5	C4	C17	109.0(2)	C46	C47	H47	119.7
C6	C5	C10	118.8(3)	C47	C48	C49	119.3(3)
C6	C5	C4	122.9(2)	C47	C48	H48	120.4
C10	C5	C4	118.3(2)	C49	C48	H48	120.4
C5	C6	C7	120.7(3)	C48	C49	C50	120.1(3)
C5	C6	H6	119.7	C48	C49	H49	119.9
C7	C6	H6	119.7	C50	C49	H49	119.9
C8	C7	C6	120.5(3)	C49	C50	C45	121.4(3)
C8	C7	H7	119.8	C49	C50	H50	119.3
C6	C7	H7	119.8	C45	C50	H50	119.3
C7	C8	C9	119.1(3)	C52	C51	C56	121.2(2)
C7	C8	H8	120.5	C52	C51	N1	119.0(2)
C9	C8	H8	120.5	C56	C51	N1	119.7(2)
C10	C9	C8	120.7(3)	C51	C52	C53	119.2(2)
C10	C9	H9	119.6	C51	C52	H52	120.4

C8	C9	H9	119.6	C53	C52	H52	120.4
C9	C10	C5	120.2(3)	C52	C53	C54	121.5(3)
C9	C10	H10	119.9	C52	C53	H53	119.3
C5	C10	H10	119.9	C54	C53	H53	119.3
C12	C11	C16	117.9(3)	C55	C54	C53	117.7(2)
C12	C11	C4	122.8(2)	C55	C54	C57	123.9(2)
C16	C11	C4	119.3(2)	C53	C54	C57	118.4(2)
C11	C12	C13	120.4(3)	C54	C55	C56	121.6(2)
C11	C12	H12	119.8	C54	C55	H55	119.2
C13	C12	H12	119.8	C56	C55	H55	119.2
C14	C13	C12	120.9(3)	C51	C56	C55	118.7(3)
C14	C13	H13	119.5	C51	C56	H56	120.7
C12	C13	H13	119.5	C55	C56	H56	120.7
C13	C14	C15	119.4(3)	C54	C57	C58	110.3(2)
C13	C14	H14	120.3	C54	C57	C64	108.4(2)
C15	C14	H14	120.3	C58	C57	C64	108.2(2)
C16	C15	C14	120.3(3)	C54	C57	C70	107.3(2)
C16	C15	H15	119.8	C58	C57	C70	110.6(2)
C14	C15	H15	119.8	C64	C57	C70	112.0(2)
C15	C16	C11	121.0(3)	C59	C58	C63	117.7(3)
C15	C16	H16	119.5	C59	C58	C57	122.7(3)
C11	C16	H16	119.5	C63	C58	C57	119.5(3)
C22	C17	C18	117.9(3)	C58	C59	C60	120.9(3)
C22	C17	C4	123.0(3)	C58	C59	H59	119.6
C18	C17	C4	119.1(2)	C60	C59	H59	119.6
C19	C18	C17	121.3(3)	C61	C60	C59	120.5(3)
C19	C18	H18	119.3	C61	C60	H60	119.8
C17	C18	H18	119.3	C59	C60	H60	119.8
C20	C19	C18	120.1(3)	C60	C61	C62	119.5(3)

C20	C19	H19	119.9	C60	C61	H61	120.2
C18	C19	H19	119.9	C62	C61	H61	120.2
C19	C20	C21	119.5(3)	C61	C62	C63	119.9(3)
C19	C20	H20	120.3	C61	C62	H62	120.1
C21	C20	H20	120.3	C63	C62	H62	120.1
C20	C21	C22	120.4(3)	C62	C63	C58	121.5(3)
C20	C21	H21	119.8	C62	C63	H63	119.2
C22	C21	H21	119.8	C58	C63	H63	119.2
C17	C22	C21	120.7(3)	C69	C64	C65	117.2(3)
C17	C22	H22	119.6	C69	C64	C57	123.4(2)
C21	C22	H22	119.6	C65	C64	C57	119.4(2)
N1	C1	N2	105.6(2)	C66	C65	C64	121.2(3)
N1	C1	Pd1	129.04(19)	C66	C65	H65	119.4
N2	C1	Pd1	125.06(19)	C64	C65	H65	119.4
C25	C24	N1	107.1(2)	C67	C66	C65	120.9(3)
C25	C24	H24	126.5	C67	C66	H66	119.6
N1	C24	H24	126.5	C65	C66	H66	119.6
C24	C25	N2	106.7(2)	C66	C67	C68	119.1(3)
C24	C25	H25	126.6	C66	C67	H67	120.5
N2	C25	H25	126.6	C68	C67	H67	120.5
C31	C26	C27	120.5(2)	C67	C68	C69	120.4(3)
C31	C26	N2	120.8(2)	C67	C68	H68	119.8
C27	C26	N2	118.6(2)	C69	C68	H68	119.8
C28	C27	C26	119.6(2)	C64	C69	C68	121.2(3)
C28	C27	H27	120.2	C64	C69	H69	119.4
C26	C27	H27	120.2	C68	C69	H69	119.4
C27	C28	C29	121.2(2)	C75	C70	C71	117.1(3)
C27	C28	H28	119.4	C75	C70	C57	124.7(2)
C29	C28	H28	119.4	C71	C70	C57	118.2(2)

C30	C29	C28	117.9(2)	C72	C71	C70	121.7(3)
C30	C29	C32	125.5(2)	C72	C71	H71	119.1
C28	C29	C32	116.6(2)	C70	C71	H71	119.1
C29	C30	C31	121.0(2)	C73	C72	C71	119.8(3)
C29	C30	H30	119.5	C73	C72	H72	120.1
C31	C30	H30	119.5	C71	C72	H72	120.1
C26	C31	C30	119.5(3)	C74	C73	C72	119.3(3)
C26	C31	H31	120.3	C74	C73	H73	120.3
C30	C31	H31	120.3	C72	C73	H73	120.3
C45	C32	C33	112.0(2)	C73	C74	C75	120.7(3)
C45	C32	C29	105.1(2)	C73	C74	H74	119.6
C33	C32	C29	112.4(2)	C75	C74	H74	119.6
C45	C32	C39	112.3(2)	C70	C75	C74	121.3(3)
C33	C32	C39	105.9(2)	C70	C75	H75	119.3
C29	C32	C39	109.3(2)	C74	C75	H75	119.3
C38	C33	C34	117.4(2)	Cl3	C76	Cl4	111.2(3)
C38	C33	C32	123.2(3)	Cl3	C76	H76A	109.4
C34	C33	C32	119.2(2)	Cl4	C76	H76A	109.4
C35	C34	C33	121.7(3)	Cl3	C76	H76B	109.4
C35	C34	H34	119.1	Cl4	C76	H76B	109.4
C33	C34	H34	119.1	H76A	C76	H76B	108.0
C34	C35	C36	120.0(3)	Cl5	C77	Cl6	110.6(2)
C34	C35	H35	120.0	Cl5	C77	H77A	109.5
C36	C35	H35	120.0	Cl6	C77	H77A	109.5
C37	C36	C35	119.1(3)	Cl5	C77	H77B	109.5
C37	C36	H36	120.4	Cl6	C77	H77B	109.5
C35	C36	H36	120.4	H77A	C77	H77B	108.1

Table S6. Torsion Angles for Complex **4.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	N3	C23	N4	0.5(3)	C38	C33	C34	C35	-1.6(5)
Pd1	N3	C23	N4	-169.68(17)	C32	C33	C34	C35	-176.3(3)
C3	N4	C23	N3	-0.8(3)	C33	C34	C35	C36	1.3(5)
C4	N4	C23	N3	-174.5(2)	C34	C35	C36	C37	0.1(5)
C23	N3	C2	C3	0.0(3)	C35	C36	C37	C38	-1.0(5)
Pd1	N3	C2	C3	170.00(18)	C34	C33	C38	C37	0.7(4)
N3	C2	C3	N4	-0.4(3)	C32	C33	C38	C37	175.1(3)
C23	N4	C3	C2	0.7(3)	C36	C37	C38	C33	0.6(5)
C4	N4	C3	C2	174.1(2)	C45	C32	C39	C40	111.0(3)
C23	N4	C4	C11	-39.7(3)	C33	C32	C39	C40	-126.5(3)
C3	N4	C4	C11	147.9(2)	C29	C32	C39	C40	-5.3(4)
C23	N4	C4	C5	82.0(3)	C45	C32	C39	C44	-71.8(3)
C3	N4	C4	C5	-90.3(3)	C33	C32	C39	C44	50.7(3)
C23	N4	C4	C17	-160.1(2)	C29	C32	C39	C44	171.9(2)
C3	N4	C4	C17	27.6(3)	C44	C39	C40	C41	1.7(4)
N4	C4	C5	C6	-13.0(4	C32	C39	C40	C41	178.9(3)
C11	C4	C5	C6	104.7(3)	C39	C40	C41	C42	-1.5(5)
C17	C4	C5	C6	-130.2(3)	C40	C41	C42	C43	0.3(5)
N4	C4	C5	C10	165.8(3)	C41	C42	C43	C44	0.6(5)
C11	C4	C5	C10	-76.4(3)	C42	C43	C44	C39	-0.5(5)
C17	C4	C5	C10	48.7(3)	C40	C39	C44	C43	-0.7(4)
C10	C5	C6	C7	-0.5(4)	C32	C39	C44	C43	-178.0(3)
C4	C5	C6	C7	178.4(3)	C33	C32	C45	C46	-117.6(3)
C5	C6	C7	C8	0.4(5)	C29	C32	C45	C46	120.1(3)
C6	C7	C8	C9	0.0(5)	C39	C32	C45	C46	1.4(3)
C7	C8	C9	C10	-0.2(5)	C33	C32	C45	C50	67.2(3)
C8	C9	C10	C5	0.1(5)	C29	C32	C45	C50	-55.1(3)
C6	C5	C10	C9	0.3(5)	C39	C32	C45	C50	-173.8(2)

C4	C5	C10	C9	-178.6(3)	C50	C45	C46	C47	0.6(4)
N4	C4	C11	C12	133.2(3)	C32	C45	C46	C47	-174.6(2)
C5	C4	C11	C12	14.3(4)	C45	C46	C47	C48	0.1(4)
C17	C4	C11	C12	-109.2(3)	C46	C47	C48	C49	-0.8(5)
N4	C4	C11	C16	-47.7(3)	C47	C48	C49	C50	0.9(5)
C5	C4	C11	C16	-166.6(2)	C48	C49	C50	C45	-0.1(4)
C17	C4	C11	C16	69.9(3)	C46	C45	C50	C49	-0.6(4)
C16	C11	C12	C13	-2.6(4)	C32	C45	C50	C49	174.9(2)
C4	C11	C12	C13	176.6(3)	C1	N1	C51	C52	-45.6(4)
C11	C12	C13	C14	0.7(5)	C24	N1	C51	C52	135.8(3)
C12	C13	C14	C15	1.2(5)	C1	N1	C51	C56	132.5(3)
C13	C14	C15	C16	-1.0(5)	C24	N1	C51	C56	-46.1(4)
C14	C15	C16	C11	-1.0(5)	C56	C51	C52	C53	-3.3(4)
C12	C11	C16	C15	2.7(4)	N1	C51	C52	C53	174.7(2)
C4	C11	C16	C15	-176.5(3)	C51	C52	C53	C54	0.9(4)
N4	C4	C17	C22	102.7(3)	C52	C53	C54	C55	2.4(4)
C11	C4	C17	C22	-14.1(4)	C52	C53	C54	C57	-174.1(3)
C5	C4	C17	C22	-139.7(3)	C53	C54	C55	C56	-3.4(4)
N4	C4	C17	C18	-76.2(3)	C57	C54	C55	C56	172.9(3)
C11	C4	C17	C18	166.9(2)	C52	C51	C56	C55	2.4(4)
C5	C4	C17	C18	41.3(3)	N1	C51	C56	C55	-175.7(2)
C22	C17	C18	C19	-1.9(4)	C54	C55	C56	C51	1.1(4)
C4	C17	C18	C19	177.1(2)	C55	C54	C57	C58	18.4(4)
C17	C18	C19	C20	-0.2(4)	C53	C54	C57	C58	-165.3(2)
C18	C19	C20	C21	2.3(5)	C55	C54	C57	C64	-99.8(3)
C19	C20	C21	C22	-2.2(5)	C53	C54	C57	C64	76.5(3)
C18	C17	C22	C21	2.0(4)	C55	C54	C57	C70	139.0(3)
C4	C17	C22	C21	-177.0(3)	C53	C54	C57	C70	-44.7(3)
C20	C21	C22	C17	0.1(5)	C54	C57	C58	C59	102.6(3)

C24	N1	C1	N2	0.9(3)	C64	C57	C58	C59	-139.0(3)
C51	N1	C1	N2	-177.9(2)	C70	C57	C58	C59	-16.0(3)
C24	N1	C1	Pd1	-173.2(2)	C54	C57	C58	C63	-74.1(3)
C51	N1	C1	Pd1	8.0(4)	C64	C57	C58	C63	44.3(3)
C25	N2	C1	N1	-0.9(3)	C70	C57	C58	C63	167.3(2)
C26	N2	C1	N1	-178.3(2)	C63	C58	C59	C60	2.1(4)
C25	N2	C1	Pd1	173.4(2)	C57	C58	C59	C60	-174.6(3)
C26	N2	C1	Pd1	-3.9(4)	C58	C59	C60	C61	0.1(4)
C1	N1	C24	C25	-0.5(3)	C59	C60	C61	C62	-1.2(5)
C51	N1	C24	C25	178.3(3)	C60	C61	C62	C63	0.1(4)
N1	C24	C25	N2	-0.1(3)	C61	C62	C63	C58	2.2(4)
C1	N2	C25	C24	0.7(3)	C59	C58	C63	C62	-3.2(4)
C26	N2	C25	C24	177.9(3)	C57	C58	C63	C62	173.6(2)
C1	N2	C26	C31	130.0(3)	C54	C57	C64	C69	-6.6(4)
C25	N2	C26	C31	-46.8(4)	C58	C57	C64	C69	-126.1(3)
C1	N2	C26	C27	-45.6(4)	C70	C57	C64	C69	111.7(3)
C25	N2	C26	C27	137.5(3)	C54	C57	C64	C65	171.9(2)
C31	C26	C27	C28	-3.2(4)	C58	C57	C64	C65	52.3(3)
N2	C26	C27	C28	172.5(2)	C70	C57	C64	C65	-69.9(3)
C26	C27	C28	C29	-1.5(4)	C69	C64	C65	C66	-2.7(4)
C27	C28	C29	C30	5.8(4)	C57	C64	C65	C66	178.8(3)
C27	C28	C29	C32	-173.5(3)	C64	C65	C66	C67	1.3(5)
C28	C29	C30	C31	-5.7(4)	C65	C66	C67	C68	0.8(5)
C32	C29	C30	C31	173.6(3)	C66	C67	C68	C69	-1.5(5)
C27	C26	C31	C30	3.3(4)	C65	C64	C69	C68	1.9(4)
N2	C26	C31	C30	-172.3(3)	C57	C64	C69	C68	-179.6(3)
C29	C30	C31	C26	1.2(4)	C67	C68	C69	C64	0.1(5)
C30	C29	C32	C45	129.5(3)	C54	C57	C70	C75	134.5(3)
C28	C29	C32	C45	-51.3(3)	C58	C57	C70	C75	-105.2(3)

C30	C29	C32	C33	7.5(4)	C64	C57	C70	C75	15.6(3)
C28	C29	C32	C33	-173.3(2)	C54	C57	C70	C71	-45.4(3)
C30	C29	C32	C39	-109.8(3)	C58	C57	C70	C71	74.9(3)
C28	C29	C32	C39	69.5(3)	C64	C57	C70	C71	-164.3(2)
C45	C32	C33	C38	2.1(4)	C75	C70	C71	C72	0.1(4)
C29	C32	C33	C38	120.1(3)	C57	C70	C71	C72	-180.0(2)
C39	C32	C33	C38	-120.6(3)	C70	C71	C72	C73	-0.4(4)
C45	C32	C33	C34	176.4(3)	C71	C72	C73	C74	0.4(4)
C29	C32	C33	C34	-65.6(3)	C72	C73	C74	C75	-0.3(4)
C39	C32	C33	C34	53.7(3)	C71	C70	C75	C74	0.0(4)
C57	C70	C75	C74	-179.9(3)	C73	C74	C75	C70	0.0(4)

Table S7. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **4.**

	X	*y*	*z*	U(eq)
H23	1868	2116	3047	18
H2	-1078	888	3028	20
H3	306	-126	3980	17
H6	864	1643	4497	20
H7	505	1944	5604	25
H8	1730	1305	6670	30
H9	3324	359	6624	30
H10	3679	49	5530	26
H12	4393	1431	4471	25
H13	6131	1993	3734	33
H14	6467	1916	2538	36
H15	5019	1305	2047	33
H16	3287	750	2764	25
H18	1268	-625	5258	20
H19	1317	-2095	5655	24

H20	2709	-2775	5092	28
H21	4142	-1982	4187	30
H22	4100	-505	3786	23
H24	-2532	5306	-112	19
H25	-1156	4693	-854	20
H27	1564	3340	818	15
H28	2920	2313	686	16
H30	748	2025	-875	20
H31	-620	3067	-748	20
H34	869	486	-201	27
H35	422	-140	-1054	34
H36	1849	-144	-2016	31
H37	3694	480	-2102	28
H38	4132	1146	-1264	20
H40	1483	1073	1299	21
H41	1331	-93	2453	29
H42	2366	-1375	2609	31
H43	3589	-1476	1596	32
H44	3790	-305	458	25
H46	4895	826	822	22
H47	6740	1506	627	31
H48	7064	2728	-462	36
H49	5542	3251	-1377	30
H50	3704	2577	-1184	23
H52	-2737	3299	2114	19
H53	-3530	3527	3187	19
H55	-3044	6038	2113	16
H56	-2190	5812	1042	17
H59	-5951	5767	3452	23

H60	-6407	7212	3123	32
H61	-4848	8169	2845	31
H62	-2818	7671	2932	29
H63	-2360	6223	3300	24
H65	-3508	5014	4905	24
H66	-1964	4572	5789	33
H67	-170	3933	5534	37
H68	83	3761	4360	32
H69	-1481	4178	3474	23
H71	-5693	4745	2811	21
H72	-7415	3936	3213	27
H73	-7646	3022	4498	29
H74	-6157	2943	5370	29
H75	-4440	3754	4972	22
H76A	421	5439	3064	87
H76B	-116	5786	2217	87
H77A	4564	3618	2065	43
H77B	3267	3776	1667	43

Table S8. Crystal data and structure refinement for complex **5.**

Identification code	**5**
Empirical formula	$C_{47.20}\ H_{36.80}\ Cl_4\ N_{2.40}\ Pd_{0.80}$
Formula weight	864.51
Temperature/K	173(2)
Crystal system	Monoclinic
Space group	P 21
a/Å	9.1629(5)
b/Å	31.1003(17)
c/Å	17.7075(9)
α/°	90

β/°	97.4920(10)
γ/°	90
Volume/Å^3	5003.0(5)
Z	5
ρ_{calc}g/cm^3	1.435
μ/mm^{-1}	0.681
F(000)	2208
Crystal size/mm^3	0.18 × 0.17 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.309 to 28.272
Index ranges	-10 ≤ h ≤ 12, -33 ≤ k ≤ 41, -23 ≤ l ≤ 23
Reflections collected	37510
Independent reflections	19535 [R(int) = 0.0639]
Data/restraints/parameters	19535 / 13 / 1226
Goodness-of-fit on F^2	1.061
Final R indexes [I>=2σ (I)]	R1 = 0.0606, wR2 = 0.1301
Final R indexes [all data]	R1 = 0.0962, wR2 = 0.1467
Largest diff. peak/hole / e Å^{-3}	2.178 -1.067

