Supporting Information

Adaptable Ligand Donor Strength: Tracking Transannular Bond Interactions in Tris(2-pyridylmethyl)-azaphosphatrane (TPAP)

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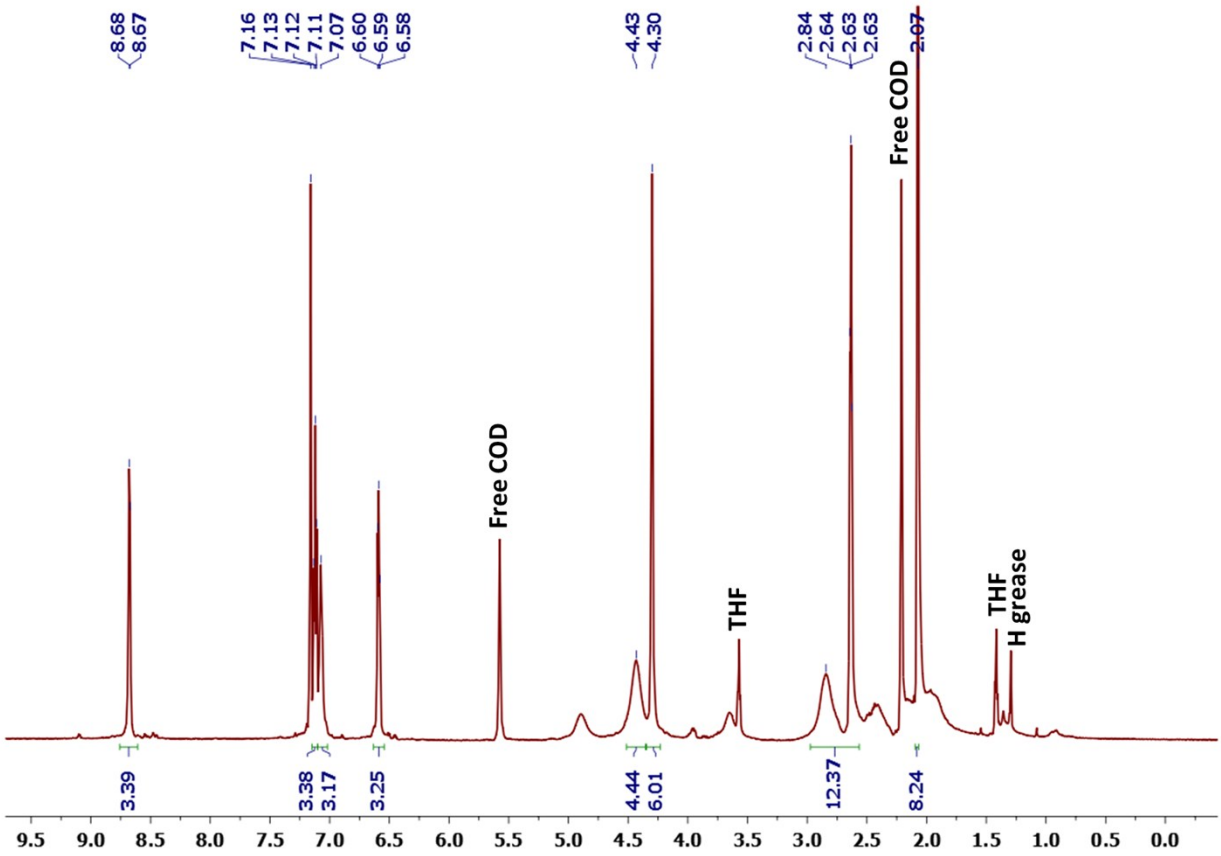

Figure S1. ^{1}H NMR spectrum of [NiTPAP(COD)] (**3**) in C_6D_6.

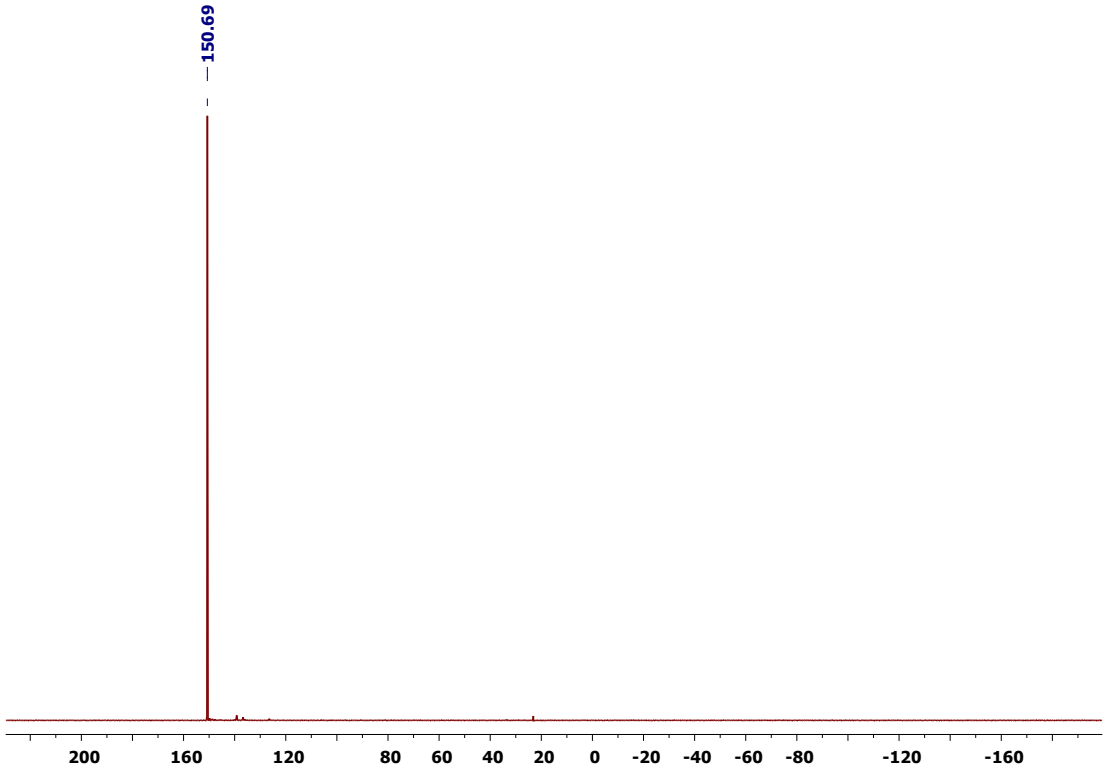

Figure S2. $^{31}P\{^{1}H\}$ spectrum of [NiTPAP(COD)] (**3**) in C_6D_6.

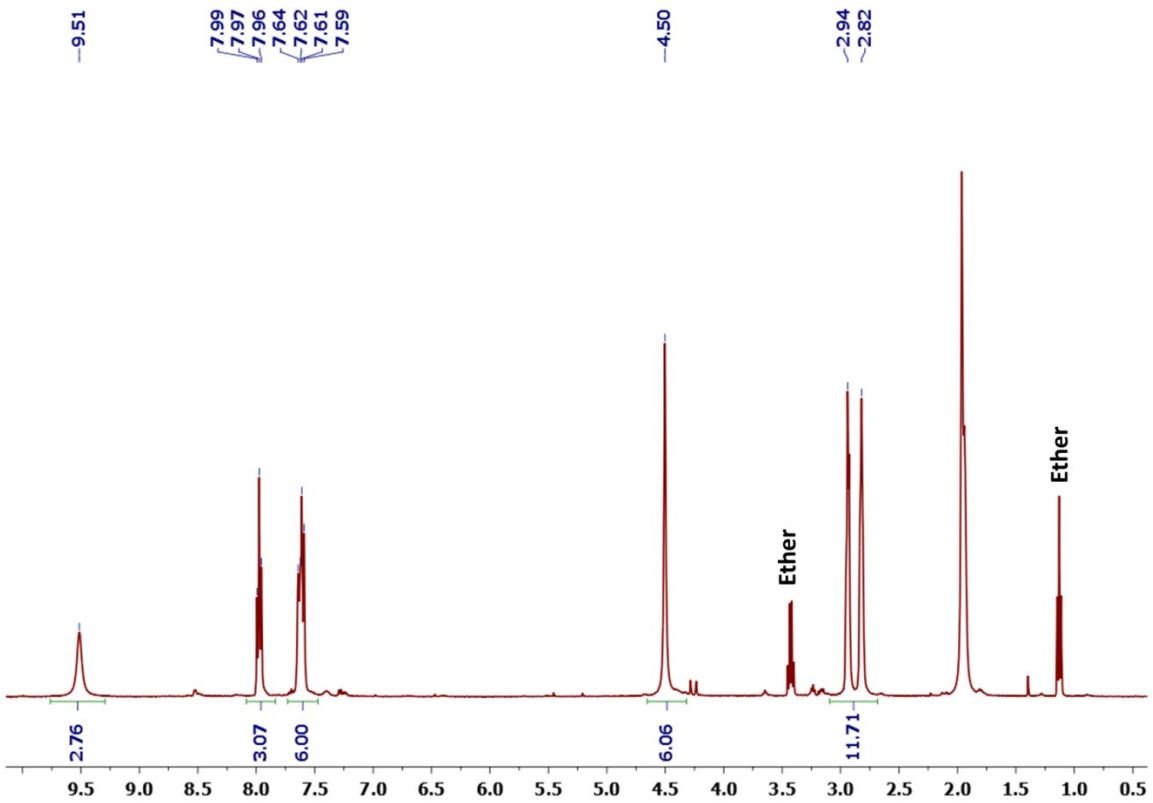

Figure S3. ^{1}H NMR of spectrum of $[NiTPAP(CH_3CN)][BF_4]_2$ (**4**) in CD_3CN.

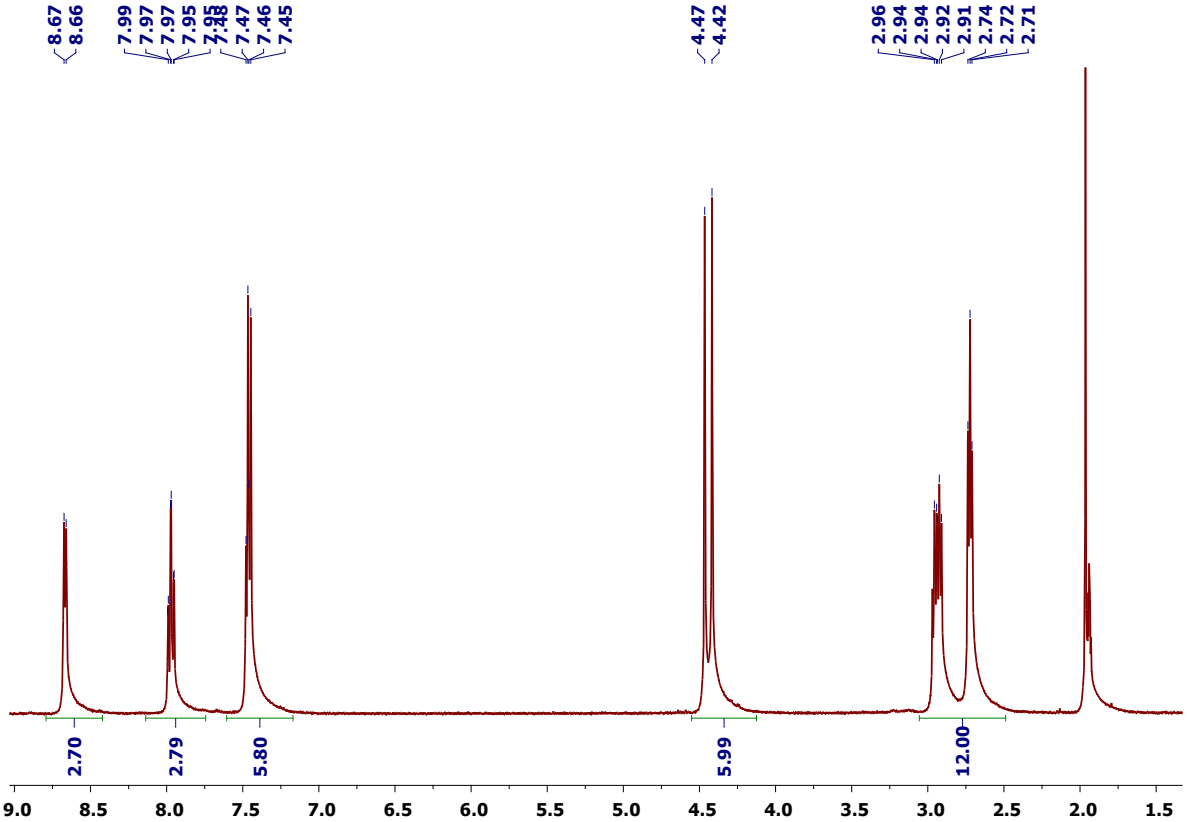

Figure S4. ^{1}H NMR spectrum of $[PdTPAP(CH_3CN)][BF_4]_2$ (**5**) in CD_3CN.

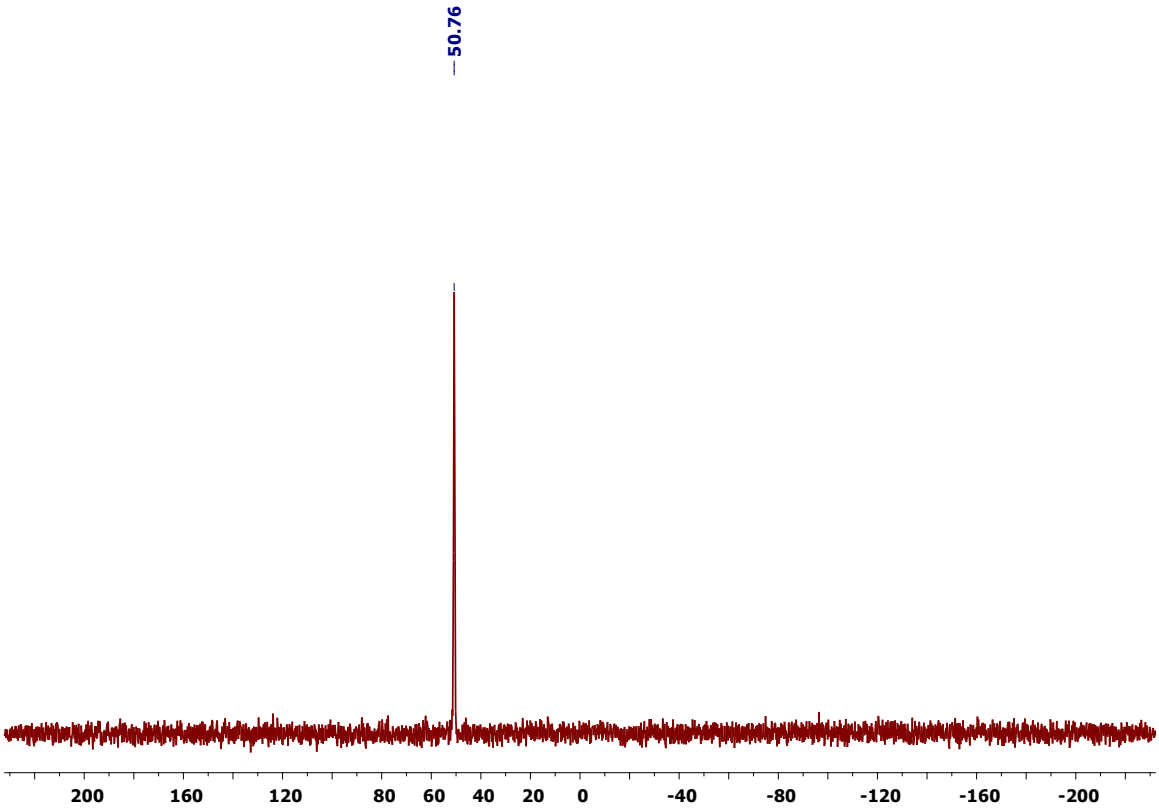

Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of $[PdTPAP(CH_3CN)][BF_4]_2$ (**5**) in CD_3CN.

