Synthesis of New Mixed Phosphine~Iminophosphorane Bidentate Ligands and their Coordination to Group 10 Metal Centers

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Crystallographic data for **5a, 5c, 5e, 5'e, 6c, 6e and 7a**

Figure S1: Molecular structure of **5a**

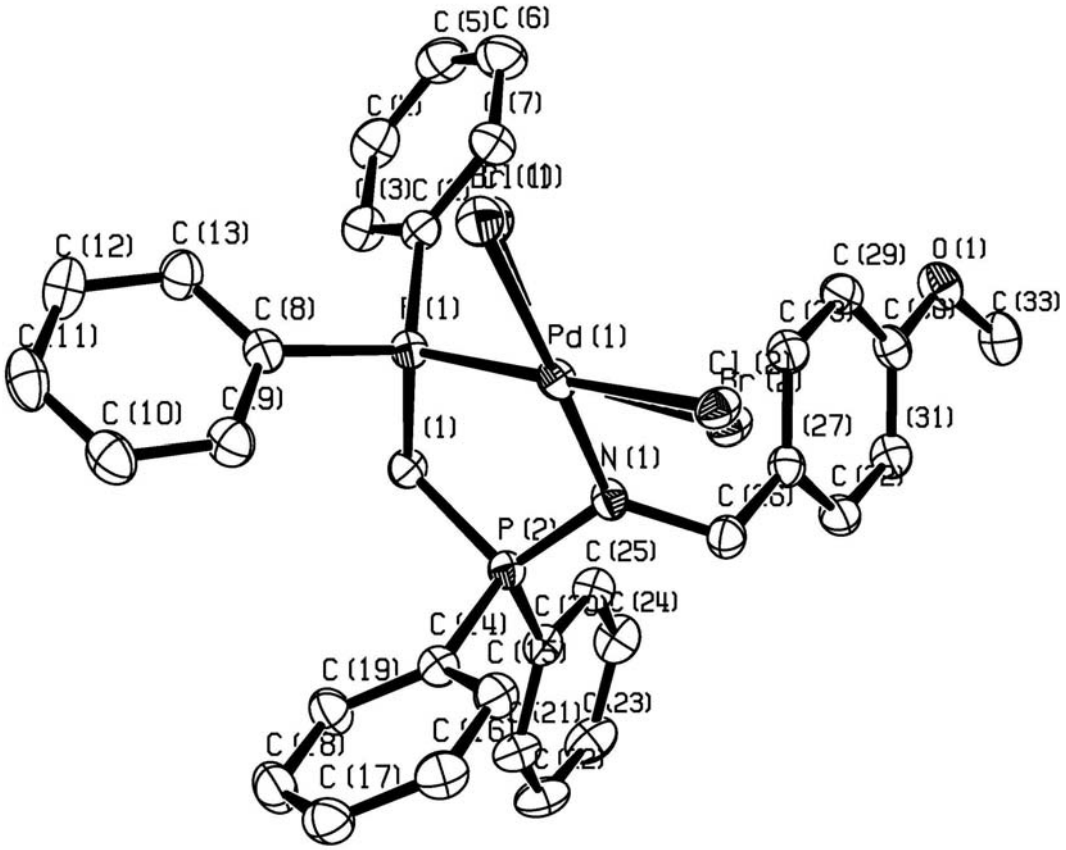

Table S1-1. Crystal data for **5a**

Compound	pdmeobenziminop
Molecular formula	$C_{33}H_{31}BrClNOP_2Pd,C_4H_8O$
Molecular weight	813.39
Crystal habit	orange block
Crystal dimensions(mm)	0.18x0.18x0.18
Crystal system	triclinic
Space group	Pbar1
a(Å)	9.5450(10)
b(Å)	10.5560(10)
c(Å)	18.1810(10)
α(°)	93.1420(10)
β(°)	102.6860(10)
γ(°)	106.8090(10)
V(Å^3)	1697.0(3)
Z	2
d(g-cm^{-3})	1.592
F(000)	824
μ(cm^{-1})	1.932
Absorption corrections	multi-scan ; 0.7224 min, 0.7224 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-8 13 ; -14 13 ; -25 22
Reflections measured	13220
Unique data	9834
Rint	0.0150
Reflections used	8631
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	414
Reflections / parameter	20
wR2	0.0863
R1	0.0312
Weights a, b	0.0395 ; 1.5250
GoF	1.021
difference peak / hole (e Å^{-3})	1.436(0.079) / -0.955(0.079)

Table S1-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a**

atom	x	y	z	U(eq)
Pd(1)	-2263(1)	1176(1)	2732(1)	21(1)
Br(1)	-2970(5)	-1011(2)	2015(2)	27(1)
Br(2)	-3759(3)	300(2)	3654(1)	23(1)
Cl(2)	-3794(8)	118(5)	3553(3)	23(1)
Cl(1)	-3050(10)	-868(6)	2001(6)	27(1)
P(1)	-814(1)	1963(1)	1954(1)	20(1)
P(2)	157(1)	3857(1)	3350(1)	20(1)
O(1)	-6701(2)	5822(2)	1992(1)	33(1)
N(1)	-1604(2)	3121(2)	3263(1)	22(1)
C(1)	430(2)	3645(2)	2405(1)	22(1)
C(2)	-1784(2)	2230(2)	1029(1)	23(1)
C(3)	-1014(3)	3121(2)	604(1)	29(1)
C(4)	-1776(3)	3334(3)	-97(1)	36(1)
C(5)	-3304(3)	2672(3)	-373(1)	37(1)
C(6)	-4077(3)	1798(3)	45(1)	37(1)
C(7)	-3318(3)	1575(2)	753(1)	29(1)
C(8)	528(2)	1113(2)	1805(1)	23(1)
C(9)	1395(3)	782(2)	2447(1)	30(1)
C(10)	2563(3)	285(2)	2380(2)	34(1)
C(11)	2865(3)	102(2)	1680(2)	35(1)
C(12)	1978(3)	382(3)	1041(2)	37(1)
C(13)	806(3)	890(2)	1100(1)	30(1)
C(14)	1399(2)	3160(2)	3980(1)	23(1)
C(15)	793(3)	2306(2)	4470(1)	26(1)
C(16)	1708(3)	1728(2)	4951(1)	30(1)
C(17)	3205(3)	1985(2)	4939(1)	31(1)
C(18)	3811(3)	2834(3)	4453(2)	34(1)
C(19)	2914(3)	3424(2)	3974(1)	30(1)
C(20)	710(2)	5622(2)	3644(1)	24(1)
C(21)	1959(3)	6280(2)	4230(1)	29(1)
C(22)	2362(3)	7658(2)	4404(1)	37(1)
C(23)	1517(3)	8368(2)	4002(2)	38(1)
C(24)	255(3)	7719(2)	3420(2)	35(1)
C(25)	-145(3)	6346(2)	3235(1)	28(1)
C(26)	-2468(2)	3618(2)	3724(1)	25(1)
C(27)	-3582(2)	4220(2)	3262(1)	23(1)
C(28)	-4587(3)	3544(2)	2583(1)	27(1)
C(29)	-5608(3)	4103(2)	2171(1)	29(1)
C(30)	-5636(2)	5359(2)	2432(1)	27(1)
C(31)	-4636(3)	6053(2)	3103(1)	28(1)
C(32)	-3627(3)	5466(2)	3512(1)	28(1)
C(33)	-6877(3)	7025(3)	2308(2)	37(1)
O(2)	-1033(3)	5958(2)	1342(1)	52(1)
C(34)	-2643(4)	5484(3)	1216(3)	63(1)
C(35)	-3183(5)	6119(4)	494(4)	116(2)
C(36)	-1901(5)	7328(4)	517(2)	66(1)
C(37)	-707(4)	7260(3)	1206(2)	53(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S1-3. Bond lengths (A) and angles (deg) for **5a**

Pd(1)-N(1)	2.077(2)	Pd(1)-P(1)	2.2197(5)
Pd(1)-Cl(1)	2.301(5)	Pd(1)-Cl(2)	2.410(6)
Pd(1)-Br(1)	2.422(2)	Pd(1)-Br(2)	2.482(2)
P(1)-C(2)	1.811(2)	P(1)-C(8)	1.819(2)
P(1)-C(1)	1.851(2)	P(2)-N(1)	1.603(2)
P(2)-C(20)	1.798(2)	P(2)-C(14)	1.806(2)
P(2)-C(1)	1.806(2)	O(1)-C(30)	1.374(3)
O(1)-C(33)	1.434(3)	N(1)-C(26)	1.470(3)
C(2)-C(7)	1.389(3)	C(2)-C(3)	1.397(3)
C(3)-C(4)	1.387(3)	C(4)-C(5)	1.385(4)
C(5)-C(6)	1.380(4)	C(6)-C(7)	1.400(3)
C(8)-C(13)	1.387(3)	C(8)-C(9)	1.399(3)
C(9)-C(10)	1.387(3)	C(10)-C(11)	1.381(4)
C(11)-C(12)	1.381(4)	C(12)-C(13)	1.394(3)
C(14)-C(19)	1.393(3)	C(14)-C(15)	1.398(3)
C(15)-C(16)	1.390(3)	C(16)-C(17)	1.381(3)
C(17)-C(18)	1.389(3)	C(18)-C(19)	1.387(3)
C(20)-C(21)	1.386(3)	C(20)-C(25)	1.399(3)
C(21)-C(22)	1.391(3)	C(22)-C(23)	1.378(4)
C(23)-C(24)	1.385(4)	C(24)-C(25)	1.390(3)
C(26)-C(27)	1.516(3)	C(27)-C(32)	1.383(3)
C(27)-C(28)	1.393(3)	C(28)-C(29)	1.385(3)
C(29)-C(30)	1.393(3)	C(30)-C(31)	1.387(3)
C(31)-C(32)	1.394(3)	O(2)-C(37)	1.368(4)
O(2)-C(34)	1.432(4)	C(34)-C(35)	1.560(7)
C(35)-C(36)	1.482(6)	C(36)-C(37)	1.518(5)

N(1)-Pd(1)-P(1)	86.84(5)	N(1)-Pd(1)-Cl(1)	72.8(3)
P(1)-Pd(1)-Cl(1)	88.3(3)	N(1)-Pd(1)-Cl(2)	98.1(1)
P(1)-Pd(1)-Cl(2)	174.5(1)	Cl(1)-Pd(1)-Cl(2)	87.1(3)
N(1)-Pd(1)-Br(1)	175.0(1)	P(1)-Pd(1)-Br(1)	88.5(1)
Cl(1)-Pd(1)-Br(1)	3.5(3)	Cl(2)-Pd(1)-Br(1)	86.7(2)
N(1)-Pd(1)-Br(2)	92.55(6)	P(1)-Pd(1)-Br(2)	176.90(6)
Cl(1)-Pd(1)-Br(2)	92.6(3)	Cl(2)-Pd(1)-Br(2)	5.6(1)
Br(1)-Pd(1)-Br(2)	92.2(1)	C(2)-P(1)-C(8)	107.5(1)
C(2)-P(1)-C(1)	104.6(1)	C(8)-P(1)-C(1)	102.6(1)
C(2)-P(1)-Pd(1)	115.99(7)	C(8)-P(1)-Pd(1)	117.80(7)
C(1)-P(1)-Pd(1)	106.73(7)	N(1)-P(2)-C(20)	113.3(1)
N(1)-P(2)-C(14)	114.2(1)	C(20)-P(2)-C(14)	108.4(1)
N(1)-P(2)-C(1)	104.9(1)	C(20)-P(2)-C(1)	107.1(1)
C(14)-P(2)-C(1)	108.5(1)	C(30)-O(1)-C(33)	116.1(2)
C(26)-N(1)-P(2)	121.7(1)	C(26)-N(1)-Pd(1)	123.8(1)
P(2)-N(1)-Pd(1)	111.7(1)	P(2)-C(1)-P(1)	107.0(1)
C(7)-C(2)-C(3)	119.8(2)	C(7)-C(2)-P(1)	119.5(2)
C(3)-C(2)-P(1)	120.6(2)	C(4)-C(3)-C(2)	120.0(2)
C(5)-C(4)-C(3)	120.0(2)	C(6)-C(5)-C(4)	120.3(2)
C(5)-C(6)-C(7)	120.1(2)	C(2)-C(7)-C(6)	119.7(2)
C(13)-C(8)-C(9)	119.5(2)	C(13)-C(8)-P(1)	122.7(2)
C(9)-C(8)-P(1)	117.5(2)	C(10)-C(9)-C(8)	120.0(2)
C(11)-C(10)-C(9)	120.2(2)	C(10)-C(11)-C(12)	120.0(2)
C(11)-C(12)-C(13)	120.4(2)	C(8)-C(13)-C(12)	119.8(2)
C(19)-C(14)-C(15)	120.0(2)	C(19)-C(14)-P(2)	121.9(2)
C(15)-C(14)-P(2)	118.1(2)	C(16)-C(15)-C(14)	119.7(2)
C(17)-C(16)-C(15)	120.1(2)	C(16)-C(17)-C(18)	120.3(2)
C(19)-C(18)-C(17)	120.2(2)	C(18)-C(19)-C(14)	119.7(2)
C(21)-C(20)-C(25)	119.8(2)	C(21)-C(20)-P(2)	122.8(2)
C(25)-C(20)-P(2)	117.3(2)	C(20)-C(21)-C(22)	119.8(2)
C(23)-C(22)-C(21)	120.3(2)	C(22)-C(23)-C(24)	120.5(2)
C(23)-C(24)-C(25)	119.7(2)	C(24)-C(25)-C(20)	119.9(2)
N(1)-C(26)-C(27)	112.7(2)	C(32)-C(27)-C(28)	118.2(2)
C(32)-C(27)-C(26)	120.3(2)	C(28)-C(27)-C(26)	121.5(2)
C(29)-C(28)-C(27)	120.8(2)	C(28)-C(29)-C(30)	120.1(2)
O(1)-C(30)-C(31)	124.1(2)	O(1)-C(30)-C(29)	115.9(2)
C(31)-C(30)-C(29)	119.9(2)	C(30)-C(31)-C(32)	119.0(2)
C(27)-C(32)-C(31)	121.9(2)	C(37)-O(2)-C(34)	105.1(2)
O(2)-C(34)-C(35)	102.6(3)	C(36)-C(35)-C(34)	104.3(3)

C(35)-C(36)-C(37)	103.5(3)	O(2)-C(37)-C(36)	107.4(3)

Table S1-4. Anisotropic displacement parameters (A^2 x 10^3) for **5a**

atom	U11	U22	U33	U23	U13	U12
Pd(1)	19(1)	19(1)	24(1)	5(1)	6(1)	4(1)
Br(1)	29(1)	17(1)	36(1)	2(1)	9(1)	6(1)
Br(2)	27(1)	20(1)	20(1)	2(1)	8(1)	2(1)
Cl(2)	27(1)	20(1)	20(1)	2(1)	8(1)	2(1)
Cl(1)	29(1)	17(1)	36(1)	2(1)	9(1)	6(1)
P(1)	20(1)	18(1)	22(1)	3(1)	6(1)	5(1)
P(2)	20(1)	18(1)	23(1)	3(1)	6(1)	5(1)
O(1)	30(1)	34(1)	38(1)	14(1)	7(1)	14(1)
N(1)	19(1)	20(1)	27(1)	3(1)	7(1)	6(1)
C(1)	23(1)	20(1)	23(1)	3(1)	8(1)	4(1)
C(2)	27(1)	23(1)	21(1)	4(1)	6(1)	11(1)
C(3)	33(1)	29(1)	29(1)	8(1)	11(1)	10(1)
C(4)	49(2)	35(1)	30(1)	13(1)	15(1)	19(1)
C(5)	48(2)	40(1)	27(1)	5(1)	3(1)	21(1)
C(6)	35(1)	41(1)	32(1)	3(1)	-1(1)	16(1)
C(7)	26(1)	30(1)	29(1)	5(1)	4(1)	8(1)
C(8)	21(1)	18(1)	31(1)	3(1)	7(1)	6(1)
C(9)	30(1)	26(1)	33(1)	5(1)	6(1)	12(1)
C(10)	29(1)	27(1)	44(1)	6(1)	4(1)	12(1)
C(11)	29(1)	26(1)	58(2)	10(1)	17(1)	13(1)
C(12)	43(1)	36(1)	45(1)	9(1)	24(1)	20(1)
C(13)	33(1)	32(1)	31(1)	7(1)	11(1)	15(1)
C(14)	23(1)	21(1)	24(1)	3(1)	6(1)	6(1)
C(15)	25(1)	24(1)	27(1)	4(1)	8(1)	5(1)
C(16)	35(1)	26(1)	26(1)	6(1)	7(1)	8(1)
C(17)	33(1)	32(1)	28(1)	4(1)	2(1)	15(1)
C(18)	26(1)	45(1)	36(1)	10(1)	8(1)	15(1)
C(19)	23(1)	36(1)	31(1)	9(1)	7(1)	9(1)
C(20)	27(1)	20(1)	25(1)	4(1)	10(1)	6(1)
C(21)	37(1)	24(1)	23(1)	2(1)	6(1)	6(1)
C(22)	48(2)	27(1)	27(1)	-3(1)	5(1)	2(1)
C(23)	55(2)	21(1)	36(1)	0(1)	14(1)	7(1)
C(24)	45(1)	25(1)	39(1)	7(1)	14(1)	14(1)
C(25)	31(1)	23(1)	31(1)	5(1)	9(1)	8(1)
C(26)	24(1)	28(1)	25(1)	5(1)	9(1)	9(1)
C(27)	22(1)	22(1)	26(1)	4(1)	9(1)	6(1)
C(28)	25(1)	22(1)	33(1)	1(1)	8(1)	7(1)
C(29)	25(1)	29(1)	29(1)	1(1)	4(1)	7(1)
C(30)	22(1)	28(1)	32(1)	11(1)	9(1)	9(1)
C(31)	29(1)	22(1)	35(1)	4(1)	9(1)	9(1)
C(32)	26(1)	25(1)	31(1)	-1(1)	5(1)	7(1)
C(33)	36(1)	37(1)	47(2)	17(1)	15(1)	21(1)
O(2)	47(1)	59(1)	51(1)	9(1)	9(1)	20(1)
C(34)	53(2)	41(2)	100(3)	11(2)	30(2)	14(1)
C(35)	52(2)	64(2)	200(6)	-52(3)	-38(3)	33(2)
C(36)	77(3)	66(2)	75(3)	25(2)	34(2)	37(2)
C(37)	40(2)	56(2)	63(2)	-4(2)	12(1)	17(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S1-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a**

atom	x	y	z	U(eq)
H(1A)	1498	3721	2430	27
H(1B)	161	4336	2108	27
H(3)	32	3582	796	35
H(4)	-1249	3933	-388	43
H(5)	-3823	2821	-854	45
H(6)	-5125	1347	-147	44
H(7)	-3850	978	1044	35
H(9)	1184	899	2928	36
H(10)	3157	69	2818	40
H(11)	3682	-217	1639	42
H(12)	2168	228	557	45
H(13)	200	1083	658	36
H(15)	-240	2122	4474	31
H(16)	1303	1155	5289	36
H(17)	3824	1579	5264	37
H(18)	4844	3010	4449	41
H(19)	3328	4005	3642	36
H(21)	2538	5792	4511	35
H(22)	3224	8111	4802	44
H(23)	1801	9308	4123	46
H(24)	-333	8211	3150	42
H(25)	-998	5898	2831	34
H(26A)	-1758	4300	4138	30
H(26B)	-3024	2872	3959	30
H(28)	-4571	2689	2400	33
H(29)	-6290	3629	1710	34
H(31)	-4638	6915	3282	34
H(32)	-2951	5935	3975	33
H(33A)	-7034.9995	6925	2819	55
H(33B)	-7751	7199	1985	55
H(33C)	-5966	7773	2337	55
H(34A)	-2972	5794	1653	75
H(34B)	-3028	4498	1121	75
H(35A)	-3396	5498	26	139
H(35B)	-4106	6357	514	139
H(36A)	-2193	8148	579	79
H(36B)	-1537	7309	49	79
H(37A)	308	7572	1106	63
H(37B)	-722	7833	1652	63