Table S9. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Complex **5**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Pd1	5712(1)	9079(1)	3562(1)	17(1)
Pd2	2445(1)	6630(1)	3495(1)	16(1)
Cl1	3807(2)	9576(1)	3317(2)	22(1)
Cl2	7479(2)	8545(1)	3815(1)	18(1)
Cl3	7224(2)	10626(1)	5169(1)	18(1)
Cl4	627(2)	7152(1)	3314(1)	16(1)
Cl5	4453(2)	6170(1)	3622(1)	22(1)
Cl6	1002(3)	5059(1)	1847(1)	21(1)

Cl7	3757(6)	9899(2)	10838(4)	128(2)
Cl8	2840(10)	9565(3)	9326(5)	177(4)
Cl9	4547(7)	1049(3)	2199(4)	157(3)
Cl10	7051(6)	473(3)	2445(3)	158(4)
N1	3223(8)	8447(2)	3481(4)	14(2)
N2	4356(8)	8429(2)	2495(4)	16(2)
N3	7243(8)	9562(3)	3956(4)	22(2)
N4	4887(8)	7274(3)	3628(4)	16(2)
N5	3719(8)	7278(2)	4605(4)	14(2)
N6	952(9)	6142(3)	3091(4)	20(2)
C28	1533(8)	8993(3)	6358(5)	10(2)
C2	1794(9)	8648(3)	6977(5)	13(2)
C3	2516(10)	8260(3)	6898(5)	19(2)
C4	2682(10)	7966(3)	7486(5)	20(2)
C5	2181(10)	8037(3)	8167(5)	18(2)
C6	1494(9)	8428(3)	8270(5)	20(2)
C7	1293(9)	8725(3)	7679(5)	17(2)
C8	2532(10)	9391(3)	6537(5)	18(2)
C9	3388(10)	9448(3)	7249(5)	18(2)
C10	4352(11)	9794(3)	7389(6)	23(2)
C11	4460(11)	10095(3)	6828(6)	23(2)
C12	3598(10)	10054(3)	6127(6)	23(2)
C13	2666(11)	9701(3)	5977(6)	20(2)
C14	-107(8)	9113(3)	6281(4)	14(2)
C15	-633(10)	9534(3)	6322(5)	18(2)
C16	-2124(10)	9620(3)	6245(5)	21(2)
C17	-3150(10)	9292(3)	6146(5)	18(2)
C18	-2649(10)	8870(3)	6126(5)	19(2)
C19	-1163(10)	8788(3)	6193(5)	15(2)

C20	1913(9)	8826(3)	5585(5)	14(2)
C21	3400(9)	8763(3)	5503(5)	14(2)
C22	3842(9)	8640(3)	4824(5)	18(2)
C23	2787(9)	8567(3)	4198(5)	15(2)
C24	1320(10)	8619(3)	4263(5)	20(2)
C25	887(9)	8748(3)	4952(5)	16(2)
C26	2535(9)	8135(3)	2998(5)	15(2)
C27	3234(10)	8121(3)	2389(5)	19(2)
C1	4327(10)	8627(3)	3169(5)	17(2)
C29	5397(9)	8525(3)	1980(5)	15(2)
C30	5385(11)	8925(3)	1665(6)	22(2)
C31	6399(10)	9026(3)	1182(5)	23(2)
C32	7434(10)	8724(3)	994(5)	18(2)
C33	7400(10)	8322(3)	1317(5)	21(2)
C34	6359(10)	8213(3)	1803(5)	21(2)
C35	8514(9)	8871(3)	436(5)	15(2)
C36	9690(10)	8530(3)	352(5)	20(2)
C37	9271(10)	8132(3)	13(5)	21(2)
C38	10267(11)	7812(3)	-105(5)	23(2)
C39	11781(11)	7895(4)	114(5)	27(2)
C40	12223(11)	8283(4)	429(5)	28(2)
C41	11201(10)	8598(3)	543(5)	24(2)
C42	7670(9)	8922(3)	-369(5)	15(2)
C43	6190(10)	8811(3)	-556(5)	21(2)
C44	5509(11)	8804(4)	-1319(5)	27(2)
C45	6326(11)	8903(3)	-1893(5)	23(2)
C46	7779(10)	9025(3)	-1729(5)	22(2)
C47	8441(9)	9024(3)	-991(5)	20(2)
C48	9159(10)	9291(3)	765(5)	21(2)

C49	9929(11)	9308(4)	1503(6)	25(2)
C50	10455(12)	9680(4)	1842(6)	34(3)
C51	10207(12)	10070(4)	1470(6)	38(3)
C52	9435(11)	10073(4)	751(6)	34(2)
C53	8919(10)	9693(3)	389(6)	25(2)
C54	6854(12)	9888(3)	4355(6)	28(2)
C55	7845(11)	10210(4)	4614(6)	28(2)
C56	9282(12)	10183(4)	4444(6)	33(3)
C57	9653(12)	9850(4)	4025(6)	33(3)
C58	8635(11)	9541(4)	3784(6)	28(2)
C59	6620(9)	6699(3)	785(4)	18(2)
C60	6309(9)	7023(3)	125(5)	16(2)
C61	5595(9)	7420(3)	191(5)	19(2)
C62	5402(10)	7705(3)	-409(5)	19(2)
C63	5902(10)	7613(3)	-1089(5)	22(2)
C64	6638(10)	7232(3)	-1164(5)	22(2)
C65	6833(9)	6945(3)	-570(5)	16(2)
C66	5658(9)	6292(3)	630(5)	16(2)
C67	5515(11)	6017(3)	1249(6)	25(2)
C68	4618(11)	5650(3)	1156(6)	28(2)
C69	3904(11)	5551(3)	447(6)	28(2)
C70	4056(11)	5808(3)	-167(6)	26(2)
C71	4926(10)	6184(3)	-67(5)	20(2)
C72	8263(9)	6581(3)	837(5)	17(2)
C73	9309(9)	6917(3)	921(5)	16(2)
C74	10793(10)	6823(3)	976(5)	22(2)
C75	11253(10)	6397(3)	911(5)	23(2)
C76	10249(10)	6077(3)	801(5)	21(2)
C77	8755(10)	6162(3)	782(5)	20(2)

C78	6247(10)	6885(3)	1544(5)	18(2)
C79	7257(10)	6969(3)	2170(5)	16(2)
C80	6805(10)	7103(3)	2863(5)	16(2)
C81	5328(9)	7157(3)	2903(5)	14(2)
C82	4288(10)	7094(3)	2287(5)	16(2)
C83	4737(10)	6959(3)	1600(5)	19(2)
C84	5553(10)	7582(3)	4121(5)	18(2)
C85	4815(10)	7582(3)	4720(5)	20(2)
C86	3777(9)	7084(3)	3926(5)	14(2)
C87	2705(10)	7165(3)	5124(5)	18(2)
C88	1707(10)	7468(3)	5299(5)	19(2)
C89	702(10)	7355(3)	5802(5)	18(2)
C90	669(10)	6947(3)	6112(5)	17(2)
C91	1673(9)	6647(3)	5903(5)	20(2)
C92	2690(10)	6750(3)	5408(5)	18(2)
C93	-369(10)	6812(3)	6681(5)	15(2)
C94	-1104(10)	6388(3)	6391(5)	16(2)
C95	-1859(11)	6376(3)	5647(6)	26(2)
C96	-2667(12)	6019(4)	5361(6)	29(2)
C97	-2728(11)	5664(3)	5821(6)	29(2)
C98	-1950(11)	5656(3)	6542(6)	26(2)
C99	-1129(11)	6017(3)	6825(5)	20(2)
C100	496(10)	6770(3)	7497(5)	17(2)
C101	-280(10)	6670(3)	8107(5)	21(2)
C102	424(10)	6654(4)	8837(5)	25(2)
C103	1933(11)	6740(3)	8992(5)	25(2)
C104	2700(11)	6825(3)	8398(6)	26(2)
C105	1999(10)	6834(3)	7658(5)	20(2)
C106	-1554(10)	7160(3)	6775(5)	16(2)

C107	-1099(10)	7549(3)	7127(5)	17(2)
C108	-2119(10)	7862(3)	7221(5)	21(2)
C109	-3586(11)	7805(3)	7001(5)	21(2)
C110	-4046(10)	7419(3)	6688(5)	21(2)
C111	-3061(10)	7096(3)	6567(5)	19(2)
C112	414(13)	5488(3)	2424(6)	31(3)
C113	1370(11)	5812(3)	2665(5)	23(2)
C114	-416(10)	6145(3)	3272(6)	26(2)
C115	-1422(12)	5825(4)	3040(6)	29(2)
C116	-1031(12)	5484(4)	2610(6)	35(3)
C117	2774(15)	9995(6)	9914(10)	76(5)
C118	5351(18)	617(8)	2695(13)	135(10)

Table S10. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **5**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Pd1	15(1)	18(1)	18(1)	-1(1)	3(1)	-2(1)
Pd2	15(1)	17(1)	16(1)	-2(1)	3(1)	-1(1)
Cl1	17(1)	12(1)	36(1)	-4(1)	-3(1)	4(1)
Cl2	8(1)	18(1)	29(1)	2(1)	-2(1)	-2(1)
Cl3	28(1)	9(1)	18(1)	-4(1)	3(1)	-3(1)
Cl4	7(1)	12(1)	27(1)	-2(1)	-2(1)	-1(1)
Cl5	17(1)	17(1)	30(1)	-1(1)	0(1)	6(1)
Cl6	35(1)	11(1)	17(1)	-4(1)	9(1)	-3(1)
Cl7	89(4)	145(5)	157(5)	85(4)	37(4)	46(3)
Cl8	237(9)	127(6)	197(8)	-44(5)	143(7)	-9(6)
Cl9	111(4)	186(7)	193(7)	122(6)	89(5)	51(4)
Cl10	78(3)	277(9)	127(5)	130(6)	46(3)	61(4)

N1	16(4)	15(4)	12(3)	-2(3)	2(3)	-2(3)
N2	12(4)	19(4)	16(4)	0(3)	4(3)	2(3)
N3	18(4)	27(5)	22(4)	2(4)	3(3)	-1(4)
N4	14(4)	25(5)	11(3)	-2(3)	7(3)	-3(3)
N5	14(4)	20(4)	11(3)	-3(3)	9(3)	-6(3)
N6	24(4)	15(4)	20(4)	4(3)	-1(3)	-1(3)
C28	7(4)	7(4)	15(4)	-3(3)	2(3)	4(3)
C2	9(4)	15(5)	14(4)	-2(4)	0(3)	1(3)
C3	19(5)	15(5)	23(5)	2(4)	5(4)	3(4)
C4	20(5)	19(5)	22(5)	2(4)	-2(4)	5(4)
C5	20(5)	18(5)	14(4)	8(4)	2(4)	2(4)
C6	13(4)	24(5)	24(5)	3(4)	6(4)	-1(4)
C7	15(4)	23(5)	12(4)	-5(4)	-1(3)	-2(4)
C8	18(5)	18(5)	17(4)	1(4)	3(4)	9(4)
C9	22(5)	11(5)	21(5)	1(4)	6(4)	7(4)
C10	24(5)	13(5)	29(5)	-4(4)	-10(4)	-1(4)
C11	24(5)	13(5)	32(6)	-6(4)	-3(4)	-3(4)
C12	18(5)	19(5)	33(6)	10(4)	13(4)	2(4)
C13	18(5)	24(6)	19(5)	4(4)	1(4)	2(4)
C14	7(4)	23(5)	11(4)	0(4)	-2(3)	-7(4)
C15	19(5)	18(5)	17(4)	0(4)	6(4)	-1(4)
C16	18(5)	21(5)	25(5)	0(4)	4(4)	10(4)
C17	13(4)	22(5)	19(4)	0(4)	5(4)	-1(4)
C18	13(4)	26(6)	17(4)	0(4)	-1(4)	3(4)
C19	19(5)	10(4)	16(4)	0(4)	0(4)	-2(4)
C20	10(4)	17(5)	12(4)	5(4)	-5(3)	0(4)
C21	10(4)	15(5)	16(4)	-1(4)	1(3)	-7(3)
C22	11(4)	27(5)	17(4)	5(4)	8(4)	0(4)
C23	14(4)	20(5)	12(4)	1(4)	8(3)	3(4)

C24	16(5)	28(6)	17(4)	2(4)	1(4)	-3(4)
C25	9(4)	21(5)	18(4)	2(4)	2(4)	0(4)
C26	13(4)	14(5)	20(4)	2(4)	4(4)	-1(4)
C27	21(5)	21(5)	16(4)	-5(4)	3(4)	-7(4)
C1	14(4)	23(5)	13(4)	0(4)	2(4)	-1(4)
C29	13(4)	23(5)	11(4)	-3(4)	6(3)	0(4)
C30	21(5)	20(5)	26(5)	4(4)	6(4)	4(4)
C31	30(5)	16(5)	25(5)	3(4)	12(4)	2(4)
C32	10(4)	28(6)	16(4)	-2(4)	4(4)	0(4)
C33	21(5)	23(5)	18(5)	4(4)	3(4)	3(4)
C34	24(5)	22(5)	18(4)	0(4)	6(4)	0(4)
C35	14(4)	18(5)	17(4)	-1(4)	10(4)	2(4)
C36	21(5)	27(6)	11(4)	7(4)	6(4)	6(4)
C37	14(4)	29(6)	20(5)	4(4)	3(4)	0(4)
C38	26(5)	22(5)	23(5)	8(4)	9(4)	1(4)
C39	28(5)	34(6)	21(5)	5(5)	8(4)	16(5)
C40	18(5)	48(7)	18(5)	1(5)	0(4)	8(5)
C41	22(5)	29(6)	20(5)	-2(4)	4(4)	1(4)
C42	18(4)	7(4)	20(4)	0(3)	5(4)	5(3)
C43	17(5)	26(5)	20(5)	6(4)	4(4)	1(4)
C44	24(5)	32(6)	22(5)	7(4)	-4(4)	-5(4)
C45	23(5)	24(5)	18(5)	3(4)	-9(4)	7(4)
C46	18(4)	27(6)	22(4)	5(4)	4(4)	2(4)
C47	9(4)	35(6)	16(4)	2(4)	-2(3)	-3(4)
C48	21(5)	28(6)	15(4)	-1(4)	5(4)	4(4)
C49	27(5)	26(6)	22(5)	0(4)	3(4)	-1(5)
C50	36(6)	46(7)	18(5)	-7(5)	-3(4)	-4(5)
C51	42(7)	40(7)	31(6)	-17(5)	3(5)	-12(5)
C52	35(6)	29(6)	40(6)	2(5)	10(5)	0(5)

C53	23(5)	30(6)	23(5)	0(4)	4(4)	1(4)
C54	33(6)	22(6)	27(5)	0(5)	2(5)	-1(5)
C55	28(6)	33(6)	23(5)	-5(5)	3(4)	-4(5)
C56	33(6)	38(7)	26(5)	1(5)	-2(5)	-15(5)
C57	28(6)	28(6)	42(6)	7(5)	5(5)	-9(5)
C58	24(5)	33(6)	27(5)	-6(5)	0(4)	-5(5)
C59	18(4)	28(6)	5(3)	4(4)	-2(3)	-2(4)
C60	7(4)	26(5)	16(4)	2(4)	3(3)	-3(4)
C61	12(4)	26(5)	20(5)	4(4)	4(4)	3(4)
C62	19(5)	16(5)	23(5)	4(4)	3(4)	9(4)
C63	16(4)	29(6)	18(5)	10(4)	0(4)	0(4)
C64	21(5)	31(6)	15(4)	4(4)	3(4)	2(4)
C65	17(4)	13(5)	19(4)	2(4)	2(4)	5(4)
C66	12(4)	12(5)	26(5)	-3(4)	7(4)	1(4)
C67	29(5)	21(5)	25(5)	4(4)	5(4)	-2(4)
C68	27(5)	22(5)	37(6)	10(5)	8(5)	4(4)
C69	25(5)	19(5)	40(6)	-2(5)	0(5)	-5(4)
C70	25(5)	23(5)	29(5)	-5(4)	3(4)	-7(4)
C71	18(4)	26(5)	15(4)	2(4)	-1(4)	-1(4)
C72	22(4)	16(5)	15(4)	3(4)	8(4)	6(4)
C73	13(4)	20(5)	16(4)	1(4)	2(4)	3(4)
C74	21(5)	27(6)	19(5)	5(4)	6(4)	-6(4)
C75	16(5)	29(6)	23(5)	8(4)	0(4)	9(4)
C76	27(5)	15(5)	22(5)	-1(4)	6(4)	3(4)
C77	17(5)	22(5)	23(5)	1(4)	4(4)	-4(4)
C78	15(4)	15(5)	24(5)	-5(4)	8(4)	1(4)
C79	14(4)	21(5)	15(4)	2(4)	5(4)	1(4)
C80	18(4)	18(5)	11(4)	-3(4)	2(4)	-1(4)
C81	16(4)	17(5)	9(4)	-4(4)	2(3)	0(4)

C82	15(4)	9(4)	25(5)	-1(4)	5(4)	-2(3)
C83	19(5)	26(5)	10(4)	-1(4)	-3(4)	3(4)
C84	15(4)	27(5)	11(4)	-5(4)	2(4)	-1(4)
C85	29(5)	16(5)	15(4)	-1(4)	1(4)	3(4)
C86	8(4)	23(5)	11(4)	4(4)	2(3)	3(4)
C87	21(5)	18(5)	15(4)	3(4)	8(4)	0(4)
C88	29(5)	12(5)	16(4)	5(4)	4(4)	-2(4)
C89	20(5)	17(5)	18(4)	-1(4)	9(4)	5(4)
C90	19(5)	16(5)	13(4)	0(4)	0(4)	-2(4)
C91	29(5)	16(5)	19(4)	-2(4)	15(4)	0(4)
C92	25(5)	11(5)	19(4)	-7(4)	7(4)	0(4)
C93	14(4)	20(5)	13(4)	0(4)	4(4)	5(4)
C94	16(4)	20(5)	12(4)	-3(4)	4(4)	-7(4)
C95	34(6)	22(6)	22(5)	-5(4)	7(5)	-6(5)
C96	34(6)	29(6)	22(5)	-10(5)	0(4)	2(5)
C97	30(6)	20(5)	39(6)	-10(5)	10(5)	-4(4)
C98	34(6)	15(5)	29(5)	-1(4)	7(5)	-3(4)
C99	22(5)	24(5)	14(4)	1(4)	2(4)	4(4)
C100	18(5)	23(5)	10(4)	0(4)	0(4)	0(4)
C101	19(4)	27(6)	18(4)	3(4)	9(4)	2(4)
C102	27(5)	33(6)	18(4)	6(5)	12(4)	4(5)
C103	28(5)	30(6)	16(4)	-3(4)	0(4)	6(4)
C104	18(5)	31(6)	29(5)	0(5)	-1(4)	-1(4)
C105	15(4)	25(5)	21(5)	2(4)	3(4)	-1(4)
C106	16(4)	21(5)	12(4)	1(4)	4(4)	-2(4)
C107	13(4)	17(5)	21(5)	0(4)	6(4)	3(4)
C108	25(5)	24(5)	15(4)	-1(4)	10(4)	3(4)
C109	26(5)	26(6)	13(4)	1(4)	5(4)	5(4)
C110	14(4)	29(6)	17(4)	7(4)	-2(4)	2(4)

C111	21(5)	27(6)	10(4)	2(4)	0(4)	-7(4)
C112	55(7)	11(5)	29(6)	-2(4)	11(5)	-8(5)
C113	29(5)	20(5)	21(5)	1(4)	3(4)	-5(4)
C114	17(5)	29(6)	32(6)	9(5)	7(4)	-6(4)
C115	25(6)	23(6)	38(6)	2(5)	-1(5)	-7(5)
C116	40(7)	27(6)	37(6)	0(5)	3(5)	-19(5)
C117	45(8)	79(12)	110(13)	44(10)	34(9)	30(8)
C118	63(11)	190(20)	160(20)	117(19)	51(13)	53(13)