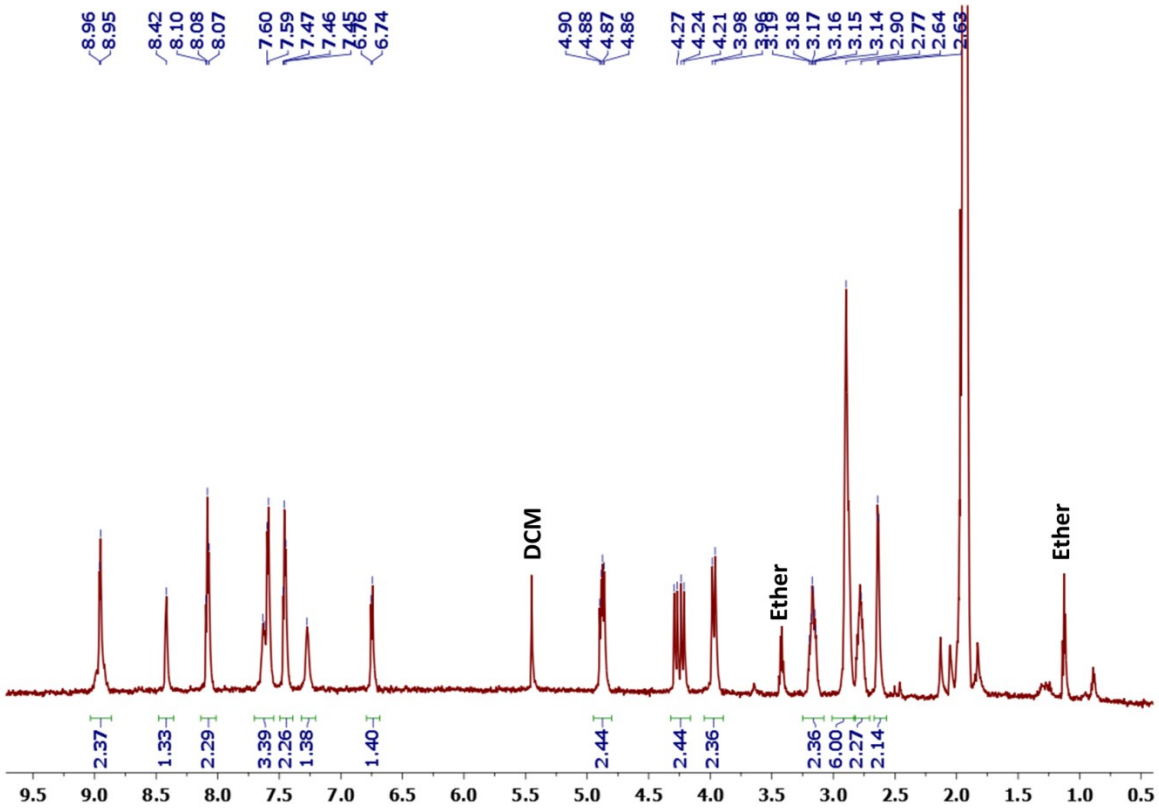

Figure S6. ^{1}H NMR spectrum of $[PtTPAPCl][PF_6]_2$ (**6**) in CD_3CN.

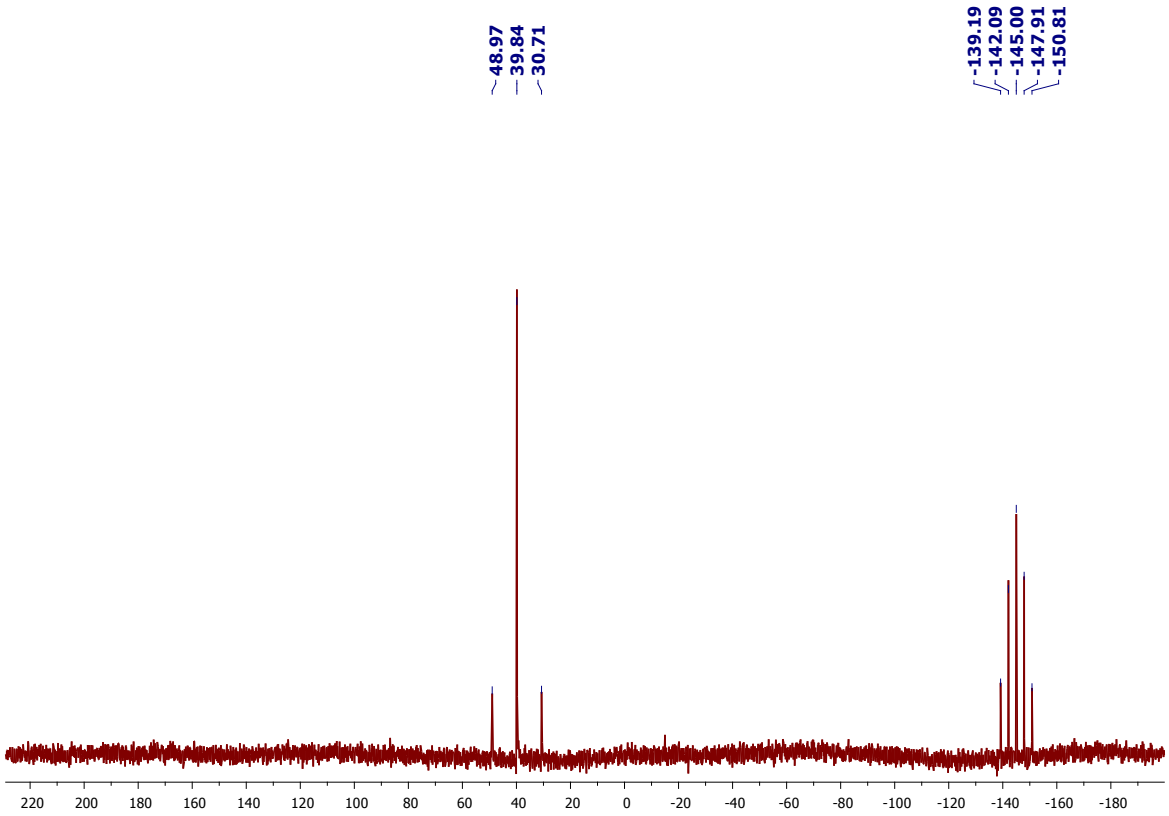

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of $[PtTPAPCl][PF_6]_2$ (**6**) in CD_3CN.

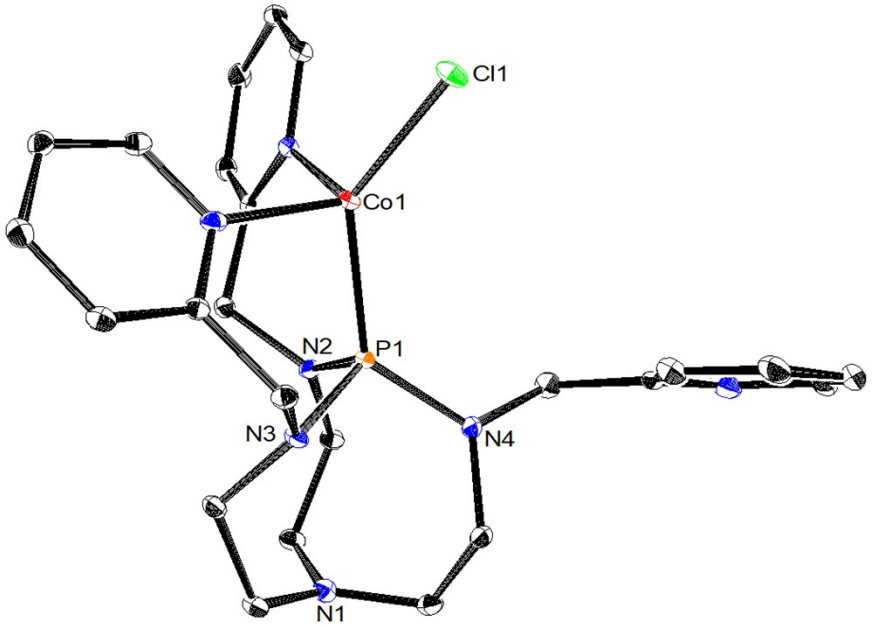

Figure S8. ORTEP of complexes **1b** Thermal ellipsoids drawn at 50% probability. Hydrogen atoms are omitted for clarity. Grown from a pentane diffusion into a concentrated THF solution.

Table S1. Crystal data and structure refinement for **1b**

Identification code	15073z	
Empirical formula	C_{24} H_{30} Cl Co N_7 P	
Formula weight	541.90	
Temperature	123(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.8827(5) Å	α = 90°.
	b = 14.0100(7) Å	β = 100.490(2)°.
	c = 17.8800(9) Å	γ = 90°.
Volume	2434.2(2) $Å^3$	
Z	4	
Density (calculated)	1.479 Mg/m^3	
Absorption coefficient	7.379 mm^{-1}	
F(000)	1128	
Crystal color	Purple	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	4.035 to 68.429°	
Index ranges	$-11 \le h \le 11$, $-16 \le k \le 16$, $-16 \le l \le 21$	
Reflections collected	17925	
Independent reflections	4398 [R(int) = 0.0486]	
Completeness to theta = 67.679°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7531 and 0.3350	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4398 / 0 / 307	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I) = 4161 data]	R1 = 0.0420, wR2 = 0.1070	
R indices (all data, 0.83 Å)	R1 = 0.0445, wR2 = 0.1092	
Largest diff. peak and hole	0.561 and -0.856 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Co(1)	5061(1)	8383(1)	1946(1)	16(1)
Cl(1)	5434(1)	7064(1)	2669(1)	25(1)
P(1)	4399(1)	9843(1)	2090(1)	15(1)
N(1)	3779(2)	12184(2)	1926(1)	22(1)
N(2)	3319(2)	10174(2)	1290(1)	17(1)
N(3)	5811(2)	10554(2)	2163(1)	17(1)
N(4)	3634(2)	10291(2)	2786(1)	19(1)
N(5)	3801(2)	8072(2)	930(1)	18(1)
N(6)	6823(2)	8747(2)	1578(1)	19(1)
N(7)	1293(3)	9517(2)	4025(2)	32(1)
C(1)	2813(3)	11943(2)	1246(2)	22(1)
C(2)	2268(3)	10917(2)	1229(2)	19(1)
C(3)	5222(3)	12274(2)	1892(2)	21(1)
C(4)	5899(3)	11370(2)	1659(2)	20(1)
C(5)	3361(3)	12090(2)	2654(2)	22(1)
C(6)	3963(3)	11234(2)	3130(1)	20(1)
C(7)	3618(3)	9758(2)	583(1)	19(1)
C(8)	3154(3)	8734(2)	441(1)	17(1)
C(9)	2165(3)	8489(2)	-183(2)	23(1)
C(10)	1862(3)	7536(2)	-336(2)	26(1)
C(11)	2549(3)	6855(2)	143(2)	25(1)
C(12)	3492(3)	7148(2)	772(2)	21(1)
C(13)	7108(3)	10077(2)	2471(2)	19(1)
C(14)	7652(3)	9461(2)	1896(1)	16(1)
C(15)	8934(3)	9627(2)	1701(2)	20(1)
C(16)	9394(3)	9046(2)	1172(2)	23(1)
C(17)	8544(3)	8321(2)	841(2)	22(1)
C(18)	7278(3)	8199(2)	1052(2)	21(1)
C(19)	2395(3)	9837(2)	2944(2)	24(1)
C(20)	2507(3)	9540(2)	3773(2)	23(1)
C(21)	3731(3)	9316(2)	4221(2)	27(1)
C(22)	3771(4)	9082(2)	4960(2)	34(1)
C(23)	2566(4)	9067(2)	5246(2)	34(1)
C(24)	1359(4)	9260(2)	4768(2)	36(1)

Table S3. Bond lengths [Å] and angles [°] for **1b**

Co(1)-N(6)	2.036(2)	N(6)-Co(1)-N(5)	100.57(8)
Co(1)-N(5)	2.054(2)	N(6)-Co(1)-P(1)	95.54(6)
Co(1)-P(1)	2.1768(7)	N(5)-Co(1)-P(1)	99.07(6)
Co(1)-Cl(1)	2.2470(7)	N(6)-Co(1)-Cl(1)	109.37(6)
P(1)-N(2)	1.687(2)	N(5)-Co(1)-Cl(1)	110.09(6)
P(1)-N(4)	1.689(2)	P(1)-Co(1)-Cl(1)	136.55(3)
P(1)-N(3)	1.700(2)	N(2)-P(1)-N(4)	102.95(11)
P(1)-N(1)	3.339(2)	N(2)-P(1)-N(3)	106.70(11)
N(1)-C(5)	1.442(3)	N(4)-P(1)-N(3)	101.35(10)
N(1)-C(1)	1.443(3)	N(2)-P(1)-Co(1)	108.36(8)
N(1)-C(3)	1.444(3)	N(4)-P(1)-Co(1)	128.35(8)
N(2)-C(2)	1.461(3)	N(3)-P(1)-Co(1)	107.43(8)
N(2)-C(7)	1.471(3)	N(2)-P(1)-N(1)	65.05(8)
N(3)-C(13)	1.462(3)	N(4)-P(1)-N(1)	66.44(8)
N(3)-C(4)	1.467(3)	N(3)-P(1)-N(1)	64.27(8)
N(4)-C(19)	1.453(3)	Co(1)-P(1)-N(1)	165.15(5)
N(4)-C(6)	1.468(3)	C(5)-N(1)-C(1)	119.0(2)
N(5)-C(12)	1.349(3)	C(5)-N(1)-C(3)	119.6(2)
N(5)-C(8)	1.353(3)	C(1)-N(1)-C(3)	119.4(2)
N(6)-C(14)	1.352(3)	C(5)-N(1)-P(1)	84.83(14)
N(6)-C(18)	1.352(3)	C(1)-N(1)-P(1)	85.82(14)
N(7)-C(20)	1.356(4)	C(3)-N(1)-P(1)	85.57(14)
N(7)-C(24)	1.367(4)	C(2)-N(2)-C(7)	118.0(2)
C(1)-C(2)	1.533(4)	C(2)-N(2)-P(1)	126.19(17)
C(3)-C(4)	1.525(4)	C(7)-N(2)-P(1)	115.18(17)
C(5)-C(6)	1.528(4)	C(13)-N(3)-C(4)	116.2(2)
C(7)-C(8)	1.513(4)	C(13)-N(3)-P(1)	114.32(16)
C(8)-C(9)	1.386(4)	C(4)-N(3)-P(1)	123.34(17)
C(9)-C(10)	1.384(4)	C(19)-N(4)-C(6)	116.2(2)
C(10)-C(11)	1.377(4)	C(19)-N(4)-P(1)	119.11(18)
C(11)-C(12)	1.385(4)	C(6)-N(4)-P(1)	123.27(17)
C(13)-C(14)	1.514(3)	C(12)-N(5)-C(8)	117.4(2)
C(14)-C(15)	1.393(4)	C(12)-N(5)-Co(1)	117.89(17)
C(15)-C(16)	1.384(4)	C(8)-N(5)-Co(1)	124.40(17)
C(16)-C(17)	1.381(4)	C(14)-N(6)-C(18)	117.3(2)
C(17)-C(18)	1.381(4)	C(14)-N(6)-Co(1)	122.55(17)
C(19)-C(20)	1.524(4)	C(18)-N(6)-Co(1)	119.71(18)
C(20)-C(21)	1.360(4)	C(20)-N(7)-C(24)	116.1(3)
C(21)-C(22)	1.356(4)	N(1)-C(1)-C(2)	114.3(2)
C(22)-C(23)	1.379(5)	N(2)-C(2)-C(1)	115.1(2)
C(23)-C(24)	1.362(5)	N(1)-C(3)-C(4)	115.1(2)
		N(3)-C(4)-C(3)	113.6(2)