Figure S2: Molecular structure of **5c**

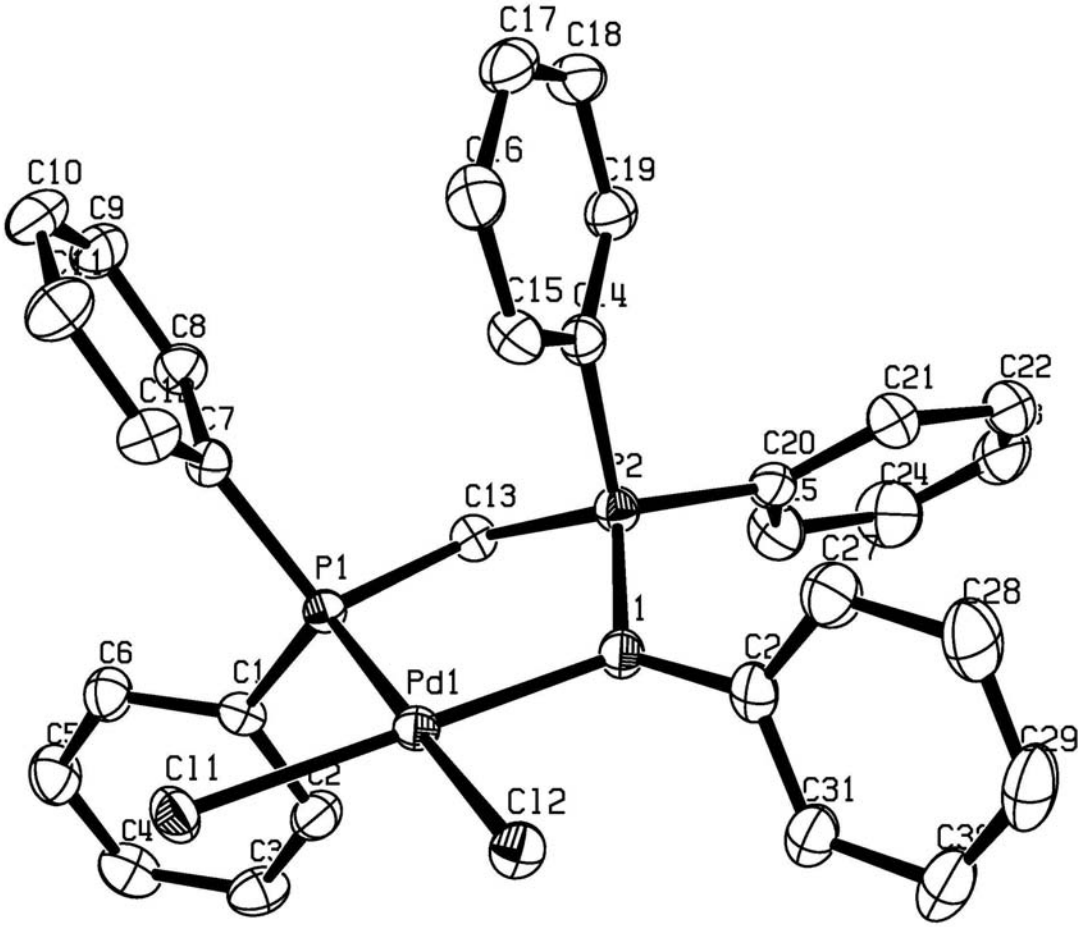

Table S2-1. Crystal data for **5c**

Compound	**5c**
Molecular formula	$C_{31}H_{27}Cl_2NP_2Pd$
Molecular weight	652.78
Crystal habit	orange needle
Crystal dimensions(mm)	0.22x0.16x0.14
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	11.3600(10)
b(Å)	14.8220(10)
c(Å)	17.0950(10)
α(°)	90.00
β(°)	105.1700(10)
γ(°)	90.00
V(Å^3)	2778.1(3)
Z	4
d(g-cm^{-3})	1.561
F(000)	1320
μ(cm^{-1})	0.998
Absorption corrections	multi-scan ; 0.8104 min, 0.8730 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	29.99
HKL ranges	-15 15 ; -19 20 ; -24 24
Reflections measured	14300
Unique data	8054
Rint	0.0224
Reflections used	6288
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	334
Reflections / parameter	18
wR2	0.0939
R1	0.0341
Weights a, b	0.0484 ; 0.0000
GoF	1.019
difference peak / hole (e Å^{-3})	1.096(0.092) / -1.123(0.092)

Table S2-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5c**

atom	x	y	z	U(eq)
Pd(1)	1249(1)	3062(1)	2450(1)	17(1)
Cl(1)	-755(1)	3042(1)	1698(1)	25(1)
Cl(2)	1955(1)	2919(1)	1270(1)	21(1)
P(1)	554(1)	3061(1)	3544(1)	17(1)
P(2)	3189(1)	2756(1)	4105(1)	19(1)
N(1)	3011(2)	3144(1)	3196(1)	20(1)
C(1)	-421(2)	3991(1)	3664(1)	20(1)
C(2)	25(2)	4873(1)	3672(1)	28(1)
C(3)	-702(2)	5604(2)	3728(1)	32(1)
C(4)	-1885(2)	5460(2)	3775(1)	32(1)
C(5)	-2334(2)	4600(2)	3777(2)	33(1)
C(6)	-1606(2)	3857(2)	3717(1)	27(1)
C(7)	-172(2)	2024(1)	3718(1)	20(1)
C(8)	-365(2)	1852(1)	4482(1)	25(1)
C(9)	-858(2)	1037(2)	4633(2)	31(1)
C(10)	-1170(2)	389(2)	4031(2)	33(1)
C(11)	-994(2)	556(2)	3274(2)	34(1)
C(12)	-493(2)	1373(1)	3116(1)	27(1)
C(13)	1900(2)	3192(1)	4413(1)	20(1)
C(14)	3147(2)	1544(1)	4195(1)	21(1)
C(15)	2615(2)	1033(1)	3512(1)	25(1)
C(16)	2498(2)	112(2)	3580(1)	29(1)
C(17)	2940(2)	-306(1)	4319(2)	29(1)
C(18)	3472(2)	200(2)	4998(1)	29(1)
C(19)	3574(2)	1130(1)	4947(1)	25(1)
C(20)	4582(2)	3129(1)	4795(1)	23(1)
C(21)	5679(2)	2675(2)	4825(2)	30(1)
C(22)	6759(2)	2980(2)	5333(2)	37(1)
C(23)	6766(2)	3710(2)	5826(2)	44(1)
C(24)	5702(3)	4160(2)	5806(2)	44(1)
C(25)	4609(2)	3877(2)	5292(1)	33(1)
C(26)	4016(2)	3158(2)	2844(1)	24(1)
C(27)	4726(2)	2410(2)	2806(2)	33(1)
C(28)	5700(2)	2461(2)	2456(2)	40(1)
C(29)	5951(2)	3257(2)	2126(2)	41(1)
C(30)	5242(2)	4009(2)	2142(2)	37(1)
C(31)	4283(2)	3968(2)	2503(1)	29(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S2-3. Bond lengths (A) and angles (deg) for **5c**

Pd(1)-N(1)	2.076(2)	Pd(1)-P(1)	2.2135(6)
Pd(1)-Cl(1)	2.3035(6	Pd(1)-Cl(2)	2.3668(5)
P(1)-C(7)	1.805(2)	P(1)-C(1)	1.813(2)
P(1)-C(13)	1.842(2)	P(2)-N(1)	1.619(2)
P(2)-C(20)	1.797(2)	P(2)-C(13)	1.800(2)
P(2)-C(14)	1.804(2)	N(1)-C(26)	1.422(3)
C(1)-C(6)	1.387(3)	C(1)-C(2)	1.402(3)
C(2)-C(3)	1.380(3)	C(3)-C(4)	1.383(3)
C(4)-C(5)	1.374(3)	C(5)-C(6)	1.396(3)
C(7)-C(12)	1.388(3)	C(7)-C(8)	1.404(3)
C(8)-C(9)	1.383(3)	C(9)-C(10)	1.384(3)
C(10)-C(11)	1.382(3)	C(11)-C(12)	1.395(3)
C(14)-C(15)	1.390(3)	C(14)-C(19)	1.391(3)
C(15)-C(16)	1.380(3)	C(16)-C(17)	1.379(3)
C(17)-C(18)	1.382(3)	C(18)-C(19)	1.388(3)
C(20)-C(25)	1.392(3)	C(20)-C(21)	1.406(3)
C(21)-C(22)	1.381(3)	C(22)-C(23)	1.371(4)
C(23)-C(24)	1.373(4)	C(24)-C(25)	1.384(3)
C(26)-C(27)	1.384(3)	C(26)-C(31)	1.401(3)
C(27)-C(28)	1.391(3)	C(28)-C(29)	1.369(4)
C(29)-C(30)	1.381(4)	C(30)-C(31)	1.387(3)

N(1)-Pd(1)-P(1)	88.90(5)	N(1)-Pd(1)-Cl(1)	175.35(5)
P(1)-Pd(1)-Cl(1)	87.25(2)	N(1)-Pd(1)-Cl(2)	92.39(5)
P(1)-Pd(1)-Cl(2)	174.71(2)	Cl(1)-Pd(1)-Cl(2)	91.67(2)
C(7)-P(1)-C(1)	108.1(1)	C(7)-P(1)-C(13)	106.1(1)
C(1)-P(1)-C(13)	103.4(1)	C(7)-P(1)-Pd(1)	114.75(7)
C(1)-P(1)-Pd(1)	117.27(7)	C(13)-P(1)-Pd(1)	106.03(7)
N(1)-P(2)-C(20)	112.8(1)	N(1)-P(2)-C(13)	104.2(1)
C(20)-P(2)-C(13)	109.9(1)	N(1)-P(2)-C(14)	115.9(1)
C(20)-P(2)-C(14)	106.8(1)	C(13)-P(2)-C(14)	106.9(1)
C(26)-N(1)-P(2)	119.9(2)	C(26)-N(1)-Pd(1)	119.5(1)
P(2)-N(1)-Pd(1)	115.2(1)	C(6)-C(1)-C(2)	119.2(2)
C(6)-C(1)-P(1)	122.1(2)	C(2)-C(1)-P(1)	118.7(2)
C(3)-C(2)-C(1)	120.7(2)	C(2)-C(3)-C(4)	119.5(2)
C(5)-C(4)-C(3)	120.7(2)	C(4)-C(5)-C(6)	120.2(2)
C(1)-C(6)-C(5)	119.7(2)	C(12)-C(7)-C(8)	119.3(2)
C(12)-C(7)-P(1)	120.8(2)	C(8)-C(7)-P(1)	119.8(2)
C(9)-C(8)-C(7)	120.1(2)	C(8)-C(9)-C(10)	120.4(2)
C(11)-C(10)-C(9)	120.0(2)	C(10)-C(11)-C(12)	120.2(2)
C(7)-C(12)-C(11)	120.1(2)	P(2)-C(13)-P(1)	107.1(1)
C(15)-C(14)-C(19)	120.4(2)	C(15)-C(14)-P(2)	119.0(2)
C(19)-C(14)-P(2)	120.5(2)	C(16)-C(15)-C(14)	119.9(2)
C(17)-C(16)-C(15)	120.1(2)	C(16)-C(17)-C(18)	120.0(2)
C(17)-C(18)-C(19)	120.7(2)	C(18)-C(19)-C(14)	118.8(2)
C(25)-C(20)-C(21)	118.8(2)	C(25)-C(20)-P(2)	121.5(2)
C(21)-C(20)-P(2)	119.8(2)	C(22)-C(21)-C(20)	120.0(2)
C(23)-C(22)-C(21)	120.4(3)	C(22)-C(23)-C(24)	120.3(2)
C(23)-C(24)-C(25)	120.4(2)	C(24)-C(25)-C(20)	120.1(2)
C(27)-C(26)-C(31)	118.3(2)	C(27)-C(26)-N(1)	123.4(2)
C(31)-C(26)-N(1)	118.3(2)	C(26)-C(27)-C(28)	121.1(2)
C(29)-C(28)-C(27)	120.0(3)	C(28)-C(29)-C(30)	120.1(2)
C(29)-C(30)-C(31)	120.2(2)	C(30)-C(31)-C(26)	120.3(2)

Table S2-4. Anisotropic displacement parameters (A^2 x 10^3) for **5c**

atom	U11	U22	U33	U23	U13	U12
Pd(1)	18(1)	18(1)	15(1)	1(1)	4(1)	0(1)
Cl(1)	19(1)	32(1)	21(1)	2(1)	0(1)	1(1)
Cl(2)	24(1)	27(1)	14(1)	-2(1)	6(1)	-2(1)
P(1)	17(1)	18(1)	16(1)	0(1)	5(1)	0(1)
P(2)	18(1)	21(1)	17(1)	0(1)	4(1)	0(1)
N(1)	18(1)	26(1)	17(1)	1(1)	4(1)	-1(1)
C(1)	22(1)	20(1)	18(1)	1(1)	5(1)	3(1)
C(2)	28(1)	23(1)	34(1)	2(1)	13(1)	-1(1)
C(3)	42(2)	20(1)	36(1)	0(1)	15(1)	1(1)
C(4)	38(1)	32(1)	29(1)	-2(1)	11(1)	13(1)
C(5)	25(1)	34(1)	41(1)	-2(1)	12(1)	5(1)
C(6)	23(1)	25(1)	33(1)	-2(1)	9(1)	0(1)
C(7)	19(1)	20(1)	22(1)	1(1)	6(1)	0(1)
C(8)	27(1)	26(1)	22(1)	0(1)	6(1)	-1(1)
C(9)	32(1)	31(1)	31(1)	5(1)	13(1)	-4(1)
C(10)	37(1)	23(1)	40(1)	2(1)	14(1)	-7(1)
C(11)	42(2)	25(1)	37(1)	-5(1)	14(1)	-7(1)
C(12)	34(1)	24(1)	26(1)	-1(1)	12(1)	-1(1)
C(13)	21(1)	20(1)	19(1)	-2(1)	5(1)	1(1)
C(14)	18(1)	22(1)	24(1)	0(1)	7(1)	0(1)
C(15)	24(1)	24(1)	25(1)	0(1)	4(1)	4(1)
C(16)	27(1)	25(1)	33(1)	-8(1)	6(1)	-1(1)
C(17)	30(1)	20(1)	41(1)	0(1)	16(1)	0(1)
C(18)	31(1)	27(1)	31(1)	8(1)	11(1)	2(1)
C(19)	25(1)	25(1)	27(1)	0(1)	10(1)	1(1)
C(20)	22(1)	25(1)	20(1)	4(1)	3(1)	-3(1)
C(21)	24(1)	32(1)	32(1)	4(1)	4(1)	1(1)
C(22)	23(1)	42(2)	40(2)	12(1)	-2(1)	-4(1)
C(23)	30(1)	51(2)	39(2)	13(1)	-8(1)	-17(1)
C(24)	44(2)	41(2)	38(2)	-9(1)	-3(1)	-11(1)
C(25)	32(1)	32(1)	32(1)	-5(1)	2(1)	-2(1)
C(26)	19(1)	37(1)	14(1)	-3(1)	2(1)	-3(1)
C(27)	31(1)	39(1)	32(1)	3(1)	14(1)	4(1)
C(28)	29(1)	57(2)	38(2)	-4(1)	15(1)	6(1)
C(29)	28(1)	65(2)	36(2)	-6(1)	16(1)	-9(1)
C(30)	32(1)	52(2)	31(1)	-1(1)	12(1)	-16(1)
C(31)	25(1)	37(1)	24(1)	-1(1)	8(1)	-6(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S2-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5c**

atom	x	y	z	U(eq)
H(2)	837	4970	3638	33
H(3)	-393.0000	6200	3734	38
H(4)	-2392	5960	3806	39
H(5)	-3143	4509	3820	40
H(6)	-1921	3263	3712	32
H(8)	-157	2295	4897	30
H(9)	-983	922	5151	37
H(10)	-1505	-170.0000	4138	39
H(11)	-1216	111	2860	40
H(12)	-370	1483	2595	33
H(13A)	2029	3837	4564	24
H(13B)	1787	2852	4887	24
H(15)	2333	1318	2999	30
H(16)	2113	-235.0000	3116	34
H(17)	2878	-942	4362	35
H(18)	3771	-91	5506	35
H(19)	3930	1478	5416	30
H(21)	5677	2158	4496	36
H(22)	7501	2681	5340	44
H(23)	7511	3906	6184	52
H(24)	5715	4669	6146	52
H(25)	3877	4194	5279	39
H(27)	4547	1852	3023	39
H(28)	6190	1944	2445	48
H(29)	6615	3291	1885	49
H(30)	5411	4558	1904	45
H(31)	3805	4490	2520	34