Table S11. Bond Lengths for Complex **5.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	C1	1.959(10)	C50	H50	0.9500
Pd1	N3	2.110(8)	C51	C52	1.373(15)
Pd1	Cl2	2.323(2)	C51	H51	0.9500
Pd1	Cl1	2.329(2)	C52	C53	1.398(15)
Pd2	C86	1.956(9)	C52	H52	0.9500
Pd2	N6	2.103(8)	C53	H53	0.9500
Pd2	Cl5	2.318(2)	C54	C55	1.390(15)
Pd2	Cl4	2.320(2)	C54	H54	0.9500
Cl3	C55	1.764(11)	C55	C56	1.391(14)
Cl6	C112	1.806(10)	C56	C57	1.343(15)
Cl7	C117	1.786(17)	C56	H56	0.9500
Cl8	C117	1.701(19)	C57	C58	1.369(14)
Cl9	C118	1.719(19)	C57	H57	0.9500
Cl10	C118	1.732(16)	C58	H58	0.9500
N1	C1	1.337(11)	C59	C72	1.540(12)
N1	C26	1.390(11)	C59	C78	1.542(12)
N1	C23	1.430(10)	C59	C60	1.541(12)

N2	C1	1.347(11)	C59	C66	1.547(13)
N2	C27	1.398(11)	C60	C65	1.400(12)
N2	C29	1.435(10)	C60	C61	1.411(13)
N3	C54	1.311(13)	C61	C62	1.377(13)
N3	C58	1.351(12)	C61	H61	0.9500
N4	C86	1.342(11)	C62	C63	1.373(12)
N4	C84	1.382(12)	C62	H62	0.9500
N4	C81	1.443(10)	C63	C64	1.378(14)
N5	C86	1.352(11)	C63	H63	0.9500
N5	C85	1.376(12)	C64	C65	1.374(12)
N5	C87	1.433(10)	C64	H64	0.9500
N6	C114	1.335(12)	C65	H65	0.9500
N6	C113	1.360(12)	C66	C71	1.367(13)
C28	C2	1.530(12)	C66	C67	1.409(13)
C28	C14	1.536(11)	C67	C68	1.403(14)
C28	C20	1.545(11)	C67	H67	0.9500
C28	C8	1.548(13)	C68	C69	1.372(14)
C2	C3	1.391(12)	C68	H68	0.9500
C2	C7	1.401(11)	C69	C70	1.372(14)
C3	C4	1.379(13)	C69	H69	0.9500
C3	H3	0.9500	C70	C71	1.414(13)
C4	C5	1.364(12)	C70	H70	0.9500
C4	H4	0.9500	C71	H71	0.9500
C5	C6	1.394(13)	C72	C77	1.385(13)
C5	H5	0.9500	C72	C73	1.414(13)
C6	C7	1.390(13)	C73	C74	1.382(12)
C6	H6	0.9500	C73	H73	0.9500
C7	H7	0.9500	C74	C75	1.399(13)
C8	C13	1.399(13)	C74	H74	0.9500

C8	C9	1.407(13)	C75	C76	1.352(14)
C9	C10	1.392(13)	C75	H75	0.9500
C9	H9	0.9500	C76	C77	1.391(13)
C10	C11	1.377(14)	C76	H76	0.9500
C10	H10	0.9500	C77	H77	0.9500
C11	C12	1.387(14)	C78	C79	1.374(13)
C11	H11	0.9500	C78	C83	1.419(12)
C12	C13	1.394(14)	C79	C80	1.409(11)
C12	H12	0.9500	C79	H79	0.9500
C13	H13	0.9500	C80	C81	1.374(12)
C14	C19	1.393(12)	C80	H80	0.9500
C14	C15	1.400(13)	C81	C82	1.365(12)
C15	C16	1.382(12)	C82	C83	1.400(12)
C15	H15	0.9500	C82	H82	0.9500
C16	C17	1.383(13)	C83	H83	0.9500
C16	H16	0.9500	C84	C85	1.330(11)
C17	C18	1.394(13)	C84	H84	0.9500
C17	H17	0.9500	C85	H85	0.9500
C18	C19	1.375(12)	C87	C88	1.376(12)
C18	H18	0.9500	C87	C92	1.385(12)
C19	H19	0.9500	C88	C89	1.406(12)
C20	C25	1.388(12)	C88	H88	0.9500
C20	C21	1.403(11)	C89	C90	1.384(13)
C21	C22	1.372(11)	C89	H89	0.9500
C21	H21	0.9500	C90	C91	1.392(13)
C22	C23	1.391(12)	C90	C93	1.532(12)
C22	H22	0.9500	C91	C92	1.397(11)
C23	C24	1.374(12)	C91	H91	0.9500
C24	C25	1.390(12)	C92	H92	0.9500

C24	H24	0.9500	C93	C94	1.539(13)
C25	H25	0.9500	C93	C106	1.556(13)
C26	C27	1.324(12)	C93	C100	1.559(12)
C26	H26	0.9500	C94	C99	1.389(14)
C27	H27	0.9500	C94	C95	1.407(13)
C29	C30	1.362(13)	C95	C96	1.391(15)
C29	C34	1.376(12)	C95	H95	0.9500
C30	C31	1.379(12)	C96	C97	1.379(15)
C30	H30	0.9500	C96	H96	0.9500
C31	C32	1.404(13)	C97	C98	1.379(14)
C31	H31	0.9500	C97	H97	0.9500
C32	C33	1.379(14)	C98	C99	1.405(14)
C32	C35	1.554(12)	C98	H98	0.9500
C33	C34	1.407(12)	C99	H99	0.9500
C33	H33	0.9500	C100	C105	1.384(12)
C34	H34	0.9500	C100	C101	1.403(11)
C35	C48	1.518(13)	C101	C102	1.368(12)
C35	C36	1.533(12)	C101	H101	0.9500
C35	C42	1.540(13)	C102	C103	1.400(13)
C36	C41	1.398(13)	C102	H102	0.9500
C36	C37	1.405(14)	C103	C104	1.365(13)
C37	C38	1.383(13)	C103	H103	0.9500
C37	H37	0.9500	C104	C105	1.383(13)
C38	C39	1.414(14)	C104	H104	0.9500
C38	H38	0.9500	C105	H105	0.9500
C39	C40	1.369(16)	C106	C111	1.396(12)
C39	H39	0.9500	C106	C107	1.399(13)
C40	C41	1.388(14)	C107	C108	1.375(12)
C40	H40	0.9500	C107	H107	0.9500

C41	H41	0.9500	C108	C109	1.362(13)
C42	C43	1.396(13)	C108	H108	0.9500
C42	C47	1.419(12)	C109	C110	1.366(14)
C43	C44	1.412(13)	C109	H109	0.9500
C43	H43	0.9500	C110	C111	1.384(13)
C44	C45	1.375(13)	C110	H110	0.9500
C44	H44	0.9500	C111	H111	0.9500
C45	C46	1.378(13)	C112	C116	1.406(15)
C45	H45	0.9500	C113	H113	0.9500
C46	C47	1.367(12)	C114	C115	1.382(14)
C46	H46	0.9500	C114	H114	0.9500
C47	H47	0.9500	C115	H115	0.9500
C48	C49	1.403(13)	C116	H116	0.9500
C48	C53	1.421(14)	C117	H11A	0.9900
C49	C50	1.360(15)	C117	H11B	0.9900
C49	H49	0.9500	C118	H11C	0.9900
C50	C51	1.385(16)	C118	H11D	0.9900

Table S12. Bond Angles for Complex **5**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Pd1	N3	178.2(3)	C57	C56	H56	120.6
C1	Pd1	Cl2	87.6(3)	C55	C56	H56	120.6
N3	Pd1	Cl2	91.7(2)	C56	C57	C58	120.2(10)
C1	Pd1	Cl1	88.6(3)	C56	C57	H57	119.9
N3	Pd1	Cl1	92.2(2)	C58	C57	H57	119.9
Cl2	Pd1	Cl1	175.72(9)	N3	C58	C57	121.3(10)
C86	Pd2	N6	176.6(3)	N3	C58	H58	119.3
C86	Pd2	Cl5	87.8(3)	C57	C58	H58	119.3

N6	Pd2	Cl5	93.5(2)	C72	C59	C78	111.3(7)
C86	Pd2	Cl4	87.0(3)	C72	C59	C60	106.5(7)
N6	Pd2	Cl4	92.0(2)	C78	C59	C60	112.0(8)
Cl5	Pd2	Cl4	172.95(9)	C72	C59	C66	110.2(8)
C1	N1	C26	110.2(7)	C78	C59	C66	106.0(7)
C1	N1	C23	124.9(8)	C60	C59	C66	110.8(7)
C26	N1	C23	124.9(7)	C65	C60	C61	116.1(8)
C1	N2	C27	109.5(7)	C65	C60	C59	120.2(8)
C1	N2	C29	123.9(8)	C61	C60	C59	123.5(8)
C27	N2	C29	126.5(7)	C62	C61	C60	120.9(8)
C54	N3	C58	119.4(9)	C62	C61	H61	119.5
C54	N3	Pd1	120.8(7)	C60	C61	H61	119.5
C58	N3	Pd1	119.8(7)	C63	C62	C61	121.3(9)
C86	N4	C84	110.6(7)	C63	C62	H62	119.4
C86	N4	C81	123.6(8)	C61	C62	H62	119.4
C84	N4	C81	125.8(7)	C62	C63	C64	119.1(9)
C86	N5	C85	109.0(7)	C62	C63	H63	120.5
C86	N5	C87	124.4(7)	C64	C63	H63	120.5
C85	N5	C87	126.6(7)	C65	C64	C63	120.2(8)
C114	N6	C113	118.7(9)	C65	C64	H64	119.9
C114	N6	Pd2	120.2(7)	C63	C64	H64	119.9
C113	N6	Pd2	121.1(6)	C64	C65	C60	122.3(9)
C2	C28	C14	107.0(6)	C64	C65	H65	118.9
C2	C28	C20	111.4(7)	C60	C65	H65	118.9
C14	C28	C20	109.6(7)	C71	C66	C67	118.0(9)
C2	C28	C8	112.4(7)	C71	C66	C59	124.2(8)
C14	C28	C8	111.7(7)	C67	C66	C59	117.8(8)
C20	C28	C8	104.8(6)	C68	C67	C66	120.9(10)
C3	C2	C7	116.9(8)	C68	C67	H67	119.5

C3	C2	C28	124.7(7)	C66	C67	H67	119.5
C7	C2	C28	118.5(8)	C69	C68	C67	119.5(10)
C4	C3	C2	120.5(8)	C69	C68	H68	120.2
C4	C3	H3	119.7	C67	C68	H68	120.2
C2	C3	H3	119.7	C70	C69	C68	120.5(10)
C5	C4	C3	122.9(9)	C70	C69	H69	119.7
C5	C4	H4	118.6	C68	C69	H69	119.7
C3	C4	H4	118.6	C69	C70	C71	119.8(9)
C4	C5	C6	117.8(8)	C69	C70	H70	120.1
C4	C5	H5	121.1	C71	C70	H70	120.1
C6	C5	H5	121.1	C66	C71	C70	121.2(9)
C7	C6	C5	119.9(8)	C66	C71	H71	119.4
C7	C6	H6	120.0	C70	C71	H71	119.4
C5	C6	H6	120.0	C77	C72	C73	118.7(8)
C6	C7	C2	121.9(9)	C77	C72	C59	123.0(9)
C6	C7	H7	119.0	C73	C72	C59	118.3(8)
C2	C7	H7	119.0	C74	C73	C72	119.9(9)
C13	C8	C9	117.2(9)	C74	C73	H73	120.1
C13	C8	C28	120.6(8)	C72	C73	H73	120.1
C9	C8	C28	122.1(8)	C73	C74	C75	120.0(9)
C10	C9	C8	121.6(9)	C73	C74	H74	120.0
C10	C9	H9	119.2	C75	C74	H74	120.0
C8	C9	H9	119.2	C76	C75	C74	120.2(9)
C11	C10	C9	120.0(9)	C76	C75	H75	119.9
C11	C10	H10	120.0	C74	C75	H75	119.9
C9	C10	H10	120.0	C75	C76	C77	120.8(9)
C10	C11	C12	119.8(9)	C75	C76	H76	119.6
C10	C11	H11	120.1	C77	C76	H76	119.6
C12	C11	H11	120.1	C72	C77	C76	120.4(9)

C11	C12	C13	120.4(9)	C72	C77	H77	119.8
C11	C12	H12	119.8	C76	C77	H77	119.8
C13	C12	H12	119.8	C79	C78	C83	118.2(8)
C12	C13	C8	121.0(9)	C79	C78	C59	124.9(8)
C12	C13	H13	119.5	C83	C78	C59	116.8(8)
C8	C13	H13	119.5	C78	C79	C80	121.1(8)
C19	C14	C15	116.4(8)	C78	C79	H79	119.4
C19	C14	C28	119.5(8)	C80	C79	H79	119.4
C15	C14	C28	124.1(8)	C81	C80	C79	118.9(8)
C16	C15	C14	121.3(9)	C81	C80	H80	120.5
C16	C15	H15	119.4	C79	C80	H80	120.5
C14	C15	H15	119.4	C82	C81	C80	122.1(8)
C15	C16	C17	121.1(9)	C82	C81	N4	119.9(7)
C15	C16	H16	119.5	C80	C81	N4	117.9(8)
C17	C16	H16	119.5	C81	C82	C83	118.9(8)
C16	C17	C18	118.5(8)	C81	C82	H82	120.6
C16	C17	H17	120.7	C83	C82	H82	120.6
C18	C17	H17	120.7	C82	C83	C78	120.6(9)
C19	C18	C17	119.9(9)	C82	C83	H83	119.7
C19	C18	H18	120.1	C78	C83	H83	119.7
C17	C18	H18	120.1	C85	C84	N4	106.0(8)
C18	C19	C14	122.8(9)	C85	C84	H84	127.0
C18	C19	H19	118.6	N4	C84	H84	127.0
C14	C19	H19	118.6	C84	C85	N5	108.5(8)
C25	C20	C21	117.1(8)	C84	C85	H85	125.7
C25	C20	C28	124.5(7)	N5	C85	H85	125.7
C21	C20	C28	118.3(7)	N4	C86	N5	105.8(8)
C22	C21	C20	122.1(8)	N4	C86	Pd2	129.2(6)
C22	C21	H21	118.9	N5	C86	Pd2	125.0(6)

C20	C21	H21	118.9	C88	C87	C92	121.2(8)
C21	C22	C23	119.4(8)	C88	C87	N5	118.8(8)
C21	C22	H22	120.3	C92	C87	N5	120.0(8)
C23	C22	H22	120.3	C87	C88	C89	118.7(8)
C24	C23	C22	120.0(8)	C87	C88	H88	120.6
C24	C23	N1	119.7(8)	C89	C88	H88	120.6
C22	C23	N1	120.3(7)	C90	C89	C88	122.0(8)
C23	C24	C25	120.1(9)	C90	C89	H89	119.0
C23	C24	H24	119.9	C88	C89	H89	119.0
C25	C24	H24	119.9	C89	C90	C91	117.3(8)
C20	C25	C24	121.3(8)	C89	C90	C93	124.0(8)
C20	C25	H25	119.4	C91	C90	C93	118.7(8)
C24	C25	H25	119.4	C90	C91	C92	122.1(9)
C27	C26	N1	107.1(8)	C90	C91	H91	119.0
C27	C26	H26	126.4	C92	C91	H91	119.0
N1	C26	H26	126.4	C87	C92	C91	118.7(8)
C26	C27	N2	107.1(8)	C87	C92	H92	120.6
C26	C27	H27	126.5	C91	C92	H92	120.6
N2	C27	H27	126.5	C90	C93	C94	107.3(7)
N1	C1	N2	106.1(8)	C90	C93	C106	112.5(8)
N1	C1	Pd1	130.0(6)	C94	C93	C106	110.4(7)
N2	C1	Pd1	123.9(6)	C90	C93	C100	110.4(7)
C30	C29	C34	121.5(8)	C94	C93	C100	112.5(7)
C30	C29	N2	118.7(8)	C106	C93	C100	103.8(7)
C34	C29	N2	119.7(8)	C99	C94	C95	117.0(9)
C29	C30	C31	119.5(9)	C99	C94	C93	124.5(8)
C29	C30	H30	120.3	C95	C94	C93	118.5(9)
C31	C30	H30	120.3	C96	C95	C94	122.4(10)
C30	C31	C32	121.7(9)	C96	C95	H95	118.8

C30	C31	H31	119.2	C94	C95	H95	118.8
C32	C31	H31	119.2	C97	C96	C95	118.9(10)
C33	C32	C31	117.1(8)	C97	C96	H96	120.5
C33	C32	C35	125.5(8)	C95	C96	H96	120.5
C31	C32	C35	117.4(9)	C96	C97	C98	120.4(10)
C32	C33	C34	121.8(9)	C96	C97	H97	119.8
C32	C33	H33	119.1	C98	C97	H97	119.8
C34	C33	H33	119.1	C97	C98	C99	120.3(10)
C29	C34	C33	118.3(9)	C97	C98	H98	119.8
C29	C34	H34	120.8	C99	C98	H98	119.8
C33	C34	H34	120.8	C94	C99	C98	120.8(9)
C48	C35	C36	112.9(8)	C94	C99	H99	119.6
C48	C35	C42	113.0(7)	C98	C99	H99	119.6
C36	C35	C42	104.8(7)	C105	C100	C101	117.6(8)
C48	C35	C32	104.9(7)	C105	C100	C93	123.4(8)
C36	C35	C32	111.9(8)	C101	C100	C93	119.0(8)
C42	C35	C32	109.5(7)	C102	C101	C100	120.8(8)
C41	C36	C37	116.4(9)	C102	C101	H101	119.6
C41	C36	C35	123.8(9)	C100	C101	H101	119.6
C37	C36	C35	119.6(8)	C101	C102	C103	120.7(8)
C38	C37	C36	123.2(9)	C101	C102	H102	119.7
C38	C37	H37	118.4	C103	C102	H102	119.7
C36	C37	H37	118.4	C104	C103	C102	118.7(9)
C37	C38	C39	118.1(10)	C104	C103	H103	120.6
C37	C38	H38	121.0	C102	C103	H103	120.6
C39	C38	H38	121.0	C103	C104	C105	120.8(9)
C40	C39	C38	119.9(9)	C103	C104	H104	119.6
C40	C39	H39	120.0	C105	C104	H104	119.6
C38	C39	H39	120.0	C104	C105	C100	121.3(8)

C39	C40	C41	120.8(10)	C104	C105	H105	119.4
C39	C40	H40	119.6	C100	C105	H105	119.4
C41	C40	H40	119.6	C111	C106	C107	117.8(9)
C40	C41	C36	121.5(10)	C111	C106	C93	123.7(9)
C40	C41	H41	119.3	C107	C106	C93	118.4(8)
C36	C41	H41	119.3	C108	C107	C106	119.9(9)
C43	C42	C47	116.0(8)	C108	C107	H107	120.0
C43	C42	C35	123.3(8)	C106	C107	H107	120.0
C47	C42	C35	120.0(7)	C109	C108	C107	122.3(10)
C42	C43	C44	121.7(8)	C109	C108	H108	118.9
C42	C43	H43	119.2	C107	C108	H108	118.9
C44	C43	H43	119.2	C108	C109	C110	118.1(9)
C45	C44	C43	119.2(9)	C108	C109	H109	120.9
C45	C44	H44	120.4	C110	C109	H109	120.9
C43	C44	H44	120.4	C109	C110	C111	121.8(9)
C44	C45	C46	120.7(9)	C109	C110	H110	119.1
C44	C45	H45	119.7	C111	C110	H110	119.1
C46	C45	H45	119.7	C110	C111	C106	119.9(9)
C47	C46	C45	119.8(8)	C110	C111	H111	120.0
C47	C46	H46	120.1	C106	C111	H111	120.0
C45	C46	H46	120.1	C113	C112	C116	121.3(10)
C46	C47	C42	122.6(8)	C113	C112	Cl6	119.7(8)
C46	C47	H47	118.7	C116	C112	Cl6	119.0(8)
C42	C47	H47	118.7	N6	C113	C112	121.0(9)
C49	C48	C53	115.5(10)	N6	C113	H113	119.5
C49	C48	C35	121.0(9)	C112	C113	H113	119.5
C53	C48	C35	123.3(8)	N6	C114	C115	122.3(10)
C50	C49	C48	123.4(10)	N6	C114	H114	118.8
C50	C49	H49	118.3	C115	C114	H114	118.8