N(1)-C(5)-C(6)	115.3(2)	C(15)-C(14)-C(13)	121.8(2)
N(4)-C(6)-C(5)	116.1(2)	C(16)-C(15)-C(14)	120.0(2)
N(2)-C(7)-C(8)	114.7(2)	C(17)-C(16)-C(15)	118.4(2)
N(5)-C(8)-C(9)	122.1(2)	C(18)-C(17)-C(16)	118.9(2)
N(5)-C(8)-C(7)	116.7(2)	N(6)-C(18)-C(17)	123.5(3)
C(9)-C(8)-C(7)	121.2(2)	N(4)-C(19)-C(20)	113.3(2)
C(10)-C(9)-C(8)	119.6(3)	N(7)-C(20)-C(21)	123.1(3)
C(11)-C(10)-C(9)	118.7(3)	N(7)-C(20)-C(19)	114.6(3)
C(10)-C(11)-C(12)	118.8(3)	C(21)-C(20)-C(19)	122.3(2)
N(5)-C(12)-C(11)	123.2(2)	C(22)-C(21)-C(20)	119.6(3)
N(3)-C(13)-C(14)	113.6(2)	C(21)-C(22)-C(23)	119.4(3)
N(6)-C(14)-C(15)	121.8(2)	C(24)-C(23)-C(22)	118.7(3)
N(6)-C(14)-C(13)	116.4(2)	C(23)-C(24)-N(7)	123.0(3)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	18(1)	11(1)	19(1)	2(1)	2(1)	0(1)
Cl(1)	23(1)	18(1)	31(1)	10(1)	-1(1)	1(1)
P(1)	17(1)	12(1)	16(1)	1(1)	4(1)	0(1)
N(1)	22(1)	21(1)	22(1)	0(1)	4(1)	-2(1)
N(2)	22(1)	13(1)	15(1)	-1(1)	3(1)	2(1)
N(3)	16(1)	12(1)	24(1)	3(1)	4(1)	0(1)
N(4)	20(1)	18(1)	20(1)	-2(1)	9(1)	-4(1)
N(5)	20(1)	15(1)	20(1)	1(1)	7(1)	0(1)
N(6)	24(1)	13(1)	19(1)	1(1)	1(1)	2(1)
N(7)	31(1)	21(1)	45(2)	4(1)	11(1)	1(1)
C(1)	25(1)	16(1)	25(1)	2(1)	1(1)	2(1)
C(2)	19(1)	16(1)	22(1)	2(1)	0(1)	3(1)
C(3)	21(1)	15(1)	27(1)	2(1)	4(1)	-3(1)
C(4)	21(1)	16(1)	24(1)	2(1)	6(1)	-3(1)
C(5)	22(1)	18(1)	26(1)	-5(1)	5(1)	0(1)
C(6)	22(1)	20(1)	18(1)	-4(1)	6(1)	-3(1)
C(7)	27(1)	16(1)	15(1)	2(1)	4(1)	0(1)
C(8)	21(1)	18(1)	14(1)	-1(1)	9(1)	0(1)
C(9)	30(2)	24(1)	16(1)	3(1)	5(1)	1(1)
C(10)	31(2)	30(2)	16(1)	-4(1)	2(1)	-7(1)
C(11)	36(2)	18(1)	22(1)	-5(1)	8(1)	-8(1)
C(12)	24(1)	16(1)	22(1)	2(1)	5(1)	0(1)
C(13)	18(1)	19(1)	21(1)	-2(1)	2(1)	-2(1)
C(14)	17(1)	14(1)	18(1)	3(1)	1(1)	3(1)
C(15)	17(1)	17(1)	25(1)	2(1)	-1(1)	1(1)
C(16)	19(1)	22(1)	28(1)	6(1)	5(1)	4(1)
C(17)	24(1)	20(1)	22(1)	1(1)	6(1)	6(1)
C(18)	22(1)	18(1)	23(1)	-1(1)	0(1)	2(1)
C(19)	21(1)	26(1)	25(1)	-1(1)	3(1)	-2(1)
C(20)	32(2)	13(1)	28(1)	-4(1)	16(1)	-6(1)
C(21)	28(2)	22(1)	32(2)	2(1)	6(1)	-3(1)
C(22)	42(2)	23(2)	37(2)	0(1)	7(1)	-11(1)
C(23)	58(2)	22(2)	25(1)	2(1)	16(1)	-4(1)
C(24)	47(2)	21(2)	49(2)	6(1)	31(2)	1(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **1b**

	x	y	z	U(eq)
H(1A)	3264	12039	801	27
H(1B)	2023	12388	1195	27
H(2A)	1757	10837	1652	23
H(2B)	1606	10822	748	23
H(3A)	5721	12476	2398	25
H(3B)	5330	12786	1526	25
H(4A)	5456	11195	1135	24
H(4B)	6881	11505	1654	24
H(5A)	2345	12045	2569	26
H(5B)	3629	12679	2952	26
H(6A)	4976	11303	3244	24
H(6B)	3633	11253	3621	24
H(7A)	4623	9789	596	23
H(7B)	3166	10152	149	23
H(9A)	1698	8971	-503	28
H(10A)	1193	7356	-765	31
H(11A)	2378	6195	45	30
H(12A)	3944	6674	1107	25
H(13A)	6973	9673	2906	23
H(13B)	7807	10566	2666	23
H(15A)	9492	10138	1930	24
H(16A)	10273	9144	1041	27
H(17A)	8825	7913	473	26
H(18A)	6697	7704	816	25
H(19A)	2195	9265	2618	29
H(19B)	1613	10284	2810	29
H(21A)	4554	9325	4016	32
H(22A)	4622	8929	5279	41
H(23A)	2577	8925	5767	41
H(24A)	526	9214	4959	44

Table S6. Crystal data and structure refinement for **1**

Identification code	jyy148	
Empirical formula	C_{24} H_{30} Cl Co N_7 P	
Formula weight	541.90	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 9.1020(16) Å	α = 90°.
	b = 16.434(3) Å	β = 90°.
	c = 33.454(6) Å	γ = 90°.
Volume	5004.1(16) $Å^3$	
Z	8	
Density (calculated)	1.439 Mg/m^3	
Absorption coefficient	0.884 mm^{-1}	
F(000)	2256	
Crystal color	purple	
Crystal size	0.301 x 0.180 x 0.164 mm^3	
Theta range for data collection	1.217 to 28.820°	
Index ranges	$-11 \le h \le 11$, $-22 \le k \le 21$, $-45 \le l \le 45$	
Reflections collected	56948	
Independent reflections	6257 [R(int) = 0.0358]	
Completeness to theta = 25.500°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6892	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6257 / 0 / 307	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I) = 5454 data]	R1 = 0.0315, wR2 = 0.0745	
R indices (all data, 0.74 Å)	R1 = 0.0387, wR2 = 0.0776	
Largest diff. peak and hole	0.698 and -0.284 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Co(1)	6443(1)	7590(1)	3444(1)	13(1)
Cl(1)	5402(1)	8665(1)	3133(1)	22(1)
P(1)	6610(1)	6930(1)	4003(1)	11(1)
N(1)	7494(2)	5782(1)	4763(1)	16(1)
N(2)	8112(1)	7256(1)	4265(1)	13(1)
N(3)	6968(2)	5942(1)	3904(1)	14(1)
N(4)	5286(1)	6899(1)	4356(1)	14(1)
N(5)	8622(1)	7857(1)	3415(1)	15(1)
N(6)	6150(2)	6572(1)	3095(1)	19(1)
N(7)	2603(2)	5774(1)	4410(1)	20(1)
C(1)	8832(2)	6249(1)	4786(1)	15(1)
C(2)	9262(2)	6699(1)	4402(1)	14(1)
C(3)	7411(2)	5082(1)	4502(1)	16(1)
C(4)	6455(2)	5244(1)	4134(1)	15(1)
C(5)	6165(2)	6078(1)	4947(1)	17(1)
C(6)	5581(2)	6885(1)	4787(1)	16(1)
C(7)	8621(2)	8062(1)	4137(1)	14(1)
C(8)	9415(2)	8080(1)	3740(1)	14(1)
C(9)	10871(2)	8322(1)	3708(1)	21(1)
C(10)	11550(2)	8346(1)	3337(1)	26(1)
C(11)	10735(2)	8127(1)	3004(1)	25(1)
C(12)	9291(2)	7889(1)	3056(1)	20(1)
C(13)	7754(2)	5784(1)	3531(1)	16(1)
C(14)	6730(2)	5829(1)	3177(1)	18(1)
C(15)	6366(2)	5144(1)	2956(1)	28(1)
C(16)	5371(3)	5210(1)	2645(1)	43(1)
C(17)	4767(3)	5961(1)	2564(1)	46(1)
C(18)	5179(2)	6624(1)	2793(1)	30(1)
C(19)	3782(2)	7038(1)	4217(1)	18(1)
C(20)	2960(2)	6270(1)	4106(1)	17(1)
C(21)	2609(2)	6093(1)	3711(1)	24(1)
C(22)	1847(2)	5384(1)	3624(1)	29(1)
C(23)	1465(2)	4872(1)	3936(1)	26(1)
C(24)	1872(2)	5092(1)	4320(1)	22(1)

Table S8. Bond lengths [Å] and angles [°] for **1**

Co(1)-N(5)	2.0334(14)	N(5)-Co(1)-N(6)	105.95(6)
Co(1)-N(6)	2.0568(14)	N(5)-Co(1)-P(1)	94.63(4)
Co(1)-P(1)	2.1675(5)	N(6)-Co(1)-P(1)	95.30(4)
Co(1)-Cl(1)	2.2589(5)	N(5)-Co(1)-Cl(1)	102.62(4)
P(1)-N(4)	1.6879(13)	N(6)-Co(1)-Cl(1)	108.66(4)
P(1)-N(3)	1.6892(13)	P(1)-Co(1)-Cl(1)	144.910(18)
P(1)-N(2)	1.7089(13)	N(4)-P(1)-N(3)	104.23(7)
P(1)-N(1)	3.2647(14)	N(4)-P(1)-N(2)	102.87(7)
N(1)-C(1)	1.441(2)	N(3)-P(1)-N(2)	104.30(7)
N(1)-C(5)	1.442(2)	N(4)-P(1)-Co(1)	124.66(5)
N(1)-C(3)	1.445(2)	N(3)-P(1)-Co(1)	109.00(5)
N(2)-C(2)	1.4640(19)	N(2)-P(1)-Co(1)	109.94(5)
N(2)-C(7)	1.4677(19)	N(4)-P(1)-N(1)	67.31(5)
N(3)-C(4)	1.4563(19)	N(3)-P(1)-N(1)	63.21(5)
N(3)-C(13)	1.4629(19)	N(2)-P(1)-N(1)	65.53(5)
N(4)-C(19)	1.4638(19)	Co(1)-P(1)-N(1)	167.92(3)
N(4)-C(6)	1.4651(19)	C(1)-N(1)-C(5)	120.44(13)
N(5)-C(12)	1.348(2)	C(1)-N(1)-C(3)	119.96(13)
N(5)-C(8)	1.3557(19)	C(5)-N(1)-C(3)	118.87(13)
N(6)-C(18)	1.346(2)	C(1)-N(1)-P(1)	86.71(8)
N(6)-C(14)	1.358(2)	C(5)-N(1)-P(1)	86.11(8)
N(7)-C(24)	1.337(2)	C(3)-N(1)-P(1)	88.70(8)
N(7)-C(20)	1.344(2)	C(2)-N(2)-C(7)	115.51(12)
C(1)-C(2)	1.533(2)	C(2)-N(2)-P(1)	122.42(10)
C(3)-C(4)	1.532(2)	C(7)-N(2)-P(1)	112.72(10)
C(5)-C(6)	1.527(2)	C(4)-N(3)-C(13)	117.82(12)
C(7)-C(8)	1.512(2)	C(4)-N(3)-P(1)	126.31(10)
C(8)-C(9)	1.387(2)	C(13)-N(3)-P(1)	115.61(10)
C(9)-C(10)	1.387(2)	C(19)-N(4)-C(6)	119.08(12)
C(10)-C(11)	1.384(3)	C(19)-N(4)-P(1)	116.16(10)
C(11)-C(12)	1.383(2)	C(6)-N(4)-P(1)	123.87(11)
C(13)-C(14)	1.509(2)	C(12)-N(5)-C(8)	117.63(14)
C(14)-C(15)	1.388(2)	C(12)-N(5)-Co(1)	119.42(11)
C(15)-C(16)	1.384(3)	C(8)-N(5)-Co(1)	122.66(11)
C(16)-C(17)	1.379(3)	C(18)-N(6)-C(14)	117.55(14)
C(17)-C(18)	1.382(3)	C(18)-N(6)-Co(1)	117.46(12)
C(19)-C(20)	1.515(2)	C(14)-N(6)-Co(1)	124.50(11)
C(20)-C(21)	1.389(2)	C(24)-N(7)-C(20)	117.27(15)
C(21)-C(22)	1.387(3)	N(1)-C(1)-C(2)	115.29(12)
C(22)-C(23)	1.384(3)	N(2)-C(2)-C(1)	112.43(12)
C(23)-C(24)	1.387(3)	N(1)-C(3)-C(4)	112.15(12)
		N(3)-C(4)-C(3)	112.19(13)

N(1)-C(5)-C(6)	115.72(13)	C(15)-C(14)-C(13)	121.74(15)
N(4)-C(6)-C(5)	115.02(13)	C(16)-C(15)-C(14)	119.58(18)
N(2)-C(7)-C(8)	115.08(12)	C(17)-C(16)-C(15)	118.57(18)
N(5)-C(8)-C(9)	121.54(15)	C(16)-C(17)-C(18)	119.28(19)
N(5)-C(8)-C(7)	116.36(14)	N(6)-C(18)-C(17)	123.03(18)
C(9)-C(8)-C(7)	122.10(14)	N(4)-C(19)-C(20)	114.20(13)
C(10)-C(9)-C(8)	120.28(16)	N(7)-C(20)-C(21)	122.51(16)
C(11)-C(10)-C(9)	118.18(16)	N(7)-C(20)-C(19)	116.03(14)
C(12)-C(11)-C(10)	118.90(16)	C(21)-C(20)-C(19)	121.46(15)
N(5)-C(12)-C(11)	123.46(16)	C(22)-C(21)-C(20)	119.38(16)
N(3)-C(13)-C(14)	111.09(13)	C(23)-C(22)-C(21)	118.57(17)
N(6)-C(14)-C(15)	121.98(16)	C(22)-C(23)-C(24)	118.22(17)
N(6)-C(14)-C(13)	116.25(13)	N(7)-C(24)-C(23)	124.06(16)