Figure S3: Molecular structure of **5e**

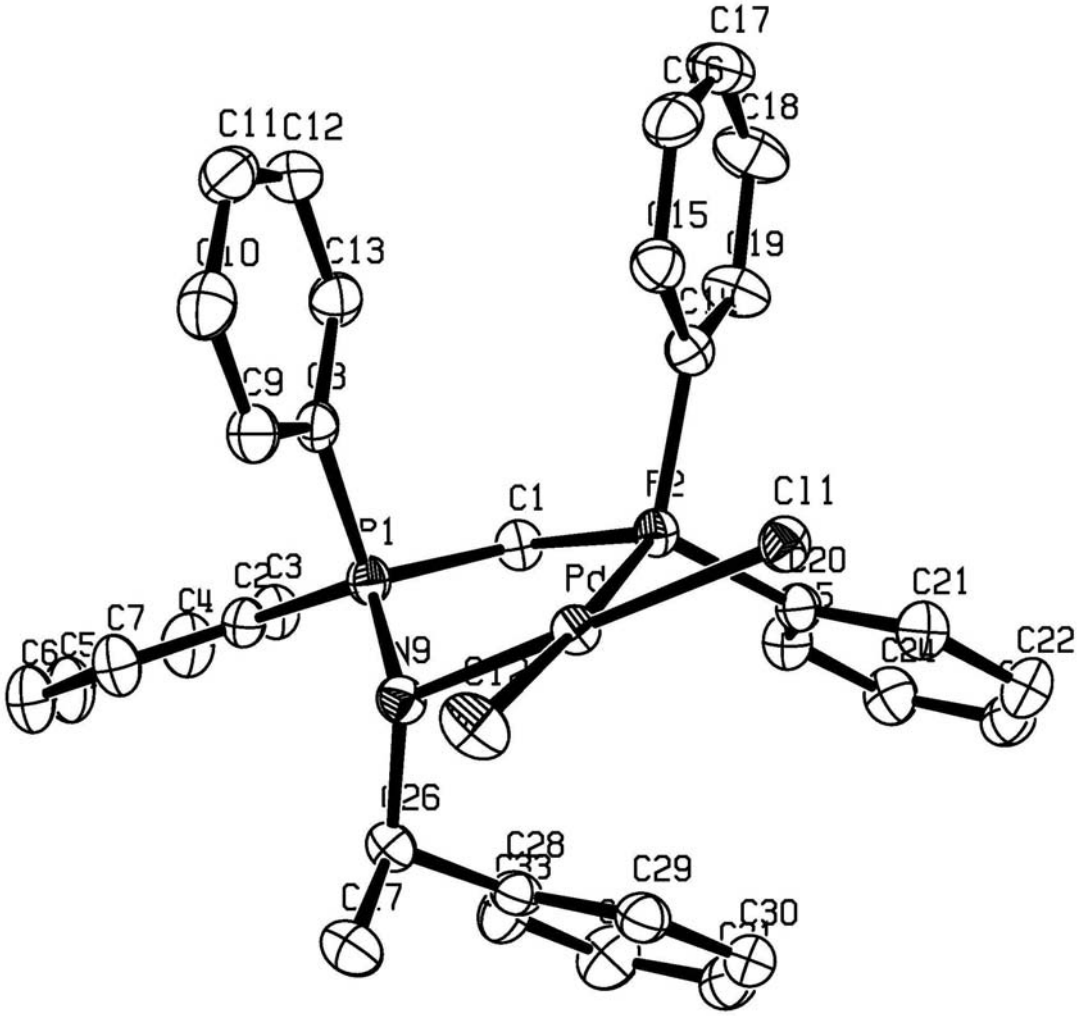

Table S3-1. Crystal data for **5e**

Compound	**5e**
Molecular formula	$C_{33}H_{31}Cl_2NP_2Pd$
Molecular weight	680.83
Crystal habit	orange plate
Crystal dimensions(mm)	0.20x0.16x0.05
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a(Å)	12.3350(10)
b(Å)	13.6480(10)
c(Å)	17.6430(10)
α(°)	90.00
β(°)	90.00
γ(°)	90.00
V(Å^3)	2970.2(4)
Z	4
d(g-cm^{-3})	1.523
F(000)	1384
μ(cm^{-1})	0.937
Absorption corrections	multi-scan ; 0.8348 min, 0.9547 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.02
HKL ranges	-17 17 ; -19 19 ; -24 24
Reflections measured	8575
Unique data	8575
Rint	0.0000
Reflections used	7398
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	354
Reflections / parameter	20
wR2	0.0819
R1	0.0337
Flack's parameter	-0.022(19)
Weights a, b	0.0427 ; 0.0000
GoF	1.008
difference peak / hole (e Å^{-3})	0.857(0.087) / -0.923(0.087)

Table S3-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5e**

atom	x	y	z	U(eq)
Pd(1)	3166(1)	32(1)	2246(1)	20(1)
Cl(1)	4993(1)	-17(1)	1919(1)	24(1)
Cl(2)	2680(1)	-155(1)	956(1)	31(1)
P(1)	1443(1)	-558(1)	3333(1)	21(1)
P(2)	3648(1)	89(1)	3471(1)	20(1)
N(9)	1535(2)	77(2)	2573(1)	22(1)
C(1)	2397(2)	-82(2)	4017(1)	23(1)
C(2)	122(2)	-537(2)	3773(2)	23(1)
C(3)	23(2)	-263(2)	4533(2)	28(1)
C(4)	-995(2)	-220(2)	4868(2)	34(1)
C(5)	-1909(3)	-443(2)	4448(2)	36(1)
C(6)	-1806(3)	-740(2)	3704(2)	36(1)
C(7)	-799(2)	-793(2)	3366(2)	30(1)
C(8)	1810(2)	-1802(2)	3116(2)	22(1)
C(9)	1673(2)	-2148(2)	2381(2)	27(1)
C(10)	1945(3)	-3114(2)	2211(2)	33(1)
C(11)	2351(2)	-3722(2)	2767(2)	35(1)
C(12)	2483(3)	-3376(2)	3498(2)	35(1)
C(13)	2213(2)	-2419(2)	3679(2)	28(1)
C(14)	4494(2)	-914(2)	3793(2)	23(1)
C(15)	4735(2)	-1701(2)	3320(2)	27(1)
C(16)	5301(3)	-2496(2)	3599(2)	33(1)
C(17)	5635(3)	-2509(2)	4333(2)	39(1)
C(18)	5410(3)	-1736(2)	4813(2)	44(1)
C(19)	4839(3)	-933(2)	4550(2)	34(1)
C(20)	4249(2)	1202(2)	3855(2)	22(1)
C(21)	5156(2)	1605(2)	3495(2)	28(1)
C(22)	5614(3)	2453(2)	3760(2)	32(1)
C(23)	5192(3)	2917(2)	4387(2)	32(1)
C(24)	4302(3)	2520(2)	4752(2)	32(1)
C(25)	3828(2)	1666(2)	4488(2)	29(1)
C(26)	885(2)	1001(2)	2501(2)	24(1)
C(27)	614(3)	1204(2)	1682(2)	32(1)
C(28)	1405(2)	1882(2)	2888(2)	25(1)
C(29)	2340(2)	2315(2)	2610(2)	29(1)
C(30)	2788(3)	3126(2)	2961(2)	35(1)
C(31)	2291(3)	3534(2)	3583(2)	38(1)
C(32)	1355(3)	3114(2)	3875(2)	40(1)
C(33)	920(3)	2287(2)	3533(2)	32(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S3-3. Bond lengths (A) and angles (deg) for **5e**

Pd(1)-N(9)	2.094(2)	Pd(1)-P(2)	2.2425(6)
Pd(1)-Cl(1)	2.3265(6	Pd(1)-Cl(2)	2.3687(7)
Pd(1)-P(1)	2.9742(7	P(1)-N(9)	1.601(2)
P(1)-C(8)	1.799(3)	P(1)-C(2)	1.805(3)
P(1)-C(1)	1.805(3)	P(2)-C(14)	1.813(3)
P(2)-C(20)	1.820(3)	P(2)-C(1)	1.834(2)
N(9)-C(26)	1.499(3)	C(2)-C(7)	1.388(4)
C(2)-C(3)	1.398(4)	C(3)-C(4)	1.389(4)
C(4)-C(5)	1.383(4)	C(5)-C(6)	1.379(4)
C(6)-C(7)	1.380(4)	C(8)-C(9)	1.391(4)
C(8)-C(13)	1.393(4)	C(9)-C(10)	1.393(4)
C(10)-C(11)	1.379(4)	C(11)-C(12)	1.384(5)
C(12)-C(13)	1.385(4)	C(14)-C(15)	1.392(4)
C(14)-C(19)	1.401(4)	C(15)-C(16)	1.381(4)
C(16)-C(17)	1.360(5)	C(17)-C(18)	1.382(5)
C(18)-C(19)	1.383(4)	C(20)-C(25)	1.385(4)
C(20)-C(21)	1.399(4)	C(21)-C(22)	1.369(4)
C(22)-C(23)	1.377(4)	C(23)-C(24)	1.383(4)
C(24)-C(25)	1.385(4)	C(26)-C(27)	1.508(4)
C(26)-C(28)	1.525(4)	C(28)-C(29)	1.386(4)
C(28)-C(33)	1.398(4)	C(29)-C(30)	1.383(4)
C(30)-C(31)	1.375(5)	C(31)-C(32)	1.388(5)
C(32)-C(33)	1.388(4)		

N(9)-Pd(1)-P(2)	89.35(6)	N(9)-Pd(1)-Cl(1)	178.39(6)
P(2)-Pd(1)-Cl(1)	89.04(2)	N(9)-Pd(1)-Cl(2)	91.37(6)
P(2)-Pd(1)-Cl(2)	175.78(3)	Cl(1)-Pd(1)-Cl(2)	90.23(2)
N(9)-Pd(1)-P(1)	31.10(6)	P(2)-Pd(1)-P(1)	65.02(2)
Cl(1)-Pd(1)-P(1)	147.62(2)	Cl(2)-Pd(1)-P(1)	114.17(2)
N(9)-P(1)-C(8)	108.3(1)	N(9)-P(1)-C(2)	114.6(1)
C(8)-P(1)-C(2)	109.5(1)	N(9)-P(1)-C(1)	108.6(1)
C(8)-P(1)-C(1)	108.5(1)	C(2)-P(1)-C(1)	107.2(1)
N(9)-P(1)-Pd(1)	42.49(8)	C(8)-P(1)-Pd(1)	86.4(1)
C(2)-P(1)-Pd(1)	156.7(1)	C(1)-P(1)-Pd(1)	82.37(8)
C(14)-P(2)-C(20)	106.2(1)	C(14)-P(2)-C(1)	102.9(1)
C(20)-P(2)-C(1)	104.7(1)	C(14)-P(2)-Pd(1)	115.3(1)
C(20)-P(2)-Pd(1)	119.7(1)	C(1)-P(2)-Pd(1)	106.14(8)
C(26)-N(9)-P(1)	119.2(2)	C(26)-N(9)-Pd(1)	121.0(2)
P(1)-N(9)-Pd(1)	106.4(1)	P(1)-C(1)-P(2)	104.1(1)
C(7)-C(2)-C(3)	119.5(3)	C(7)-C(2)-P(1)	120.8(2)
C(3)-C(2)-P(1)	119.7(2)	C(4)-C(3)-C(2)	119.8(3)
C(5)-C(4)-C(3)	120.0(3)	C(6)-C(5)-C(4)	120.0(3)
C(5)-C(6)-C(7)	120.7(3)	C(6)-C(7)-C(2)	120.0(3)
C(9)-C(8)-C(13)	120.2(2)	C(9)-C(8)-P(1)	119.2(2)
C(13)-C(8)-P(1)	120.6(2)	C(8)-C(9)-C(10)	119.5(3)
C(11)-C(10)-C(9)	120.3(3)	C(10)-C(11)-C(12)	120.0(3)
C(11)-C(12)-C(13)	120.5(3)	C(12)-C(13)-C(8)	119.5(3)
C(15)-C(14)-C(19)	119.4(3)	C(15)-C(14)-P(2)	121.2(2)
C(19)-C(14)-P(2)	119.2(2)	C(16)-C(15)-C(14)	120.0(3)
C(17)-C(16)-C(15)	120.2(3)	C(16)-C(17)-C(18)	120.9(3)
C(17)-C(18)-C(19)	120.0(3)	C(18)-C(19)-C(14)	119.4(3)
C(25)-C(20)-C(21)	119.0(2)	C(25)-C(20)-P(2)	121.9(2)
C(21)-C(20)-P(2)	119.0(2)	C(22)-C(21)-C(20)	120.5(3)
C(21)-C(22)-C(23)	120.5(3)	C(22)-C(23)-C(24)	119.6(3)
C(23)-C(24)-C(25)	120.5(3)	C(24)-C(25)-C(20)	119.9(3)
N(9)-C(26)-C(27)	110.8(2)	N(9)-C(26)-C(28)	113.6(2)
C(27)-C(26)-C(28)	112.1(2)	C(29)-C(28)-C(33)	118.4(3)
C(29)-C(28)-C(26)	121.8(3)	C(33)-C(28)-C(26)	119.8(3)
C(30)-C(29)-C(28)	121.0(3)	C(31)-C(30)-C(29)	120.1(3)
C(30)-C(31)-C(32)	120.1(3)	C(33)-C(32)-C(31)	119.7(3)
C(32)-C(33)-C(28)	120.6(3)		

Table S3-4. Anisotropic displacement parameters (A^2 x 10^3) for **5e**

atom	U11	U22	U33	U23	U13	U12
Pd(1)	21(1)	23(1)	17(1)	0(1)	1(1)	0(1)
Cl(1)	21(1)	25(1)	24(1)	-1(1)	5(1)	0(1)
Cl(2)	31(1)	45(1)	17(1)	-2(1)	0(1)	6(1)
P(1)	20(1)	23(1)	19(1)	-1(1)	0(1)	-2(1)
P(2)	20(1)	23(1)	19(1)	0(1)	1(1)	-1(1)
N(9)	20(1)	25(1)	21(1)	1(1)	2(1)	1(1)
C(1)	23(1)	27(1)	19(1)	-1(1)	2(1)	-1(1)
C(2)	21(1)	24(1)	23(1)	0(1)	1(1)	-3(1)
C(3)	26(1)	32(1)	26(1)	-2(1)	2(1)	-2(1)
C(4)	30(2)	44(2)	27(1)	-7(1)	11(1)	-4(1)
C(5)	26(2)	47(2)	36(2)	-5(1)	7(1)	-5(1)
C(6)	26(2)	47(2)	33(2)	-3(1)	2(1)	-8(1)
C(7)	24(2)	39(2)	26(2)	-2(1)	1(1)	-4(1)
C(8)	19(1)	23(1)	24(1)	0(1)	0(1)	-4(1)
C(9)	25(2)	29(1)	26(2)	-1(1)	1(1)	-2(1)
C(10)	32(2)	33(1)	35(2)	-9(1)	5(2)	-3(1)
C(11)	30(2)	25(1)	52(2)	1(1)	7(2)	-1(1)
C(12)	32(2)	27(1)	45(2)	8(1)	-4(2)	1(1)
C(13)	29(2)	30(1)	25(1)	4(1)	-1(1)	-3(1)
C(14)	22(1)	26(1)	22(1)	0(1)	1(1)	0(1)
C(15)	25(2)	27(1)	28(2)	-1(1)	1(1)	1(1)
C(16)	33(2)	25(1)	42(2)	-3(1)	9(2)	2(1)
C(17)	34(2)	38(2)	45(2)	12(2)	4(2)	11(1)
C(18)	45(2)	53(2)	32(2)	9(2)	-7(2)	16(2)
C(19)	37(2)	38(2)	27(2)	-1(1)	-3(1)	13(1)
C(20)	23(2)	23(1)	21(1)	-2(1)	-4(1)	-2(1)
C(21)	28(2)	32(1)	24(2)	-2(1)	3(1)	-2(1)
C(22)	34(2)	29(1)	32(2)	-1(1)	3(1)	-8(1)
C(23)	38(2)	27(1)	31(2)	0(1)	-6(1)	-4(1)
C(24)	34(2)	34(1)	29(2)	-8(1)	-2(1)	-1(1)
C(25)	29(2)	33(1)	24(1)	-2(1)	0(1)	-4(1)
C(26)	21(1)	26(1)	25(1)	-1(1)	-1(1)	2(1)
C(27)	31(2)	35(2)	31(2)	0(1)	-6(1)	6(1)
C(28)	22(1)	25(1)	26(2)	4(1)	1(1)	4(1)
C(29)	26(2)	29(1)	32(2)	4(1)	2(1)	3(1)
C(30)	28(2)	31(1)	46(2)	9(1)	-5(2)	-3(1)
C(31)	48(2)	30(1)	37(2)	0(1)	-13(2)	-6(1)
C(32)	49(2)	36(2)	35(2)	-9(1)	4(2)	-1(2)
C(33)	34(2)	32(2)	30(2)	-2(1)	5(1)	-4(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S3-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5e**

atom	x	y	z	U(eq)
H(1A)	2509	-553	4436	27
H(1B)	2140	548	4229	27
H(3)	651	-105	4821	34
H(4)	-1064	-38	5385	41
H(5)	-2608	-392	4671	44
H(6)	-2435	-908.9999	3422	43
H(7)	-736	-1005	2855	36
H(9)	1395	-1728	1997	32
H(10)	1851	-3353.9998	1710	40
H(11)	2541	-4379	2647	42
H(12)	2761	-3799	3880	42
H(13)	2301	-2185	4182	34
H(15)	4509	-1691	2805	32
H(16)	5457	-3035	3277	40
H(17)	6027	-3058	4519	47
H(18)	5648	-1755	5325	52
H(19)	4682	-400	4878	41
H(21)	5457	1289	3064	34
H(22)	6227	2722	3510	38
H(23)	5510	3506	4568	38
H(24)	4013	2836	5188	39
H(25)	3216	1399	4741	34
H(26)	181	879	2766	29
H(27A)	1284	1324	1399	48
H(27B)	145	1782	1650	48
H(27C)	238	637	1465	48
H(29)	2679	2050	2172	35
H(30)	3441	3402	2771	42
H(31)	2588	4103	3813	46
H(32)	1014	3391	4308	48
H(33)	286	1993	3738	39