C48	C49	H49	118.3	C116	C115	C114	120.4(10)
C49	C50	C51	120.5(10)	C116	C115	H115	119.8
C49	C50	H50	119.8	C114	C115	H115	119.8
C51	C50	H50	119.8	C115	C116	C112	116.3(10)
C52	C51	C50	118.7(10)	C115	C116	H116	121.9
C52	C51	H51	120.6	C112	C116	H116	121.9
C50	C51	H51	120.6	Cl8	C117	Cl7	112.1(9)
C51	C52	C53	121.4(11)	Cl8	C117	H11A	109.2
C51	C52	H52	119.3	Cl7	C117	H11A	109.2
C53	C52	H52	119.3	Cl8	C117	H11B	109.2
C52	C53	C48	120.5(9)	Cl7	C117	H11B	109.2
C52	C53	H53	119.7	H11A	C117	H11B	107.9
C48	C53	H53	119.7	Cl9	C118	Cl10	114.3(10)
N3	C54	C55	121.5(10)	Cl9	C118	H11C	108.7
N3	C54	H54	119.2	Cl10	C118	H11C	108.7
C55	C54	H54	119.2	Cl9	C118	H11D	108.7
C54	C55	C56	118.8(10)	Cl10	C118	H11D	108.7
C54	C55	Cl3	117.9(8)	H11C	C118	H11D	107.6

Table S13. Torsion Angles for Complex **5.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C14	C28	C2	C3	130.1(9)	C56	C57	C58	N3	0.3(17)
C20	C28	C2	C3	10.4(12)	C72	C59	C60	C65	45.9(11)
C8	C28	C2	C3	106.9(10	C78	C59	C60	C65	167.9(8)
C14	C28	C2	C7	50.7(10)	C66	C59	C60	C65	73.9(10)
C20	C28	C2	C7	170.4(8)	C72	C59	C60	C61	129.4(9)
C8	C28	C2	C7	72.3(10)	C78	C59	C60	C61	7.4(12)
C7	C2	C3	C4	1.7(13)	C66	C59	C60	C61	110.8(9)

C28	C2	C3	C4	179.1(8)	C65	C60	C61	C62	1.7(13)
C2	C3	C4	C5	0.9(15)	C59	C60	C61	C62	177.2(8)
C3	C4	C5	C6	1.1(15)	C60	C61	C62	C63	0.3(15)
C4	C5	C6	C7	2.3(14)	C61	C62	C63	C64	1.4(15)
C5	C6	C7	C2	1.5(14)	C62	C63	C64	C65	1.6(15)
C3	C2	C7	C6	0.4(13)	C63	C64	C65	C60	0.1(15)
C28	C2	C7	C6	179.7(8)	C61	C60	C65	C64	1.5(13)
C2	C28	C8	C13	167.3(8)	C59	C60	C65	C64	177.2(8)
C14	C28	C8	C13	72.3(10)	C72	C59	C66	C71	102.0(10
C20	C28	C8	C13	46.2(10)	C78	C59	C66	C71	137.4(9)
C2	C28	C8	C9	9.8(11)	C60	C59	C66	C71	15.6(12)
C14	C28	C8	C9	110.5(9)	C72	C59	C66	C67	78.7(9)
C20	C28	C8	C9	130.9(8)	C78	C59	C66	C67	41.9(10)
C13	C8	C9	C10	1.3(13)	C60	C59	C66	C67	163.7(8)
C28	C8	C9	C10	175.9(8)	C71	C66	C67	C68	1.6(14)
C8	C9	C10	C11	1.5(14)	C59	C66	C67	C68	177.7(8)
C9	C10	C11	C12	0.4(15)	C66	C67	C68	C69	1.9(15)
C10	C11	C12	C13	2.5(15)	C67	C68	C69	C70	0.3(15)
C11	C12	C13	C8	2.7(14)	C68	C69	C70	C71	1.6(15)
C9	C8	C13	C12	0.8(13)	C67	C66	C71	C70	0.3(13)
C28	C8	C13	C12	178.1(8)	C59	C66	C71	C70	179.6(8)
C2	C28	C14	C19	50.5(9)	C69	C70	C71	C66	1.9(14)
C20	C28	C14	C19	70.4(9)	C78	C59	C72	C77	114.7(10
C8	C28	C14	C19	173.9(7)	C60	C59	C72	C77	122.9(9)
C2	C28	C14	C15	127.1(8)	C66	C59	C72	C77	2.7(11)
C20	C28	C14	C15	112.0(9)	C78	C59	C72	C73	67.2(10)
C8	C28	C14	C15	3.7(11)	C60	C59	C72	C73	55.2(10)
C19	C14	C15	C16	2.7(12)	C66	C59	C72	C73	175.5(7)
C28	C14	C15	C16	179.6(8)	C77	C72	C73	C74	2.4(13)

C14	C15	C16	C17	1.9(14)	C59	C72	C73	C74	179.4(7)
C15	C16	C17	C18	0.0(14)	C72	C73	C74	C75	3.1(14)
C16	C17	C18	C19	1.0(14)	C73	C74	C75	C76	0.6(15)
C17	C18	C19	C14	0.0(14)	C74	C75	C76	C77	2.7(15)
C15	C14	C19	C18	1.8(12)	C73	C72	C77	C76	0.8(13)
C28	C14	C19	C18	179.5(8)	C59	C72	C77	C76	177.3(8)
C2	C28	C20	C25	111.1(10	C75	C76	C77	C72	3.4(14)
C14	C28	C20	C25	7.1(12)	C72	C59	C78	C79	4.9(13)
C8	C28	C20	C25	127.2(9)	C60	C59	C78	C79	114.2(10
C2	C28	C20	C21	71.5(10)	C66	C59	C78	C79	124.8(10
C14	C28	C20	C21	170.2(8)	C72	C59	C78	C83	172.8(8)
C8	C28	C20	C21	50.2(10)	C60	C59	C78	C83	68.1(11)
C25	C20	C21	C22	1.7(14)	C66	C59	C78	C83	52.9(11)
C28	C20	C21	C22	175.9(8)	C83	C78	C79	C80	3.2(14)
C20	C21	C22	C23	1.3(14)	C59	C78	C79	C80	174.4(9)
C21	C22	C23	C24	0.2(14)	C78	C79	C80	C81	1.0(14)
C21	C22	C23	N1	178.8(8)	C79	C80	C81	C82	1.8(14)
C1	N1	C23	C24	134.9(10	C79	C80	C81	N4	177.0(8)
C26	N1	C23	C24	43.2(13)	C86	N4	C81	C82	44.9(13)
C1	N1	C23	C22	43.6(13)	C84	N4	C81	C82	137.1(10
C26	N1	C23	C22	138.2(9)	C86	N4	C81	C80	133.9(9)
C22	C23	C24	C25	0.4(15)	C84	N4	C81	C80	44.1(13)
N1	C23	C24	C25	178.1(8)	C80	C81	C82	C83	2.1(14)
C21	C20	C25	C24	1.0(14)	N4	C81	C82	C83	176.7(8)
C28	C20	C25	C24	176.4(8)	C81	C82	C83	C78	0.4(14)
C23	C24	C25	C20	0.0(15)	C79	C78	C83	C82	3.0(14)
C1	N1	C26	C27	0.6(11)	C59	C78	C83	C82	174.8(8)
C23	N1	C26	C27	179.0(8)	C86	N4	C84	C85	1.0(11)
N1	C26	C27	N2	0.3(10)	C81	N4	C84	C85	179.2(8)

C1	N2	C27	C26	0.1(11)	N4	C84	C85	N5	0.5(11)
C29	N2	C27	C26	179.7(8)	C86	N5	C85	C84	0.2(11)
C26	N1	C1	N2	0.6(10)	C87	N5	C85	C84	177.7(9)
C23	N1	C1	N2	179.0(8)	C84	N4	C86	N5	1.1(10)
C26	N1	C1	Pd1	179.5(7)	C81	N4	C86	N5	179.3(8)
C23	N1	C1	Pd1	2.1(14)	C84	N4	C86	Pd2	180.0(7)
C27	N2	C1	N1	0.4(10)	C81	N4	C86	Pd2	1.8(13)
C29	N2	C1	N1	179.4(8)	C85	N5	C86	N4	0.8(10)
C27	N2	C1	Pd1	179.4(7)	C87	N5	C86	N4	178.4(8)
C29	N2	C1	Pd1	0.4(13)	C85	N5	C86	Pd2	179.7(6
C1	N2	C29	C30	63.6(12)	C87	N5	C86	Pd2	2.7(13)
C27	N2	C29	C30	116.6(11	C86	N5	C87	C88	117.8(10
C1	N2	C29	C34	117.8(10	C85	N5	C87	C88	65.0(13)
C27	N2	C29	C34	62.0(12)	C86	N5	C87	C92	58.8(13)
C34	C29	C30	C31	2.8(15)	C85	N5	C87	C92	118.4(11
N2	C29	C30	C31	178.6(8)	C92	C87	C88	C89	2.8(14)
C29	C30	C31	C32	1.2(15)	N5	C87	C88	C89	179.4(8)
C30	C31	C32	C33	0.4(14)	C87	C88	C89	C90	1.4(14)
C30	C31	C32	C35	179.3(9)	C88	C89	C90	C91	0.3(14)
C31	C32	C33	C34	1.3(14)	C88	C89	C90	C93	178.0(9)
C35	C32	C33	C34	178.4(9)	C89	C90	C91	C92	0.7(14)
C30	C29	C34	C33	3.6(14)	C93	C90	C91	C92	177.7(8)
N2	C29	C34	C33	177.8(8)	C88	C87	C92	C91	2.4(14)
C32	C33	C34	C29	2.8(14)	N5	C87	C92	C91	179.0(8)
C33	C32	C35	C48	129.5(10	C90	C91	C92	C87	0.6(14)
C31	C32	C35	C48	50.7(11)	C89	C90	C93	C94	130.9(10
C33	C32	C35	C36	6.8(13)	C91	C90	C93	C94	50.8(11)
C31	C32	C35	C36	173.5(8)	C89	C90	C93	C106	9.3(13)
C33	C32	C35	C42	109.0(10	C91	C90	C93	C106	172.5(8)

C31	C32	C35	C42	70.8(10)	C89	C90	C93	C100	106.1(10
C48	C35	C36	C41	1.1(12)	C91	C90	C93	C100	72.1(11)
C42	C35	C36	C41	122.3(9)	C90	C93	C94	C99	127.5(9)
C32	C35	C36	C41	119.2(9)	C106	C93	C94	C99	109.6(10
C48	C35	C36	C37	176.3(8)	C100	C93	C94	C99	5.9(12)
C42	C35	C36	C37	52.9(10)	C90	C93	C94	C95	55.2(11)
C32	C35	C36	C37	65.6(11)	C106	C93	C94	C95	67.8(10)
C41	C36	C37	C38	2.5(13)	C100	C93	C94	C95	176.8(8)
C35	C36	C37	C38	178.0(8)	C99	C94	C95	C96	3.4(14)
C36	C37	C38	C39	1.3(14)	C93	C94	C95	C96	174.1(9)
C37	C38	C39	C40	0.2(14)	C94	C95	C96	C97	0.3(15)
C38	C39	C40	C41	0.4(15)	C95	C96	C97	C98	2.6(15)
C39	C40	C41	C36	1.0(15)	C96	C97	C98	C99	2.3(15)
C37	C36	C41	C40	2.3(13)	C95	C94	C99	C98	3.8(14)
C35	C36	C41	C40	177.6(8)	C93	C94	C99	C98	173.6(8)
C48	C35	C42	C43	121.9(9)	C97	C98	C99	C94	1.1(14)
C36	C35	C42	C43	114.8(9)	C90	C93	C100	C105	1.8(13)
C32	C35	C42	C43	5.4(12)	C94	C93	C100	C105	118.0(10
C48	C35	C42	C47	68.0(10)	C106	C93	C100	C105	122.6(10
C36	C35	C42	C47	55.3(11)	C90	C93	C100	C101	176.7(9)
C32	C35	C42	C47	175.5(8)	C94	C93	C100	C101	63.5(11)
C47	C42	C43	C44	0.3(14)	C106	C93	C100	C101	55.9(11)
C35	C42	C43	C44	170.8(9)	C105	C100	C101	C102	2.3(15)
C42	C43	C44	C45	0.8(16)	C93	C100	C101	C102	176.2(10
C43	C44	C45	C46	2.4(16)	C100	C101	C102	C103	0.6(17
C44	C45	C46	C47	3.7(16)	C101	C102	C103	C104	2.3(17
C45	C46	C47	C42	3.3(16)	C102	C103	C104	C105	1.1(16)
C43	C42	C47	C46	1.6(15)	C103	C104	C105	C100	1.9(16)
C35	C42	C47	C46	172.4(9)	C101	C100	C105	C104	3.6(15)

C36	C35	C48	C49	63.2(11)	C93	C100	C105	C104	174.9(9)
C42	C35	C48	C49	178.1(8)	C90	C93	C106	C111	115.4(9)
C32	C35	C48	C49	58.9(10)	C94	C93	C106	C111	4.4(11)
C36	C35	C48	C53	122.9(9)	C100	C93	C106	C111	125.3(9)
C42	C35	C48	C53	4.2(11)	C90	C93	C106	C107	68.3(10)
C32	C35	C48	C53	115.0(9)	C94	C93	C106	C107	171.8(8)
C53	C48	C49	C50	1.7(14)	C100	C93	C106	C107	51.0(10)
C35	C48	C49	C50	176.1(9)	C111	C106	C107	C108	3.3(13)
C48	C49	C50	C51	2.0(16)	C93	C106	C107	C108	179.8(8)
C49	C50	C51	C52	0.6(16)	C106	C107	C108	C109	1.7(14)
C50	C51	C52	C53	0.9(15)	C107	C108	C109	C110	1.2(14)
C51	C52	C53	C48	1.2(15)	C108	C109	C110	C111	2.5(14)
C49	C48	C53	C52	0.1(13)	C109	C110	C111	C106	0.9(14)
C35	C48	C53	C52	174.3(8)	C107	C106	C111	C110	2.1(13)
C58	N3	C54	C55	0.8(15)	C93	C106	C111	C110	178.3(8)
Pd1	N3	C54	C55	179.5(8)	C114	N6	C113	C112	0.1(14)
N3	C54	C55	C56	0.1(16)	Pd2	N6	C113	C112	177.9(8)
N3	C54	C55	Cl3	178.2(8)	C116	C112	C113	N6	0.2(16)
C54	C55	C56	C57	1.1(16)	Cl6	C112	C113	N6	179.0(7)
Cl3	C55	C56	C57	179.0(9)	C113	N6	C114	C115	0.2(15)
C55	C56	C57	C58	1.2(16)	Pd2	N6	C114	C115	178.0(8)
C54	N3	C58	C57	0.7(15)	N6	C114	C115	C116	0.4(16)
Pd1	N3	C58	C57	179.5(8)	C114	C115	C116	C112	0.5(16)

Table S14. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **5.**

Atom	x	Y	z	U(eq)
H23	1868	2116	3047	18
H2	-1078	888	3028	20

H3	306	-126	3980	17
H6	864	1643	4497	20
H7	505	1944	5604	25
H8	1730	1305	6670	30
H9	3324	359	6624	30
H10	3679	49	5530	26
H12	4393	1431	4471	25
H13	6131	1993	3734	33
H14	6467	1916	2538	36
H15	5019	1305	2047	33
H16	3287	750	2764	25
H18	1268	-625	5258	20
H19	1317	-2095	5655	24
H20	2709	-2775	5092	28
H21	4142	-1982	4187	30
H22	4100	-505	3786	23
H24	-2532	5306	-112	19
H25	-1156	4693	-854	20
H27	1564	3340	818	15
H28	2920	2313	686	16
H30	748	2025	-875	20
H31	-620	3067	-748	20
H34	869	486	-201	27
H35	422	-140	-1054	34
H36	1849	-144	-2016	31
H37	3694	480	-2102	28
H38	4132	1146	-1264	20
H40	1483	1073	1299	21
H41	1331	-93	2453	29

H42	2366	-1375	2609	31
H43	3589	-1476	1596	32
H44	3790	-305	458	25
H46	4895	826	822	22
H47	6740	1506	627	31
H48	7064	2728	-462	36
H49	5542	3251	-1377	30
H50	3704	2577	-1184	23
H52	-2737	3299	2114	19
H53	-3530	3527	3187	19
H55	-3044	6038	2113	16
H56	-2190	5812	1042	17
H59	-5951	5767	3452	23
H60	-6407	7212	3123	32
H61	-4848	8169	2845	31
H62	-2818	7671	2932	29
H63	-2360	6223	3300	24
H65	-3508	5014	4905	24
H66	-1964	4572	5789	33
H67	-170	3933	5534	37
H68	83	3761	4360	32
H69	-1481	4178	3474	23
H71	-5693	4745	2811	21
H72	-7415	3936	3213	27
H73	-7646	3022	4498	29
H74	-6157	2943	5370	29
H75	-4440	3754	4972	22
H76A	421	5439	3064	87
H76B	-116	5786	2217	87

H77A	4564	3618	2065	43
H77B	3267	3776	1667	43

Table S15. Crystal data and structure refinement for complex **6.**

Identification code	**6**
Empirical formula	C_{62} H_{53} Cl_2 N_3 O_2 Pd
Formula weight	1049.37
Temperature/K	173(2)
Crystal system	Triclinic
Space group	P-1
a/Å	12.6752(9)
b/Å	13.2902(9)
c/Å	16.9619(13)
α/°	92.605(2)
β/°	108.9860(10)
γ/°	107.7310(10)
Volume/Å^3	2540.2(3)
Z	2
ρ_{calc}g/cm^3	1.372
μ/mm^{-1}	0.519
F(000)	1084
Crystal size/mm^3	0.15 × 0.14 × 0.13
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.63 to 25.01
Index ranges	-14 ≤ h ≤ 15, -13 ≤ k ≤ 15, -20 ≤ l ≤ 18
Reflections collected	14815
Independent reflections	8930 [R(int) = 0.0380]
Data/restraints/parameters	8930 / 0 / 633
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R1 = 0.0445, wR2 = 0.0890
Final R indexes [all data]	R1 = 0.0618, wR2 = 0.0976
Largest diff. peak/hole / e Å^{-3}	0.453-0.666

Table S16. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **6**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	Y	z	U(eq)
Pd1	1835(1)	3185(1)	5243(1)	14(1)
Cl1	2135(1)	1796(1)	5950(1)	21(1)
Cl2	1661(1)	4615(1)	4547(1)	26(1)
O1	1299(2)	3358(2)	666(2)	36(1)
O2	2119(3)	3562(2)	2071(2)	41(1)
N1	4284(2)	3552(2)	5231(2)	12(1)
N2	4288(2)	4632(2)	6208(2)	13(1)
N3	-6(2)	2519(2)	4913(2)	20(1)
C1	2745(3)	12(3)	2532(2)	13(1)
C2	1413(3)	-583(3)	2373(2)	16(1)
C3	1067(3)	-801(3)	3060(2)	24(1)
C4	-99(3)	-1394(3)	2956(3)	31(1)
C5	-938(3)	-1768(3)	2154(3)	30(1)
C6	-611(3)	-1539(3)	1467(3)	30(1)
C7	557(3)	-944(3)	1576(2)	23(1)
C8	3451(3)	-765(3)	2774(2)	13(1)
C9	4637(3)	-427(3)	2821(2)	14(1)
C10	5307(3)	-1089(3)	3020(2)	15(1)
C11	4804(3)	-2118(3)	3155(2)	17(1)
C12	3633(3)	-2466(3)	3095(2)	21(1)
C13	2966(3)	-1790(3)	2915(2)	17(1)
C14	2932(3)	421(3)	1734(2)	13(1)
C15	2805(3)	-323(3)	1062(2)	17(1)