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	14(1)	12(1)	13(1)	2(1)	-2(1)	0(1)
Cl(1)	21(1)	20(1)	25(1)	9(1)	0(1)	4(1)
P(1)	12(1)	9(1)	12(1)	0(1)	0(1)	0(1)
N(1)	16(1)	14(1)	16(1)	-1(1)	3(1)	0(1)
N(2)	14(1)	10(1)	14(1)	1(1)	-1(1)	-1(1)
N(3)	19(1)	10(1)	12(1)	-1(1)	1(1)	0(1)
N(4)	12(1)	17(1)	14(1)	1(1)	2(1)	1(1)
N(5)	16(1)	13(1)	15(1)	0(1)	-1(1)	-1(1)
N(6)	23(1)	18(1)	15(1)	1(1)	-3(1)	-4(1)
N(7)	15(1)	24(1)	21(1)	4(1)	0(1)	1(1)
C(1)	18(1)	16(1)	12(1)	1(1)	-2(1)	1(1)
C(2)	13(1)	15(1)	16(1)	1(1)	-2(1)	0(1)
C(3)	19(1)	12(1)	17(1)	2(1)	0(1)	1(1)
C(4)	19(1)	9(1)	18(1)	1(1)	-1(1)	-1(1)
C(5)	20(1)	18(1)	13(1)	3(1)	4(1)	1(1)
C(6)	19(1)	17(1)	13(1)	-2(1)	4(1)	3(1)
C(7)	18(1)	11(1)	15(1)	-1(1)	-1(1)	-3(1)
C(8)	17(1)	10(1)	16(1)	1(1)	-2(1)	-1(1)
C(9)	19(1)	20(1)	23(1)	0(1)	-4(1)	-5(1)
C(10)	18(1)	28(1)	32(1)	1(1)	4(1)	-6(1)
C(11)	24(1)	28(1)	22(1)	0(1)	9(1)	-1(1)
C(12)	22(1)	23(1)	15(1)	-2(1)	1(1)	0(1)
C(13)	17(1)	15(1)	16(1)	-3(1)	2(1)	1(1)
C(14)	22(1)	18(1)	14(1)	-2(1)	2(1)	-3(1)
C(15)	46(1)	19(1)	20(1)	-4(1)	-2(1)	-4(1)
C(16)	74(2)	28(1)	28(1)	-6(1)	-18(1)	-15(1)
C(17)	71(2)	35(1)	31(1)	3(1)	-33(1)	-14(1)
C(18)	41(1)	25(1)	23(1)	4(1)	-16(1)	-6(1)
C(19)	13(1)	18(1)	22(1)	2(1)	1(1)	3(1)
C(20)	10(1)	21(1)	21(1)	1(1)	2(1)	4(1)
C(21)	24(1)	30(1)	19(1)	2(1)	3(1)	2(1)
C(22)	27(1)	36(1)	23(1)	-7(1)	-3(1)	3(1)
C(23)	18(1)	21(1)	38(1)	-4(1)	-2(1)	2(1)
C(24)	16(1)	22(1)	29(1)	6(1)	0(1)	3(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **1**

	x	y	z	U(eq)
H(1A)	9644	5877	4860	19
H(1B)	8729	6653	5003	19
H(2A)	10175	7010	4450	17
H(2B)	9465	6295	4189	17
H(3A)	7000	4616	4652	19
H(3B)	8414	4933	4414	19
H(4A)	6460	4756	3960	18
H(4B)	5430	5342	4220	18
H(5A)	6346	6139	5238	20
H(5B)	5391	5660	4914	20
H(6A)	4661	7019	4930	20
H(6B)	6304	7317	4849	20
H(7A)	9286	8282	4345	17
H(7B)	7761	8430	4120	17
H(9)	11404	8472	3940	25
H(10)	12548	8508	3311	31
H(11)	11161	8141	2745	30
H(12)	8741	7739	2826	24
H(13A)	8207	5237	3542	19
H(13B)	8550	6189	3498	19
H(15)	6797	4632	3017	34
H(16)	5110	4747	2490	52
H(17)	4075	6024	2354	55
H(18)	4758	7139	2734	36
H(19A)	3813	7401	3981	21
H(19B)	3229	7323	4430	21
H(21)	2889	6454	3503	29
H(22)	1591	5253	3356	34
H(23)	939	4382	3887	31
H(24)	1615	4737	4533	26

Table S11. Crystal data and structure refinement for **3**

Identification code	jyy18	
Empirical formula	C_{32} H_{42} N_7 Ni P	
Formula weight	614.40	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.5307(6) Å	α = 90°.
	b = 28.5152(19) Å	β = 106.0248(9)°.
	c = 11.3412(8) Å	γ = 90°.
Volume	2962.4(3) Å^3	
Z	4	
Density (calculated)	1.378 Mg/m^3	
Absorption coefficient	0.744 mm^{-1}	
F(000)	1304	
Crystal color	green	
Crystal size	0.182 x 0.137 x 0.125 mm^3	
Theta range for data collection	1.428 to 26.412°	
Index ranges	$-11 \le h \le 11$, $-35 \le k \le 35$, $-14 \le l \le 14$	
Reflections collected	32225	
Independent reflections	6048 [R(int) = 0.0422]	
Completeness to theta = 25.500°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8013 and 0.7475	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6048 / 0 / 370	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I) = 4981 data]	R1 = 0.0331, wR2 = 0.0764	
R indices (all data, 0.80 Å)	R1 = 0.0449, wR2 = 0.0819	
Largest diff. peak and hole	0.400 and -0.260 e.Å^{-3}	

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Ni(1)	3519(1)	8963(1)	9984(1)	17(1)
P(1)	4828(1)	8605(1)	8981(1)	14(1)
N(1)	7382(2)	7988(1)	8062(2)	19(1)
N(2)	6603(2)	8658(1)	9842(1)	17(1)
N(3)	4997(2)	8768(1)	7588(1)	17(1)
N(4)	4501(2)	8020(1)	8767(1)	16(1)
N(5)	4895(2)	8837(1)	11636(2)	20(1)
N(6)	2037(2)	9262(1)	5074(2)	33(1)
N(7)	2227(2)	7165(1)	9789(2)	28(1)
C(1)	8342(2)	8123(1)	9235(2)	20(1)
C(2)	7589(2)	8257(1)	10204(2)	19(1)
C(3)	7074(2)	8318(1)	7060(2)	21(1)
C(4)	6386(2)	8788(1)	7274(2)	19(1)
C(5)	6408(2)	7596(1)	8004(2)	21(1)
C(6)	4818(2)	7731(1)	7797(2)	19(1)
C(7)	6854(2)	9043(1)	10729(2)	18(1)
C(8)	6351(2)	8920(1)	11839(2)	20(1)
C(9)	7333(2)	8870(1)	12989(2)	24(1)
C(10)	6848(3)	8717(1)	13971(2)	30(1)
C(11)	5378(3)	8626(1)	13767(2)	30(1)
C(12)	4451(2)	8694(1)	12610(2)	25(1)
C(13)	3656(2)	8787(1)	6599(2)	18(1)
C(14)	3275(2)	9261(1)	5998(2)	20(1)
C(15)	4112(2)	9659(1)	6368(2)	24(1)
C(16)	3662(3)	10078(1)	5764(2)	32(1)
C(17)	2393(3)	10086(1)	4823(2)	40(1)
C(18)	1628(3)	9675(1)	4516(2)	41(1)
C(19)	3955(2)	7763(1)	9646(2)	19(1)
C(20)	2518(2)	7513(1)	9102(2)	19(1)
C(21)	1562(2)	7644(1)	7985(2)	20(1)
C(22)	237(2)	7418(1)	7587(2)	24(1)
C(23)	-93(2)	7067(1)	8305(2)	27(1)
C(24)	931(2)	6951(1)	9378(2)	33(1)
C(25)	3028(2)	9639(1)	9165(2)	22(1)
C(26)	3384(2)	9676(1)	10427(2)	23(1)
C(27)	2319(2)	9711(1)	11194(2)	28(1)
C(28)	1061(2)	9352(1)	10824(2)	28(1)
C(29)	1517(2)	8895(1)	10337(2)	24(1)

C(30)	1384(2)	8818(1)	9100(2)	23(1)
C(31)	749(2)	9170(1)	8093(2)	26(1)
C(32)	1475(2)	9656(1)	8340(2)	28(1)

Table S13. Bond lengths [Å] and angles [°] for **3**

Ni(1)-N(5)	2.0008(17)	C(23)-C(24)	1.374(3)
Ni(1)-C(30)	2.047(2)	C(25)-C(26)	1.381(3)
Ni(1)-C(29)	2.0636(19)	C(25)-C(32)	1.519(3)
Ni(1)-C(26)	2.1057(19)	C(26)-C(27)	1.512(3)
Ni(1)-C(25)	2.134(2)	C(27)-C(28)	1.543(3)
Ni(1)-P(1)	2.1642(5)	C(28)-C(29)	1.525(3)
P(1)-N(3)	1.6965(16)	C(29)-C(30)	1.391(3)
P(1)-N(4)	1.7007(16)	C(30)-C(31)	1.516(3)
P(1)-N(2)	1.7101(16)	C(31)-C(32)	1.539(3)
P(1)-N(1)	3.3915(17)		
N(1)-C(3)	1.441(2)	N(5)-Ni(1)-C(30)	136.72(8)
N(1)-C(1)	1.443(2)	N(5)-Ni(1)-C(29)	101.74(8)
N(1)-C(5)	1.444(2)	C(30)-Ni(1)-C(29)	39.55(8)
N(2)-C(2)	1.463(2)	N(5)-Ni(1)-C(26)	91.04(7)
N(2)-C(7)	1.465(2)	C(30)-Ni(1)-C(26)	101.22(8)
N(3)-C(13)	1.450(2)	C(29)-Ni(1)-C(26)	85.65(8)
N(3)-C(4)	1.464(2)	N(5)-Ni(1)-C(25)	125.36(7)
N(4)-C(19)	1.446(2)	C(30)-Ni(1)-C(25)	84.31(8)
N(4)-C(6)	1.472(2)	C(29)-Ni(1)-C(25)	93.80(8)
N(5)-C(12)	1.350(3)	C(26)-Ni(1)-C(25)	38.00(8)
N(5)-C(8)	1.363(3)	N(5)-Ni(1)-P(1)	94.76(5)
N(6)-C(18)	1.341(3)	C(30)-Ni(1)-P(1)	106.64(6)
N(6)-C(14)	1.344(3)	C(29)-Ni(1)-P(1)	139.09(6)
N(7)-C(20)	1.337(3)	C(26)-Ni(1)-P(1)	131.56(6)
N(7)-C(24)	1.341(3)	C(25)-Ni(1)-P(1)	106.66(6)
C(1)-C(2)	1.519(3)	N(3)-P(1)-N(4)	101.36(8)
C(3)-C(4)	1.540(3)	N(3)-P(1)-N(2)	100.03(8)
C(5)-C(6)	1.518(3)	N(4)-P(1)-N(2)	106.35(8)
C(7)-C(8)	1.507(3)	N(3)-P(1)-Ni(1)	125.20(6)
C(8)-C(9)	1.387(3)	N(4)-P(1)-Ni(1)	115.38(6)
C(9)-C(10)	1.389(3)	N(2)-P(1)-Ni(1)	106.33(6)
C(10)-C(11)	1.380(3)	N(3)-P(1)-N(1)	66.15(6)
C(11)-C(12)	1.378(3)	N(4)-P(1)-N(1)	64.35(6)
C(13)-C(14)	1.513(3)	N(2)-P(1)-N(1)	62.65(6)
C(14)-C(15)	1.384(3)	Ni(1)-P(1)-N(1)	166.82(3)
C(15)-C(16)	1.384(3)	C(3)-N(1)-C(1)	119.56(16)
C(16)-C(17)	1.375(3)	C(3)-N(1)-C(5)	118.75(16)
C(17)-C(18)	1.374(4)	C(1)-N(1)-C(5)	118.92(16)
C(19)-C(20)	1.515(3)	C(3)-N(1)-P(1)	84.06(10)
C(20)-C(21)	1.392(3)	C(1)-N(1)-P(1)	84.56(10)
C(21)-C(22)	1.378(3)	C(5)-N(1)-P(1)	84.74(10)
C(22)-C(23)	1.382(3)	C(2)-N(2)-C(7)	114.96(15)

C(2)-N(2)-P(1)	123.28(13)	C(15)-C(14)-C(13)	123.34(18)
C(7)-N(2)-P(1)	113.99(12)	C(14)-C(15)-C(16)	118.9(2)
C(13)-N(3)-C(4)	118.23(15)	C(17)-C(16)-C(15)	119.0(2)
C(13)-N(3)-P(1)	116.15(12)	C(18)-C(17)-C(16)	118.3(2)
C(4)-N(3)-P(1)	124.18(13)	N(6)-C(18)-C(17)	124.3(2)
C(19)-N(4)-C(6)	114.71(15)	N(4)-C(19)-C(20)	114.47(16)
C(19)-N(4)-P(1)	119.05(12)	N(7)-C(20)-C(21)	122.72(18)
C(6)-N(4)-P(1)	126.10(12)	N(7)-C(20)-C(19)	114.86(17)
C(12)-N(5)-C(8)	116.66(18)	C(21)-C(20)-C(19)	122.41(17)
C(12)-N(5)-Ni(1)	123.23(14)	C(22)-C(21)-C(20)	118.90(18)
C(8)-N(5)-Ni(1)	120.01(13)	C(21)-C(22)-C(23)	118.90(19)
C(18)-N(6)-C(14)	116.6(2)	C(24)-C(23)-C(22)	118.37(19)
C(20)-N(7)-C(24)	117.08(18)	N(7)-C(24)-C(23)	124.0(2)
N(1)-C(1)-C(2)	115.35(15)	C(26)-C(25)-C(32)	123.73(19)
N(2)-C(2)-C(1)	112.92(16)	C(26)-C(25)-Ni(1)	69.90(12)
N(1)-C(3)-C(4)	116.53(16)	C(32)-C(25)-Ni(1)	110.91(13)
N(3)-C(4)-C(3)	117.24(16)	C(25)-C(26)-C(27)	126.14(19)
N(1)-C(5)-C(6)	114.40(16)	C(25)-C(26)-Ni(1)	72.09(11)
N(4)-C(6)-C(5)	115.35(16)	C(27)-C(26)-Ni(1)	107.15(14)
N(2)-C(7)-C(8)	111.69(15)	C(26)-C(27)-C(28)	113.27(17)
N(5)-C(8)-C(9)	122.17(19)	C(29)-C(28)-C(27)	112.76(16)
N(5)-C(8)-C(7)	116.33(17)	C(30)-C(29)-C(28)	123.0(2)
C(9)-C(8)-C(7)	121.42(18)	C(30)-C(29)-Ni(1)	69.57(11)
C(8)-C(9)-C(10)	119.9(2)	C(28)-C(29)-Ni(1)	111.16(14)
C(11)-C(10)-C(9)	118.2(2)	C(29)-C(30)-C(31)	124.14(19)
C(12)-C(11)-C(10)	119.2(2)	C(29)-C(30)-Ni(1)	70.88(12)
N(5)-C(12)-C(11)	123.9(2)	C(31)-C(30)-Ni(1)	111.77(13)
N(3)-C(13)-C(14)	115.65(16)	C(30)-C(31)-C(32)	113.17(17)
N(6)-C(14)-C(15)	122.87(19)	C(25)-C(32)-C(31)	113.29(17)
N(6)-C(14)-C(13)	113.78(17)		