Figure S4: Molecular structure of **5'e**

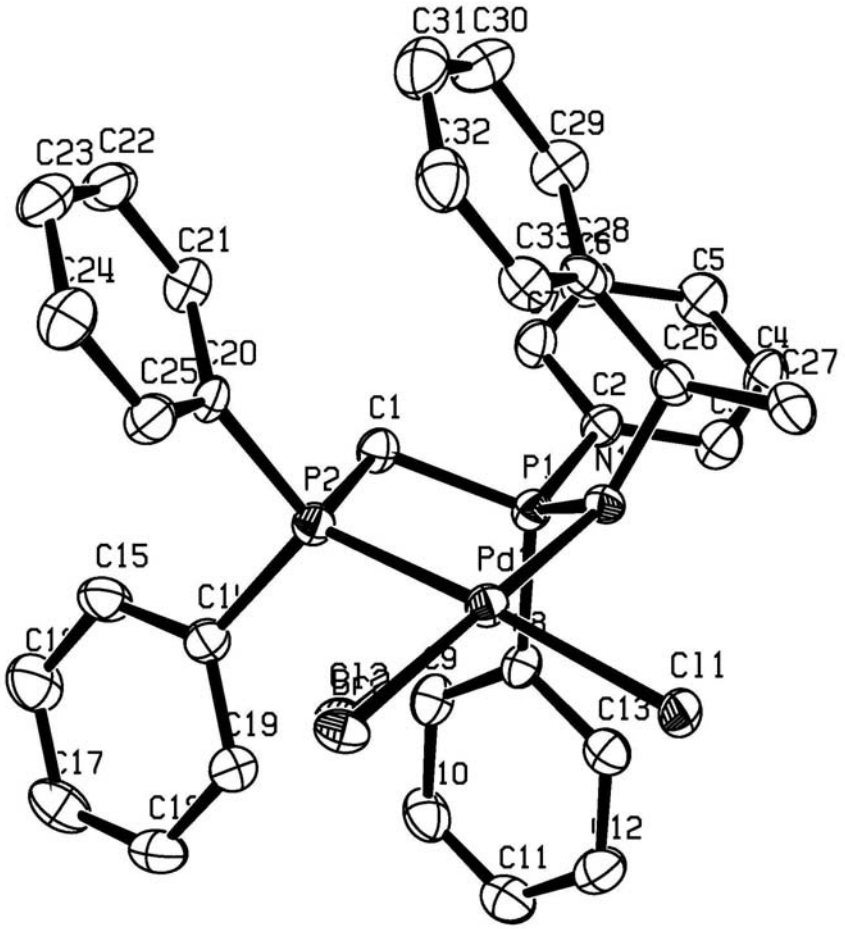

Table S4-1. Crystal data for **5'e**

Compound	**5'e**
Molecular formula	$C_{33}H_{31}Br_{0.16}Cl_{1.84}NP_2Pd$
Molecular weight	688.05
Crystal habit	orange plate
Crystal dimensions(mm)	0.12x0.10x0.04
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a(Å)	12.3220(10)
b(Å)	13.6670(10)
c(Å)	17.6790(10)
α(°)	90.00
β(°)	90.00
γ(°)	90.00
V(Å^3)	2977.2(4)
Z	4
d(g-cm^{-3})	1.535
F(000)	1396
μ(cm^{-1})	1.138
Absorption corrections	multi-scan ; 0.8755 min, 0.9559 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-17 17 ; -19 19 ; -24 24
Reflections measured	8674
Unique data	8674
Rint	0.0000
Reflections used	6885
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	364
Reflections / parameter	18
wR2	0.0930
R1	0.0398
Flack's parameter	0.01(2)
Weights a, b	0.0457 ; 0.0000
GoF	1.005
difference peak / hole (e Å^{-3})	0.999(0.103) / -1.117(0.103)

Table 4-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5'e**

atom	x	y	z	U(eq)
Pd(1)	1840(1)	34(1)	2752(1)	19(1)
Cl(1)	2334(1)	-161(1)	4047(1)	24(1)
Br(2)	-40(20)	0(10)	3130(10)	22(2)
Cl(2)	10(8)	-20(5)	3064(6)	25(1)
P(1)	3564(1)	-555(1)	1667(1)	20(1)
P(2)	1356(1)	92(1)	1529(1)	20(1)
N(1)	3476(2)	79(2)	2431(1)	19(1)
C(1)	2610(2)	-81(3)	988(2)	21(1)
C(2)	4891(3)	-540(3)	1227(2)	22(1)
C(3)	5808(3)	-794(3)	1638(2)	29(1)
C(4)	6819(3)	-728(3)	1298(2)	34(1)
C(5)	6919(3)	-437(3)	562(2)	35(1)
C(6)	6004(3)	-223(3)	139(2)	32(1)
C(7)	4993(3)	-260(3)	469(2)	27(1)
C(8)	3201(3)	-1795(2)	1881(2)	21(1)
C(9)	2801(3)	-2415(3)	1320(2)	27(1)
C(10)	2520(3)	-3367(3)	1497(2)	34(1)
C(11)	2652(3)	-3715(3)	2222(2)	33(1)
C(12)	3062(3)	-3111(3)	2780(2)	32(1)
C(13)	3329(3)	-2146(3)	2613(2)	25(1)
C(14)	510(3)	-910(3)	1211(2)	23(1)
C(15)	169(3)	-933(3)	454(2)	32(1)
C(16)	-400(4)	-1729(3)	189(2)	42(1)
C(17)	-638(4)	-2497(3)	660(2)	39(1)
C(18)	-304(3)	-2493(3)	1402(2)	31(1)
C(19)	272(3)	-1696(3)	1675(2)	26(1)
C(20)	755(3)	1202(3)	1148(2)	22(1)
C(21)	1172(3)	1661(3)	516(2)	27(1)
C(22)	709(3)	2517(3)	247(2)	32(1)
C(23)	-196(3)	2909(3)	609(2)	31(1)
C(24)	-615(3)	2446(3)	1236(2)	32(1)
C(25)	-156(3)	1603(3)	1504(2)	27(1)
C(26)	4122(3)	999(3)	2499(2)	23(1)
C(27)	4392(3)	1207(3)	3315(2)	30(1)
C(28)	3600(3)	1885(2)	2111(2)	22(1)
C(29)	4087(3)	2289(3)	1469(2)	32(1)
C(30)	3649(4)	3117(3)	1129(2)	39(1)
C(31)	2712(4)	3532(3)	1417(3)	38(1)
C(32)	2218(3)	3121(3)	2043(2)	34(1)
C(33)	2664(3)	2315(3)	2391(2)	28(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S4-3. Bond lengths (A) and angles (deg) for **5'e**

Pd(1)-N(1)	2.095(2)	Pd(1)-P(2)	2.2444(8)
Pd(1)-Cl(2)	2.323(9)	Pd(1)-Cl(1)	2.3830(8)
Pd(1)-Br(2)	2.41(2)	Pd(1)-P(1)	2.974(1)
P(1)-N(1)	1.608(3)	P(1)-C(8)	1.793(3)
P(1)-C(1)	1.801(3)	P(1)-C(2)	1.810(3)
P(2)-C(14)	1.810(4)	P(2)-C(20)	1.819(4)
P(2)-C(1)	1.833(3)	N(1)-C(26)	1.494(4)
C(2)-C(3)	1.387(5)	C(2)-C(7)	1.400(5)
C(3)-C(4)	1.386(5)	C(4)-C(5)	1.367(5)
C(5)-C(6)	1.384(5)	C(6)-C(7)	1.376(5)
C(8)-C(13)	1.390(5)	C(8)-C(9)	1.394(5)
C(9)-C(10)	1.382(6)	C(10)-C(11)	1.376(6)
C(11)-C(12)	1.383(5)	C(12)-C(13)	1.391(5)
C(14)-C(19)	1.383(5)	C(14)-C(15)	1.403(5)
C(15)-C(16)	1.375(5)	C(16)-C(17)	1.372(6)
C(17)-C(18)	1.374(6)	C(18)-C(19)	1.387(5)
C(20)-C(21)	1.382(5)	C(20)-C(25)	1.398(5)
C(21)-C(22)	1.385(5)	C(22)-C(23)	1.393(5)
C(23)-C(24)	1.377(5)	C(24)-C(25)	1.368(5)
C(26)-C(27)	1.507(5)	C(26)-C(28)	1.534(5)
C(28)-C(33)	1.386(5)	C(28)-C(29)	1.397(5)
C(29)-C(30)	1.390(5)	C(30)-C(31)	1.384(6)
C(31)-C(32)	1.381(6)	C(32)-C(33)	1.377(5)

N(1)-Pd(1)-P(2)	89.61(7)	N(1)-Pd(1)-Cl(2)	178.0(3)
P(2)-Pd(1)-Cl(2)	88.4(3)	N(1)-Pd(1)-Cl(1)	91.02(7)
P(2)-Pd(1)-Cl(1)	175.55(4)	Cl(2)-Pd(1)-Cl(1)	91.0(3)
N(1)-Pd(1)-Br(2)	179.3(4)	P(2)-Pd(1)-Br(2)	90.9(5)
Cl(2)-Pd(1)-Br(2)	2.6(7)	Cl(1)-Pd(1)-Br(2)	88.5(5)
N(1)-Pd(1)-P(1)	31.31(7)	P(2)-Pd(1)-P(1)	65.01(3)
Cl(2)-Pd(1)-P(1)	146.9(2)	Cl(1)-Pd(1)-P(1)	114.00(3)
Br(2)-Pd(1)-P(1)	149.4(4)	N(1)-P(1)-C(8)	108.4(2)
N(1)-P(1)-C(1)	108.8(2)	C(8)-P(1)-C(1)	108.5(2)
N(1)-P(1)-C(2)	114.6(2)	C(8)-P(1)-C(2)	109.1(2)
C(1)-P(1)-C(2)	107.4(2)	N(1)-P(1)-Pd(1)	42.6(1)
C(8)-P(1)-Pd(1)	86.7(1)	C(1)-P(1)-Pd(1)	82.3(1)
C(2)-P(1)-Pd(1)	156.8(1)	C(14)-P(2)-C(20)	106.3(2)
C(14)-P(2)-C(1)	103.0(2)	C(20)-P(2)-C(1)	104.9(2)
C(14)-P(2)-Pd(1)	115.2(1)	C(20)-P(2)-Pd(1)	119.6(1)
C(1)-P(2)-Pd(1)	106.0(1)	C(26)-N(1)-P(1)	119.0(2)
C(26)-N(1)-Pd(1)	121.1(2)	P(1)-N(1)-Pd(1)	106.1(1)
P(1)-C(1)-P(2)	104.4(2)	C(3)-C(2)-C(7)	119.8(3)
C(3)-C(2)-P(1)	120.5(2)	C(7)-C(2)-P(1)	119.7(3)
C(4)-C(3)-C(2)	119.2(3)	C(5)-C(4)-C(3)	120.9(4)
C(4)-C(5)-C(6)	120.1(4)	C(7)-C(6)-C(5)	120.1(3)
C(6)-C(7)-C(2)	119.8(3)	C(13)-C(8)-C(9)	119.6(3)
C(13)-C(8)-P(1)	119.6(3)	C(9)-C(8)-P(1)	120.8(3)
C(10)-C(9)-C(8)	119.9(3)	C(11)-C(10)-C(9)	120.5(4)
C(10)-C(11)-C(12)	120.1(4)	C(11)-C(12)-C(13)	120.0(3)
C(8)-C(13)-C(12)	119.9(3)	C(19)-C(14)-C(15)	119.0(4)
C(19)-C(14)-P(2)	121.7(3)	C(15)-C(14)-P(2)	119.1(3)
C(16)-C(15)-C(14)	119.7(4)	C(17)-C(16)-C(15)	120.5(4)
C(16)-C(17)-C(18)	120.8(4)	C(17)-C(18)-C(19)	119.2(4)
C(14)-C(19)-C(18)	120.8(4)	C(21)-C(20)-C(25)	119.0(3)
C(21)-C(20)-P(2)	121.8(3)	C(25)-C(20)-P(2)	119.2(3)
C(20)-C(21)-C(22)	120.5(3)	C(21)-C(22)-C(23)	119.8(3)
C(24)-C(23)-C(22)	119.6(4)	C(25)-C(24)-C(23)	120.7(4)
C(24)-C(25)-C(20)	120.4(4)	N(1)-C(26)-C(27)	110.7(3)
N(1)-C(26)-C(28)	113.9(3)	C(27)-C(26)-C(28)	111.8(3)
C(33)-C(28)-C(29)	118.7(3)	C(33)-C(28)-C(26)	121.6(3)
C(29)-C(28)-C(26)	119.7(3)	C(30)-C(29)-C(28)	120.4(4)
C(31)-C(30)-C(29)	119.9(4)	C(32)-C(31)-C(30)	119.8(4)
C(33)-C(32)-C(31)	120.5(4)	C(32)-C(33)-C(28)	120.8(4)

Table S4-4. Anisotropic displacement parameters (A^2 x 10^3) for **5'e**

atom	U11	U22	U33	U23	U13	U12
Pd(1)	20(1)	22(1)	17(1)	0(1)	1(1)	0(1)
Cl(1)	24(1)	36(1)	11(1)	1(1)	0(1)	-6(1)
Br(2)	23(3)	19(3)	22(3)	-2(2)	7(2)	-2(3)
Cl(2)	22(1)	30(2)	25(2)	0(1)	5(1)	3(1)
P(1)	19(1)	22(1)	18(1)	1(1)	1(1)	2(1)
P(2)	19(1)	22(1)	19(1)	1(1)	1(1)	1(1)
N(1)	17(1)	21(1)	18(1)	2(1)	1(1)	-3(1)
C(1)	23(1)	25(2)	16(1)	-1(2)	1(1)	1(2)
C(2)	22(2)	22(2)	23(2)	1(1)	0(1)	3(1)
C(3)	25(2)	36(2)	26(2)	4(2)	2(2)	5(2)
C(4)	24(2)	44(2)	35(2)	3(2)	-3(2)	10(2)
C(5)	22(2)	47(2)	37(2)	4(2)	8(2)	5(2)
C(6)	30(2)	39(3)	27(2)	7(2)	11(2)	3(2)
C(7)	23(2)	33(2)	26(2)	2(1)	-2(1)	3(1)
C(8)	22(2)	19(2)	22(2)	-1(1)	-2(2)	6(2)
C(9)	30(2)	29(2)	23(2)	-4(2)	-3(2)	5(2)
C(10)	33(2)	25(2)	44(3)	-7(2)	-8(2)	-2(2)
C(11)	27(2)	23(2)	48(2)	1(2)	4(2)	2(2)
C(12)	31(2)	33(2)	32(2)	9(2)	3(2)	5(2)
C(13)	22(2)	25(2)	28(2)	-2(1)	2(2)	1(1)
C(14)	24(2)	26(2)	19(2)	0(1)	2(2)	-1(2)
C(15)	36(2)	36(2)	25(2)	3(2)	2(2)	-12(2)
C(16)	46(3)	50(3)	29(2)	-5(2)	-5(2)	-14(2)
C(17)	38(2)	32(2)	45(2)	-12(2)	5(2)	-12(2)
C(18)	30(2)	23(2)	41(2)	4(2)	9(2)	0(2)
C(19)	27(2)	26(2)	26(2)	2(2)	0(2)	-1(2)
C(20)	20(2)	22(2)	23(2)	4(1)	-6(1)	4(1)
C(21)	27(2)	29(2)	23(2)	-1(1)	-1(2)	6(2)
C(22)	36(2)	29(2)	29(2)	9(2)	1(2)	1(2)
C(23)	43(2)	22(2)	29(2)	2(2)	-5(2)	5(2)
C(24)	34(2)	28(2)	34(2)	-3(2)	1(2)	10(2)
C(25)	27(2)	28(2)	27(2)	5(2)	1(2)	3(2)
C(26)	20(2)	25(2)	22(2)	-1(1)	0(1)	-3(1)
C(27)	31(2)	30(2)	29(2)	-2(2)	-5(2)	-8(2)
C(28)	23(2)	22(2)	23(2)	-4(1)	0(2)	-6(2)
C(29)	34(2)	32(2)	30(2)	-2(2)	4(2)	5(2)
C(30)	49(3)	35(2)	32(2)	11(2)	0(2)	3(2)
C(31)	45(3)	27(2)	43(2)	-4(2)	-14(2)	7(2)
C(32)	31(2)	30(2)	41(2)	-6(2)	-9(2)	5(2)
C(33)	27(2)	28(2)	30(2)	-3(2)	1(2)	-2(2)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S4-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5'e**

atom	x	y	z	U(eq)
H(1A)	2497	-552	569	26
H(1B)	2867	547	775	26
H(3)	5743	-1011	2147	35
H(4)	7450	-886.9999	1581	41
H(5)	7619	-382.0000	339	42
H(6)	6074	-50	-379	39
H(7)	4366	-97	182	33
H(9)	2721	-2183	816	33
H(10)	2235	-3784	1116	41
H(11)	2460	-4371	2339	39
H(12)	3162	-3355	3278	38
H(13)	3599	-1728	2998	30
H(15)	329	-402	126	38
H(16)	-629	-1746	-324	50
H(17)	-1038	-3037.9998	471	46
H(18)	-467	-3028.9998	1724	38
H(19)	507	-1690	2187	32
H(21)	1782	1388	263	32
H(22)	1007	2834	-183	38
H(23)	-522	3492	424	38
H(24)	-1229	2716	1485	38
H(25)	-458	1289	1934	33
H(26)	4827	878	2235	27
H(27A)	3721	1322	3599	45
H(27B)	4855	1789	3345	45
H(27C)	4777	646	3532	45
H(29)	4720	1995	1263	38
H(30)	3993	3398	700	46
H(31)	2410	4097	1186	46
H(32)	1565	3397	2234	41
H(33)	2326	2050	2829	34