C16	2948(3)	-7(3)	331(2)	20(1)
C17	3235(3)	1060(3)	236(2)	20(1)
C18	3369(3)	1803(3)	893(2)	19(1)
C19	3229(3)	1487(3)	1628(2)	17(1)
C20	3191(3)	954(3)	3268(2)	13(1)
C21	4180(3)	1132(3)	3988(2)	15(1)
C22	4543(3)	1982(3)	4631(2)	15(1)
C23	3906(3)	2677(3)	4556(2)	13(1)
C24	2902(3)	2520(3)	3849(2)	14(1)
C25	2544(3)	1654(3)	3217(2)	16(1)
C26	5455(3)	4211(3)	5643(2)	13(1)
C27	5460(3)	4881(3)	6260(2)	15(1)
C28	3553(3)	3817(3)	5567(2)	13(1)
C29	3894(3)	5129(3)	6779(2)	13(1)
C30	4129(3)	6222(3)	6878(2)	18(1)
C31	3720(3)	6685(3)	7424(2)	17(1)
C32	3090(3)	6072(3)	7869(2)	14(1)
C33	2875(3)	4965(3)	7757(2)	18(1)
C34	3272(3)	4498(3)	7220(2)	17(1)
C35	2649(3)	6551(3)	8502(2)	15(1)
C36	3546(3)	6725(3)	9412(2)	15(1)
C37	4459(3)	6301(3)	9635(2)	16(1)
C38	5242(3)	6491(3)	10459(2)	21(1)
C39	5121(3)	7090(3)	11095(2)	22(1)
C40	4197(3)	7501(3)	10882(2)	21(1)
C41	3427(3)	7324(3)	10057(2)	18(1)
C42	2550(3)	7661(3)	8305(2)	17(1)
C43	3584(3)	8558(3)	8569(2)	18(1)
C44	3565(4)	9562(3)	8414(2)	26(1)

C45	2506(4)	9704(3)	7985(3)	30(1)
C46	1469(4)	8838(3)	7715(3)	35(1)
C47	1497(3)	7823(3)	7877(2)	25(1)
C48	1433(3)	5737(3)	8425(2)	15(1)
C49	1202(3)	5321(3)	9111(2)	18(1)
C50	107(3)	4572(3)	9015(3)	25(1)
C51	-780(3)	4238(3)	8236(3)	30(1)
C52	-556(3)	4632(3)	7542(3)	33(1)
C53	533(3)	5358(3)	7631(2)	25(1)
C54	-649(3)	3136(3)	4962(3)	31(1)
C55	-1860(3)	2719(3)	4781(3)	47(1)
C56	-2423(3)	1631(3)	4540(3)	51(2)
C57	-1768(3)	991(3)	4489(3)	40(1)
C58	-570(3)	1461(3)	4673(3)	26(1)
C59	3193(4)	4608(3)	1294(3)	42(1)
C60	2177(3)	3808(3)	1403(3)	29(1)
C61	203(3)	2582(3)	686(3)	38(1)
C62	279(3)	1511(3)	798(3)	34(1)

Table S17. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **6**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Pd1	13(1)	13(1)	16(1)	0(1)	6(1)	5(1)
Cl1	16(1)	19(1)	30(1)	8(1)	9(1)	7(1)
Cl2	23(1)	23(1)	35(1)	13(1)	11(1)	12(1)
O1	32(2)	42(2)	32(2)	11(1)	7(1)	13(1)
O2	57(2)	34(2)	29(2)	5(1)	12(2)	16(2)
N1	14(1)	11(2)	11(2)	0(1)	6(1)	6(1)
N2	18(1)	11(2)	9(2)	-1(1)	7(1)	4(1)

N3	18(2)	20(2)	19(2)	-1(1)	4(1)	8(1)
C1	12(2)	12(2)	15(2)	-1(1)	5(1)	3(1)
C2	14(2)	15(2)	20(2)	1(2)	7(2)	7(2)
C3	17(2)	32(2)	23(2)	0(2)	8(2)	6(2)
C4	30(2)	33(3)	34(3)	7(2)	21(2)	8(2)
C5	14(2)	28(2)	49(3)	8(2)	16(2)	3(2)
C6	16(2)	31(2)	32(3)	1(2)	-1(2)	4(2)
C7	18(2)	23(2)	24(2)	5(2)	8(2)	4(2)
C8	16(2)	14(2)	9(2)	-2(1)	4(1)	4(1)
C9	18(2)	12(2)	12(2)	-2(1)	8(2)	2(1)
C10	13(2)	23(2)	9(2)	-1(2)	3(1)	7(2)
C11	19(2)	18(2)	12(2)	-1(2)	1(2)	10(2)
C12	20(2)	17(2)	20(2)	3(2)	3(2)	4(2)
C13	14(2)	15(2)	21(2)	1(2)	7(2)	2(1)
C14	7(2)	14(2)	16(2)	1(1)	2(1)	3(1)
C15	17(2)	15(2)	18(2)	-1(2)	5(2)	5(2)
C16	26(2)	21(2)	17(2)	-1(2)	10(2)	10(2)
C17	20(2)	27(2)	19(2)	7(2)	11(2)	9(2)
C18	22(2)	16(2)	23(2)	4(2)	10(2)	8(2)
C19	15(2)	19(2)	19(2)	0(2)	9(2)	5(2)
C20	14(2)	11(2)	13(2)	2(1)	7(1)	2(1)
C21	18(2)	16(2)	14(2)	0(1)	7(2)	10(2)
C22	12(2)	19(2)	11(2)	-2(1)	3(1)	4(1)
C23	17(2)	11(2)	13(2)	1(1)	10(2)	3(1)
C24	15(2)	14(2)	18(2)	3(1)	9(2)	7(1)
C25	14(2)	22(2)	13(2)	1(2)	4(1)	7(2)
C26	12(2)	16(2)	13(2)	3(1)	6(1)	5(1)
C27	14(2)	14(2)	15(2)	0(1)	5(1)	3(1)
C28	17(2)	12(2)	9(2)	1(1)	6(1)	6(1)

C29	14(2)	14(2)	9(2)	-3(1)	2(1)	5(1)
C30	18(2)	13(2)	19(2)	-3(2)	9(2)	2(2)
C31	18(2)	10(2)	19(2)	-4(1)	5(2)	2(1)
C32	14(2)	10(2)	13(2)	-2(1)	2(1)	3(1)
C33	22(2)	15(2)	17(2)	0(2)	10(2)	2(2)
C34	24(2)	9(2)	18(2)	0(1)	9(2)	6(2)
C35	17(2)	15(2)	14(2)	0(1)	8(2)	6(2)
C36	18(2)	11(2)	15(2)	2(1)	7(2)	2(1)
C37	21(2)	11(2)	18(2)	1(1)	10(2)	4(2)
C38	16(2)	22(2)	26(2)	6(2)	7(2)	7(2)
C39	25(2)	19(2)	13(2)	1(2)	-2(2)	4(2)
C40	27(2)	18(2)	14(2)	-4(2)	8(2)	4(2)
C41	20(2)	14(2)	16(2)	-3(2)	6(2)	4(2)
C42	25(2)	19(2)	15(2)	3(2)	13(2)	13(2)
C43	26(2)	17(2)	16(2)	-1(2)	11(2)	10(2)
C44	43(2)	16(2)	29(2)	2(2)	25(2)	11(2)
C45	53(3)	25(2)	36(3)	19(2)	34(2)	26(2)
C46	38(2)	48(3)	41(3)	28(2)	25(2)	33(2)
C47	24(2)	31(2)	23(2)	9(2)	11(2)	11(2)
C48	20(2)	16(2)	11(2)	0(1)	7(2)	7(2)
C49	18(2)	17(2)	16(2)	-1(2)	4(2)	4(2)
C50	28(2)	23(2)	24(2)	5(2)	14(2)	3(2)
C51	24(2)	32(3)	30(3)	0(2)	11(2)	1(2)
C52	21(2)	37(3)	26(3)	-1(2)	2(2)	-3(2)
C53	25(2)	27(2)	18(2)	1(2)	9(2)	2(2)
C54	18(2)	14(2)	57(3)	-2(2)	11(2)	5(2)
C55	18(2)	34(3)	88(4)	-5(2)	15(2)	12(2)
C56	15(2)	31(3)	91(4)	-8(3)	9(2)	0(2)
C57	19(2)	27(3)	55(3)	-9(2)	-3(2)	4(2)

C58	22(2)	17(2)	33(3)	-5(2)	2(2)	7(2)
C59	46(3)	36(3)	39(3)	8(2)	14(2)	9(2)
C60	31(2)	31(3)	25(3)	2(2)	5(2)	16(2)
C61	18(2)	45(3)	48(3)	10(2)	13(2)	8(2)
C62	22(2)	44(3)	29(3)	6(2)	6(2)	7(2)

Table S18. Bond Lengths for Complex **6**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	C28	1.954(3)	C29	C34	1.387(5)
Pd1	N3	2.095(3)	C30	C31	1.400(4)
Pd1	Cl1	2.3076(9)	C30	H30	0.9500
Pd1	Cl2	2.3115(10)	C31	C32	1.386(5)
O1	C60	1.334(5)	C31	H31	0.9500
O1	C61	1.468(5)	C32	C33	1.405(4)
O2	C60	1.212(5)	C32	C35	1.553(4)
N1	C28	1.354(4)	C33	C34	1.380(4)
N1	C26	1.392(4)	C33	H33	0.9500
N1	C23	1.441(4)	C34	H34	0.9500
N2	C28	1.357(4)	C35	C36	1.548(5)
N2	C27	1.392(4)	C35	C48	1.551(5)
N2	C29	1.443(4)	C35	C42	1.560(5)
N3	C54	1.337(4)	C36	C37	1.390(4)
N3	C58	1.341(4)	C36	C41	1.398(5)
C1	C14	1.542(5)	C37	C38	1.383(5)
C1	C8	1.548(4)	C37	H37	0.9500
C1	C20	1.554(4)	C38	C39	1.388(5)
C1	C2	1.556(4)	C38	H38	0.9500
C2	C7	1.381(5)	C39	C40	1.390(5)

C2	C3	1.385(5)	C39	H39	0.9500
C3	C4	1.395(5)	C40	C41	1.381(5)
C3	H3	0.9500	C40	H40	0.9500
C4	C5	1.380(6)	C41	H41	0.9500
C4	H4	0.9500	C42	C47	1.384(5)
C5	C6	1.376(6)	C42	C43	1.399(5)
C5	H5	0.9500	C43	C44	1.378(5)
C6	C7	1.395(5)	C43	H43	0.9500
C6	H6	0.9500	C44	C45	1.378(5)
C7	H7	0.9500	C44	H44	0.9500
C8	C13	1.381(5)	C45	C46	1.378(6)
C8	C9	1.405(4)	C45	H45	0.9500
C9	C10	1.381(4)	C46	C47	1.397(5)
C9	H9	0.9500	C46	H46	0.9500
C10	C11	1.386(5)	C47	H47	0.9500
C10	H10	0.9500	C48	C49	1.388(5)
C11	C12	1.380(5)	C48	C53	1.400(5)
C11	H11	0.9500	C49	C50	1.393(5)
C12	C13	1.392(5)	C49	H49	0.9500
C12	H12	0.9500	C50	C51	1.372(5)
C13	H13	0.9500	C50	H50	0.9500
C14	C19	1.387(5)	C51	C52	1.386(6)
C14	C15	1.409(4)	C51	H51	0.9500
C15	C16	1.377(5)	C52	C53	1.378(5)
C15	H15	0.9500	C52	H52	0.9500
C16	C17	1.383(5)	C53	H53	0.9500
C16	H16	0.9500	C54	C55	1.385(5)
C17	C18	1.384(5)	C54	H54	0.9500
C17	H17	0.9500	C55	C56	1.377(6)

C18	C19	1.382(5)	C55	H55	0.9500
C18	H18	0.9500	C56	C57	1.375(5)
C19	H19	0.9500	C56	H56	0.9500
C20	C21	1.384(4)	C57	C58	1.375(5)
C20	C25	1.404(4)	C57	H57	0.9500
C21	C22	1.387(4)	C58	H58	0.9500
C21	H21	0.9500	C59	C60	1.470(6)
C22	C23	1.384(4)	C59	H59A	0.9800
C22	H22	0.9500	C59	H59B	0.9800
C23	C24	1.387(4)	C59	H59C	0.9800
C24	C25	1.391(4)	C61	C62	1.472(6)
C24	H24	0.9500	C61	H61A	0.9900
C25	H25	0.9500	C61	H61B	0.9900
C26	C27	1.340(4)	C62	H62A	0.9800
C26	H26	0.9500	C62	H62B	0.9800
C27	H27	0.9500	C62	H62C	0.9800

Table S19. Bond Angles for Complex **6**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C 28	Pd 1	N 3	179.11(13)	C 32	C 31	C 30	121.5(3)
C 28	Pd 1	Cl 1	88.12(10)	C 32	C 31	H 31	119.3
N 3	Pd 1	Cl 1	91.79(9)	C 30	C 31	H 31	119.3
C 28	Pd 1	Cl 2	88.29(10)	C 31	C 32	C 33	117.8(3)
N 3	Pd 1	Cl 2	91.81(9)	C 31	C 32	C 35	123.4(3)
Cl 1	Pd 1	Cl 2	176.37(3)	C 33	C 32	C 35	118.7(3)
C 60	O 1	C 61	117.6(3)	C 34	C 33	C 32	121.3(3)
C 28	N 1	C 26	111.1(3)	C 34	C 33	H 33	119.3
C 28	N 1	C 23	124.5(3)	C 32	C 33	H 33	119.3

C 26	N 1	C 23	124.4(3)	C 33	C 34	C 29	119.6(3)
C 28	N 2	C 27	111.2(3)	C 33	C 34	H 34	120.2
C 28	N 2	C 29	123.6(3)	C 29	C 34	H 34	120.2
C 27	N 2	C 29	125.2(3)	C 36	C 35	C 48	109.9(3)
C 54	N 3	C 58	118.1(3)	C 36	C 35	C 32	109.9(3)
C 54	N 3	Pd 1	120.7(2)	C 48	C 35	C 32	107.4(3)
C 58	N 3	Pd 1	121.2(2)	C 36	C 35	C 42	107.6(3)
C 14	C 1	C 8	106.8(3)	C 48	C 35	C 42	111.5(3)
C 14	C 1	C 20	111.1(3)	C 32	C 35	C 42	110.5(3)
C 8	C 1	C 20	110.5(3)	C 37	C 36	C 41	117.4(3)
C 14	C 1	C 2	111.9(3)	C 37	C 36	C 35	123.8(3)
C 8	C 1	C 2	109.7(3)	C 41	C 36	C 35	118.8(3)
C 20	C 1	C 2	106.9(2)	C 38	C 37	C 36	121.3(3)
C 7	C 2	C 3	117.9(3)	C 38	C 37	H 37	119.3
C 7	C 2	C 1	123.2(3)	C 36	C 37	H 37	119.3
C 3	C 2	C 1	118.9(3)	C 37	C 38	C 39	120.9(3)
C 2	C 3	C 4	121.5(4)	C 37	C 38	H 38	119.5
C 2	C 3	H 3	119.2	C 39	C 38	H 38	119.5
C 4	C 3	H 3	119.2	C 38	C 39	C 40	118.2(3)
C 5	C 4	C 3	119.8(4)	C 38	C 39	H 39	120.9
C 5	C 4	H 4	120.1	C 40	C 39	H 39	120.9
C 3	C 4	H 4	120.1	C 41	C 40	C 39	120.7(3)
C 6	C 5	C 4	119.3(4)	C 41	C 40	H 40	119.6
C 6	C 5	H 5	120.4	C 39	C 40	H 40	119.6
C 4	C 5	H 5	120.4	C 40	C 41	C 36	121.3(3)
C 5	C 6	C 7	120.6(4)	C 40	C 41	H 41	119.3
C 5	C 6	H 6	119.7	C 36	C 41	H 41	119.3
C 7	C 6	H 6	119.7	C 47	C 42	C 43	117.0(3)
C 2	C 7	C 6	120.9(4)	C 47	C 42	C 35	124.2(3)

C 2	C 7	H 7	119.5	C 43	C 42	C 35	118.7(3)
C 6	C 7	H 7	119.5	C 44	C 43	C 42	121.9(3)
C 13	C 8	C 9	118.0(3)	C 44	C 43	H 43	119.0
C 13	C 8	C 1	123.6(3)	C 42	C 43	H 43	119.0
C 9	C 8	C 1	118.4(3)	C 45	C 44	C 43	120.0(4)
C 10	C 9	C 8	121.1(3)	C 45	C 44	H 44	120.0
C 10	C 9	H 9	119.4	C 43	C 44	H 44	120.0
C 8	C 9	H 9	119.4	C 44	C 45	C 46	119.7(4)
C 9	C 10	C 11	120.1(3)	C 44	C 45	H 45	120.2
C 9	C 10	H 10	119.9	C 46	C 45	H 45	120.2
C 11	C 10	H 10	119.9	C 45	C 46	C 47	120.0(4)
C 12	C 11	C 10	119.3(3)	C 45	C 46	H 46	120.0
C 12	C 11	H 11	120.4	C 47	C 46	H 46	120.0
C 10	C 11	H 11	120.4	C 42	C 47	C 46	121.4(4)
C 11	C 12	C 13	120.7(3)	C 42	C 47	H 47	119.3
C 11	C 12	H 12	119.7	C 46	C 47	H 47	119.3
C 13	C 12	H 12	119.7	C 49	C 48	C 53	117.5(3)
C 8	C 13	C 12	120.8(3)	C 49	C 48	C 35	122.9(3)
C 8	C 13	H 13	119.6	C 53	C 48	C 35	119.6(3)
C 12	C 13	H 13	119.6	C 48	C 49	C 50	121.3(3)
C 19	C 14	C 15	116.8(3)	C 48	C 49	H 49	119.4
C 19	C 14	C 1	124.4(3)	C 50	C 49	H 49	119.4
C 15	C 14	C 1	118.8(3)	C 51	C 50	C 49	120.5(4)
C 16	C 15	C 14	121.4(3)	C 51	C 50	H 50	119.8
C 16	C 15	H 15	119.3	C 49	C 50	H 50	119.8
C 14	C 15	H 15	119.3	C 50	C 51	C 52	118.9(4)
C 15	C 16	C 17	120.8(3)	C 50	C 51	H 51	120.5
C 15	C 16	H 16	119.6	C 52	C 51	H 51	120.5
C 17	C 16	H 16	119.6	C 53	C 52	C 51	120.8(4)

C 16	C 17	C 18	118.5(4)	C 53	C 52	H 52	119.6
C 16	C 17	H 17	120.7	C 51	C 52	H 52	119.6
C 18	C 17	H 17	120.7	C 52	C 53	C 48	121.0(4)
C 19	C 18	C 17	120.8(3)	C 52	C 53	H 53	119.5
C 19	C 18	H 18	119.6	C 48	C 53	H 53	119.5
C 17	C 18	H 18	119.6	N 3	C 54	C 55	122.3(4)
C 18	C 19	C 14	121.7(3)	N 3	C 54	H 54	118.8
C 18	C 19	H 19	119.2	C 55	C 54	H 54	118.8
C 14	C 19	H 19	119.2	C 56	C 55	C 54	118.8(4)
C 21	C 20	C 25	117.6(3)	C 56	C 55	H 55	120.6
C 21	C 20	C 1	123.7(3)	C 54	C 55	H 55	120.6
C 25	C 20	C 1	118.6(3)	C 57	C 56	C 55	119.2(4)
C 20	C 21	C 22	121.7(3)	C 57	C 56	H 56	120.4
C 20	C 21	H 21	119.1	C 55	C 56	H 56	120.4
C 22	C 21	H 21	119.1	C 58	C 57	C 56	118.8(4)
C 23	C 22	C 21	119.6(3)	C 58	C 57	H 57	120.6
C 23	C 22	H 22	120.2	C 56	C 57	H 57	120.6
C 21	C 22	H 22	120.2	N 3	C 58	C 57	122.8(3)
C 22	C 23	C 24	120.6(3)	N 3	C 58	H 58	118.6
C 22	C 23	N 1	119.2(3)	C 57	C 58	H 58	118.6
C 24	C 23	N 1	120.2(3)	C 60	C 59	H 59A	109.5
C 23	C 24	C 25	119.0(3)	C 60	C 59	H 59B	109.5
C 23	C 24	H 24	120.5	H 59A	C 59	H 59B	109.5
C 25	C 24	H 24	120.5	C 60	C 59	H 59C	109.5
C 24	C 25	C 20	121.5(3)	H 59A	C 59	H 59C	109.5
C 24	C 25	H 25	119.2	H 59B	C 59	H 59C	109.5
C 20	C 25	H 25	119.2	O 2	C 60	O 1	122.5(4)
C 27	C 26	N 1	106.8(3)	O 2	C 60	C 59	125.6(4)
C 27	C 26	H 26	126.6	O 1	C 60	C 59	111.9(4)