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	15(1)	17(1)	20(1)	-2(1)	7(1)	0(1)
P(1)	14(1)	14(1)	15(1)	0(1)	5(1)	0(1)
N(1)	20(1)	20(1)	18(1)	2(1)	5(1)	1(1)
N(2)	15(1)	17(1)	18(1)	-3(1)	5(1)	-1(1)
N(3)	16(1)	18(1)	17(1)	3(1)	6(1)	0(1)
N(4)	19(1)	15(1)	16(1)	-1(1)	7(1)	-2(1)
N(5)	23(1)	18(1)	19(1)	-1(1)	9(1)	2(1)
N(6)	36(1)	29(1)	27(1)	6(1)	-2(1)	7(1)
N(7)	27(1)	26(1)	28(1)	9(1)	1(1)	-10(1)
C(1)	15(1)	22(1)	22(1)	0(1)	4(1)	3(1)
C(2)	16(1)	22(1)	18(1)	2(1)	2(1)	3(1)
C(3)	20(1)	25(1)	18(1)	1(1)	9(1)	2(1)
C(4)	20(1)	21(1)	19(1)	3(1)	9(1)	-1(1)
C(5)	25(1)	18(1)	20(1)	-1(1)	6(1)	4(1)
C(6)	21(1)	15(1)	19(1)	-2(1)	5(1)	-2(1)
C(7)	16(1)	19(1)	19(1)	-2(1)	2(1)	-2(1)
C(8)	23(1)	14(1)	22(1)	-4(1)	6(1)	2(1)
C(9)	26(1)	21(1)	24(1)	-6(1)	5(1)	5(1)
C(10)	42(1)	28(1)	18(1)	-1(1)	5(1)	12(1)
C(11)	44(1)	29(1)	20(1)	2(1)	16(1)	9(1)
C(12)	31(1)	25(1)	25(1)	0(1)	14(1)	2(1)
C(13)	18(1)	18(1)	18(1)	1(1)	4(1)	1(1)
C(14)	24(1)	20(1)	17(1)	1(1)	8(1)	5(1)
C(15)	26(1)	23(1)	27(1)	2(1)	13(1)	3(1)
C(16)	40(1)	18(1)	43(1)	5(1)	20(1)	4(1)
C(17)	54(2)	28(1)	42(2)	16(1)	15(1)	17(1)
C(18)	49(2)	33(1)	31(1)	10(1)	-2(1)	13(1)
C(19)	21(1)	18(1)	18(1)	3(1)	4(1)	-3(1)
C(20)	21(1)	16(1)	21(1)	0(1)	6(1)	-2(1)
C(21)	24(1)	18(1)	20(1)	1(1)	7(1)	-1(1)
C(22)	24(1)	23(1)	22(1)	-3(1)	3(1)	1(1)
C(23)	23(1)	24(1)	33(1)	-3(1)	5(1)	-7(1)
C(24)	34(1)	26(1)	37(1)	8(1)	6(1)	-13(1)
C(25)	22(1)	14(1)	33(1)	0(1)	10(1)	0(1)
C(26)	19(1)	16(1)	34(1)	-4(1)	8(1)	0(1)
C(27)	26(1)	28(1)	33(1)	-11(1)	10(1)	4(1)
C(28)	20(1)	38(1)	32(1)	-9(1)	14(1)	1(1)
C(29)	16(1)	28(1)	32(1)	-3(1)	12(1)	-4(1)

C(30)	13(1)	23(1)	34(1)	-5(1)	7(1)	-5(1)
C(31)	16(1)	33(1)	28(1)	-6(1)	4(1)	2(1)
C(32)	23(1)	28(1)	33(1)	2(1)	7(1)	6(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3**

	x	y	z	U(eq)
H(1A)	8942	8391	9108	24
H(1B)	9015	7858	9553	24
H(2A)	7026	7985	10367	22
H(2B)	8339	8335	10975	22
H(3A)	6409	8165	6335	25
H(3B)	7997	8386	6855	25
H(4A)	7099	8956	7941	23
H(4B)	6238	8979	6521	23
H(5A)	6731	7417	8781	25
H(5B)	6488	7385	7332	25
H(6A)	4493	7903	7011	22
H(6B)	4231	7440	7711	22
H(7A)	6324	9325	10331	22
H(7B)	7909	9119	10992	22
H(9A)	8336	8942	13106	29
H(10A)	7509	8675	14760	36
H(11A)	5009	8519	14416	36
H(12A)	3440	8636	12490	31
H(13A)	2842	8685	6923	22
H(13B)	3731	8559	5961	22
H(15A)	4982	9645	7025	29
H(16A)	4221	10356	5997	39
H(17A)	2053	10369	4396	49
H(18A)	752	9683	3865	49
H(19A)	3831	7983	10284	23
H(19B)	4695	7528	10054	23
H(21A)	1819	7885	7504	24
H(22A)	-438	7503	6832	28
H(23A)	-1005	6909	8062	33
H(24A)	708	6704	9859	39
H(25A)	3781	9766	8787	27
H(26A)	4350	9828	10804	28
H(27A)	1903	10031	11116	34
H(27B)	2853	9661	12067	34
H(28A)	703	9283	11546	34
H(28B)	245	9493	10184	34
H(29A)	1408	8609	10813	29
H(30A)	1199	8483	8840	27

H(31A)	-309	9204	8004	32
H(31B)	864	9048	7308	32
H(32A)	1481	9801	7548	34
H(32B)	883	9859	8726	34

Table S16. Crystal data and structure refinement for **4**

Identification code	jyy156	
Empirical formula	C_{28} H_{36} B_2 F_8 N_9 Ni P	
Formula weight	761.96	
Temperature	88(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.0563(17) Å	α = 90°.
	b = 20.118(4) Å	β = 98.9026(17)°.
	c = 18.435(4) Å	γ = 90°.
Volume	3318.3(11) $Å^3$	
Z	4	
Density (calculated)	1.525 Mg/m^3	
Absorption coefficient	0.714 mm^{-1}	
F(000)	1568	
Crystal color	orange	
Crystal size	0.437 x 0.238 x 0.178 mm^3	
Theta range for data collection	2.025 to 29.077°	
Index ranges	$-12 \le h \le 11$, $-26 \le k \le 26$, $-24 \le l \le 24$	
Reflections collected	40781	
Independent reflections	8456 [R(int) = 0.0386]	
Completeness to theta = 25.500°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6681	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8456 / 0 / 462	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I) = 6941 data]	R1 = 0.0454, wR2 = 0.1187	
R indices (all data, ? Å)	R1 = 0.0583, wR2 = 0.1267	
Largest diff. peak and hole	1.173 and -0.945 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Ni(1)	6792(1)	3464(1)	6670(1)	21(1)
P(1)	6114(1)	3006(1)	5607(1)	18(1)
F(1)	-830(2)	3759(1)	9515(1)	67(1)
F(2)	1598(2)	3476(1)	9901(1)	49(1)
F(3)	46(2)	2749(1)	9234(1)	48(1)
F(4)	764(2)	3695(1)	8703(1)	43(1)
F(5)	-858(2)	5668(1)	5636(1)	57(1)
F(6)	-2898(3)	5266(2)	6050(1)	104(1)
F(7)	-318(5)	4975(2)	6539(3)	61(1)
F(7B)	-1338(6)	4612(2)	6070(3)	73(1)
F(8)	-1553(5)	5913(2)	6687(3)	60(1)
F(8B)	-892(6)	5429(3)	6901(3)	85(2)
N(1)	5185(2)	2472(1)	4118(1)	25(1)
N(2)	7484(2)	3114(1)	5123(1)	26(1)
N(3)	4613(2)	3397(1)	5193(1)	20(1)
N(4)	5793(2)	2203(1)	5666(1)	19(1)
N(5)	8660(2)	3003(1)	6746(1)	23(1)
N(6)	4781(2)	3718(1)	6741(1)	24(1)
N(7)	4402(2)	1233(1)	7111(1)	25(1)
N(8)	7511(2)	4041(1)	7502(1)	30(1)
N(9)	5134(7)	4897(2)	9001(3)	107(2)
B(1)	387(3)	3420(2)	9342(2)	29(1)
B(2)	-1426(4)	5354(2)	6199(2)	39(1)
C(1)	6507(3)	2736(1)	3867(1)	27(1)
C(2)	7169(3)	3317(1)	4345(1)	29(1)
C(3)	3804(2)	2846(1)	4007(1)	23(1)
C(4)	3354(2)	3054(1)	4743(1)	20(1)
C(5)	5181(3)	1795(1)	4380(1)	26(1)
C(6)	6186(3)	1720(1)	5124(1)	24(1)
C(7)	9032(3)	3222(2)	5483(1)	31(1)
C(8)	9434(2)	2856(1)	6194(1)	26(1)
C(9)	10594(3)	2401(1)	6294(1)	31(1)
C(10)	11013(3)	2097(1)	6968(2)	32(1)
C(11)	10253(3)	2266(1)	7542(1)	30(1)
C(12)	9094(3)	2717(1)	7411(1)	26(1)
C(13)	4362(3)	4066(1)	5472(1)	23(1)
C(14)	3805(3)	3994(1)	6196(1)	23(1)
C(15)	2355(3)	4152(1)	6299(2)	29(1)

C(16)	1906(3)	4015(1)	6973(2)	36(1)
C(17)	2898(3)	3724(1)	7523(2)	36(1)
C(18)	4328(3)	3585(1)	7392(1)	32(1)
C(19)	4729(2)	1976(1)	6135(1)	19(1)
C(20)	5407(2)	1510(1)	6740(1)	19(1)
C(21)	6930(3)	1384(1)	6900(1)	24(1)
C(22)	7444(3)	951(1)	7471(1)	31(1)
C(23)	6420(4)	664(1)	7852(1)	36(1)
C(24)	4919(3)	814(1)	7660(1)	33(1)
C(25)	7925(3)	4465(1)	7893(1)	35(1)
C(26)	8460(4)	5017(2)	8381(2)	57(1)
C(27)	3866(6)	4937(2)	9188(3)	69(1)
C(28)	2427(5)	5004(2)	9453(3)	91(2)

Table S18. Bond lengths [Å] and angles [°] for **4**

Ni(1)-N(6)	1.915(2)	C(9)-C(10)	1.385(4)
Ni(1)-N(5)	1.916(2)	C(10)-C(11)	1.391(4)
Ni(1)-N(8)	1.953(2)	C(11)-C(12)	1.380(4)
Ni(1)-P(1)	2.1670(7)	C(13)-C(14)	1.504(3)
P(1)-N(4)	1.649(2)	C(14)-C(15)	1.393(3)
P(1)-N(2)	1.6500(19)	C(15)-C(16)	1.392(4)
P(1)-N(3)	1.6511(19)	C(16)-C(17)	1.378(4)
P(1)-N(1)	2.948(2)	C(17)-C(18)	1.382(4)
F(1)-B(1)	1.374(3)	C(19)-C(20)	1.513(3)
F(2)-B(1)	1.388(3)	C(20)-C(21)	1.389(3)
F(3)-B(1)	1.394(4)	C(21)-C(22)	1.390(3)
F(4)-B(1)	1.389(3)	C(22)-C(23)	1.374(4)
F(5)-B(2)	1.381(4)	C(23)-C(24)	1.385(4)
F(6)-B(2)	1.331(4)	C(25)-C(26)	1.465(4)
F(7)-F(8B)	1.288(8)	C(27)-C(28)	1.467(7)
F(7)-B(2)	1.337(4)		
F(7B)-B(2)	1.514(6)	N(6)-Ni(1)-N(5)	164.27(9)
F(8)-F(8B)	1.178(7)	N(6)-Ni(1)-N(8)	89.59(8)
F(8)-B(2)	1.458(5)	N(5)-Ni(1)-N(8)	92.69(8)
F(8B)-B(2)	1.319(5)	N(6)-Ni(1)-P(1)	92.06(6)
N(1)-C(3)	1.446(3)	N(5)-Ni(1)-P(1)	89.06(6)
N(1)-C(5)	1.446(3)	N(8)-Ni(1)-P(1)	167.53(7)
N(1)-C(1)	1.450(3)	N(4)-P(1)-N(2)	108.66(10)
N(2)-C(7)	1.472(3)	N(4)-P(1)-N(3)	110.83(9)
N(2)-C(2)	1.477(3)	N(2)-P(1)-N(3)	108.74(10)
N(3)-C(13)	1.472(3)	N(4)-P(1)-Ni(1)	112.67(7)
N(3)-C(4)	1.473(3)	N(2)-P(1)-Ni(1)	107.53(7)
N(4)-C(19)	1.464(3)	N(3)-P(1)-Ni(1)	108.30(7)
N(4)-C(6)	1.476(3)	N(4)-P(1)-N(1)	71.09(7)
N(5)-C(8)	1.355(3)	N(2)-P(1)-N(1)	71.04(8)
N(5)-C(12)	1.355(3)	N(3)-P(1)-N(1)	69.30(8)
N(6)-C(14)	1.352(3)	Ni(1)-P(1)-N(1)	176.21(5)
N(6)-C(18)	1.353(3)	F(8B)-F(7)-B(2)	60.3(3)
N(7)-C(20)	1.341(3)	F(8B)-F(8)-B(2)	58.9(3)
N(7)-C(24)	1.345(3)	F(8)-F(8B)-F(7)	129.7(5)
N(8)-C(25)	1.141(3)	F(8)-F(8B)-B(2)	71.2(4)
N(9)-C(27)	1.252(7)	F(7)-F(8B)-B(2)	61.7(3)
C(1)-C(2)	1.528(4)	C(3)-N(1)-C(5)	119.33(19)
C(3)-C(4)	1.535(3)	C(3)-N(1)-C(1)	120.2(2)
C(5)-C(6)	1.531(3)	C(5)-N(1)-C(1)	119.8(2)
C(7)-C(8)	1.498(3)	C(3)-N(1)-P(1)	93.31(13)
C(8)-C(9)	1.385(4)	C(5)-N(1)-P(1)	92.67(12)