Figure S5: Molecular structure of **6c**

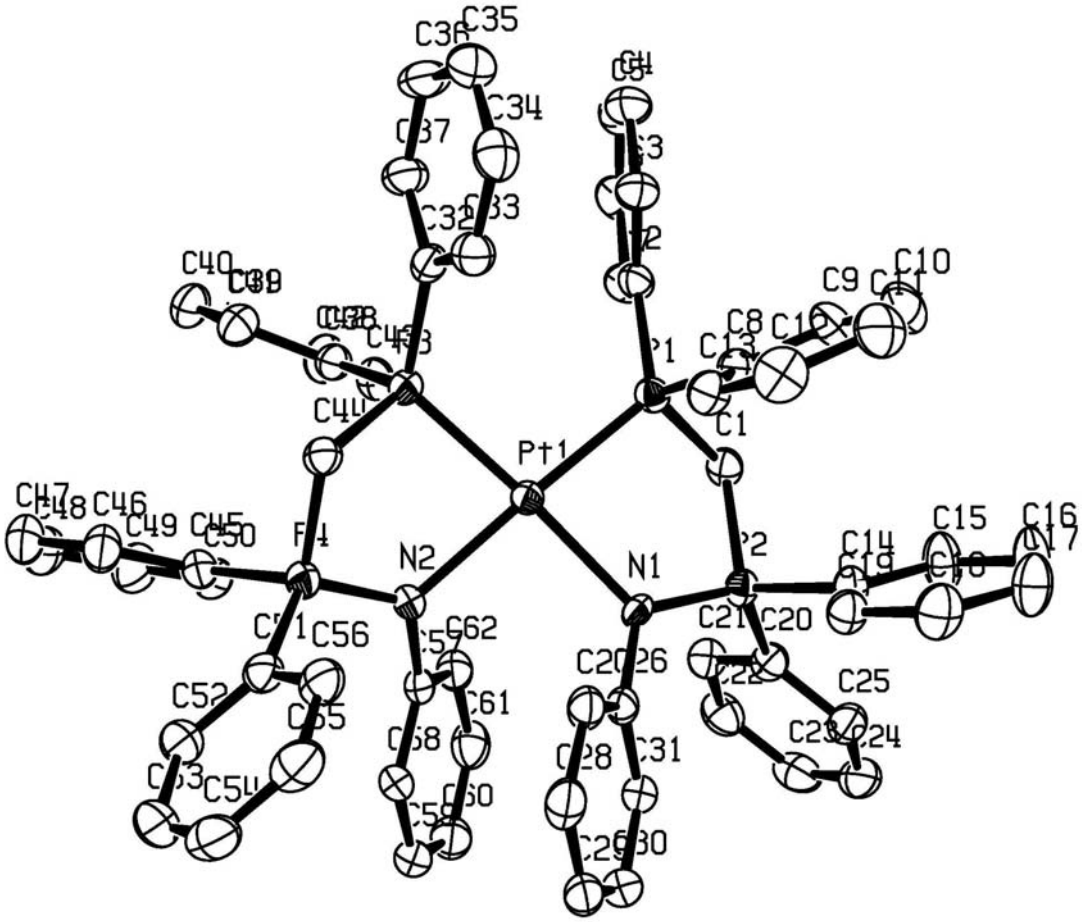

Table S5-1. Crystal data for **6c**

Compound	**6c**
Molecular formula	$C_{62}H_{54}N_2P_4Pt$,2.5 (CH_2Cl_2), (Br), (Cl)
Molecular weight	1473.72
Crystal habit	colorless block
Crystal dimensions(mm)	0.20x0.20x0.20
Crystal system	triclinic
Space group	Pbar1
a(Å)	12.4100(10)
b(Å)	12.6440(10)
c(Å)	21.6810(10)
α(°)	75.6000(10)
β(°)	75.8500(10)
γ(°)	81.0400(10)
V(Å^3)	3178.8(4)
Z	2
d(g-cm^{-3})	1.540
F000	1470
μ(cm^{-1})	3.229
Absorption corrections	multi-scan ; 0.5644 min, 0.5644 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.03
HKL ranges	-17 12 ; -17 17 ; -30 29
Reflections measured	25128
Unique data	18447
Rint	0.0209
Reflections used	15385
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	722
Reflections / parameter	21
wR2	0.1012
R1	0.0379
Weights a, b	0.0546 ; 0.0000
GoF	1.058
difference peak / hole (e Å^{-3})	1.985(0.118) / -1.871(0.118)

Note; An highly disorderd half CH2Cl2 molecule was accounted for using the Platon SQUEEZE function.

Table S5-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6c**

atom	x	y	z	U(eq)
Pt(1)	324(1)	2056(1)	7352(1)	21(1)
Cl(1)	-1967(5)	2628(8)	9293(4)	36(1)
Br(1)	-1717(2)	2693(3)	9233(2)	36(1)
Cl(2)	2570(20)	1310(20)	5397(8)	37(1)
Br(2)	2434(4)	1254(5)	5457(2)	37(1)
P(1)	-863(1)	2698(1)	6697(1)	23(1)
P(2)	628(1)	4447(1)	6336(1)	24(1)
P(3)	-311(1)	440(1)	7850(1)	23(1)
P(4)	1444(1)	494(1)	8528(1)	25(1)
N(1)	911(2)	3642(2)	6994(1)	22(1)
N(2)	1617(2)	1446(2)	7868(1)	23(1)
C(1)	-14(3)	3583(3)	6007(1)	27(1)
C(2)	-1392(3)	1832(3)	6309(2)	27(1)
C(3)	-2473(3)	1536(3)	6553(2)	32(1)
C(4)	-2906(3)	907(3)	6252(2)	38(1)
C(5)	-2265(3)	574(3)	5697(2)	42(1)
C(6)	-1197(3)	866(3)	5458(2)	42(1)
C(7)	-737(3)	1486(3)	5756(2)	33(1)
C(8)	-2052(2)	3592(3)	7002(1)	25(1)
C(9)	-2690(3)	4265(3)	6576(2)	35(1)
C(10)	-3558(3)	4997(3)	6806(2)	43(1)
C(11)	-3810(3)	5040(3)	7456(2)	44(1)
C(12)	-3180(3)	4380(3)	7875(2)	41(1)
C(13)	-2294(3)	3653(3)	7648(2)	31(1)
C(14)	-339(3)	5634(3)	6451(1)	28(1)
C(15)	-692(3)	6339(3)	5913(2)	43(1)
C(16)	-1440(4)	7255(3)	5988(2)	51(1)
C(17)	-1842(3)	7472(3)	6600(2)	47(1)
C(18)	-1497(3)	6780(3)	7135(2)	42(1)
C(19)	-758(3)	5858(3)	7067(2)	31(1)
C(20)	1804(3)	4928(3)	5714(1)	28(1)
C(21)	2591(3)	4137(3)	5450(2)	33(1)
C(22)	3535(3)	4461(3)	4999(2)	39(1)
C(23)	3717(3)	5561(4)	4796(2)	43(1)
C(24)	2948(3)	6341(3)	5047(2)	42(1)
C(25)	1998(3)	6028(3)	5508(2)	34(1)
C(26)	1419(3)	4059(2)	7404(1)	25(1)
C(27)	916(3)	3916(3)	8070(2)	31(1)
C(28)	1406(3)	4270(3)	8484(2)	38(1)
C(29)	2376(3)	4778(3)	8248(2)	43(1)
C(30)	2863(3)	4947(3)	7587(2)	40(1)
C(31)	2388(3)	4571(3)	7167(2)	31(1)
C(32)	-1782(3)	247(3)	8008(1)	26(1)
C(33)	-2578(3)	886(3)	8372(2)	32(1)
C(34)	-3690(3)	767(3)	8472(2)	38(1)
C(35)	-4039(3)	-7(3)	8225(2)	43(1)
C(36)	-3257(3)	-668(3)	7887(2)	42(1)
C(37)	-2128(3)	-540(3)	7764(2)	35(1)
C(38)	427(2)	-701(3)	7505(2)	27(1)
C(39)	413(3)	-1773(3)	7878(2)	33(1)
C(40)	959(3)	-2632(3)	7596(2)	40(1)
C(41)	1531(3)	-2411(3)	6943(2)	43(1)
C(42)	1548(3)	-1362(3)	6582(2)	40(1)
C(43)	997(3)	-491(3)	6861(2)	32(1)
C(44)	6(2)	256(3)	8657(1)	26(1)
C(45)	2291(3)	-781(3)	8462(2)	29(1)
C(46)	2182(3)	-1659(3)	9015(2)	37(1)
C(47)	2808(3)	-2650(3)	8980(2)	45(1)
C(48)	3544(3)	-2790(3)	8414(2)	46(1)
C(49)	3644(3)	-1950(3)	7867(2)	45(1)
C(50)	3022(3)	-929(3)	7891(2)	36(1)
C(51)	1668(3)	846(3)	9239(2)	31(1)
C(52)	2601(3)	387(3)	9503(2)	38(1)

C(53)	2804(4)	753(4)	10011(2)	47(1)
C(54)	2079(4)	1561(4)	10270(2)	46(1)
C(55)	1145(4)	2007(3)	10018(2)	44(1)
C(56)	935(3)	1654(3)	9501(2)	36(1)
C(57)	2708(2)	1801(3)	7560(2)	26(1)
C(58)	3373(3)	2138(3)	7901(2)	29(1)
C(59)	4394(3)	2529(3)	7571(2)	37(1)
C(60)	4751(3)	2594(3)	6913(2)	41(1)
C(61)	4114(3)	2235(3)	6569(2)	39(1)
C(62)	3102(3)	1833(3)	6899(2)	30(1)
C(63)	5241(4)	1211(5)	4369(2)	69(1)
Cl(3)	4847(8)	810(10)	3766(4)	142(3)
Cl(4)	5617(4)	2599(3)	3993(2)	57(1)
Cl(5)	5034(8)	604(5)	3821(4)	71(2)
Cl(6)	5686(7)	2370(20)	4280(10)	175(6)
C(64)	-4659(6)	3017(7)	9757(3)	109(2)
Cl(7)	-5605(1)	3353(2)	9238(1)	92(1)
Cl(8)	-5005(3)	8136(3)	9650(2)	231(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S5-3. Bond lengths (A) and angles (deg) for **6c**

Pt(1)-N(2)	2.118(2)	Pt(1)-N(1)	2.135(2)
Pt(1)-P(1)	2.2191(7	Pt(1)-P(3)	2.2251(8)
P(1)-C(8)	1.807(3)	P(1)-C(2)	1.812(3)
P(1)-C(1)	1.834(3)	P(2)-N(1)	1.614(2)
P(2)-C(20)	1.795(3)	P(2)-C(14)	1.798(3)
P(2)-C(1)	1.808(3)	P(3)-C(38)	1.807(3)
P(3)-C(32)	1.817(3)	P(3)-C(44)	1.837(3)
P(4)-N(2)	1.616(3)	P(4)-C(44)	1.799(3)
P(4)-C(45)	1.799(3)	P(4)-C(51)	1.801(3)
N(1)-C(26)	1.442(4)	N(2)-C(57)	1.443(4)
C(2)-C(3)	1.390(5)	C(2)-C(7)	1.402(4)
C(3)-C(4)	1.383(5)	C(4)-C(5)	1.391(5)
C(5)-C(6)	1.371(6)	C(6)-C(7)	1.389(5)
C(8)-C(13)	1.379(4)	C(8)-C(9)	1.400(4)
C(9)-C(10)	1.386(4)	C(10)-C(11)	1.380(5)
C(11)-C(12)	1.378(5)	C(12)-C(13)	1.393(5)
C(14)-C(19)	1.393(4)	C(14)-C(15)	1.399(4)
C(15)-C(16)	1.384(5)	C(16)-C(17)	1.378(5)
C(17)-C(18)	1.383(5)	C(18)-C(19)	1.382(5)
C(20)-C(25)	1.391(5)	C(20)-C(21)	1.410(4)
C(21)-C(22)	1.374(5)	C(22)-C(23)	1.388(6)
C(23)-C(24)	1.377(6)	C(24)-C(25)	1.386(5)
C(26)-C(31)	1.379(5)	C(26)-C(27)	1.404(4)
C(27)-C(28)	1.388(4)	C(28)-C(29)	1.378(6)
C(29)-C(30)	1.390(5)	C(30)-C(31)	1.402(5)
C(32)-C(33)	1.392(4)	C(32)-C(37)	1.400(4)
C(33)-C(34)	1.371(5)	C(34)-C(35)	1.392(5)
C(35)-C(36)	1.373(5)	C(36)-C(37)	1.389(5)
C(38)-C(43)	1.383(4)	C(38)-C(39)	1.395(5)
C(39)-C(40)	1.382(5)	C(40)-C(41)	1.401(5)
C(41)-C(42)	1.363(5)	C(42)-C(43)	1.393(5)
C(45)-C(50)	1.380(5)	C(45)-C(46)	1.413(5)
C(46)-C(47)	1.376(5)	C(47)-C(48)	1.372(6)
C(48)-C(49)	1.375(6)	C(49)-C(50)	1.403(5)
C(51)-C(56)	1.392(5)	C(51)-C(52)	1.397(5)
C(52)-C(53)	1.384(5)	C(53)-C(54)	1.385(6)
C(54)-C(55)	1.382(6)	C(55)-C(56)	1.397(5)
C(57)-C(62)	1.389(4)	C(57)-C(58)	1.403(4)
C(58)-C(59)	1.392(5)	C(59)-C(60)	1.372(5)
C(60)-C(61)	1.398(5)	C(61)-C(62)	1.388(5)
C(63)-Cl(6)	1.59(1)	C(63)-Cl(5)	1.652(9)
C(63)-Cl(3)	1.712(8)	C(63)-Cl(4)	1.822(7)
C(64)-Cl(8)#2	1.716(8)	C(64)-Cl(7)	1.755(6)
Cl(8)-C(64)#2	1.715(8)		

N(2)-Pt(1)-N(1)	92.9(1)	N(2)-Pt(1)-P(1)	172.76(7)
N(1)-Pt(1)-P(1)	84.55(7)	N(2)-Pt(1)-P(3)	83.47(7)
N(1)-Pt(1)-P(3)	172.80(6)	P(1)-Pt(1)-P(3)	99.75(3)
C(8)-P(1)-C(2)	106.1(1)	C(8)-P(1)-C(1)	105.3(2)
C(2)-P(1)-C(1)	103.2(1)	C(8)-P(1)-Pt(1)	115.3(1)
C(2)-P(1)-Pt(1)	122.9(1)	C(1)-P(1)-Pt(1)	101.8(1)
N(1)-P(2)-C(20)	116.2(1)	N(1)-P(2)-C(14)	115.5(1)
C(20)-P(2)-C(14)	106.7(2)	N(1)-P(2)-C(1)	103.2(1)
C(20)-P(2)-C(1)	106.5(1)	C(14)-P(2)-C(1)	108.2(2)
C(38)-P(3)-C(32)	105.3(1)	C(38)-P(3)-C(44)	107.4(1)
C(32)-P(3)-C(44)	105.3(1)	C(38)-P(3)-Pt(1)	114.8(1)
C(32)-P(3)-Pt(1)	121.8(1)	C(44)-P(3)-Pt(1)	100.9(1)
N(2)-P(4)-C(44)	103.1(1)	N(2)-P(4)-C(45)	114.7(1)
C(44)-P(4)-C(45)	107.9(2)	N(2)-P(4)-C(51)	115.5(2)
C(44)-P(4)-C(51)	109.4(2)	C(45)-P(4)-C(51)	106.0(2)
C(26)-N(1)-P(2)	119.4(2)	C(26)-N(1)-Pt(1)	118.4(2)
P(2)-N(1)-Pt(1)	121.5(1)	C(57)-N(2)-P(4)	120.6(2)
C(57)-N(2)-Pt(1)	117.0(2)	P(4)-N(2)-Pt(1)	121.8(1)
P(2)-C(1)-P(1)	107.6(1)	C(3)-C(2)-C(7)	119.7(3)
C(3)-C(2)-P(1)	119.4(2)	C(7)-C(2)-P(1)	120.9(2)
C(4)-C(3)-C(2)	120.4(3)	C(3)-C(4)-C(5)	120.2(3)
C(6)-C(5)-C(4)	119.3(3)	C(5)-C(6)-C(7)	121.8(3)