N 1	C 26	H 26	126.6	O 1	C 61	C 62	113.6(3)
C 26	C 27	N 2	106.6(3)	O 1	C 61	H 61A	108.8
C 26	C 27	H 27	126.7	C 62	C 61	H 61A	108.8
N 2	C 27	H 27	126.7	O 1	C 61	H 61B	108.8
N 1	C 28	N 2	104.3(3)	C 62	C 61	H 61B	108.8
N 1	C 28	Pd 1	129.3(2)	H 61A	C 61	H 61B	107.7
N 2	C 28	Pd 1	126.4(2)	C 61	C 62	H 62A	109.5
C 30	C 29	C 34	120.6(3)	C 61	C 62	H 62B	109.5
C 30	C 29	N 2	120.1(3)	H 62A	C 62	H 62B	109.5
C 34	C 29	N 2	119.3(3)	C 61	C 62	H 62C	109.5
C 29	C 30	C 31	119.1(3)	H 62A	C 62	H 62C	109.5
C 29	C 30	H 30	120.4	H 62B	C 62	H 62C	109.5

Table S20. Torsion Angles for Complex **6.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C28	Pd1	N3	C54	54(9)	C29	N2	C28	Pd1	2.9(5)
Cl1	Pd1	N3	C54	137.6(3)	N3	Pd1	C28	N1	162(9)
Cl2	Pd1	N3	C54	42.9(3)	Cl1	Pd1	C28	N1	78.2(3)
C28	Pd1	N3	C58	124(9)	Cl2	Pd1	C28	N1	101.3(3)
Cl1	Pd1	N3	C58	40.3(3)	N3	Pd1	C28	N2	17(9)
Cl2	Pd1	N3	C58	139.2(3)	Cl1	Pd1	C28	N2	100.8(3)
C14	C1	C2	C7	15.9(4)	Cl2	Pd1	C28	N2	79.7(3)
C8	C1	C2	C7	102.4(4)	C28	N2	C29	C30	124.6(4)
C20	C1	C2	C7	137.7(3)	C27	N2	C29	C30	58.7(5)
C14	C1	C2	C3	166.6(3)	C28	N2	C29	C34	54.9(5)
C8	C1	C2	C3	75.1(4)	C27	N2	C29	C34	121.8(4)
C20	C1	C2	C3	44.8(4)	C34	C29	C30	C31	0.6(5)
C7	C2	C3	C4	2.0(5)	N2	C29	C30	C31	178.9(3)

C1	C2	C3	C4	175.7(3)	C29	C30	C31	C32	0.2(5)
C2	C3	C4	C5	0.7(6)	C30	C31	C32	C33	0.2(5)
C3	C4	C5	C6	0.6(6)	C30	C31	C32	C35	178.2(3)
C4	C5	C6	C7	0.5(6)	C31	C32	C33	C34	0.2(5)
C3	C2	C7	C6	2.0(5)	C35	C32	C33	C34	178.3(3)
C1	C2	C7	C6	175.5(3)	C32	C33	C34	C29	0.2(5)
C5	C6	C7	C2	0.8(6)	C30	C29	C34	C33	0.6(5)
C14	C1	C8	C13	128.1(3)	N2	C29	C34	C33	178.9(3)
C20	C1	C8	C13	111.0(4)	C31	C32	C35	C36	96.1(4)
C2	C1	C8	C13	6.7(4)	C33	C32	C35	C36	81.9(4)
C14	C1	C8	C9	49.3(4)	C31	C32	C35	C48	144.4(3)
C20	C1	C8	C9	71.6(4)	C33	C32	C35	C48	37.6(4)
C2	C1	C8	C9	170.7(3)	C31	C32	C35	C42	22.5(4)
C13	C8	C9	C10	1.4(5)	C33	C32	C35	C42	159.4(3)
C1	C8	C9	C10	179.0(3)	C48	C35	C36	C37	105.3(4)
C8	C9	C10	C11	1.9(5)	C32	C35	C36	C37	12.6(5)
C9	C10	C11	C12	0.6(5)	C42	C35	C36	C37	133.0(3)
C10	C11	C12	C13	1.1(5)	C48	C35	C36	C41	73.4(4)
C9	C8	C13	C12	0.2(5)	C32	C35	C36	C41	168.6(3)
C1	C8	C13	C12	177.2(3)	C42	C35	C36	C41	48.2(4)
C11	C12	C13	C8	1.5(5)	C41	C36	C37	C38	1.8(5)
C8	C1	C14	C19	132.7(3)	C35	C36	C37	C38	179.5(3)
C20	C1	C14	C19	12.2(4)	C36	C37	C38	C39	1.6(6)
C2	C1	C14	C19	107.2(3)	C37	C38	C39	C40	0.3(6)
C8	C1	C14	C15	46.8(4)	C38	C39	C40	C41	0.6(6)
C20	C1	C14	C15	167.4(3)	C39	C40	C41	C36	0.4(6)
C2	C1	C14	C15	73.2(3)	C37	C36	C41	C40	0.8(5)
C19	C14	C15	C16	1.2(5)	C35	C36	C41	C40	179.6(3)
C1	C14	C15	C16	179.3(3)	C36	C35	C42	C47	138.8(3)

C14	C15	C16	C17	0.6(5)	C48	C35	C42	C47	18.2(5)
C15	C16	C17	C18	0.2(5)	C32	C35	C42	C47	101.2(4)
C16	C17	C18	C19	0.4(5)	C36	C35	C42	C43	41.5(4)
C17	C18	C19	C14	1.0(5)	C48	C35	C42	C43	162.1(3)
C15	C14	C19	C18	1.3(5)	C32	C35	C42	C43	78.5(4)
C1	C14	C19	C18	179.2(3)	C47	C42	C43	C44	0.0(5)
C14	C1	C20	C21	110.6(4)	C35	C42	C43	C44	179.7(3)
C8	C1	C20	C21	7.8(5)	C42	C43	C44	C45	0.1(5)
C2	C1	C20	C21	127.1(3)	C43	C44	C45	C46	0.2(6)
C14	C1	C20	C25	71.0(4)	C44	C45	C46	C47	0.1(6)
C8	C1	C20	C25	170.7(3)	C43	C42	C47	C46	0.2(5)
C2	C1	C20	C25	51.3(4)	C35	C42	C47	C46	179.5(3)
C25	C20	C21	C22	1.3(5)	C45	C46	C47	C42	0.1(6)
C1	C20	C21	C22	179.8(3)	C36	C35	C48	C49	5.1(4)
C20	C21	C22	C23	0.2(5)	C32	C35	C48	C49	124.6(3)
C21	C22	C23	C24	0.9(5)	C42	C35	C48	C49	114.3(4)
C21	C22	C23	N1	179.5(3)	C36	C35	C48	C53	172.1(3)
C28	N1	C23	C22	132.9(4)	C32	C35	C48	C53	52.6(4)
C26	N1	C23	C22	44.5(5)	C42	C35	C48	C53	68.6(4)
C28	N1	C23	C24	45.7(5)	C53	C48	C49	C50	1.3(5)
C26	N1	C23	C24	136.9(3)	C35	C48	C49	C50	178.5(3)
C22	C23	C24	C25	0.0(5)	C48	C49	C50	C51	1.0(5)
N1	C23	C24	C25	178.6(3)	C49	C50	C51	C52	2.0(6)
C23	C24	C25	C20	1.6(5)	C50	C51	C52	C53	0.8(6)
C21	C20	C25	C24	2.3(5)	C51	C52	C53	C48	1.5(6)
C1	C20	C25	C24	179.2(3)	C49	C48	C53	C52	2.5(5)
C28	N1	C26	C27	1.5(4)	C35	C48	C53	C52	179.8(3)
C23	N1	C26	C27	176.2(3)	C58	N3	C54	C55	0.6(6)
N1	C26	C27	N2	0.9(4)	Pd1	N3	C54	C55	177.4(4)

C28	N2	C27	C26	0.1(4)	N3	C54	C55	C56	0.2(8)
C29	N2	C27	C26	177.1(3)	C54	C55	C56	C57	0.3(8)
C26	N1	C28	N2	1.4(4)	C55	C56	C57	C58	0.6(8)
C23	N1	C28	N2	176.3(3)	C54	N3	C58	C57	0.9(6)
C26	N1	C28	Pd1	179.4(3)	Pd1	N3	C58	C57	177.0(3)
C23	N1	C28	Pd1	2.9(5)	C56	C57	C58	N3	1.0(7)
C27	N2	C28	N1	0.8(4)	C61	O1	C60	O2	3.5(5)
C29	N2	C28	N1	176.3(3)	C61	O1	C60	C59	177.0(3)
C27	N2	C28	Pd1	180.0(2)	C60	O1	C61	C62	79.5(5)

Table S21. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **6.**

Atom	x	y	z	U(eq)
H3	1637	-540	3614	29
H4	-315	-1540	3436	37
H5	-1733	-2178	2077	36
H6	-1186	-1789	913	36
H7	765	-786	1095	27
H9	4983	270	2713	17
H10	6114	-840	3065	18
H11	5259	-2579	3287	20
H12	3279	-3175	3177	25
H13	2167	-2036	2889	20
H15	2616	-1060	1115	20
H16	2850	-527	-114	24
H17	3336	1279	-267	24
H18	3561	2538	837	23
H19	3339	2014	2073	21
H21	4623	660	4043	18

H22	5223	2087	5120	18
H24	2466	2997	3798	17
H25	1845	1533	2739	19
H26	6123	4191	5512	16
H27	6133	5420	6656	18
H30	4561	6654	6579	21
H31	3878	7436	7492	20
H33	2448	4528	8056	22
H34	3121	3748	7153	20
H37	4548	5874	9213	19
H38	5870	6206	10591	25
H39	5656	7217	11661	27
H40	4093	7907	11309	25
H41	2805	7616	9925	21
H43	4321	8472	8865	22
H44	4282	10156	8603	31
H45	2490	10395	7875	36
H46	736	8932	7419	42
H47	777	7232	7689	30
H49	1802	5551	9657	22
H50	-27	4290	9492	30
H51	-1535	3745	8172	36
H52	-1161	4399	6999	39
H53	674	5606	7146	30
H54	-261	3887	5127	37
H55	-2295	3176	4823	57
H56	-3254	1326	4410	61
H57	-2137	238	4329	48
H58	-122	1018	4628	31

H59A	3221	5327	1481	62
H59B	3107	4531	697	62
H59C	3927	4497	1632	62
H61A	-452	2520	152	45
H61B	8	2856	1154	45
H62A	568	1270	380	51
H62B	-508	1008	721	51
H62C	827	1541	1368	51

Table S22. Crystal data and structure refinement for complex **7.**

Identification code	**7**
Empirical formula	$C_{118}\ H_{92}\ Br_6\ Cl_4\ N_6\ Pd_2$
Formula weight	2428.03
Temperature/K	173(2)
Crystal system	Monoclinic
Space group	P 21
a/Å	9.2472(4)
b/Å	31.4274(13) A
c/Å	17.7065(8) A
α/°	90
β/°	97.3590(10)
γ/°	90
Volume/Å^3	5103.4(4)
Z	2
ρ_{calc}g/cm^3	1.580
μ/mm^{-1}	2.859
F(000)	2424
Crystal size/mm^3	0.18 × 0.17 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.33 to 28.32
Index ranges	$-12 \le h \le 12$, $-40 \le k \le 41$, $-23 \le l \le 20$

Reflections collected	38498
Independent reflections	23942 [R(int) = 0.0485]
Data/restraints/parameters	23942 / 397 / 1226
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R1 = 0.0653, wR2 = 0.1580
Final R indexes [all data]	R1 = 0.0915, wR2 = 0.1735
Largest diff. peak/hole / e $Å^{-3}$	2.793 -2.584

Table S23. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **7**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
H2	5095	3046	-144	16
H3	3738	3038	986	20
H5	8389	3031	-68	16
H6	10011	2864	-929	16
H8	8399	1672	-1109	16
H9	6706	1842	-287	16
H12	13440	2135	-1325	18
H13	15093	2663	-1516	20
H14	14277	3330	-2014	20
H15	11784	3419	-2447	18
H16	10135	2889	-2287	15
H18	11835	1912	-327	26
H19	13141	1304	108	31
H20	13238	720	-688	32
H21	11902	716	-1889	29
H22	10611	1314	-2340	18
H24	7492	2184	-2257	17
H25	6356	2183	-3512	23
H26	7658	2040	-4518	26
H27	10167	1900	-4259	19
H28	11354	1942	-3027	18

Table S24. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Complex **7**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
Pd1	8(1)	17(1)	8(1)	4(1)	3(1)	-1(1)
Br1	18(1)	29(1)	37(1)	2(1)	0(1)	1(1)
Br2	35(1)	39(1)	48(1)	7(1)	-1(1)	-10(1)
Br3	67(1)	22(1)	29(1)	7(1)	15(1)	6(1)
N1	8(4)	15(4)	12(4)	3(3)	5(3)	2(3)
N2	12(3)	17(3)	12(3)	0(2)	4(2)	1(2)
N3	22(5)	10(4)	18(5)	-2(4)	2(4)	3(4)
C1	11(3)	17(3)	9(3)	1(2)	6(2)	-2(2)
C2	9(5)	20(5)	12(5)	6(4)	1(4)	4(4)
C3	18(3)	19(3)	14(3)	-1(2)	3(2)	2(2)
C4	15(2)	17(2)	10(2)	1(2)	6(2)	0(2)
C5	15(2)	17(2)	10(2)	0(2)	6(2)	0(2)
C6	15(2)	17(2)	10(2)	1(2)	6(2)	0(2)
C7	15(2)	16(2)	10(2)	0(2)	5(2)	0(2)
C8	16(2)	17(2)	10(2)	1(2)	5(2)	0(2)
C9	15(2)	17(2)	10(2)	1(2)	6(2)	0(2)
C10	9(3)	9(3)	6(3)	1(2)	3(2)	0(2)
C11	12(4)	13(4)	7(4)	-1(3)	6(3)	4(3)
C12	14(5)	25(6)	7(5)	2(4)	0(4)	-1(5)
C13	14(3)	20(3)	14(3)	-2(2)	1(2)	-1(2)
C14	16(6)	18(6)	16(5)	-3(4)	6(4)	-12(5)
C15	21(6)	15(5)	12(5)	-3(4)	12(4)	1(4)
C16	11(4)	19(4)	9(4)	-4(3)	6(3)	1(4)
C17	6(5)	19(6)	15(5)	5(4)	4(4)	2(4)

C18	15(6)	36(7)	15(6)	3(5)	4(5)	-6(5)
C19	34(8)	25(6)	18(6)	4(5)	-1(5)	0(6)
C20	21(6)	26(7)	33(7)	3(5)	10(5)	4(5)
C21	31(7)	11(5)	31(7)	0(5)	8(5)	1(5)
C22	17(6)	18(5)	11(5)	9(4)	7(4)	1(4)
C23	19(6)	10(5)	10(5)	-1(4)	5(4)	-4(4)
C24	14(5)	10(5)	19(5)	-2(4)	5(4)	-1(4)
C25	10(5)	30(6)	16(5)	-1(5)	0(4)	-3(5)
C26	21(6)	27(6)	16(5)	2(5)	-4(5)	-6(5)
C27	14(5)	27(6)	9(4)	2(5)	7(4)	-3(5)
C28	9(5)	24(6)	13(5)	-5(4)	6(4)	-3(4)
C29	6(3)	22(3)	10(2)	-1(2)	4(2)	1(2)
C30	6(2)	22(3)	11(2)	-1(2)	3(2)	1(2)
C31	6(2)	22(2)	10(2)	-1(2)	3(2)	1(2)
C32	6(2)	23(3)	11(2)	-1(2)	3(2)	2(2)
C33	6(3)	23(3)	10(2)	-1(2)	3(2)	1(2)
C34	10(5)	26(6)	6(5)	3(4)	1(4)	1(4)
C35	9(3)	10(3)	8(3)	0(2)	3(2)	-2(2)
C36	7(4)	15(4)	6(4)	-1(3)	2(3)	3(3)
C37	12(5)	27(6)	8(5)	6(4)	6(4)	0(4)
C38	11(4)	22(5)	20(4)	-2(4)	5(4)	1(4)
C39	16(5)	27(6)	6(5)	-6(4)	-1(4)	-2(5)
C40	18(4)	30(5)	7(4)	-1(4)	5(4)	-1(4)
C41	10(5)	23(5)	12(5)	1(4)	6(4)	-4(4)
C42	10(5)	18(5)	15(5)	2(4)	4(4)	-2(4)
C43	23(6)	12(5)	12(5)	-3(4)	3(4)	1(4)
C44	19(6)	21(6)	29(6)	4(5)	-7(5)	2(5)
C45	24(7)	21(6)	48(8)	1(6)	13(6)	5(5)
C46	22(6)	24(6)	34(7)	-12(5)	11(5)	7(5)

C47	28(7)	18(5)	16(5)	-3(4)	6(5)	7(5)
C48	13(2)	21(2)	11(2)	-2(2)	5(2)	-3(2)
C49	13(2)	21(2)	11(2)	-2(2)	5(2)	-3(2)
C50	13(2)	22(2)	11(2)	-2(2)	4(2)	-2(2)
C51	13(2)	22(2)	12(2)	-2(2)	4(2)	-3(2)
C52	13(2)	22(2)	12(2)	-2(2)	4(2)	-3(2)
C53	13(2)	21(2)	12(2)	-2(2)	4(2)	-3(2)
C107	21(6)	11(5)	15(5)	2(4)	5(4)	1(4)
C108	33(7)	25(6)	7(5)	2(4)	5(5)	9(5)
C109	30(7)	25(7)	33(7)	-8(6)	-5(6)	15(6)
C110	18(6)	16(6)	38(7)	-1(5)	12(5)	3(5)
C111	16(6)	18(6)	28(6)	-8(5)	8(5)	3(5)
Pd2	8(1)	18(1)	10(1)	0(1)	2(1)	-4(1)
Br4	30(1)	33(1)	48(1)	-4(1)	-2(1)	6(1)
Br5	19(1)	37(1)	40(1)	4(1)	-1(1)	-3(1)
Br6	61(1)	24(1)	33(1)	-7(1)	10(1)	-3(1)
N4	5(4)	18(4)	7(4)	-4(3)	-1(3)	-6(3)
N5	9(3)	11(3)	7(2)	-1(2)	4(2)	-1(2)
N6	14(5)	31(6)	20(5)	-2(4)	4(4)	-10(4)
C54	12(3)	15(3)	12(3)	1(2)	3(2)	0(2)
C55	19(6)	16(5)	10(5)	-2(4)	6(4)	-4(4)
C56	12(5)	24(6)	11(5)	-4(4)	5(4)	-7(4)
C57	10(2)	14(2)	7(2)	1(2)	3(2)	0(2)
C58	10(2)	14(2)	8(2)	1(2)	3(2)	0(2)
C59	10(2)	14(2)	7(2)	1(2)	4(2)	0(2)
C60	10(2)	13(2)	7(2)	1(2)	3(2)	0(2)
C61	10(2)	14(2)	7(2)	1(2)	3(2)	0(2)
C62	10(2)	14(2)	8(2)	1(2)	3(2)	-1(2)
C63	3(4)	11(4)	6(4)	-1(3)	1(3)	2(3)