C(1)-N(1)-P(1)	91.85(13)	F(5)-B(2)-F(7B)	107.4(3)
C(7)-N(2)-C(2)	115.14(18)	N(1)-C(1)-C(2)	111.47(19)
C(7)-N(2)-P(1)	121.30(15)	N(2)-C(2)-C(1)	110.5(2)
C(2)-N(2)-P(1)	120.88(15)	N(1)-C(3)-C(4)	111.07(17)
C(13)-N(3)-C(4)	118.52(17)	N(3)-C(4)-C(3)	109.66(18)
C(13)-N(3)-P(1)	115.71(14)	N(1)-C(5)-C(6)	111.1(2)
C(4)-N(3)-P(1)	123.18(15)	N(4)-C(6)-C(5)	111.68(18)
C(19)-N(4)-C(6)	116.42(18)	N(2)-C(7)-C(8)	114.0(2)
C(19)-N(4)-P(1)	118.92(14)	N(5)-C(8)-C(9)	121.0(2)
C(6)-N(4)-P(1)	122.46(15)	N(5)-C(8)-C(7)	117.8(2)
C(8)-N(5)-C(12)	118.4(2)	C(9)-C(8)-C(7)	121.2(2)
C(8)-N(5)-Ni(1)	127.18(16)	C(10)-C(9)-C(8)	120.5(2)
C(12)-N(5)-Ni(1)	113.63(16)	C(9)-C(10)-C(11)	118.4(2)
C(14)-N(6)-C(18)	119.2(2)	C(12)-C(11)-C(10)	118.7(2)
C(14)-N(6)-Ni(1)	125.33(16)	N(5)-C(12)-C(11)	122.9(2)
C(18)-N(6)-Ni(1)	115.49(17)	N(3)-C(13)-C(14)	108.28(18)
C(20)-N(7)-C(24)	117.3(2)	N(6)-C(14)-C(15)	120.9(2)
C(25)-N(8)-Ni(1)	167.6(2)	N(6)-C(14)-C(13)	115.4(2)
F(1)-B(1)-F(2)	110.9(3)	C(15)-C(14)-C(13)	123.5(2)
F(1)-B(1)-F(4)	108.1(2)	C(16)-C(15)-C(14)	119.2(3)
F(2)-B(1)-F(4)	109.1(2)	C(17)-C(16)-C(15)	119.7(2)
F(1)-B(1)-F(3)	110.2(2)	C(16)-C(17)-C(18)	118.5(3)
F(2)-B(1)-F(3)	108.4(2)	N(6)-C(18)-C(17)	122.5(3)
F(4)-B(1)-F(3)	110.0(2)	N(4)-C(19)-C(20)	113.59(17)
F(8B)-B(2)-F(6)	114.8(4)	N(7)-C(20)-C(21)	123.1(2)
F(8B)-B(2)-F(7)	58.0(4)	N(7)-C(20)-C(19)	113.79(19)
F(8B)-B(2)-F(5)	124.2(4)	C(21)-C(20)-C(19)	123.1(2)
F(6)-B(2)-F(5)	112.6(2)	C(20)-C(21)-C(22)	118.7(2)
F(7)-B(2)-F(5)	105.9(3)	C(23)-C(22)-C(21)	118.6(2)
F(8B)-B(2)-F(8)	49.9(4)	C(22)-C(23)-C(24)	119.4(2)
F(7)-B(2)-F(8)	106.0(4)	N(7)-C(24)-C(23)	122.9(3)
F(5)-B(2)-F(8)	100.6(3)	N(8)-C(25)-C(26)	178.8(3)
F(8B)-B(2)-F(7B)	104.3(4)	N(9)-C(27)-C(28)	176.2(5)
F(6)-B(2)-F(7B)	85.0(3)		

Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	18(1)	31(1)	13(1)	-2(1)	0(1)	-2(1)
P(1)	15(1)	26(1)	12(1)	1(1)	0(1)	-1(1)
F(1)	47(1)	64(1)	101(2)	29(1)	48(1)	20(1)
F(2)	53(1)	44(1)	43(1)	10(1)	-19(1)	-7(1)
F(3)	40(1)	43(1)	57(1)	4(1)	-3(1)	-11(1)
F(4)	48(1)	54(1)	29(1)	3(1)	13(1)	-6(1)
F(5)	41(1)	65(1)	67(1)	21(1)	19(1)	10(1)
F(6)	62(2)	193(3)	48(1)	44(2)	-17(1)	-61(2)
F(7)	49(2)	65(3)	71(3)	29(2)	15(2)	37(2)
F(7B)	96(4)	45(2)	87(3)	7(2)	41(3)	24(2)
F(8)	74(3)	49(2)	60(3)	-16(2)	22(2)	6(2)
F(8B)	71(3)	122(5)	52(3)	10(3)	-24(2)	-58(3)
N(1)	19(1)	34(1)	20(1)	3(1)	1(1)	3(1)
N(2)	16(1)	46(1)	14(1)	4(1)	0(1)	-5(1)
N(3)	19(1)	22(1)	17(1)	0(1)	-3(1)	0(1)
N(4)	18(1)	24(1)	15(1)	1(1)	3(1)	4(1)
N(5)	18(1)	33(1)	16(1)	-2(1)	-2(1)	-4(1)
N(6)	23(1)	28(1)	21(1)	-5(1)	4(1)	-3(1)
N(7)	32(1)	20(1)	22(1)	1(1)	3(1)	-2(1)
N(8)	26(1)	40(1)	22(1)	-5(1)	-1(1)	2(1)
N(9)	150(5)	80(3)	101(3)	32(2)	46(3)	51(3)
B(1)	19(1)	39(2)	29(1)	6(1)	4(1)	0(1)
B(2)	30(2)	52(2)	33(2)	10(1)	3(1)	18(1)
C(1)	22(1)	45(1)	13(1)	2(1)	2(1)	2(1)
C(2)	23(1)	49(2)	14(1)	5(1)	2(1)	-5(1)
C(3)	20(1)	30(1)	16(1)	2(1)	-4(1)	2(1)
C(4)	17(1)	24(1)	18(1)	1(1)	-2(1)	1(1)
C(5)	29(1)	31(1)	17(1)	-4(1)	0(1)	5(1)
C(6)	26(1)	30(1)	17(1)	-3(1)	2(1)	8(1)
C(7)	18(1)	58(2)	17(1)	2(1)	0(1)	-9(1)
C(8)	17(1)	42(1)	17(1)	-4(1)	-1(1)	-6(1)
C(9)	17(1)	48(2)	26(1)	-10(1)	-1(1)	-3(1)
C(10)	17(1)	40(1)	36(1)	-6(1)	-5(1)	-2(1)
C(11)	20(1)	41(1)	26(1)	3(1)	-7(1)	-5(1)
C(12)	20(1)	39(1)	18(1)	0(1)	-2(1)	-6(1)
C(13)	24(1)	20(1)	25(1)	2(1)	0(1)	-1(1)
C(14)	24(1)	18(1)	28(1)	-5(1)	3(1)	-3(1)
C(15)	24(1)	21(1)	42(1)	-10(1)	5(1)	-4(1)

C(16)	29(1)	31(1)	52(2)	-16(1)	17(1)	-10(1)
C(17)	36(1)	41(2)	34(1)	-12(1)	16(1)	-13(1)
C(18)	33(1)	41(1)	23(1)	-7(1)	8(1)	-7(1)
C(19)	17(1)	24(1)	17(1)	3(1)	0(1)	2(1)
C(20)	24(1)	17(1)	15(1)	-1(1)	0(1)	2(1)
C(21)	26(1)	26(1)	19(1)	-2(1)	-2(1)	7(1)
C(22)	38(1)	30(1)	23(1)	-3(1)	-8(1)	14(1)
C(23)	62(2)	20(1)	24(1)	4(1)	-4(1)	10(1)
C(24)	52(2)	22(1)	24(1)	4(1)	3(1)	-4(1)
C(25)	32(1)	40(1)	28(1)	-5(1)	-9(1)	10(1)
C(26)	66(2)	42(2)	52(2)	-18(2)	-28(2)	16(2)
C(27)	84(3)	39(2)	78(3)	5(2)	-9(2)	0(2)
C(28)	57(3)	48(2)	158(5)	12(3)	-9(3)	-15(2)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4**

	x	y	z	U(eq)
H(1A)	6244	2889	3352	32
H(1B)	7265	2380	3879	32
H(2A)	8105	3466	4181	35
H(2B)	6457	3693	4290	35
H(3A)	3001	2570	3731	27
H(3B)	3927	3247	3711	27
H(4A)	2477	3353	4656	24
H(4B)	3073	2656	5007	24
H(5A)	5537	1494	4019	31
H(5B)	4147	1664	4429	31
H(6A)	6088	1264	5311	29
H(6B)	7241	1787	5059	29
H(7A)	9187	3704	5576	37
H(7B)	9720	3082	5144	37
H(9)	11107	2296	5896	37
H(10)	11801	1780	7037	39
H(11)	10527	2076	8015	36
H(12)	8578	2833	7804	31
H(13A)	3616	4306	5118	28
H(13B)	5307	4323	5538	28
H(15)	1680	4352	5915	35
H(16)	921	4121	7052	43
H(17)	2605	3620	7983	43
H(18)	5018	3389	7772	38
H(19A)	3889	1747	5827	23
H(19B)	4316	2368	6359	23
H(21)	7608	1590	6625	29
H(22)	8480	856	7596	38
H(23)	6740	365	8244	44
H(24)	4223	611	7927	39
H(26A)	9252	5256	8182	86
H(26B)	8856	4844	8869	86
H(26C)	7630	5322	8419	86
H(28A)	1761	4642	9254	136
H(28B)	1971	5432	9291	136
H(28C)	2586	4984	9990	136

Table S21. Crystal data and structure refinement for **5**

Identification code	jyy24	
Empirical formula	C_{28} H_{36} B_2 F_8 N_9 P Pd	
Formula weight	809.65	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.9669(6) Å	α = 77.9589(6)°.
	b = 12.4170(7) Å	β = 87.3208(7)°.
	c = 25.3468(14) Å	γ = 81.2206(7)°.
Volume	3335.7(3) $Å^3$	
Z	4	
Density (calculated)	1.612 Mg/m^3	
Absorption coefficient	0.685 mm^{-1}	
F(000)	1640	
Crystal color	orange	
Crystal size	0.410 x 0.265 x 0.136 mm^3	
Theta range for data collection	1.643 to 28.734°	
Index ranges	$-14 \le h \le 14$, $-16 \le k \le 15$, $-32 \le l \le 32$	
Reflections collected	39746	
Independent reflections	15613 [R(int) = 0.0192]	
Completeness to theta = 25.500°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8015 and 0.7163	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15613 / 0 / 934	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I) = 13905 data]	R1 = 0.0288, wR2 = 0.0659	
R indices (all data, 0.74 Å)	R1 = 0.0340, wR2 = 0.0682	
Largest diff. peak and hole	0.862 and -0.344 $e.Å^{-3}$	

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Pd(1)	8222(1)	12881(1)	1230(1)	16(1)
P(1)	6760(1)	14040(1)	1551(1)	16(1)
N(1)	4884(2)	15382(2)	1894(1)	22(1)
N(2)	7202(2)	15301(1)	1430(1)	20(1)
N(3)	6582(2)	13540(1)	2203(1)	20(1)
N(4)	5546(1)	14011(1)	1191(1)	18(1)
N(5)	8371(1)	14148(1)	575(1)	18(1)
N(6)	7982(2)	11561(1)	1857(1)	18(1)
N(7)	6516(2)	12069(2)	617(1)	33(1)
N(8)	9675(2)	11853(1)	884(1)	22(1)
C(1)	5430(2)	16403(2)	1788(1)	25(1)
C(2)	6819(2)	16078(2)	1799(1)	25(1)
C(3)	4816(2)	14792(2)	2448(1)	26(1)
C(4)	5366(2)	13579(2)	2478(1)	23(1)
C(5)	3936(2)	15307(2)	1526(1)	24(1)
C(6)	4614(2)	14987(2)	1026(1)	23(1)
C(7)	8450(2)	15392(2)	1184(1)	22(1)
C(8)	8470(2)	15191(2)	623(1)	20(1)
C(9)	8579(2)	16024(2)	173(1)	25(1)
C(10)	8570(2)	15793(2)	-337(1)	26(1)
C(11)	8452(2)	14721(2)	-384(1)	25(1)
C(12)	8356(2)	13920(2)	79(1)	22(1)
C(13)	7644(2)	12815(2)	2482(1)	20(1)
C(14)	7748(2)	11658(2)	2375(1)	20(1)
C(15)	7567(2)	10749(2)	2772(1)	25(1)
C(16)	7614(2)	9715(2)	2641(1)	30(1)
C(17)	7859(2)	9614(2)	2112(1)	27(1)
C(18)	8035(2)	10553(2)	1730(1)	23(1)
C(19)	5139(2)	12914(2)	1238(1)	21(1)
C(20)	5355(2)	12463(2)	727(1)	21(1)
C(21)	4381(2)	12443(2)	403(1)	35(1)
C(22)	4619(2)	12016(2)	-60(1)	44(1)
C(23)	5821(2)	11622(2)	-182(1)	39(1)
C(24)	6726(2)	11655(2)	168(1)	40(1)
C(25)	10481(2)	11375(2)	693(1)	26(1)
C(26)	11524(3)	10781(2)	444(1)	46(1)
Pd(2)	12267(1)	6932(1)	3842(1)	16(1)
P(2)	11161(1)	5881(1)	3494(1)	15(1)

N(9)	9783(2)	4600(1)	3139(1)	23(1)
N(10)	11816(2)	4581(1)	3702(1)	21(1)
N(11)	11208(2)	6280(1)	2823(1)	18(1)
N(12)	9751(2)	6167(1)	3740(1)	19(1)
N(13)	12937(1)	5630(1)	4459(1)	18(1)
N(14)	11544(2)	8258(1)	3268(1)	22(1)
N(15)	10100(2)	7303(2)	4886(1)	35(1)
N(16)	13295(2)	8005(1)	4150(1)	22(1)
C(27)	10434(2)	3512(2)	3383(1)	26(1)
C(28)	11086(2)	3663(2)	3874(1)	26(1)
C(29)	9951(2)	5007(2)	2566(1)	22(1)
C(30)	11170(2)	5453(2)	2479(1)	23(1)
C(31)	8599(2)	4958(2)	3375(1)	27(1)
C(32)	8633(2)	6139(2)	3447(1)	25(1)
C(33)	13129(2)	4388(2)	3830(1)	22(1)
C(34)	13314(2)	4586(2)	4386(1)	19(1)
C(35)	13789(2)	3743(2)	4803(1)	24(1)
C(36)	13886(2)	3973(2)	5312(1)	26(1)
C(37)	13498(2)	5040(2)	5387(1)	25(1)
C(38)	13022(2)	5849(2)	4954(1)	21(1)
C(39)	12014(2)	7123(2)	2592(1)	23(1)
C(40)	11557(2)	8220(2)	2740(1)	24(1)
C(41)	11160(2)	9160(2)	2353(1)	34(1)
C(42)	10752(2)	10154(2)	2511(1)	44(1)
C(43)	10713(2)	10182(2)	3052(1)	42(1)
C(44)	11104(2)	9218(2)	3423(1)	33(1)
C(45)	9626(2)	6092(2)	4325(1)	22(1)
C(46)	9395(2)	7215(2)	4487(1)	22(1)
C(47)	8509(2)	8064(2)	4250(1)	41(1)
C(48)	8310(2)	9044(2)	4436(1)	45(1)
C(49)	8996(3)	9136(2)	4859(1)	42(1)
C(50)	9888(3)	8261(2)	5063(1)	48(1)
C(51)	13920(2)	8534(2)	4292(1)	24(1)
C(52)	14745(3)	9186(2)	4478(1)	39(1)
N(17)	6104(4)	9109(3)	1063(2)	89(1)
C(53)	5330(5)	9396(3)	1337(2)	69(1)
C(54)	4617(8)	9823(8)	1725(4)	76(3)
C(54B)	4026(11)	9542(9)	1648(4)	75(3)
N(18)	12750(3)	1275(3)	3792(1)	74(1)
C(55)	13327(3)	1041(2)	3439(1)	47(1)
C(56)	14066(3)	705(2)	3003(1)	52(1)
B(1)	1723(2)	12881(2)	1852(1)	24(1)
F(1)	2175(1)	12137(1)	1522(1)	41(1)
F(2)	593(1)	12651(1)	2071(1)	40(1)