C(6)-C(7)-C(2)	118.7(3)	C(13)-C(8)-C(9)	119.9(3)
C(13)-C(8)-P(1)	119.9(2)	C(9)-C(8)-P(1)	120.1(2)
C(10)-C(9)-C(8)	119.7(3)	C(11)-C(10)-C(9)	120.1(3)
C(12)-C(11)-C(10)	120.2(3)	C(11)-C(12)-C(13)	120.3(3)
C(8)-C(13)-C(12)	119.7(3)	C(19)-C(14)-C(15)	119.2(3)
C(19)-C(14)-P(2)	121.3(2)	C(15)-C(14)-P(2)	119.5(2)
C(16)-C(15)-C(14)	120.7(3)	C(17)-C(16)-C(15)	119.5(3)
C(16)-C(17)-C(18)	120.2(3)	C(19)-C(18)-C(17)	120.9(3)
C(18)-C(19)-C(14)	119.5(3)	C(25)-C(20)-C(21)	119.1(3)
C(25)-C(20)-P(2)	123.1(2)	C(21)-C(20)-P(2)	117.7(3)
C(22)-C(21)-C(20)	119.8(3)	C(21)-C(22)-C(23)	120.5(3)
C(24)-C(23)-C(22)	120.1(3)	C(23)-C(24)-C(25)	120.2(4)
C(24)-C(25)-C(20)	120.3(3)	C(31)-C(26)-C(27)	119.4(3)
C(31)-C(26)-N(1)	122.2(3)	C(27)-C(26)-N(1)	118.4(3)
C(28)-C(27)-C(26)	119.9(3)	C(29)-C(28)-C(27)	120.9(3)
C(28)-C(29)-C(30)	119.5(3)	C(29)-C(30)-C(31)	120.1(4)
C(26)-C(31)-C(30)	120.2(3)	C(33)-C(32)-C(37)	119.3(3)
C(33)-C(32)-P(3)	120.2(2)	C(37)-C(32)-P(3)	120.5(2)
C(34)-C(33)-C(32)	120.2(3)	C(33)-C(34)-C(35)	120.7(3)
C(36)-C(35)-C(34)	119.5(3)	C(35)-C(36)-C(37)	120.7(3)
C(36)-C(37)-C(32)	119.5(3)	C(43)-C(38)-C(39)	120.5(3)
C(43)-C(38)-P(3)	118.6(2)	C(39)-C(38)-P(3)	120.9(2)
C(40)-C(39)-C(38)	119.5(3)	C(39)-C(40)-C(41)	119.5(4)
C(42)-C(41)-C(40)	120.8(3)	C(41)-C(42)-C(43)	120.1(3)
C(38)-C(43)-C(42)	119.5(3)	P(4)-C(44)-P(3)	107.2(2)
C(50)-C(45)-C(46)	119.5(3)	C(50)-C(45)-P(4)	122.3(3)
C(46)-C(45)-P(4)	118.2(2)	C(47)-C(46)-C(45)	119.7(3)
C(48)-C(47)-C(46)	120.6(4)	C(47)-C(48)-C(49)	120.4(4)
C(48)-C(49)-C(50)	120.2(4)	C(45)-C(50)-C(49)	119.6(3)
C(56)-C(51)-C(52)	119.5(3)	C(56)-C(51)-P(4)	118.8(2)
C(52)-C(51)-P(4)	121.5(3)	C(53)-C(52)-C(51)	119.9(4)
C(52)-C(53)-C(54)	120.6(4)	C(55)-C(54)-C(53)	119.8(3)
C(54)-C(55)-C(56)	120.3(4)	C(51)-C(56)-C(55)	119.9(3)
C(62)-C(57)-C(58)	119.0(3)	C(62)-C(57)-N(2)	118.6(3)
C(58)-C(57)-N(2)	122.3(3)	C(59)-C(58)-C(57)	119.9(3)
C(60)-C(59)-C(58)	120.3(3)	C(59)-C(60)-C(61)	120.6(3)
C(62)-C(61)-C(60)	119.1(3)	C(61)-C(62)-C(57)	121.0(3)
Cl(6)-C(63)-Cl(5)	130(1)	Cl(6)-C(63)-Cl(3)	124(1)
Cl(5)-C(63)-Cl(3)	11.3(6)	Cl(6)-C(63)-Cl(4)	20(1)
Cl(5)-C(63)-Cl(4)	110.9(4)	Cl(3)-C(63)-Cl(4)	103.9(5)
Cl(8)#2-C(64)-Cl(7)	110.4(4)		

Table S5-4. Anisotropic displacement parameters (A^2 x 10^3) for **6c**

atom	U11	U22	U33	U23	U13	U12
Pt(1)	24(1)	20(1)	21(1)	-4(1)	-7(1)	-2(1)
Cl(1)	35(1)	44(1)	30(1)	-8(1)	-7(1)	-2(1)
Br(1)	35(1)	44(1)	30(1)	-8(1)	-7(1)	-2(1)
Cl(2)	48(1)	39(1)	25(1)	-6(1)	-6(1)	-12(1)
Br(2)	48(1)	39(1)	25(1)	-6(1)	-6(1)	-12(1)
P(1)	25(1)	24(1)	22(1)	-6(1)	-7(1)	-1(1)
P(2)	28(1)	21(1)	21(1)	-4(1)	-6(1)	-1(1)
P(3)	26(1)	20(1)	25(1)	-4(1)	-7(1)	-3(1)
P(4)	29(1)	23(1)	23(1)	-3(1)	-9(1)	-3(1)
N(1)	28(1)	14(1)	25(1)	-3(1)	-8(1)	-5(1)
N(2)	24(1)	22(1)	25(1)	-2(1)	-10(1)	-2(1)
C(1)	33(2)	26(2)	22(1)	-7(1)	-9(1)	-1(1)
C(2)	28(2)	25(2)	31(2)	-9(1)	-13(1)	0(1)
C(3)	32(2)	34(2)	33(2)	-10(1)	-9(1)	-6(1)
C(4)	38(2)	38(2)	45(2)	-13(2)	-15(2)	-8(2)
C(5)	55(2)	31(2)	51(2)	-18(2)	-24(2)	1(2)
C(6)	42(2)	43(2)	50(2)	-29(2)	-18(2)	9(2)
C(7)	31(2)	36(2)	37(2)	-17(2)	-8(1)	0(1)
C(8)	23(1)	24(2)	28(1)	-9(1)	-5(1)	-1(1)
C(9)	31(2)	42(2)	34(2)	-14(2)	-14(1)	6(2)
C(10)	35(2)	44(2)	52(2)	-14(2)	-17(2)	10(2)
C(11)	34(2)	43(2)	55(2)	-21(2)	-5(2)	8(2)
C(12)	43(2)	45(2)	32(2)	-15(2)	2(2)	-2(2)
C(13)	33(2)	30(2)	30(2)	-9(1)	-5(1)	-2(1)
C(14)	33(2)	25(2)	25(1)	-3(1)	-8(1)	1(1)
C(15)	58(2)	39(2)	28(2)	-5(2)	-13(2)	12(2)
C(16)	65(3)	40(2)	38(2)	0(2)	-17(2)	17(2)
C(17)	54(2)	31(2)	51(2)	-12(2)	-9(2)	14(2)
C(18)	51(2)	37(2)	37(2)	-14(2)	-6(2)	3(2)
C(19)	36(2)	28(2)	28(2)	-7(1)	-8(1)	-2(1)
C(20)	34(2)	28(2)	23(1)	-5(1)	-7(1)	-5(1)
C(21)	34(2)	31(2)	33(2)	-6(1)	-8(1)	-3(1)
C(22)	29(2)	49(2)	36(2)	-7(2)	-5(1)	-1(2)
C(23)	34(2)	62(3)	29(2)	3(2)	-7(1)	-19(2)
C(24)	51(2)	40(2)	36(2)	8(2)	-17(2)	-19(2)
C(25)	42(2)	29(2)	32(2)	-5(1)	-10(1)	-6(2)
C(26)	32(2)	18(2)	27(1)	-6(1)	-12(1)	2(1)
C(27)	40(2)	24(2)	28(2)	-3(1)	-12(1)	-2(1)
C(28)	60(2)	27(2)	29(2)	-8(1)	-17(2)	1(2)
C(29)	65(3)	24(2)	54(2)	-9(2)	-39(2)	-1(2)
C(30)	43(2)	28(2)	57(2)	-6(2)	-26(2)	-5(2)
C(31)	35(2)	23(2)	38(2)	-2(1)	-16(1)	-4(1)
C(32)	29(2)	21(2)	27(1)	-4(1)	-6(1)	-4(1)
C(33)	32(2)	34(2)	29(2)	-6(1)	-7(1)	-5(1)
C(34)	35(2)	39(2)	35(2)	-6(2)	-3(1)	3(2)
C(35)	31(2)	45(2)	49(2)	-3(2)	-9(2)	-7(2)
C(36)	36(2)	38(2)	58(2)	-14(2)	-12(2)	-13(2)
C(37)	31(2)	32(2)	47(2)	-13(2)	-10(1)	-5(1)
C(38)	25(1)	22(2)	34(2)	-9(1)	-8(1)	0(1)
C(39)	34(2)	29(2)	35(2)	-7(1)	-6(1)	-4(1)
C(40)	42(2)	23(2)	54(2)	-6(2)	-13(2)	-1(2)
C(41)	48(2)	27(2)	55(2)	-18(2)	-13(2)	6(2)
C(42)	44(2)	35(2)	37(2)	-11(2)	-4(2)	2(2)
C(43)	35(2)	29(2)	30(2)	-7(1)	-9(1)	1(1)
C(44)	29(2)	27(2)	23(1)	-3(1)	-6(1)	-6(1)
C(45)	31(2)	24(2)	32(2)	-4(1)	-13(1)	-1(1)
C(46)	42(2)	29(2)	37(2)	-1(1)	-11(2)	-2(2)
C(47)	56(2)	29(2)	50(2)	1(2)	-24(2)	-2(2)
C(48)	46(2)	28(2)	64(3)	-12(2)	-16(2)	5(2)
C(49)	43(2)	35(2)	53(2)	-11(2)	-6(2)	2(2)
C(50)	37(2)	28(2)	42(2)	-6(2)	-11(2)	-4(1)
C(51)	39(2)	28(2)	27(1)	-2(1)	-10(1)	-10(1)
C(52)	49(2)	37(2)	34(2)	-2(2)	-18(2)	-9(2)
C(53)	60(3)	47(3)	40(2)	2(2)	-29(2)	-13(2)

C(54)	67(3)	49(3)	28(2)	-1(2)	-14(2)	-29(2)
C(55)	66(3)	39(2)	29(2)	-8(2)	-7(2)	-17(2)
C(56)	47(2)	33(2)	26(2)	-3(1)	-8(1)	-10(2)
C(57)	24(1)	19(2)	34(2)	-2(1)	-11(1)	1(1)
C(58)	29(2)	25(2)	36(2)	-2(1)	-16(1)	-2(1)
C(59)	34(2)	30(2)	50(2)	1(2)	-20(2)	-7(1)
C(60)	25(2)	38(2)	52(2)	2(2)	-7(2)	-6(2)
C(61)	33(2)	35(2)	40(2)	-2(2)	-3(1)	2(2)
C(62)	30(2)	28(2)	31(2)	-4(1)	-7(1)	0(1)
C(63)	68(3)	74(4)	69(3)	-25(3)	-22(3)	2(3)
Cl(3)	127(4)	247(8)	87(3)	-60(4)	5(3)	-128(5)
Cl(4)	52(2)	44(2)	77(2)	-28(2)	0(1)	-10(1)
Cl(5)	97(4)	51(3)	72(3)	-38(2)	11(3)	-36(2)
Cl(6)	53(3)	200(10)	350(20)	-220(10)	-23(7)	-5(5)
C(64)	84(4)	133(7)	105(5)	-2(5)	-33(4)	-21(4)
Cl(7)	67(1)	130(2)	70(1)	-13(1)	-10(1)	-6(1)
Cl(8)	173(3)	273(4)	243(3)	112(3)	-140(3)	-130(3)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S5-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6c**

atom	x	y	z	U(eq)
H(1A)	567	3132	5755	32
H(1B)	-489	4040	5714	32
H(3)	-2918	1767	6929	38
H(4)	-3643.0002	700	6424	46
H(5)	-2563	150	5486	51
H(6)	-762	638	5079	50
H(7)	8	1672	5587	40
H(9)	-2530	4220	6131	41
H(10)	-3978.9998	5470	6516	52
H(11)	-4420	5526	7616	53
H(12)	-3349	4422	8320	49
H(13)	-1860	3201	7937	37
H(15)	-416	6187	5491	52
H(16)	-1676	7731	5621	61
H(17)	-2357	8098	6655	57
H(18)	-1771	6942	7554	50
H(19)	-538	5378	7439	37
H(21)	2469	3383	5585	39
H(22)	4066	3926	4824	47
H(23)	4373	5777	4484	51
H(24)	3070	7094	4903	51
H(25)	1476	6567	5685	41
H(27)	241	3577	8237	37
H(28)	1069	4161	8935	45
H(29)	2710	5011	8536	52
H(30)	3518	5317	7419	48
H(31)	2735	4669	6717	38
H(33)	-2349	1405	8551	38
H(34)	-4229	1218	8712	46
H(35)	-4812	-77	8291	51
H(36)	-3491	-1219	7735	50
H(37)	-1593	-983	7516	42
H(39)	30	-1912	8322	40
H(40)	946	-3366	7843	48
H(41)	1912	-3000	6749	51
H(42)	1936	-1224	6138	48
H(43)	1012	241	6610	38
H(44A)	-486	783	8898	31
H(44B)	-113	-498	8914	31
H(46)	1679	-1566	9410	44
H(47)	2728	-3243	9351	54
H(48)	3987	-3471	8399	55
H(49)	4136	-2061	7472	54
H(50)	3103	-343	7516	43
H(52)	3096	-176	9333	46
H(53)	3446	447	10183	56
H(54)	2223	1807	10619	55
H(55)	643	2556	10197	52
H(56)	295	1965	9328	43
H(58)	3125	2099	8356	35
H(59)	4846	2751	7802	45
H(60)	5437	2885	6689	49
H(61)	4371	2266	6115	46
H(62)	2673	1576	6669	36
H(63A)	5887	724	4505	82
H(63B)	4617	1208	4754	82
H(63C)	4513	1241	4682	82
H(63D)	5751	673	4607	82
H(64A)	-3893	2885	9500	130
H(64B)	-4677	3637	9963	130

Figure S6: Molecular structure of **6e**

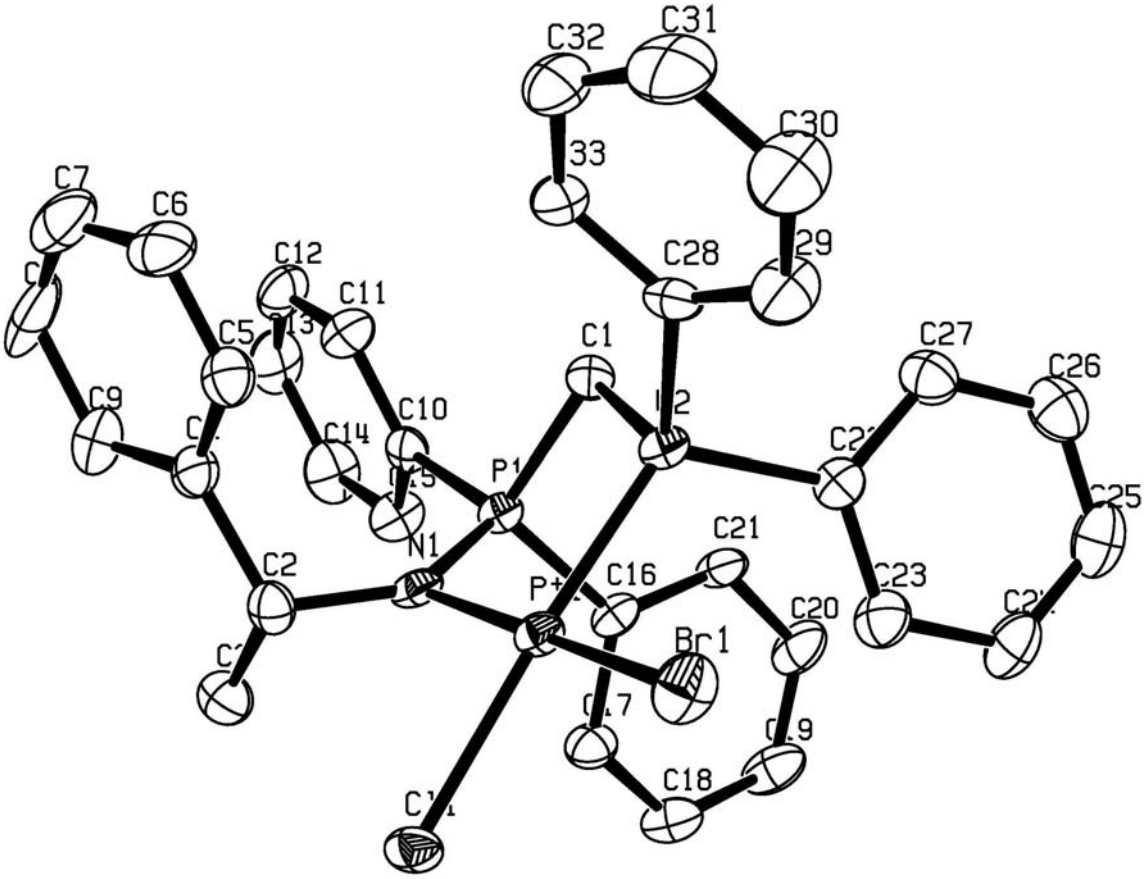

Table S6-1. Crystal data for **6e**

Compound	**6e**
Molecular formula	$C_{33}H_{31}BrClNP_2Pt,C_4H_8O,CH_2Cl_2$
Molecular weight	971.01
Crystal habit	yellow plate
Crystal dimensions(mm)	0.20x0.18x0.05
Crystal system	monoclinic
Space group	$P2_1$
a(Å)	8.5010(10)
b(Å)	16.3370(10)
c(Å)	13.5450(10)
α(°)	90.00
β(°)	94.0500(10)
γ(°)	90.00
V(Å^3)	1876.4(3)
Z	2
d(g-cm^{-3})	1.719
F000	956
μ(cm^{-1})	5.134
Absorption corrections	multi-scan ; 0.4266 min, 0.7834 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.02
HKL ranges	-11 11 ; -22 20 ; -19 19
Reflections measured	10110
Unique data	10110
Rint	0.0000
Reflections used	9116
Criterion	>2sigma(I)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	400
Reflections / parameter	22
wR2	0.1001
R1	0.0390
Flack's parameter	0.016(5)
Weights a, b	0.0641 ; 0.0000
GoF	1.005
difference peak / hole (e Å^{-3})	1.405(0.157) / -2.506(0.157)