C64	8(3)	11(3)	7(3)	1(2)	4(2)	1(2)
C65	13(5)	13(5)	15(5)	1(4)	5(4)	2(4)
C66	17(6)	15(5)	23(6)	3(4)	9(4)	10(4)
C67	10(5)	31(6)	7(5)	-5(4)	3(4)	9(5)
C68	9(4)	20(4)	12(4)	0(4)	1(3)	-3(4)
C69	8(5)	13(5)	8(4)	0(4)	-2(4)	2(4)
C70	9(2)	13(2)	9(2)	1(2)	3(2)	0(2)
C71	10(2)	13(2)	9(2)	2(2)	3(2)	0(2)
C72	10(2)	14(2)	10(2)	2(2)	3(2)	-1(2)
C73	10(2)	14(2)	10(2)	2(2)	3(2)	-1(2)
C74	10(2)	13(2)	10(2)	2(2)	3(2)	-1(2)
C75	9(2)	13(2)	9(2)	1(2)	3(2)	0(2)
C76	7(4)	15(4)	9(4)	-1(3)	4(3)	1(3)
C77	14(6)	21(6)	14(5)	5(4)	1(4)	0(5)
C78	23(5)	16(4)	12(4)	8(4)	8(4)	2(4)
C79	17(6)	11(5)	36(7)	1(5)	8(5)	1(4)
C80	10(5)	21(6)	23(6)	-1(5)	0(4)	-2(5)
C81	10(5)	11(5)	13(5)	1(4)	-3(4)	1(4)
C82	9(4)	20(4)	9(4)	-2(3)	6(3)	-2(4)
C83	16(6)	19(5)	21(6)	8(4)	12(5)	4(5)
C84	22(6)	24(6)	16(5)	3(5)	13(4)	10(5)
C85	8(5)	21(5)	3(4)	0(4)	2(4)	5(4)
C86	13(5)	28(6)	13(5)	1(4)	1(4)	7(5)
C87	19(4)	18(4)	11(4)	3(3)	8(4)	1(4)
C88	12(5)	18(5)	9(5)	5(4)	2(4)	-1(4)
C89	13(6)	30(6)	9(5)	-4(4)	4(4)	-3(5)
C90	31(7)	33(7)	13(6)	-2(5)	4(5)	-8(6)
C91	30(7)	49(9)	19(6)	-12(6)	-2(5)	0(6)
C92	35(8)	35(7)	27(7)	-15(6)	0(6)	-15(6)

C93	33(7)	22(6)	32(7)	-7(5)	8(6)	-1(6)
C94	12(5)	21(5)	15(5)	1(4)	2(4)	-5(4)
C95	12(3)	16(3)	9(3)	2(2)	5(2)	1(2)
C96	13(6)	35(7)	13(5)	8(5)	1(4)	-2(5)
C97	20(3)	26(3)	20(3)	4(2)	5(2)	-1(2)
C98	20(6)	43(8)	17(6)	19(5)	10(5)	13(6)
C99	20(3)	21(3)	18(3)	1(2)	5(2)	1(2)
C100	14(3)	17(3)	14(3)	0(2)	4(2)	-1(2)
C101	7(3)	10(3)	7(3)	2(2)	3(2)	1(2)
C102	18(6)	22(6)	13(5)	5(4)	8(4)	0(5)
C103	14(6)	26(6)	20(6)	8(5)	-3(5)	-4(5)
C104	15(6)	22(6)	15(5)	-4(4)	-2(4)	8(5)
C105	16(5)	23(6)	6(4)	2(4)	5(4)	7(5)
C106	14(5)	16(5)	12(5)	-1(4)	1(4)	-2(4)
C112	26(7)	37(7)	12(6)	3(5)	-4(5)	-6(6)
C113	41(8)	26(7)	15(6)	-4(5)	-1(5)	-5(6)
C114	29(7)	39(8)	24(7)	4(6)	1(6)	-14(6)
C115	30(8)	34(7)	29(7)	3(6)	9(6)	-11(6)
C116	26(7)	23(6)	28(7)	-6(5)	9(5)	-6(5)
Cl1	192(8)	117(5)	130(6)	2(5)	85(6)	-40(6)
Cl2	90(4)	91(4)	124(5)	-32(4)	32(4)	-35(4)
C117	42(11)	82(14)	86(15)	-27(12)	31(10)	-15(10)
Cl3	73(4)	159(6)	92(4)	59(4)	25(3)	23(4)
Cl4	85(4)	142(6)	181(7)	95(6)	65(5)	18(4)
C118	94(19)	110(20)	140(20)	54(19)	55(18)	-11(17)

Table S25. Bond Lengths for Complex **7.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å

Pd1	C1	1.951(11)	Pd2	Br4	2.4201(16)
Pd1	N3	2.108(9)	Br6	C113	1.872(13)
Pd1	Br2	2.4046(16)	N4	C54	1.352(13)
Pd1	Br1	2.4069(15)	N4	C56	1.382(13)
Br3	C108	1.904(12)	N4	C57	1.440(12)
N1	C1	1.346(13)	N5	C54	1.368(13)
N1	C2	1.374(13)	N5	C55	1.372(14)
N1	C4	1.447(13)	N5	C82	1.449(12)
N2	C3	1.377(14)	N6	C112	1.310(16)
N2	C1	1.383(13)	N6	C116	1.354(16)
N2	C29	1.416(13)	C55	C56	1.342(14)
N3	C107	1.362(14)	C55	H55	0.9500
N3	C111	1.366(14)	C56	H56	0.9500
C2	C3	1.365(14)	C57	C58	1.390(14)
C2	H2	0.9500	C57	C62	1.399(14)
C3	H3	0.9500	C58	C59	1.433(13)
C4	C5	1.375(15)	C58	H58	0.9500
C4	C9	1.385(15)	C59	C60	1.364(14)
C5	C6	1.384(14)	C59	H59	0.9500
C5	H5	0.9500	C60	C61	1.380(14)
C6	C7	1.393(15)	C60	C63	1.572(13)
C6	H6	0.9500	C61	C62	1.401(13)
C7	C8	1.382(15)	C61	H61	0.9500
C7	C10	1.559(13)	C62	H62	0.9500
C8	C9	1.386(13)	C63	C70	1.524(13)
C8	H8	0.9500	C63	C76	1.526(15)
C9	H9	0.9500	C63	C64	1.563(13)
C10	C23	1.536(14)	C64	C65	1.377(14)

C10	C11	1.544(14)	C64	C69	1.412(14)
C10	C17	1.564(15)	C65	C66	1.381(15)
C11	C16	1.406(15)	C65	H65	0.9500
C11	C12	1.417(15)	C66	C67	1.342(17)
C12	C13	1.375(15)	C66	H66	0.9500
C12	H12	0.9500	C67	C68	1.424(15)
C13	C14	1.403(16)	C67	H67	0.9500
C13	H13	0.9500	C68	C69	1.366(14)
C14	C15	1.395(16)	C68	H68	0.9500
C14	H14	0.9500	C69	H69	0.9500
C15	C16	1.371(15)	C70	C75	1.395(14)
C15	H15	0.9500	C70	C71	1.399(14)
C16	H16	0.9500	C71	C72	1.391(14)
C17	C22	1.388(16)	C71	H71	0.9500
C17	C18	1.413(16)	C72	C73	1.391(14)
C18	C19	1.388(18)	C72	H72	0.9500
C18	H18	0.9500	C73	C74	1.369(14)
C19	C20	1.378(17)	C73	H73	0.9500
C19	H19	0.9500	C74	C75	1.397(14)
C20	C21	1.370(18)	C74	H74	0.9500
C20	H20	0.9500	C75	H75	0.9500
C21	C22	1.374(16)	C76	C81	1.385(15)
C21	H21	0.9500	C76	C77	1.424(15)
C22	H22	0.9500	C77	C78	1.390(17)
C23	C28	1.403(14)	C77	H77	0.9500
C23	C24	1.405(16)	C78	C79	1.399(17)
C24	C25	1.400(15)	C78	H78	0.9500
C24	H24	0.9500	C79	C80	1.385(16)
C25	C26	1.369(16)	C79	H79	0.9500

C25	H25	0.9500	C80	C81	1.425(15)
C26	C27	1.392(16)	C80	H80	0.9500
C26	H26	0.9500	C81	H81	0.9500
C27	C28	1.385(14)	C82	C87	1.372(15)
C27	H27	0.9500	C82	C83	1.384(15)
C28	H28	0.9500	C83	C84	1.387(14)
C29	C30	1.369(14)	C83	H83	0.9500
C29	C34	1.392(15)	C84	C85	1.434(14)
C30	C31	1.407(14)	C84	H84	0.9500
C30	H30	0.9500	C85	C86	1.384(15)
C31	C32	1.414(15)	C85	C88	1.537(14)
C31	H31	0.9500	C86	C87	1.379(14)
C32	C33	1.385(14)	C86	H86	0.9500
C32	C35	1.537(13)	C87	H87	0.9500
C33	C34	1.391(14)	C88	C95	1.540(15)
C33	H33	0.9500	C88	C101	1.541(14)
C34	H34	0.9500	C88	C89	1.563(16)
C35	C48	1.548(14)	C89	C94	1.393(16)
C35	C36	1.548(13)	C89	C90	1.416(16)
C35	C42	1.572(15)	C90	C91	1.341(19)
C36	C41	1.396(13)	C90	H90	0.9500
C36	C37	1.402(15)	C91	C92	1.41(2)
C37	C38	1.364(15)	C91	H91	0.9500
C37	H37	0.9500	C92	C93	1.375(18)
C38	C39	1.390(15)	C92	H92	0.9500
C38	H38	0.9500	C93	C94	1.371(16)
C39	C40	1.389(16)	C93	H93	0.9500
C39	H39	0.9500	C94	H94	0.9500
C40	C41	1.382(15)	C95	C96	1.396(15)

C40	H40	0.9500	C95	C100	1.401(15)
C41	H41	0.9500	C96	C97	1.396(17)
C42	C47	1.373(15)	C96	H96	0.9500
C42	C43	1.378(15)	C97	C98	1.370(19)
C43	C44	1.400(16)	C97	H97	0.9500
C43	H43	0.9500	C98	C99	1.401(18)
C44	C45	1.361(18)	C98	H98	0.9500
C44	H44	0.9500	C99	C100	1.374(16)
C45	C46	1.413(19)	C99	H99	0.9500
C45	H45	0.9500	C100	H100	0.9500
C46	C47	1.383(16)	C101	C102	1.374(15)
C46	H46	0.9500	C101	C106	1.400(13)
C47	H47	0.9500	C102	C103	1.404(15)
C48	C53	1.382(16)	C102	H102	0.9500
C48	C49	1.386(16)	C103	C104	1.367(16)
C49	C50	1.402(15)	C103	H103	0.9500
C49	H49	0.9500	C104	C105	1.402(16)
C50	C51	1.341(15)	C104	H104	0.9500
C50	H50	0.9500	C105	C106	1.390(14)
C51	C52	1.406(16)	C105	H105	0.9500
C51	H51	0.9500	C106	H106	0.9500
C52	C53	1.411(15)	C112	C113	1.410(18)
C52	H52	0.9500	C112	H112	0.9500
C53	H53	0.9500	C114	H114	0.9500
C107	C108	1.358(16)	C115	C116	1.374(18)
C107	H107	0.9500	C115	H115	0.9500
C108	C109	1.384(18)	C116	H116	0.9500
C109	C110	1.386(18)	Cl1	C117	1.78(2)
C109	H109	0.9500	Cl2	C117	1.76(2)

C110	C111	1.367(17)	C117	H11'	0.9900
C110	H110	0.9500	C117	H11"	0.9900
C111	H111	0.9500	Cl3	C118	1.73(3)
Pd2	C54	1.934(11)	Cl4	C118	1.71(3)
Pd2	N6	2.100(10)	C118	H18"	0.9900
Pd2	Br5	2.4101(16)	C118	H18'	0.9900

Table S26. Bond Angles for Complex **7**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Pd1	N3	176.3(4)	C54	N4	C56	111.7(8)
C1	Pd1	Br2	87.3(3)	C54	N4	C57	124.7(9)
N3	Pd1	Br2	94.2(3)	C56	N4	C57	123.6(8)
C1	Pd1	Br1	86.1(3)	C54	N5	C55	110.9(8)
N3	Pd1	Br1	92.8(3)	C54	N5	C82	122.1(9)
Br2	Pd1	Br1	171.27(6)	C55	N5	C82	126.9(8)
C1	N1	C2	110.5(8)	C112	N6	C116	120.1(11)
C1	N1	C4	124.1(9)	C112	N6	Pd2	119.7(8)
C2	N1	C4	125.3(9)	C116	N6	Pd2	120.3(8)
C3	N2	C1	109.8(9)	N4	C54	N5	103.7(9)
C3	N2	C29	126.8(9)	N4	C54	Pd2	130.6(8)
C1	N2	C29	123.3(9)	N5	C54	Pd2	125.7(7)
C107	N3	C111	116.8(10)	C56	C55	N5	107.4(9)
C107	N3	Pd1	122.5(8)	C56	C55	H55	126.3
C111	N3	Pd1	120.7(8)	N5	C55	H55	126.3
N1	C1	N2	105.5(9)	C55	C56	N4	106.2(9)
N1	C1	Pd1	126.1(7)	C55	C56	H56	126.9
N2	C1	Pd1	128.3(7)	N4	C56	H56	126.9
C3	C2	N1	107.5(9)	C58	C57	C62	121.8(9)

C3	C2	H2	126.2	C58	C57	N4	118.1(9)
N1	C2	H2	126.2	C62	C57	N4	120.1(9)
C2	C3	N2	106.6(10)	C57	C58	C59	117.8(9)
C2	C3	H3	126.7	C57	C58	H58	121.1
N2	C3	H3	126.7	C59	C58	H58	121.1
C5	C4	C9	121.0(9)	C60	C59	C58	120.8(9)
C5	C4	N1	119.0(9)	C60	C59	H59	119.6
C9	C4	N1	120.0(9)	C58	C59	H59	119.6
C4	C5	C6	119.7(10)	C59	C60	C61	120.0(9)
C4	C5	H5	120.1	C59	C60	C63	123.2(9)
C6	C5	H5	120.1	C61	C60	C63	116.6(9)
C5	C6	C7	120.7(10)	C60	C61	C62	121.7(10)
C5	C6	H6	119.6	C60	C61	H61	119.2
C7	C6	H6	119.6	C62	C61	H61	119.2
C8	C7	C6	118.1(9)	C57	C62	C61	117.9(9)
C8	C7	C10	118.0(9)	C57	C62	H62	121.0
C6	C7	C10	123.9(9)	C61	C62	H62	121.0
C7	C8	C9	122.1(10)	C70	C63	C76	112.6(8)
C7	C8	H8	118.9	C70	C63	C64	106.3(8)
C9	C8	H8	118.9	C76	C63	C64	111.7(8)
C4	C9	C8	118.3(10)	C70	C63	C60	111.5(8)
C4	C9	H9	120.8	C76	C63	C60	106.0(7)
C8	C9	H9	120.8	C64	C63	C60	108.9(8)
C23	C10	C11	105.6(8)	C65	C64	C69	116.8(9)
C23	C10	C7	111.0(9)	C65	C64	C63	124.7(9)
C11	C10	C7	111.5(8)	C69	C64	C63	118.5(8)
C23	C10	C17	111.3(8)	C64	C65	C66	121.9(10)
C11	C10	C17	110.5(8)	C64	C65	H65	119.1
C7	C10	C17	106.9(8)	C66	C65	H65	119.1

C16	C11	C12	116.9(10)	C67	C66	C65	121.6(10)
C16	C11	C10	118.4(9)	C67	C66	H66	119.2
C12	C11	C10	124.7(9)	C65	C66	H66	119.2
C13	C12	C11	121.3(10)	C66	C67	C68	118.4(10)
C13	C12	H12	119.4	C66	C67	H67	120.8
C11	C12	H12	119.4	C68	C67	H67	120.8
C12	C13	C14	120.7(10)	C69	C68	C67	120.0(10)
C12	C13	H13	119.6	C69	C68	H68	120.0
C14	C13	H13	119.6	C67	C68	H68	120.0
C15	C14	C13	118.3(10)	C68	C69	C64	121.3(9)
C15	C14	H14	120.8	C68	C69	H69	119.3
C13	C14	H14	120.8	C64	C69	H69	119.3
C16	C15	C14	120.9(11)	C75	C70	C71	116.4(9)
C16	C15	H15	119.5	C75	C70	C63	123.9(9)
C14	C15	H15	119.5	C71	C70	C63	119.7(9)
C15	C16	C11	121.8(10)	C72	C71	C70	122.5(10)
C15	C16	H16	119.1	C72	C71	H71	118.7
C11	C16	H16	119.1	C70	C71	H71	118.7
C22	C17	C18	118.3(10)	C71	C72	C73	119.5(9)
C22	C17	C10	124.0(10)	C71	C72	H72	120.2
C18	C17	C10	117.6(10)	C73	C72	H72	120.2
C19	C18	C17	119.5(12)	C74	C73	C72	119.0(9)
C19	C18	H18	120.3	C74	C73	H73	120.5
C17	C18	H18	120.3	C72	C73	H73	120.5
C20	C19	C18	120.4(12)	C73	C74	C75	121.2(10)
C20	C19	H19	119.8	C73	C74	H74	119.4
C18	C19	H19	119.8	C75	C74	H74	119.4
C21	C20	C19	120.3(12)	C70	C75	C74	121.2(9)
C21	C20	H20	119.9	C70	C75	H75	119.4

C19	C20	H20	119.9	C74	C75	H75	119.4
C20	C21	C22	120.2(11)	C81	C76	C77	118.0(10)
C20	C21	H21	119.9	C81	C76	C63	122.2(9)
C22	C21	H21	119.9	C77	C76	C63	119.7(9)
C21	C22	C17	121.2(11)	C78	C77	C76	120.3(10)
C21	C22	H22	119.4	C78	C77	H77	119.8
C17	C22	H22	119.4	C76	C77	H77	119.8
C28	C23	C24	116.8(10)	C77	C78	C79	121.7(10)
C28	C23	C10	119.5(10)	C77	C78	H78	119.2
C24	C23	C10	123.4(9)	C79	C78	H78	119.2
C25	C24	C23	120.8(10)	C80	C79	C78	118.3(11)
C25	C24	H24	119.6	C80	C79	H79	120.9
C23	C24	H24	119.6	C78	C79	H79	120.9
C26	C25	C24	121.6(11)	C79	C80	C81	120.7(11)
C26	C25	H25	119.2	C79	C80	H80	119.6
C24	C25	H25	119.2	C81	C80	H80	119.6
C25	C26	C27	118.3(10)	C76	C81	C80	120.9(10)
C25	C26	H26	120.8	C76	C81	H81	119.5
C27	C26	H26	120.8	C80	C81	H81	119.5
C28	C27	C26	121.0(9)	C87	C82	C83	120.5(9)
C28	C27	H27	119.5	C87	C82	N5	121.0(9)
C26	C27	H27	119.5	C83	C82	N5	118.5(9)
C27	C28	C23	121.5(10)	C82	C83	C84	120.4(10)
C27	C28	H28	119.2	C82	C83	H83	119.8
C23	C28	H28	119.2	C84	C83	H83	119.8
C30	C29	C34	121.3(9)	C83	C84	C85	119.9(10)
C30	C29	N2	118.1(9)	C83	C84	H84	120.0
C34	C29	N2	120.6(9)	C85	C84	H84	120.0
C29	C30	C31	119.7(10)	C86	C85	C84	117.0(9)