F(3)	2551(1)	12811(1)	2257(1)	43(1)
F(4)	1573(2)	13960(1)	1550(1)	39(1)
B(2)	10399(4)	18058(2)	1054(1)	45(1)
F(5)	9761(5)	17469(5)	1506(2)	54(1)
F(6)	10179(5)	17640(6)	615(2)	58(1)
F(7)	11667(10)	17978(9)	1142(4)	102(3)
F(8)	9728(5)	19149(4)	967(4)	55(2)
F(5B)	10353(16)	17065(8)	1327(5)	84(5)
F(6B)	10519(10)	18130(10)	485(3)	61(3)
F(7B)	11632(13)	18148(8)	1151(4)	51(3)
F(8B)	9989(10)	18941(10)	1191(4)	61(2)
B(3)	6707(3)	2127(2)	4030(1)	32(1)
F(9)	7912(2)	1967(2)	3840(1)	50(1)
F(10)	6169(2)	3197(1)	3807(1)	59(1)
F(11)	6712(2)	1965(2)	4583(1)	67(1)
F(12)	6085(2)	1363(1)	3874(1)	50(1)
B(4)	15540(2)	7463(2)	3132(1)	22(1)
F(13)	14441(1)	8046(1)	2904(1)	32(1)
F(14)	16433(1)	7407(1)	2729(1)	36(1)
F(15)	15355(2)	6402(1)	3393(1)	42(1)
F(16)	15935(1)	8020(1)	3506(1)	26(1)

Table S23. Bond lengths [Å] and angles [°] for **5**

Pd(1)-N(5)	2.0535(16)	C(25)-C(26)	1.456(3)
Pd(1)-N(6)	2.0706(16)	Pd(2)-N(14)	2.0410(17)
Pd(1)-N(8)	2.1577(17)	Pd(2)-N(13)	2.0711(16)
Pd(1)-P(1)	2.2294(5)	Pd(2)-N(16)	2.1517(17)
P(1)-N(3)	1.6528(17)	Pd(2)-P(2)	2.2394(5)
P(1)-N(4)	1.6583(16)	P(2)-N(10)	1.6515(17)
P(1)-N(2)	1.6722(17)	P(2)-N(12)	1.6561(17)
P(1)-N(1)	2.6747(18)	P(2)-N(11)	1.6691(17)
N(1)-C(3)	1.447(3)	P(2)-N(9)	2.6613(18)
N(1)-C(1)	1.453(3)	N(9)-C(29)	1.449(3)
N(1)-C(5)	1.455(3)	N(9)-C(31)	1.450(3)
N(2)-C(2)	1.482(2)	N(9)-C(27)	1.454(3)
N(2)-C(7)	1.488(2)	N(10)-C(33)	1.464(3)
N(3)-C(13)	1.469(2)	N(10)-C(28)	1.472(3)
N(3)-C(4)	1.476(2)	N(11)-C(39)	1.483(2)
N(4)-C(6)	1.462(3)	N(11)-C(30)	1.486(2)
N(4)-C(19)	1.477(2)	N(12)-C(45)	1.467(2)
N(5)-C(12)	1.346(3)	N(12)-C(32)	1.473(2)
N(5)-C(8)	1.347(3)	N(13)-C(34)	1.347(3)
N(6)-C(18)	1.347(3)	N(13)-C(38)	1.350(2)
N(6)-C(14)	1.353(2)	N(14)-C(44)	1.344(3)
N(7)-C(20)	1.331(3)	N(14)-C(40)	1.349(3)
N(7)-C(24)	1.341(3)	N(15)-C(46)	1.333(3)
N(8)-C(25)	1.134(3)	N(15)-C(50)	1.342(3)
C(1)-C(2)	1.515(3)	N(16)-C(51)	1.135(3)
C(3)-C(4)	1.522(3)	C(27)-C(28)	1.523(3)
C(5)-C(6)	1.531(3)	C(29)-C(30)	1.513(3)
C(7)-C(8)	1.492(3)	C(31)-C(32)	1.520(3)
C(8)-C(9)	1.385(3)	C(33)-C(34)	1.509(3)
C(9)-C(10)	1.383(3)	C(34)-C(35)	1.382(3)
C(10)-C(11)	1.386(3)	C(35)-C(36)	1.390(3)
C(11)-C(12)	1.384(3)	C(36)-C(37)	1.378(3)
C(13)-C(14)	1.505(3)	C(37)-C(38)	1.384(3)
C(14)-C(15)	1.380(3)	C(39)-C(40)	1.495(3)
C(15)-C(16)	1.386(3)	C(40)-C(41)	1.386(3)
C(16)-C(17)	1.382(3)	C(41)-C(42)	1.380(4)
C(17)-C(18)	1.383(3)	C(42)-C(43)	1.376(4)
C(19)-C(20)	1.512(3)	C(43)-C(44)	1.383(3)
C(20)-C(21)	1.383(3)	C(45)-C(46)	1.516(3)
C(21)-C(22)	1.384(3)	C(46)-C(47)	1.376(3)
C(22)-C(23)	1.379(4)	C(47)-C(48)	1.380(3)
C(23)-C(24)	1.371(4)	C(48)-C(49)	1.371(4)

C(49)-C(50)	1.376(4)	C(3)-N(1)-C(1)	117.82(17)
C(51)-C(52)	1.457(3)	C(3)-N(1)-C(5)	118.27(17)
N(17)-C(53)	1.133(5)	C(1)-N(1)-C(5)	116.80(18)
C(53)-C(54)	1.370(11)	C(3)-N(1)-P(1)	98.62(12)
C(53)-C(54B)	1.605(13)	C(1)-N(1)-P(1)	98.69(11)
N(18)-C(55)	1.133(4)	C(5)-N(1)-P(1)	99.52(11)
C(55)-C(56)	1.434(4)	C(2)-N(2)-C(7)	113.73(15)
B(1)-F(2)	1.380(3)	C(2)-N(2)-P(1)	120.59(14)
B(1)-F(3)	1.383(3)	C(7)-N(2)-P(1)	116.83(13)
B(1)-F(4)	1.387(3)	C(13)-N(3)-C(4)	118.70(16)
B(1)-F(1)	1.393(3)	C(13)-N(3)-P(1)	116.94(13)
B(2)-F(8B)	1.232(10)	C(4)-N(3)-P(1)	122.90(14)
B(2)-F(5B)	1.290(6)	C(6)-N(4)-C(19)	116.44(16)
B(2)-F(6)	1.369(5)	C(6)-N(4)-P(1)	122.42(13)
B(2)-F(7)	1.404(11)	C(19)-N(4)-P(1)	116.30(13)
B(2)-F(7B)	1.412(13)	C(12)-N(5)-C(8)	119.12(17)
B(2)-F(8)	1.418(6)	C(12)-N(5)-Pd(1)	118.15(14)
B(2)-F(6B)	1.427(7)	C(8)-N(5)-Pd(1)	122.73(13)
B(2)-F(5)	1.438(5)	C(18)-N(6)-C(14)	118.84(17)
B(3)-F(11)	1.374(3)	C(18)-N(6)-Pd(1)	117.01(13)
B(3)-F(12)	1.378(3)	C(14)-N(6)-Pd(1)	124.12(13)
B(3)-F(10)	1.382(3)	C(20)-N(7)-C(24)	117.4(2)
B(3)-F(9)	1.386(3)	C(25)-N(8)-Pd(1)	175.19(17)
B(4)-F(15)	1.385(3)	N(1)-C(1)-C(2)	107.50(17)
B(4)-F(14)	1.389(3)	N(2)-C(2)-C(1)	109.75(16)
B(4)-F(13)	1.391(3)	N(1)-C(3)-C(4)	108.63(16)
B(4)-F(16)	1.402(3)	N(3)-C(4)-C(3)	108.57(17)
		N(1)-C(5)-C(6)	106.42(16)
N(5)-Pd(1)-N(6)	175.70(6)	N(4)-C(6)-C(5)	109.62(17)
N(5)-Pd(1)-N(8)	88.94(6)	N(2)-C(7)-C(8)	109.60(16)
N(6)-Pd(1)-N(8)	90.78(6)	N(5)-C(8)-C(9)	121.24(19)
N(5)-Pd(1)-P(1)	87.49(5)	N(5)-C(8)-C(7)	116.34(17)
N(6)-Pd(1)-P(1)	92.86(5)	C(9)-C(8)-C(7)	122.42(19)
N(8)-Pd(1)-P(1)	176.25(5)	C(10)-C(9)-C(8)	119.9(2)
N(3)-P(1)-N(4)	113.37(9)	C(9)-C(10)-C(11)	118.64(19)
N(3)-P(1)-N(2)	112.24(9)	C(12)-C(11)-C(10)	119.0(2)
N(4)-P(1)-N(2)	112.06(9)	N(5)-C(12)-C(11)	122.1(2)
N(3)-P(1)-Pd(1)	107.91(6)	N(3)-C(13)-C(14)	110.89(16)
N(4)-P(1)-Pd(1)	102.38(6)	N(6)-C(14)-C(15)	121.35(19)
N(2)-P(1)-Pd(1)	108.21(6)	N(6)-C(14)-C(13)	116.03(17)
N(3)-P(1)-N(1)	73.70(7)	C(15)-C(14)-C(13)	122.57(18)
N(4)-P(1)-N(1)	73.38(7)	C(14)-C(15)-C(16)	119.7(2)
N(2)-P(1)-N(1)	74.40(7)	C(17)-C(16)-C(15)	119.0(2)
Pd(1)-P(1)-N(1)	175.71(4)	C(16)-C(17)-C(18)	118.8(2)

N(6)-C(18)-C(17)	122.32(19)	C(44)-N(14)-C(40)	119.31(19)
N(4)-C(19)-C(20)	113.05(16)	C(44)-N(14)-Pd(2)	118.33(16)
N(7)-C(20)-C(21)	122.7(2)	C(40)-N(14)-Pd(2)	122.26(14)
N(7)-C(20)-C(19)	116.40(18)	C(46)-N(15)-C(50)	116.8(2)
C(21)-C(20)-C(19)	120.92(19)	C(51)-N(16)-Pd(2)	174.39(17)
C(20)-C(21)-C(22)	119.0(2)	N(9)-C(27)-C(28)	106.61(16)
C(23)-C(22)-C(21)	118.8(2)	N(10)-C(28)-C(27)	108.24(17)
C(24)-C(23)-C(22)	118.3(2)	N(9)-C(29)-C(30)	108.06(16)
N(7)-C(24)-C(23)	123.9(2)	N(11)-C(30)-C(29)	109.58(16)
N(8)-C(25)-C(26)	179.0(3)	N(9)-C(31)-C(32)	106.20(16)
N(14)-Pd(2)-N(13)	176.55(7)	N(12)-C(32)-C(31)	109.53(17)
N(14)-Pd(2)-N(16)	89.40(7)	N(10)-C(33)-C(34)	110.69(16)
N(13)-Pd(2)-N(16)	89.42(6)	N(13)-C(34)-C(35)	121.65(18)
N(14)-Pd(2)-P(2)	88.03(5)	N(13)-C(34)-C(33)	115.85(17)
N(13)-Pd(2)-P(2)	93.15(5)	C(35)-C(34)-C(33)	122.44(18)
N(16)-Pd(2)-P(2)	177.43(5)	C(34)-C(35)-C(36)	119.5(2)
N(10)-P(2)-N(12)	114.22(9)	C(37)-C(36)-C(35)	118.8(2)
N(10)-P(2)-N(11)	112.30(9)	C(36)-C(37)-C(38)	119.1(2)
N(12)-P(2)-N(11)	111.59(8)	N(13)-C(38)-C(37)	122.2(2)
N(10)-P(2)-Pd(2)	106.04(6)	N(11)-C(39)-C(40)	111.44(17)
N(12)-P(2)-Pd(2)	103.96(6)	N(14)-C(40)-C(41)	121.1(2)
N(11)-P(2)-Pd(2)	108.03(6)	N(14)-C(40)-C(39)	117.20(18)
N(10)-P(2)-N(9)	73.20(7)	C(41)-C(40)-C(39)	121.7(2)
N(12)-P(2)-N(9)	73.52(7)	C(42)-C(41)-C(40)	119.4(2)
N(11)-P(2)-N(9)	75.32(7)	C(43)-C(42)-C(41)	119.2(2)
Pd(2)-P(2)-N(9)	176.49(4)	C(42)-C(43)-C(44)	119.2(2)
C(29)-N(9)-C(31)	116.80(17)	N(14)-C(44)-C(43)	121.7(2)
C(29)-N(9)-C(27)	118.36(17)	N(12)-C(45)-C(46)	113.61(16)
C(31)-N(9)-C(27)	117.46(17)	N(15)-C(46)-C(47)	122.9(2)
C(29)-N(9)-P(2)	98.13(11)	N(15)-C(46)-C(45)	114.46(19)
C(31)-N(9)-P(2)	99.85(12)	C(47)-C(46)-C(45)	122.65(19)
C(27)-N(9)-P(2)	99.38(12)	C(46)-C(47)-C(48)	119.4(2)
C(33)-N(10)-C(28)	118.89(16)	C(49)-C(48)-C(47)	118.6(2)
C(33)-N(10)-P(2)	117.63(13)	C(48)-C(49)-C(50)	118.4(2)
C(28)-N(10)-P(2)	122.07(14)	N(15)-C(50)-C(49)	123.9(3)
C(39)-N(11)-C(30)	112.59(15)	N(16)-C(51)-C(52)	178.5(3)
C(39)-N(11)-P(2)	117.19(13)	N(17)-C(53)-C(54)	166.3(6)
C(30)-N(11)-P(2)	119.91(13)	N(17)-C(53)-C(54B)	162.2(5)
C(45)-N(12)-C(32)	117.29(16)	N(18)-C(55)-C(56)	178.0(3)
C(45)-N(12)-P(2)	117.09(13)	F(2)-B(1)-F(3)	110.14(19)
C(32)-N(12)-P(2)	122.74(13)	F(2)-B(1)-F(4)	108.56(19)
C(34)-N(13)-C(38)	118.77(17)	F(3)-B(1)-F(4)	108.37(18)
C(34)-N(13)-Pd(2)	123.17(13)	F(2)-B(1)-F(1)	110.01(18)
C(38)-N(13)-Pd(2)	118.04(14)	F(3)-B(1)-F(1)	109.98(19)

F(4)-B(1)-F(1)	109.74(19)	F(11)-B(3)-F(12)	110.1(2)
F(8B)-B(2)-F(5B)	127.1(8)	F(11)-B(3)-F(10)	110.6(2)
F(6)-B(2)-F(7)	111.8(5)	F(12)-B(3)-F(10)	110.2(2)
F(8B)-B(2)-F(7B)	93.3(8)	F(11)-B(3)-F(9)	109.0(2)
F(5B)-B(2)-F(7B)	99.3(7)	F(12)-B(3)-F(9)	108.0(2)
F(6)-B(2)-F(8)	105.7(4)	F(10)-B(3)-F(9)	108.8(2)
F(7)-B(2)-F(8)	115.7(6)	F(15)-B(4)-F(14)	110.26(18)
F(8B)-B(2)-F(6B)	114.8(5)	F(15)-B(4)-F(13)	109.56(18)
F(5B)-B(2)-F(6B)	114.1(5)	F(14)-B(4)-F(13)	109.14(18)
F(7B)-B(2)-F(6B)	97.6(7)	F(15)-B(4)-F(16)	109.32(18)
F(6)-B(2)-F(5)	107.0(3)	F(14)-B(4)-F(16)	108.96(17)
F(7)-B(2)-F(5)	112.7(5)	F(13)-B(4)-F(16)	109.58(17)
F(8)-B(2)-F(5)	103.2(3)		