Table S6-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6e**

atom	x	y	z	U(eq)
Pt(1)	-218(1)	2014(1)	421(1)	20(1)
Cl(1)	-2637(1)	1632(1)	-423(1)	26(1)
Br(1)	-1542(1)	2090(1)	1959(1)	35(1)
P(1)	2639(2)	1739(1)	-774(1)	20(1)
P(2)	2085(2)	2262(1)	1212(1)	21(1)
N(1)	843(4)	2032(5)	-925(3)	22(1)
C(1)	3557(6)	2291(4)	278(4)	24(1)
C(2)	7(6)	2432(4)	-1769(4)	25(1)
C(3)	-230(7)	1858(4)	-2657(4)	33(2)
C(4)	761(6)	3265(4)	-2007(4)	27(1)
C(5)	951(7)	3835(4)	-1242(4)	30(1)
C(6)	1606(8)	4598(4)	-1391(6)	41(2)
C(7)	2080(8)	4795(5)	-2324(7)	46(2)
C(8)	1890(10)	4246(5)	-3095(7)	56(2)
C(9)	1218(8)	3462(4)	-2951(5)	35(1)
C(10)	3774(5)	1912(5)	-1829(4)	22(1)
C(11)	4441(7)	2677(4)	-1982(5)	32(1)
C(12)	5329(7)	2794(4)	-2801(5)	37(2)
C(13)	5520(7)	2172(6)	-3455(5)	44(2)
C(14)	4860(8)	1401(5)	-3308(5)	40(2)
C(15)	4003(7)	1277(4)	-2496(5)	31(1)
C(16)	2777(6)	671(3)	-492(4)	23(1)
C(17)	1567(7)	143(4)	-857(5)	28(1)
C(18)	1718(7)	-701(4)	-709(5)	34(1)
C(19)	2998(7)	-1004(4)	-175(5)	36(1)
C(20)	4155(7)	-497(4)	206(5)	36(1)
C(21)	4080(6)	341(3)	41(4)	26(1)
C(22)	2778(6)	1465(4)	2055(4)	24(1)
C(23)	1931(8)	732(4)	2094(5)	32(2)
C(24)	2489(8)	103(4)	2721(5)	38(2)
C(25)	3869(8)	212(5)	3316(5)	42(2)
C(26)	4684(8)	929(5)	3285(5)	40(2)
C(27)	4182(7)	1556(4)	2653(5)	32(1)
C(28)	2317(7)	3218(4)	1909(5)	25(1)
C(29)	2024(8)	3233(4)	2880(5)	38(1)
C(30)	2050(10)	3978(5)	3395(6)	52(2)
C(31)	2360(10)	4692(5)	2909(6)	50(2)
C(32)	2644(8)	4685(4)	1929(6)	40(2)
C(33)	2629(7)	3948(4)	1412(5)	30(1)
Cl(2)	1623(2)	1643(2)	-5087(1)	57(1)
Cl(3)	-1583(2)	1024(2)	-5046(2)	65(1)
C(34)	100(10)	1049(6)	4312(6)	55(2)
O(1)	1320(10)	-833(8)	5260(10)	131(4)
C(35)	2190(10)	-450(8)	-3850(10)	85(3)
C(36)	6470(10)	3960(8)	3430(10)	81(3)
C(37)	6570(20)	3300(10)	4230(10)	127(6)
C(38)	1830(20)	-1480(10)	5160(10)	115(5)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S6-3. Bond lengths (A) and angles (deg) for **6e**

Pt(1)-N(1)	2.090(4)	Pt(1)-P(2)	2.203(1)
Pt(1)-Cl(1)	2.364(1)	Pt(1)-Br(1)	2.4400(6)
P(1)-N(1)	1.599(4)	P(1)-C(16)	1.789(6)
P(1)-C(10)	1.803(5)	P(1)-C(1)	1.815(5)
P(2)-C(22)	1.801(6)	P(2)-C(28)	1.829(6)
P(2)-C(1)	1.842(5)	N(1)-C(2)	1.458(8)
C(2)-C(3)	1.527(8)	C(2)-C(4)	1.549(8)
C(4)-C(5)	1.394(9)	C(4)-C(9)	1.400(8)
C(5)-C(6)	1.39(1)	C(6)-C(7)	1.39(1)
C(7)-C(8)	1.38(1)	C(8)-C(9)	1.42(1)
C(10)-C(11)	1.393(9)	C(10)-C(15)	1.398(9)
C(11)-C(12)	1.398(9)	C(12)-C(13)	1.37(1)
C(13)-C(14)	1.40(1)	C(14)-C(15)	1.377(9)
C(16)-C(21)	1.388(8)	C(16)-C(17)	1.405(8)
C(17)-C(18)	1.398(9)	C(18)-C(19)	1.357(9)
C(19)-C(20)	1.359(9)	C(20)-C(21)	1.388(8)
C(22)-C(23)	1.400(9)	C(22)-C(27)	1.403(8)
C(23)-C(24)	1.395(9)	C(24)-C(25)	1.39(1)
C(25)-C(26)	1.36(1)	C(26)-C(27)	1.38(1)
C(28)-C(29)	1.356(9)	C(28)-C(33)	1.403(9)
C(29)-C(30)	1.40(1)	C(30)-C(31)	1.38(1)
C(31)-C(32)	1.37(1)	C(32)-C(33)	1.393(9)
Cl(2)-C(34)#1	1.766(9)	Cl(3)-C(34)#1	1.731(8)
C(34)-Cl(3)#1	1.731(8)	C(34)-Cl(2)#1	1.766(9)
O(1)-C(38)	1.16(2)	O(1)-C(35)#1	1.51(2)
C(35)-O(1)#1	1.51(2)	C(35)-C(36)#2	1.57(2)
C(36)-C(37)	1.53(2)	C(36)-C(35)#2	1.57(2)
C(37)-C(38)#2	1.58(2)	C(38)-C(37)#2	1.58(2)

N(1)-Pt(1)-P(2)	89.9(1)	N(1)-Pt(1)-Cl(1)	89.8(1)
P(2)-Pt(1)-Cl(1)	175.28(5)	N(1)-Pt(1)-Br(1)	175.8(2)
P(2)-Pt(1)-Br(1)	91.29(4)	Cl(1)-Pt(1)-Br(1)	89.35(4)
N(1)-P(1)-C(16)	111.5(3)	N(1)-P(1)-C(10)	114.3(2)
C(16)-P(1)-C(10)	107.0(3)	N(1)-P(1)-C(1)	107.8(3)
C(16)-P(1)-C(1)	107.4(3)	C(10)-P(1)-C(1)	108.6(3)
C(22)-P(2)-C(28)	105.8(3)	C(22)-P(2)-C(1)	104.3(2)
C(28)-P(2)-C(1)	106.2(3)	C(22)-P(2)-Pt(1)	114.5(2)
C(28)-P(2)-Pt(1)	117.9(2)	C(1)-P(2)-Pt(1)	107.1(2)
C(2)-N(1)-P(1)	130.0(3)	C(2)-N(1)-Pt(1)	118.3(3)
P(1)-N(1)-Pt(1)	110.6(2)	P(1)-C(1)-P(2)	104.6(3)
N(1)-C(2)-C(3)	111.8(5)	N(1)-C(2)-C(4)	111.8(5)
C(3)-C(2)-C(4)	114.2(5)	C(5)-C(4)-C(9)	120.1(6)
C(5)-C(4)-C(2)	117.4(5)	C(9)-C(4)-C(2)	122.5(5)
C(6)-C(5)-C(4)	121.2(6)	C(5)-C(6)-C(7)	119.1(7)
C(8)-C(7)-C(6)	120.8(7)	C(7)-C(8)-C(9)	120.6(7)
C(4)-C(9)-C(8)	118.2(7)	C(11)-C(10)-C(15)	119.5(5)
C(11)-C(10)-P(1)	120.3(5)	C(15)-C(10)-P(1)	120.2(5)
C(10)-C(11)-C(12)	119.2(6)	C(13)-C(12)-C(11)	120.6(6)
C(12)-C(13)-C(14)	120.7(6)	C(15)-C(14)-C(13)	119.1(7)
C(14)-C(15)-C(10)	120.9(6)	C(21)-C(16)-C(17)	118.8(5)
C(21)-C(16)-P(1)	121.9(4)	C(17)-C(16)-P(1)	119.2(4)
C(18)-C(17)-C(16)	119.8(6)	C(19)-C(18)-C(17)	119.9(6)
C(18)-C(19)-C(20)	120.7(6)	C(19)-C(20)-C(21)	121.1(6)
C(20)-C(21)-C(16)	119.5(5)	C(23)-C(22)-C(27)	119.2(6)
C(23)-C(22)-P(2)	119.7(4)	C(27)-C(22)-P(2)	121.1(5)
C(24)-C(23)-C(22)	120.0(6)	C(25)-C(24)-C(23)	119.8(7)
C(26)-C(25)-C(24)	120.2(6)	C(25)-C(26)-C(27)	121.4(6)
C(26)-C(27)-C(22)	119.5(6)	C(29)-C(28)-C(33)	120.2(6)
C(29)-C(28)-P(2)	119.7(5)	C(33)-C(28)-P(2)	119.7(5)
C(28)-C(29)-C(30)	120.0(7)	C(31)-C(30)-C(29)	119.7(7)
C(32)-C(31)-C(30)	120.8(7)	C(31)-C(32)-C(33)	120.0(7)
C(32)-C(33)-C(28)	119.3(6)	Cl(3)#1-C(34)-Cl(2)#1	112.7(5)
C(38)-O(1)-C(35)#1	108(1)	O(1)#1-C(35)-C(36)#2	110(1)
C(37)-C(36)-C(35)#2	100(1)	C(36)-C(37)-C(38)#2	102(1)
O(1)-C(38)-C(37)#2	117(2)		

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::
   1: x, y, z   2: -x, y+1/2, -z

Table S6-4. Anisotropic displacement parameters (A^2 x 10^3) for **6e**

atom	U11	U22	U33	U23	U13	U12
Pt(1)	18(1)	17(1)	27(1)	1(1)	4(1)	0(1)
Cl(1)	15(1)	27(1)	35(1)	0(1)	3(1)	-2(1)
Br(1)	32(1)	39(1)	35(1)	4(1)	14(1)	5(1)
P(1)	19(1)	17(1)	23(1)	0(1)	4(1)	-1(1)
P(2)	21(1)	17(1)	25(1)	-1(1)	4(1)	-1(1)
N(1)	18(2)	13(2)	36(2)	2(3)	5(1)	-1(3)
C(1)	21(2)	25(2)	25(3)	1(2)	1(2)	-2(2)
C(2)	22(2)	29(3)	25(3)	2(2)	2(2)	4(2)
C(3)	32(3)	34(5)	33(3)	-3(2)	-1(2)	0(2)
C(4)	23(2)	24(3)	33(3)	5(2)	-1(2)	3(2)
C(5)	31(3)	28(3)	30(3)	0(2)	2(2)	6(2)
C(6)	35(3)	21(3)	67(5)	-1(3)	-3(3)	2(2)
C(7)	39(4)	26(3)	74(5)	14(3)	9(3)	4(3)
C(8)	51(4)	46(5)	73(6)	42(4)	23(4)	9(3)
C(9)	42(3)	34(3)	31(3)	7(2)	8(2)	8(3)
C(10)	14(2)	27(4)	24(2)	2(2)	2(2)	3(2)
C(11)	33(3)	28(3)	36(3)	4(3)	7(2)	-4(2)
C(12)	33(3)	40(4)	40(4)	16(3)	9(3)	-6(3)
C(13)	33(3)	67(7)	34(3)	16(3)	15(2)	-1(3)
C(14)	41(4)	53(4)	27(3)	-3(3)	12(3)	6(3)
C(15)	34(3)	29(3)	31(3)	-4(2)	12(2)	0(2)
C(16)	24(2)	19(2)	26(3)	2(2)	9(2)	-1(2)
C(17)	33(3)	22(3)	29(3)	-4(2)	3(2)	-4(2)
C(18)	31(3)	25(3)	46(4)	-3(3)	8(3)	-5(2)
C(19)	31(3)	21(3)	59(4)	3(3)	16(3)	3(2)
C(20)	34(3)	22(3)	54(4)	12(3)	6(3)	6(2)
C(21)	20(2)	20(3)	39(3)	4(2)	4(2)	-4(2)
C(22)	25(2)	21(2)	26(3)	-1(2)	4(2)	3(2)
C(23)	33(3)	24(3)	38(4)	3(3)	2(3)	4(3)
C(24)	44(4)	27(3)	44(4)	13(3)	7(3)	6(3)
C(25)	49(4)	39(4)	39(4)	13(3)	7(3)	14(3)
C(26)	37(3)	43(4)	38(4)	-1(3)	-4(3)	6(3)
C(27)	27(3)	33(3)	35(3)	-2(2)	-1(2)	1(2)
C(28)	20(3)	23(3)	32(3)	-5(2)	-2(2)	-4(2)
C(29)	56(4)	29(3)	32(3)	-7(3)	12(3)	-1(3)
C(30)	78(5)	41(4)	39(4)	-11(3)	17(4)	2(4)
C(31)	64(5)	27(3)	60(5)	-15(3)	4(4)	1(3)
C(32)	46(4)	22(3)	50(4)	0(3)	-2(3)	1(3)
C(33)	32(3)	23(3)	34(3)	0(2)	-2(2)	-3(2)
Cl(2)	50(1)	77(1)	44(1)	4(1)	11(1)	-5(1)
Cl(3)	50(1)	102(2)	43(1)	-21(1)	7(1)	-14(1)
C(34)	57(5)	71(6)	38(4)	-6(4)	12(3)	5(4)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S6-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6e**

atom	x	y	z	U(eq)
H(1A)	3794	2861	95	29
H(1B)	4548	2020	528	29
H(2)	-1072	2559	-1561	30
H(3A)	778	1778	-2952	49
H(3B)	-995	2099	-3149	49
H(3C)	-625	1329	-2439	49
H(5)	625	3698	-606	36
H(6)	1729	4981	-864	50
H(7)	2542	5314	-2430	55
H(8)	2203	4394	-3730	67
H(9)	1085	3082	-3481	42
H(11)	4293	3114	-1535	39
H(12)	5804	3310	-2902	45
H(13)	6107	2265	-4016	53
H(14)	5001	969	-3763	48
H(15)	3561	754	-2388	37
H(17)	648	359	-1203	33
H(18)	926	-1062	-983	41
H(19)	3087	-1577	-66	44
H(20)	5029	-719.9999	592	44
H(21)	4915	686	291	32
H(23)	977	663	1694	38
H(24)	1925	-398	2741	46
H(25)	4248	-215	3747	51
H(26)	5616	1000	3705	48
H(27)	4784	2045	2624	38
H(29)	1799	2739	3211	46
H(30)	1858	3989	4077	62
H(31)	2382	5197	3259	60
H(32)	2850	5183	1600	48
H(33)	2827	3939	731	36
H(34A)	-158	1277	3644	66
H(34B)	491	483	4232	66
H(35A)	1441	-344	-3331	103
H(35B)	2649	79	-4032	103
H(36A)	5431	4234	3375	97
H(36B)	6697	3735	2772	97
H(37A)	6603	2744	3940	152
H(37B)	5662	3334	4650	152
H(38A)	1987	-1561	4449	138
H(38B)	1025	-1885	5338	138