C29	C30	H30	120.2	C86	C85	C88	126.4(9)
C31	C30	H30	120.2	C84	C85	C88	116.6(9)
C30	C31	C32	120.7(9)	C87	C86	C85	122.6(10)
C30	C31	H31	119.7	C87	C86	H86	118.7
C32	C31	H31	119.7	C85	C86	H86	118.7
C33	C32	C31	116.9(9)	C82	C87	C86	119.6(10)
C33	C32	C35	119.9(9)	C82	C87	H87	120.2
C31	C32	C35	123.0(9)	C86	C87	H87	120.2
C32	C33	C34	123.3(10)	C85	C88	C95	112.2(8)
C32	C33	H33	118.3	C85	C88	C101	111.0(9)
C34	C33	H33	118.3	C95	C88	C101	104.5(8)
C29	C34	C33	118.0(10)	C85	C88	C89	104.4(8)
C29	C34	H34	121.0	C95	C88	C89	112.8(9)
C33	C34	H34	121.0	C101	C88	C89	112.3(8)
C32	C35	C48	112.3(8)	C94	C89	C90	115.9(11)
C32	C35	C36	110.8(8)	C94	C89	C88	124.1(10)
C48	C35	C36	106.3(8)	C90	C89	C88	119.7(10)
C32	C35	C42	104.7(8)	C91	C90	C89	124.0(13)
C48	C35	C42	110.6(8)	C91	C90	H90	118.0
C36	C35	C42	112.2(8)	C89	C90	H90	118.0
C41	C36	C37	116.7(9)	C90	C91	C92	118.8(12)
C41	C36	C35	119.3(9)	C90	C91	H91	120.6
C37	C36	C35	123.9(8)	C92	C91	H91	120.6
C38	C37	C36	122.2(10)	C93	C92	C91	118.2(12)
C38	C37	H37	118.9	C93	C92	H92	120.9
C36	C37	H37	118.9	C91	C92	H92	120.9
C37	C38	C39	120.3(11)	C94	C93	C92	122.6(12)
C37	C38	H38	119.9	C94	C93	H93	118.7
C39	C38	H38	119.9	C92	C93	H93	118.7

C40	C39	C38	119.0(10)	C93	C94	C89	120.2(11)
C40	C39	H39	120.5	C93	C94	H94	119.9
C38	C39	H39	120.5	C89	C94	H94	119.9
C41	C40	C39	120.2(9)	C96	C95	C100	117.1(10)
C41	C40	H40	119.9	C96	C95	C88	124.1(10)
C39	C40	H40	119.9	C100	C95	C88	118.7(10)
C40	C41	C36	121.6(10)	C95	C96	C97	120.6(12)
C40	C41	H41	119.2	C95	C96	H96	119.7
C36	C41	H41	119.2	C97	C96	H96	119.7
C47	C42	C43	118.9(10)	C98	C97	C96	121.0(12)
C47	C42	C35	118.4(10)	C98	C97	H97	119.5
C43	C42	C35	122.7(9)	C96	C97	H97	119.5
C42	C43	C44	119.9(10)	C97	C98	C99	119.4(12)
C42	C43	H43	120.0	C97	C98	H98	120.3
C44	C43	H43	120.0	C99	C98	H98	120.3
C45	C44	C43	121.4(11)	C100	C99	C98	119.3(12)
C45	C44	H44	119.3	C100	C99	H99	120.4
C43	C44	H44	119.3	C98	C99	H99	120.4
C44	C45	C46	118.6(11)	C99	C100	C95	122.5(11)
C44	C45	H45	120.7	C99	C100	H100	118.7
C46	C45	H45	120.7	C95	C100	H100	118.7
C47	C46	C45	119.3(11)	C102	C101	C106	117.9(9)
C47	C46	H46	120.3	C102	C101	C88	122.8(9)
C45	C46	H46	120.3	C106	C101	C88	119.0(9)
C42	C47	C46	121.7(11)	C101	C102	C103	121.3(10)
C42	C47	H47	119.1	C101	C102	H102	119.4
C46	C47	H47	119.1	C103	C102	H102	119.4
C53	C48	C49	118.1(10)	C104	C103	C102	120.9(11)
C53	C48	C35	122.6(10)	C104	C103	H103	119.5

C49	C48	C35	119.3(9)	C102	C103	H103	119.5
C48	C49	C50	121.3(10)	C103	C104	C105	118.5(10)
C48	C49	H49	119.4	C103	C104	H104	120.7
C50	C49	H49	119.4	C105	C104	H104	120.7
C51	C50	C49	120.7(11)	C106	C105	C104	120.3(10)
C51	C50	H50	119.6	C106	C105	H105	119.8
C49	C50	H50	119.6	C104	C105	H105	119.8
C50	C51	C52	119.7(10)	C105	C106	C101	121.0(10)
C50	C51	H51	120.2	C105	C106	H106	119.5
C52	C51	H51	120.2	C101	C106	H106	119.5
C51	C52	C53	119.5(10)	N6	C112	C113	120.8(12)
C51	C52	H52	120.3	N6	C112	H112	119.6
C53	C52	H52	120.3	C113	C112	H112	119.6
C48	C53	C52	120.6(11)	C114	C113	C112	119.9(12)
C48	C53	H53	119.7	C114	C113	Br6	122.7(10)
C52	C53	H53	119.7	C112	C113	Br6	117.4(10)
C108	C107	N3	121.7(10)	C115	C114	C113	117.6(13)
C108	C107	H107	119.2	C115	C114	H114	121.2
N3	C107	H107	119.2	C113	C114	H114	121.2
C107	C108	C109	121.6(11)	C114	C115	C116	120.9(13)
C107	C108	Br3	118.6(9)	C114	C115	H115	119.6
C109	C108	Br3	119.8(9)	C116	C115	H115	119.6
C108	C109	C110	117.2(12)	N6	C116	C115	120.7(12)
C108	C109	H109	121.4	N6	C116	H116	119.6
C110	C109	H109	121.4	C115	C116	H116	119.6
C111	C110	C109	119.4(11)	Cl2	C117	Cl1	109.3(11)
C111	C110	H110	120.3	Cl2	C117	H11'	109.8
C109	C110	H110	120.3	Cl1	C117	H11'	109.8
C110	C111	N3	123.3(11)	Cl2	C117	H11"	109.8

C110	C111	H111	118.4	Cl1	C117	H11"	109.8
N3	C111	H111	118.4	H11'	C117	H11"	108.3
C54	Pd2	N6	178.0(4)	Cl4	C118	Cl3	116.3(12)
C54	Pd2	Br5	87.9(3)	Cl4	C118	H18"	108.2
N6	Pd2	Br5	91.6(3)	Cl3	C118	H18"	108.2
C54	Pd2	Br4	87.7(3)	Cl4	C118	H18'	108.2
N6	Pd2	Br4	92.9(3)	Cl3	C118	H18'	108.2
Br5	Pd2	Br4	175.30(6)	H18"	C118	H18'	107.4

Table S27. Torsion Angles for Complex **7.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	N1	C1	N2	0.5(12)	C57	N4	C54	N5	-178.8(9
C4	N1	C1	N2	-178.0(9)	C56	N4	C54	Pd2	-179.5(8
C2	N1	C1	Pd1	179.3(8)	C57	N4	C54	Pd2	3.6(16)
C4	N1	C1	Pd1	0.8(15)	C55	N5	C54	N4	2.0(11)
C3	N2	C1	N1	0.0(12)	C82	N5	C54	N4	-178.8(9
C29	N2	C1	N1	177.5(9)	C55	N5	C54	Pd2	179.8(8)
C3	N2	C1	Pd1	-178.8(8)	C82	N5	C54	Pd2	-1.1(14)
C29	N2	C1	Pd1	-1.3(15)	C54	N5	C55	C56	-1.5(12)
C1	N1	C2	C3	-0.9(13)	C82	N5	C55	C56	179.4(10
C4	N1	C2	C3	177.6(10)	N5	C55	C56	N4	0.3(12)
N1	C2	C3	N2	0.8(12)	C54	N4	C56	C55	1.0(13)
C1	N2	C3	C2	-0.5(12)	C57	N4	C56	C55	178.0(9)
C29	N2	C3	C2	-177.9(10)	C54	N4	C57	C58	132.6(11
C1	N1	C4	C5	-115.7(12)	C56	N4	C57	C58	-44.0(14
C2	N1	C4	C5	66.1(15)	C54	N4	C57	C62	-46.1(15
C1	N1	C4	C9	60.9(15)	C56	N4	C57	C62	137.3(11
C2	N1	C4	C9	-117.3(12)	C62	C57	C58	C59	0.3(15)
C9	C4	C5	C6	2.8(17)	N4	C57	C58	C59	-178.5(9

N1	C4	C5	C6	179.4(10)	C57	C58	C59	C60	-0.1(15)
C4	C5	C6	C7	-2.3(17)	C58	C59	C60	C61	0.4(15)
C5	C6	C7	C8	0.5(17)	C58	C59	C60	C63	176.3(9)
C5	C6	C7	C10	178.3(10)	C59	C60	C61	C62	-0.8(16)
C6	C7	C8	C9	0.9(16)	C63	C60	C61	C62	-177.0(9
C10	C7	C8	C9	-177.0(10)	C58	C57	C62	C61	-0.6(15)
C5	C4	C9	C8	-1.5(16)	N4	C57	C62	C61	178.1(9)
N1	C4	C9	C8	-178.0(9)	C60	C61	C62	C57	0.9(15)
C7	C8	C9	C4	-0.4(16)	C59	C60	C63	C70	111.7(11
C8	C7	C10	C23	70.8(12)	C61	C60	C63	C70	-72.3(11
C6	C7	C10	C23	-107.0(12)	C59	C60	C63	C76	-125.5(1
C8	C7	C10	C11	-171.8(9)	C61	C60	C63	C76	50.5(11)
C6	C7	C10	C11	10.4(15)	C59	C60	C63	C64	-5.2(13)
C8	C7	C10	C17	-50.9(12)	C61	C60	C63	C64	170.8(9)
C6	C7	C10	C17	131.4(11)	C70	C63	C64	C65	126.9(10
C23	C10	C11	C16	51.6(11)	C76	C63	C64	C65	3.7(13)
C7	C10	C11	C16	-69.1(11)	C60	C63	C64	C65	-112.9(1
C17	C10	C11	C16	172.1(8)	C70	C63	C64	C69	-49.5(11
C23	C10	C11	C12	-125.2(10)	C76	C63	C64	C69	-172.7(8
C7	C10	C11	C12	114.1(11)	C60	C63	C64	C69	70.7(10)
C17	C10	C11	C12	-4.7(13)	C69	C64	C65	C66	-1.5(15)
C16	C11	C12	C13	1.3(15)	C63	C64	C65	C66	-178.0(9
C10	C11	C12	C13	178.2(9)	C64	C65	C66	C67	-1.4(17)
C11	C12	C13	C14	1.7(16)	C65	C66	C67	C68	2.6(16)
C12	C13	C14	C15	-3.8(16)	C66	C67	C68	C69	-0.9(16)
C13	C14	C15	C16	3.0(16)	C67	C68	C69	C64	-2.1(15)
C14	C15	C16	C11	0.0(15)	C65	C64	C69	C68	3.2(14)
C12	C11	C16	C15	-2.2(14)	C63	C64	C69	C68	179.9(9)
C10	C11	C16	C15	-179.3(9)	C76	C63	C70	C75	-109.1(1

C23	C10	C17	C22	6.4(14)	C64	C63	C70	C75	128.3(10
C11	C10	C17	C22	-110.6(11)	C60	C63	C70	C75	9.8(14)
C7	C10	C17	C22	127.9(11)	C76	C63	C70	C71	70.9(12)
C23	C10	C17	C18	-175.9(9)	C64	C63	C70	C71	-51.6(12
C11	C10	C17	C18	67.1(11)	C60	C63	C70	C71	-170.1(9
C7	C10	C17	C18	-54.5(12)	C75	C70	C71	C72	0.5(16)
C22	C17	C18	C19	3.5(16)	C63	C70	C71	C72	-179.5(9
C10	C17	C18	C19	-174.3(10)	C70	C71	C72	C73	-1.5(16)
C17	C18	C19	C20	-0.6(18)	C71	C72	C73	C74	1.7(16)
C18	C19	C20	C21	-2.6(19)	C72	C73	C74	C75	-1.0(16)
C19	C20	C21	C22	2.8(18)	C71	C70	C75	C74	0.2(16)
C20	C21	C22	C17	0.2(17)	C63	C70	C75	C74	-179.7(1
C18	C17	C22	C21	-3.4(16)	C73	C74	C75	C70	0.0(16)
C10	C17	C22	C21	174.3(10)	C70	C63	C76	C81	-9.1(13)
C11	C10	C23	C28	52.6(12)	C64	C63	C76	C81	110.3(11
C7	C10	C23	C28	173.6(9)	C60	C63	C76	C81	-131.3(1
C17	C10	C23	C28	-67.4(12)	C70	C63	C76	C77	167.4(9)
C11	C10	C23	C24	-121.1(10)	C64	C63	C76	C77	-73.1(11
C7	C10	C23	C24	-0.1(14)	C60	C63	C76	C77	45.3(12)
C17	C10	C23	C24	118.9(11)	C81	C76	C77	C78	-0.6(16)
C28	C23	C24	C25	-0.7(15)	C63	C76	C77	C78	-177.3(1
C10	C23	C24	C25	173.2(10)	C76	C77	C78	C79	2.0(17)
C23	C24	C25	C26	1.6(17)	C77	C78	C79	C80	-1.4(17)
C24	C25	C26	C27	-0.3(18)	C78	C79	C80	C81	-0.7(17)
C25	C26	C27	C28	-1.8(18)	C77	C76	C81	C80	-1.4(15)
C26	C27	C28	C23	2.8(18)	C63	C76	C81	C80	175.2(9)
C24	C23	C28	C27	-1.4(16)	C79	C80	C81	C76	2.1(16)
C10	C23	C28	C27	-175.6(10)	C54	N5	C82	C87	115.6(12
C3	N2	C29	C30	41.6(16)	C55	N5	C82	C87	-65.4(15

C1	N2	C29	C30	-135.4(11)	C54	N5	C82	C83	-64.8(14
C3	N2	C29	C34	-136.0(12)	C55	N5	C82	C83	114.1(12
C1	N2	C29	C34	47.0(15)	C87	C82	C83	C84	-1.9(18)
C34	C29	C30	C31	-4.3(17)	N5	C82	C83	C84	178.5(10
N2	C29	C30	C31	178.1(10)	C82	C83	C84	C85	1.1(18)
C29	C30	C31	C32	1.0(16)	C83	C84	C85	C86	0.3(17)
C30	C31	C32	C33	1.1(16)	C83	C84	C85	C88	179.1(11
C30	C31	C32	C35	-173.7(10)	C84	C85	C86	C87	-0.9(17)
C31	C32	C33	C34	0.1(17)	C88	C85	C86	C87	-179.6(1
C35	C32	C33	C34	175.0(10)	C83	C82	C87	C86	1.4(17)
C30	C29	C34	C33	5.4(17)	N5	C82	C87	C86	-179.1(1
N2	C29	C34	C33	-177.1(10)	C85	C86	C87	C82	0.1(18)
C32	C33	C34	C29	-3.2(17)	C86	C85	C88	C95	-7.5(15)
C33	C32	C35	C48	-171.7(10)	C84	C85	C88	C95	173.8(9)
C31	C32	C35	C48	2.9(14)	C86	C85	C88	C101	108.9(12
C33	C32	C35	C36	69.6(12)	C84	C85	C88	C101	-69.8(12
C31	C32	C35	C36	-115.8(11)	C86	C85	C88	C89	-129.9(1
C33	C32	C35	C42	-51.6(12)	C84	C85	C88	C89	51.4(12)
C31	C32	C35	C42	123.0(11)	C85	C88	C89	C94	-115.7(1
C32	C35	C36	C41	170.9(9)	C95	C88	C89	C94	122.3(11
C48	C35	C36	C41	48.6(12)	C101	C88	C89	C94	4.5(14)
C42	C35	C36	C41	-72.5(11)	C85	C88	C89	C90	57.5(13)
C32	C35	C36	C37	-5.4(14)	C95	C88	C89	C90	-64.5(13
C48	C35	C36	C37	-127.7(10)	C101	C88	C89	C90	177.8(10
C42	C35	C36	C37	111.2(11)	C94	C89	C90	C91	-3.9(19)
C41	C36	C37	C38	1.6(16)	C88	C89	C90	C91	-177.7(1
C35	C36	C37	C38	177.9(10)	C89	C90	C91	C92	5(2)
C36	C37	C38	C39	-1.7(17)	C90	C91	C92	C93	-3(2)
C37	C38	C39	C40	0.4(17)	C91	C92	C93	C94	-1(2)

C38	C39	C40	C41	1.1(17)	C92	C93	C94	C89	2.2(19)
C39	C40	C41	C36	-1.2(17)	C90	C89	C94	C93	0.1(16)
C37	C36	C41	C40	-0.1(16)	C88	C89	C94	C93	173.6(11
C35	C36	C41	C40	-176.6(10)	C85	C88	C95	C96	-117.6(1
C32	C35	C42	C47	-45.2(12)	C101	C88	C95	C96	122.1(10
C48	C35	C42	C47	76.1(11)	C89	C88	C95	C96	-0.1(14)
C36	C35	C42	C47	-165.4(9)	C85	C88	C95	C100	66.7(12)
C32	C35	C42	C43	135.6(10)	C101	C88	C95	C100	-53.6(11
C48	C35	C42	C43	-103.1(11)	C89	C88	C95	C100	-175.8(9
C36	C35	C42	C43	15.4(13)	C100	C95	C96	C97	-2.9(15)
C47	C42	C43	C44	0.0(16)	C88	C95	C96	C97	-178.6(1
C35	C42	C43	C44	179.2(10)	C95	C96	C97	C98	2.2(17)
C42	C43	C44	C45	2.2(18)	C96	C97	C98	C99	-1.0(17)
C43	C44	C45	C46	-2.1(19)	C97	C98	C99	C100	0.7(17)
C44	C45	C46	C47	-0.2(19)	C98	C99	C100	C95	-1.5(17)
C43	C42	C47	C46	-2.3(17)	C96	C95	C100	C99	2.5(16)
C35	C42	C47	C46	178.5(10)	C88	C95	C100	C99	178.5(10
C45	C46	C47	C42	2.4(18)	C85	C88	C101	C102	-5.3(14)
C32	C35	C48	C53	116.9(11)	C95	C88	C101	C102	115.8(11
C36	C35	C48	C53	-121.8(10)	C89	C88	C101	C102	-121.6(1
C42	C35	C48	C53	0.3(13)	C85	C88	C101	C106	-178.3(9
C32	C35	C48	C49	-66.2(12)	C95	C88	C101	C106	-57.2(12
C36	C35	C48	C49	55.1(11)	C89	C88	C101	C106	65.3(12)
C42	C35	C48	C49	177.2(9)	C106	C101	C102	C103	0.8(16)
C53	C48	C49	C50	-3.4(15)	C88	C101	C102	C103	-172.3(1
C35	C48	C49	C50	179.6(9)	C101	C102	C103	C104	1.1(18)
C48	C49	C50	C51	2.2(16)	C102	C103	C104	C105	-2.0(18)
C49	C50	C51	C52	1.5(16)	C103	C104	C105	C106	1.0(17)
C50	C51	C52	C53	-3.8(16)	C104	C105	C106	C101	1.0(17)

C49	C48	C53	C52	1.0(15)	C102	C101	C106	C105	-1.9(16)
C35	C48	C53	C52	178.0(9)	C88	C101	C106	C105	171.5(10
C51	C52	C53	C48	2.5(15)	C116	N6	C112	C113	0.6(18)
C111	N3	C107	C108	-0.6(16)	Pd2	N6	C112	C113	-178.9(9
Pd1	N3	C107	C108	177.7(8)	N6	C112	C113	C114	-0.1(19)
N3	C107	C108	C109	0.5(18)	N6	C112	C113	Br6	-178.4(9
N3	C107	C108	Br3	-179.0(8)	C112	C113	C114	C115	-1.3(19)
C107	C108	C109	C110	-1.3(18)	Br6	C113	C114	C115	177.0(10
Br3	C108	C109	C110	178.2(9)	C113	C114	C115	C116	2(2)
C108	C109	C110	C111	2.3(18)	C112	N6	C116	C115	0.2(19)
C109	C110	C111	N3	-2.6(19)	Pd2	N6	C116	C115	179.8(9)

Table S28. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for Complex **7.**

Atom	*x*	*y*	*z*	U(eq)
H2	5095	3046	-144	16
H3	3738	3038	986	20
H5	8389	3031	-68	16
H6	10011	2864	-929	16
H8	8399	1672	-1109	16
H9	6706	1842	-287	16
H12	13440	2135	-1325	18
H13	15093	2663	-1516	20
H14	14277	3330	-2014	20
H15	11784	3419	-2447	18
H16	10135	2889	-2287	15
H18	11835	1912	-327	26
H19	13141	1304	108	31