Figure S6: Molecular structure of **7a**

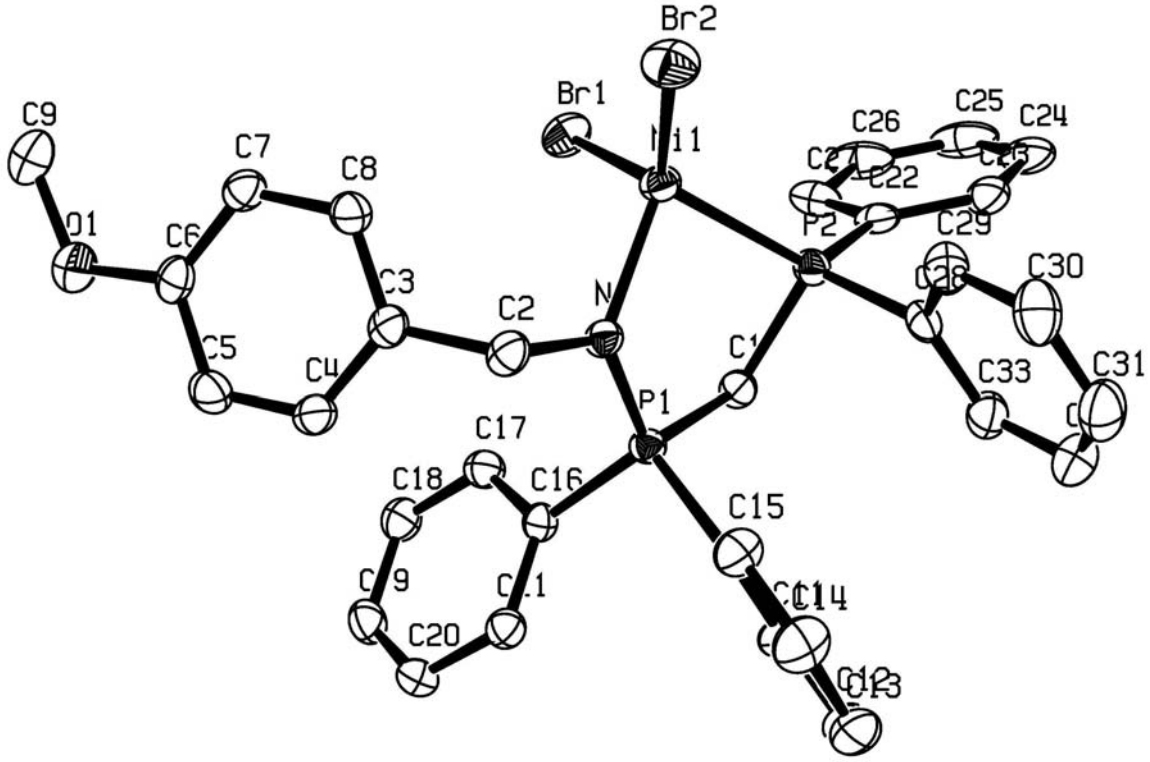

Table S7-1. Crystal data for **7a**

Compound	**7a**
Molecular formula	$C_{33}H_{31}Br_2NNiOP_2,C_4H_8O$
Molecular weight	810.16
Crystal habit	blue plate
Crystal dimensions(mm)	0.22x0.18x0.03
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	19.9970(10)
b(Å)	9.7900(10)
c(Å)	17.6700(10)
α(°)	90.00
β(°)	95.4000(10)
γ(°)	90.00
V(Å^3)	3443.9(4)
Z	4
d(g-cm^{-3})	1.563
F(000)	1648
μ(cm^{-1})	3.011
Absorption corrections	multi-scan ; 0.5571 min, 0.9151 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	27.47
HKL ranges	-25 25 ; -10 12 ; -22 22
Reflections measured	14102
Unique data	7871
Rint	0.0264
Reflections used	5916
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	407
Reflections / parameter	14
wR2	0.0903
R1	0.0350
Weights a, b	0.0425 ; 0.1060
GoF	1.039
difference peak / hole (e Å^{-3})	0.907(0.079) / -0.669(0.079)

Table S7-2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**

atom	x	y	z	U(eq)
Br(1)	1558(1)	955(1)	3056(1)	32(1)
Br(2)	3529(1)	458(1)	4046(1)	36(1)
Ni(1)	2597(1)	-229(1)	3221(1)	23(1)
P(1)	2090(1)	-3177(1)	2796(1)	19(1)
P(2)	2662(1)	-868(1)	1977(1)	21(1)
O(1)	182(1)	-1195(2)	5835(1)	37(1)
N(1)	2380(1)	-2157(2)	3451(1)	21(1)
C(1)	1994(1)	-2162(2)	1937(1)	21(1)
C(2)	2433(2)	-2624(3)	4257(1)	26(1)
C(3)	1840(1)	-2208(2)	4685(1)	23(1)
C(4)	1339(2)	-3137(3)	4814(1)	28(1)
C(5)	797(2)	-2780(3)	5197(1)	29(1)
C(6)	743(2)	-1455(3)	5473(1)	26(1)
C(7)	1237(2)	-508(3)	5353(2)	26(1)
C(8)	1782(2)	-888(3)	4962(1)	26(1)
C(9)	126(2)	112(3)	6174(2)	37(1)
C(10)	2625(1)	-4605(2)	2626(1)	20(1)
C(11)	2459(2)	-5444(3)	1996(2)	28(1)
C(12)	2863(2)	-6550(3)	1860(2)	33(1)
C(13)	3412(2)	-6864(3)	2361(2)	36(1)
C(14)	3578(2)	-6034(3)	2983(2)	37(1)
C(15)	3189(2)	-4894(3)	3105(2)	30(1)
C(16)	1283(1)	-3918(2)	2937(1)	21(1)
C(17)	724(1)	-3057(3)	2927(1)	25(1)
C(18)	110(2)	-3568(3)	3090(2)	29(1)
C(19)	56(2)	-4937(3)	3292(2)	29(1)
C(20)	604(1)	-5790(3)	3318(2)	27(1)
C(21)	1217(1)	-5285(2)	3135(1)	24(1)
C(22)	2427(2)	180(2)	1139(1)	26(1)
C(23)	2892(2)	471(3)	616(2)	34(1)
C(24)	2704(2)	1336(3)	7(2)	46(1)
C(25)	2070(2)	1898(3)	-87(2)	51(1)
C(26)	1612(2)	1621(3)	429(2)	44(1)
C(27)	1794(2)	766(3)	1046(2)	31(1)
C(28)	3413(1)	-1795(2)	1791(1)	23(1)
C(29)	4004(2)	-1541(3)	2249(2)	32(1)
C(30)	4584(2)	-2266(3)	2131(2)	41(1)
C(31)	4574(2)	-3234(3)	1564(2)	41(1)
C(32)	3990(2)	-3488(3)	1108(2)	39(1)
C(33)	3409(2)	-2775(3)	1220(2)	30(1)
O(2)	4416(2)	-8481(3)	1222(2)	81(1)
C(34)	4388(3)	-7234(5)	807(3)	114(2)
C(35)	4904(2)	-7153(5)	357(3)	89(2)
C(36)	5443(2)	-8119(4)	675(2)	61(1)
C(37)	5038(2)	-9126(3)	1102(2)	60(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table S7-3. Bond lengths (A) and angles (deg) for **7a**

Br(1)-Ni(1)	2.3743(5	Br(2)-Ni(1)	2.3545(4)
Ni(1)-N(1)	1.987(2)	Ni(1)-P(2)	2.3010(7)
P(1)-N(1)	1.596(2)	P(1)-C(10)	1.802(2)
P(1)-C(16)	1.807(3)	P(1)-C(1)	1.809(2)
P(2)-C(28)	1.810(3)	P(2)-C(22)	1.825(3)
P(2)-C(1)	1.838(3)	O(1)-C(6)	1.367(3)
O(1)-C(9)	1.421(3)	N(1)-C(2)	1.488(3)
C(2)-C(3)	1.521(4)	C(3)-C(4)	1.388(4)
C(3)-C(8)	1.391(4)	C(4)-C(5)	1.376(4)
C(5)-C(6)	1.393(4)	C(6)-C(7)	1.385(4)
C(7)-C(8)	1.396(4)	C(10)-C(15)	1.374(4)
C(10)-C(11)	1.398(4)	C(11)-C(12)	1.386(4)
C(12)-C(13)	1.379(4)	C(13)-C(14)	1.382(4)
C(14)-C(15)	1.389(4)	C(16)-C(21)	1.392(3)
C(16)-C(17)	1.399(4)	C(17)-C(18)	1.382(4)
C(18)-C(19)	1.394(4)	C(19)-C(20)	1.375(4)
C(20)-C(21)	1.387(4)	C(22)-C(27)	1.385(4)
C(22)-C(23)	1.401(4)	C(23)-C(24)	1.392(4)
C(24)-C(25)	1.379(5)	C(25)-C(26)	1.378(5)
C(26)-C(27)	1.395(4)	C(28)-C(33)	1.391(4)
C(28)-C(29)	1.392(4)	C(29)-C(30)	1.392(4)
C(30)-C(31)	1.378(4)	C(31)-C(32)	1.379(4)
C(32)-C(33)	1.384(4)	O(2)-C(34)	1.423(5)
O(2)-C(37)	1.429(5)	C(34)-C(35)	1.364(6)
C(35)-C(36)	1.502(5)	C(36)-C(37)	1.519(5)

N(1)-Ni(1)-P(2)	88.35(6)	N(1)-Ni(1)-Br(2)	108.68(6)
P(2)-Ni(1)-Br(2)	123.83(2)	N(1)-Ni(1)-Br(1)	106.44(7)
P(2)-Ni(1)-Br(1)	98.21(2)	Br(2)-Ni(1)-Br(1)	124.71(2)
N(1)-P(1)-C(10)	115.2(1)	N(1)-P(1)-C(16)	114.8(1)
C(10)-P(1)-C(16)	105.3(1)	N(1)-P(1)-C(1)	105.5(1)
C(10)-P(1)-C(1)	107.7(1)	C(16)-P(1)-C(1)	108.1(1)
C(28)-P(2)-C(22)	106.8(1)	C(28)-P(2)-C(1)	105.0(1)
C(22)-P(2)-C(1)	103.0(1)	C(28)-P(2)-Ni(1)	115.6(1)
C(22)-P(2)-Ni(1)	126.05(8)	C(1)-P(2)-Ni(1)	96.70(8)
C(6)-O(1)-C(9)	117.8(2)	C(2)-N(1)-P(1)	119.3(2)
C(2)-N(1)-Ni(1)	119.3(2)	P(1)-N(1)-Ni(1)	121.1(1)
P(1)-C(1)-P(2)	109.2(1)	N(1)-C(2)-C(3)	113.8(2)
C(4)-C(3)-C(8)	117.8(3)	C(4)-C(3)-C(2)	121.0(2)
C(8)-C(3)-C(2)	121.2(2)	C(5)-C(4)-C(3)	121.9(2)
C(4)-C(5)-C(6)	120.0(3)	O(1)-C(6)-C(7)	125.1(2)
O(1)-C(6)-C(5)	115.6(2)	C(7)-C(6)-C(5)	119.4(3)
C(6)-C(7)-C(8)	119.9(2)	C(3)-C(8)-C(7)	121.2(3)
C(15)-C(10)-C(11)	119.3(2)	C(15)-C(10)-P(1)	121.5(2)
C(11)-C(10)-P(1)	119.2(2)	C(12)-C(11)-C(10)	119.9(3)
C(13)-C(12)-C(11)	120.3(3)	C(12)-C(13)-C(14)	119.8(3)
C(13)-C(14)-C(15)	120.0(3)	C(10)-C(15)-C(14)	120.6(3)
C(21)-C(16)-C(17)	119.2(2)	C(21)-C(16)-P(1)	121.9(2)
C(17)-C(16)-P(1)	118.6(2)	C(18)-C(17)-C(16)	120.3(2)
C(17)-C(18)-C(19)	119.6(3)	C(20)-C(19)-C(18)	120.8(3)
C(19)-C(20)-C(21)	119.6(2)	C(20)-C(21)-C(16)	120.6(3)
C(27)-C(22)-C(23)	119.5(3)	C(27)-C(22)-P(2)	119.5(2)
C(23)-C(22)-P(2)	120.8(2)	C(24)-C(23)-C(22)	119.1(3)
C(25)-C(24)-C(23)	120.9(3)	C(26)-C(25)-C(24)	120.2(3)
C(25)-C(26)-C(27)	119.6(3)	C(22)-C(27)-C(26)	120.6(3)
C(33)-C(28)-C(29)	119.4(3)	C(33)-C(28)-P(2)	122.0(2)
C(29)-C(28)-P(2)	118.6(2)	C(30)-C(29)-C(28)	119.8(3)
C(31)-C(30)-C(29)	120.3(3)	C(30)-C(31)-C(32)	120.1(3)
C(31)-C(32)-C(33)	120.2(3)	C(32)-C(33)-C(28)	120.3(3)
C(34)-O(2)-C(37)	107.2(3)	C(35)-C(34)-O(2)	110.8(4)
C(34)-C(35)-C(36)	107.5(4)	C(35)-C(36)-C(37)	101.4(3)
O(2)-C(37)-C(36)	107.4(3)		

Table S7-4. Anisotropic displacement parameters (A^2 x 10^3) for **7a**

atom	U11	U22	U33	U23	U13	U12
Br(1)	32(1)	29(1)	35(1)	-4(1)	1(1)	8(1)
Br(2)	35(1)	38(1)	33(1)	-5(1)	-7(1)	-7(1)
Ni(1)	27(1)	20(1)	21(1)	-2(1)	1(1)	-1(1)
P(1)	21(1)	17(1)	18(1)	1(1)	1(1)	0(1)
P(2)	24(1)	20(1)	18(1)	1(1)	2(1)	-2(1)
O(1)	37(1)	38(1)	37(1)	-4(1)	12(1)	0(1)
N(1)	27(1)	19(1)	16(1)	0(1)	2(1)	1(1)
C(1)	25(2)	20(1)	19(1)	2(1)	2(1)	2(1)
C(2)	33(2)	26(1)	19(1)	1(1)	2(1)	5(1)
C(3)	30(2)	24(1)	16(1)	2(1)	1(1)	3(1)
C(4)	43(2)	21(1)	19(1)	0(1)	3(1)	0(1)
C(5)	38(2)	27(1)	23(1)	3(1)	3(1)	-5(1)
C(6)	30(2)	32(2)	17(1)	1(1)	2(1)	4(1)
C(7)	32(2)	22(1)	23(1)	0(1)	2(1)	4(1)
C(8)	32(2)	25(1)	22(1)	1(1)	3(1)	-3(1)
C(9)	39(2)	43(2)	30(2)	-5(1)	7(1)	9(1)
C(10)	20(2)	19(1)	23(1)	1(1)	6(1)	-1(1)
C(11)	28(2)	24(1)	31(2)	-5(1)	0(1)	0(1)
C(12)	37(2)	25(1)	39(2)	-11(1)	10(1)	-3(1)
C(13)	33(2)	26(2)	49(2)	-2(1)	11(2)	7(1)
C(14)	27(2)	39(2)	44(2)	-2(1)	-1(1)	9(1)
C(15)	27(2)	31(2)	31(2)	-4(1)	1(1)	2(1)
C(16)	22(2)	23(1)	18(1)	1(1)	3(1)	0(1)
C(17)	28(2)	23(1)	25(1)	0(1)	2(1)	0(1)
C(18)	25(2)	30(2)	32(2)	-1(1)	6(1)	3(1)
C(19)	25(2)	34(2)	31(2)	0(1)	7(1)	-6(1)
C(20)	30(2)	23(1)	30(2)	0(1)	6(1)	-6(1)
C(21)	25(2)	25(1)	23(1)	-1(1)	3(1)	0(1)
C(22)	41(2)	15(1)	19(1)	-2(1)	0(1)	-4(1)
C(23)	57(2)	23(1)	25(2)	-2(1)	13(2)	-3(1)
C(24)	93(3)	23(2)	25(2)	-1(1)	15(2)	-10(2)
C(25)	103(3)	21(2)	25(2)	3(1)	-13(2)	-5(2)
C(26)	64(2)	22(1)	41(2)	2(1)	-21(2)	2(2)
C(27)	39(2)	23(1)	30(2)	2(1)	-7(1)	-7(1)
C(28)	24(2)	25(1)	21(1)	4(1)	6(1)	-4(1)
C(29)	29(2)	39(2)	28(2)	-1(1)	4(1)	-2(1)
C(30)	24(2)	58(2)	40(2)	2(2)	5(1)	2(2)
C(31)	34(2)	45(2)	44(2)	4(1)	13(2)	9(2)
C(32)	40(2)	38(2)	40(2)	-5(1)	14(2)	5(2)
C(33)	30(2)	33(2)	27(2)	-3(1)	6(1)	-2(1)
O(2)	56(2)	71(2)	118(3)	47(2)	17(2)	6(2)
C(34)	74(4)	118(4)	158(5)	102(4)	48(4)	38(3)
C(35)	55(3)	98(3)	118(4)	67(3)	26(3)	25(3)
C(36)	47(3)	70(3)	66(3)	7(2)	5(2)	15(2)
C(37)	67(3)	35(2)	76(3)	4(2)	-2(2)	9(2)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table S7-5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**

atom	x	y	z	U(eq)
H(1A)	1549	-1710	1890	26
H(1B)	2022	-2757	1488	26
H(2A)	2849	-2244	4524	31
H(2B)	2473	-3632	4267	31
H(4)	1371	-4046	4632	33
H(5)	460	-3436	5273	35
H(7)	1204	399	5536	31
H(8)	2120	-234	4884	32
H(9A)	499	245	6567	56
H(9B)	-301	170	6403	56
H(9C)	140	820	5784	56
H(11)	2069	-5256	1662	34
H(12)	2762	-7094	1419	40
H(13)	3675	-7649.0005	2279	43
H(14)	3958	-6243	3327	45
H(15)	3313	-4309	3524	36
H(17)	767	-2118	2806	30
H(18)	-273	-2990	3065	35
H(19)	-365	-5286	3412	35
H(20)	564	-6720	3461	33
H(21)	1594	-5876	3145	29
H(23)	3328	84	675	41
H(24)	3018	1541	-349.0000	56
H(25)	1948	2479	-508	61
H(26)	1175	2010	365	53
H(27)	1481	585	1405	38
H(29)	4013	-875	2640	38
H(30)	4988	-2093	2443	49
H(31)	4971	-3728	1487	49
H(32)	3985	-4154	717	47
H(33)	3007	-2956	906	36
H(34A)	3955	-7177	487	137
H(34B)	4412	-6455	1165	137
H(35A)	5080	-6208	356	107
H(35B)	4747	-7410	-172	107
H(36A)	5784	-7646	1022	73
H(36B)	5665	-8575	267	73
H(37A)	4955	-9972	801	72
H(37B)	5286	-9368	1595	72