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	15(1)	18(1)	16(1)	-4(1)	2(1)	-1(1)
P(1)	13(1)	20(1)	17(1)	-7(1)	1(1)	-2(1)
N(1)	19(1)	27(1)	24(1)	-12(1)	-2(1)	-2(1)
N(2)	16(1)	21(1)	25(1)	-10(1)	2(1)	-4(1)
N(3)	16(1)	25(1)	17(1)	-6(1)	3(1)	-1(1)
N(4)	15(1)	21(1)	22(1)	-10(1)	-2(1)	-2(1)
N(5)	13(1)	22(1)	18(1)	-2(1)	0(1)	0(1)
N(6)	17(1)	20(1)	17(1)	-4(1)	0(1)	-3(1)
N(7)	21(1)	44(1)	42(1)	-28(1)	1(1)	-3(1)
N(8)	22(1)	21(1)	24(1)	-5(1)	1(1)	-1(1)
C(1)	22(1)	23(1)	32(1)	-15(1)	-2(1)	0(1)
C(2)	22(1)	26(1)	31(1)	-16(1)	-1(1)	-4(1)
C(3)	19(1)	36(1)	24(1)	-16(1)	4(1)	-1(1)
C(4)	18(1)	33(1)	20(1)	-7(1)	4(1)	-5(1)
C(5)	16(1)	30(1)	30(1)	-14(1)	-4(1)	2(1)
C(6)	18(1)	26(1)	26(1)	-10(1)	-6(1)	2(1)
C(7)	17(1)	25(1)	25(1)	-6(1)	0(1)	-6(1)
C(8)	10(1)	24(1)	25(1)	-5(1)	0(1)	-1(1)
C(9)	18(1)	22(1)	30(1)	1(1)	0(1)	0(1)
C(10)	18(1)	30(1)	25(1)	6(1)	0(1)	2(1)
C(11)	17(1)	34(1)	20(1)	-2(1)	1(1)	2(1)
C(12)	17(1)	28(1)	22(1)	-6(1)	1(1)	1(1)
C(13)	18(1)	25(1)	16(1)	-6(1)	-1(1)	-2(1)
C(14)	15(1)	24(1)	19(1)	-5(1)	0(1)	-3(1)
C(15)	26(1)	30(1)	18(1)	-3(1)	2(1)	-5(1)
C(16)	33(1)	28(1)	27(1)	1(1)	1(1)	-10(1)
C(17)	32(1)	22(1)	30(1)	-7(1)	1(1)	-7(1)
C(18)	24(1)	24(1)	23(1)	-9(1)	0(1)	-4(1)
C(19)	19(1)	24(1)	24(1)	-10(1)	2(1)	-7(1)
C(20)	20(1)	21(1)	25(1)	-9(1)	0(1)	-4(1)
C(21)	24(1)	48(2)	37(1)	-22(1)	-5(1)	3(1)
C(22)	38(1)	60(2)	40(1)	-27(1)	-12(1)	3(1)
C(23)	40(1)	51(2)	34(1)	-26(1)	6(1)	-11(1)
C(24)	25(1)	51(2)	53(2)	-34(1)	7(1)	-7(1)
C(25)	26(1)	18(1)	34(1)	-4(1)	4(1)	-3(1)
C(26)	39(1)	30(1)	66(2)	-9(1)	25(1)	2(1)
Pd(2)	15(1)	16(1)	19(1)	-5(1)	-2(1)	-2(1)
P(2)	14(1)	14(1)	17(1)	-3(1)	-1(1)	-2(1)

N(9)	19(1)	24(1)	25(1)	-7(1)	2(1)	-3(1)
N(10)	21(1)	17(1)	24(1)	-5(1)	-5(1)	-2(1)
N(11)	19(1)	19(1)	18(1)	-4(1)	1(1)	-6(1)
N(12)	16(1)	23(1)	20(1)	-7(1)	1(1)	-2(1)
N(13)	14(1)	22(1)	19(1)	-4(1)	0(1)	-4(1)
N(14)	18(1)	16(1)	34(1)	-4(1)	-6(1)	-3(1)
N(15)	48(1)	30(1)	30(1)	-7(1)	-8(1)	-7(1)
N(16)	24(1)	21(1)	21(1)	-6(1)	1(1)	-5(1)
C(27)	29(1)	20(1)	31(1)	-9(1)	1(1)	-7(1)
C(28)	32(1)	16(1)	29(1)	-2(1)	-1(1)	-5(1)
C(29)	20(1)	28(1)	23(1)	-10(1)	-2(1)	-5(1)
C(30)	23(1)	28(1)	21(1)	-9(1)	2(1)	-5(1)
C(31)	18(1)	35(1)	32(1)	-13(1)	5(1)	-10(1)
C(32)	14(1)	32(1)	30(1)	-12(1)	-1(1)	-2(1)
C(33)	21(1)	22(1)	20(1)	-5(1)	-2(1)	4(1)
C(34)	13(1)	24(1)	19(1)	-4(1)	1(1)	-1(1)
C(35)	20(1)	25(1)	25(1)	-2(1)	0(1)	2(1)
C(36)	20(1)	34(1)	21(1)	3(1)	-2(1)	-2(1)
C(37)	19(1)	39(1)	17(1)	-4(1)	2(1)	-9(1)
C(38)	16(1)	29(1)	21(1)	-7(1)	2(1)	-7(1)
C(39)	24(1)	25(1)	21(1)	-1(1)	1(1)	-9(1)
C(40)	20(1)	21(1)	32(1)	-1(1)	-6(1)	-8(1)
C(41)	31(1)	27(1)	42(1)	7(1)	-15(1)	-10(1)
C(42)	36(1)	23(1)	69(2)	8(1)	-29(1)	-6(1)
C(43)	32(1)	18(1)	78(2)	-12(1)	-25(1)	2(1)
C(44)	26(1)	24(1)	53(2)	-15(1)	-11(1)	-1(1)
C(45)	22(1)	23(1)	19(1)	-3(1)	2(1)	-2(1)
C(46)	20(1)	28(1)	20(1)	-7(1)	6(1)	-7(1)
C(47)	39(1)	32(1)	55(2)	-17(1)	-20(1)	2(1)
C(48)	31(1)	30(1)	77(2)	-20(1)	-6(1)	2(1)
C(49)	54(2)	32(1)	48(2)	-22(1)	13(1)	-11(1)
C(50)	79(2)	35(1)	35(1)	-11(1)	-12(1)	-14(1)
C(51)	30(1)	22(1)	21(1)	-4(1)	-1(1)	-5(1)
C(52)	51(2)	36(1)	38(1)	-12(1)	-9(1)	-22(1)
N(17)	113(3)	105(3)	64(2)	-19(2)	-24(2)	-57(3)
C(53)	118(4)	53(2)	41(2)	-5(2)	-19(2)	-28(2)
C(54)	66(6)	76(6)	69(6)	23(5)	-1(4)	-11(4)
C(54B)	117(10)	55(5)	43(4)	-1(4)	-21(6)	6(6)
N(18)	79(2)	60(2)	79(2)	-28(2)	-13(2)	29(2)
C(55)	43(2)	27(1)	70(2)	-12(1)	-20(2)	8(1)
C(56)	48(2)	36(2)	65(2)	-3(1)	-3(1)	3(1)
B(1)	22(1)	25(1)	25(1)	-1(1)	-2(1)	-6(1)
F(1)	36(1)	42(1)	50(1)	-23(1)	10(1)	-7(1)
F(2)	26(1)	26(1)	68(1)	-13(1)	16(1)	-9(1)

F(3)	36(1)	54(1)	36(1)	-6(1)	-14(1)	1(1)
F(4)	60(1)	30(1)	27(1)	3(1)	-3(1)	-17(1)
B(2)	76(2)	27(1)	33(2)	-9(1)	-4(2)	-8(2)
F(5)	71(3)	52(2)	40(2)	-2(2)	5(2)	-26(2)
F(6)	87(3)	58(3)	39(2)	-29(2)	3(2)	-17(2)
F(7)	78(5)	130(7)	84(5)	-20(4)	1(4)	28(4)
F(8)	54(3)	25(2)	86(4)	-17(2)	27(3)	-6(2)
F(5B)	138(10)	47(4)	69(6)	20(4)	-44(6)	-55(6)
F(6B)	94(5)	60(5)	26(3)	-13(3)	-1(3)	2(4)
F(7B)	85(8)	33(3)	34(4)	9(2)	-13(4)	-25(4)
F(8B)	78(5)	60(5)	48(4)	-32(4)	1(4)	12(4)
B(3)	47(2)	28(1)	23(1)	-9(1)	3(1)	-9(1)
F(9)	42(1)	66(1)	44(1)	-9(1)	-1(1)	-20(1)
F(10)	84(1)	36(1)	54(1)	-12(1)	-12(1)	3(1)
F(11)	118(2)	66(1)	21(1)	-14(1)	10(1)	-22(1)
F(12)	50(1)	53(1)	60(1)	-25(1)	8(1)	-27(1)
B(4)	23(1)	22(1)	22(1)	-6(1)	-3(1)	-4(1)
F(13)	23(1)	37(1)	36(1)	-7(1)	-8(1)	-1(1)
F(14)	27(1)	55(1)	30(1)	-22(1)	2(1)	-4(1)
F(15)	63(1)	24(1)	39(1)	-2(1)	-11(1)	-13(1)
F(16)	26(1)	31(1)	24(1)	-12(1)	-1(1)	-7(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5**

	x	y	z	U(eq)
H(1A)	5156	16845	2066	30
H(1B)	5174	16858	1430	30
H(2A)	7223	16752	1686	30
H(2B)	7078	15717	2171	30
H(3A)	3946	14842	2575	31
H(3B)	5281	15127	2682	31
H(4A)	5457	13188	2860	28
H(4B)	4814	13205	2302	28
H(5A)	3395	16031	1426	29
H(5B)	3422	14735	1696	29
H(6A)	4017	14819	784	28
H(6B)	5014	15616	826	28
H(7A)	9074	14839	1402	26
H(7B)	8658	16144	1177	26
H(9A)	8659	16752	215	30
H(10A)	8643	16357	-649	31
H(11A)	8438	14540	-730	30
H(12A)	8277	13185	46	27
H(13A)	7550	12784	2876	24
H(13B)	8410	13129	2358	24
H(15A)	7411	10832	3135	30
H(16A)	7480	9084	2910	36
H(17A)	7906	8913	2012	33
H(18A)	8200	10485	1367	27
H(19A)	4248	12980	1332	25
H(19B)	5587	12379	1536	25
H(21A)	3561	12717	497	42
H(22A)	3967	11995	-290	53
H(23A)	6018	11335	-500	47
H(24A)	7551	11367	87	48
H(26A)	11399	10909	54	70
H(26B)	11591	9983	598	70
H(26C)	12284	11052	511	70
H(27A)	11041	3232	3123	31
H(27B)	9845	2972	3492	31
H(28A)	10472	3839	4154	31
H(28B)	11633	2968	4028	31
H(29A)	9268	5605	2428	27

H(29B)	9953	4397	2369	27
H(30A)	11857	4833	2572	28
H(30B)	11268	5809	2095	28
H(31A)	8471	4464	3727	32
H(31B)	7921	4945	3133	32
H(32A)	8634	6647	3090	30
H(32B)	7891	6392	3651	30
H(33A)	13571	4894	3560	26
H(33B)	13479	3612	3812	26
H(35A)	14047	3012	4743	29
H(36A)	14214	3404	5603	32
H(37A)	13557	5219	5731	30
H(38A)	12747	6582	5008	25
H(39A)	12043	7218	2194	28
H(39B)	12863	6858	2726	28
H(41A)	11169	9121	1983	41
H(42A)	10501	10811	2250	53
H(43A)	10420	10856	3169	51
H(44A)	11061	9234	3796	40
H(45A)	10389	5662	4499	26
H(45B)	8935	5678	4463	26
H(47A)	8038	7975	3960	49
H(48A)	7710	9644	4275	54
H(49A)	8859	9787	5007	51
H(50A)	10382	8340	5347	58
H(52A)	15056	8802	4835	59
H(52B)	14294	9920	4502	59
H(52C)	15440	9276	4223	59
H(54A)	4258	9224	1966	113
H(54B)	3954	10390	1552	113
H(54C)	5129	10160	1933	113
H(54D)	3461	9121	1516	112
H(54E)	3675	10332	1583	112
H(54F)	4145	9262	2036	112
H(56A)	14895	902	3015	77
H(56B)	13685	1086	2659	77
H(56C)	14123	-101	3037	77

Table S26. Crystal data and structure refinement for **6**

Identification code	jyy160	
Empirical formula	C_{24} H_{30} Cl F_6 N_7 P_2 Pt	
Formula weight	823.03	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.4092(8) Å	α = 104.4188(9)°.
	b = 15.4825(12) Å	β = 92.0696(9)°.
	c = 19.0637(14) Å	γ = 94.3920(9)°.
Volume	2962.0(4) $Å^3$	
Z	4	
Density (calculated)	1.846 Mg/m^3	
Absorption coefficient	5.002 mm^{-1}	
F(000)	1608	
Crystal color	colorless	
Crystal size	0.238 x 0.186 x 0.160 mm^3	
Theta range for data collection	1.363 to 28.808°	
Index ranges	$-13 \le h \le 14$, $-20 \le k \le 20$, $-25 \le l \le 25$	
Reflections collected	34958	
Independent reflections	14052 [R(int) = 0.0248]	
Completeness to theta = 25.500°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4315 and 0.3191	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14052 / 0 / 757	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I) = 11631 data]	R1 = 0.0341, wR2 = 0.0740	
R indices (all data, 0.74 Å)	R1 = 0.0462, wR2 = 0.0780	
Largest diff. peak and hole	2.145 and -1.065 $e.Å^{-3}$	

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Pt(1)	9684(1)	5280(1)	7144(1)	18(1)
Pt(1B)	9622(4)	5015(2)	7238(2)	22(1)
Cl(1)	7699(1)	5815(1)	6796(1)	37(1)
P(1)	11642(1)	4999(1)	7485(1)	21(1)
N(1)	14320(4)	4729(3)	7833(2)	36(1)
N(2)	12367(3)	5946(2)	8013(2)	26(1)
N(3)	12428(3)	4683(2)	6742(2)	24(1)
N(4)	11650(3)	4237(3)	7949(2)	27(1)
N(5)	9437(3)	5857(3)	8207(2)	25(1)
N(6)	9804(3)	4539(2)	6105(2)	25(1)
N(7)	9536(4)	3682(3)	8721(2)	43(1)
C(1)	14639(4)	5661(4)	8165(3)	41(1)
C(2)	13715(4)	6241(3)	7900(3)	33(1)
C(3)	14603(4)	4367(4)	7086(3)	36(1)
C(4)	13359(4)	4005(3)	6629(3)	29(1)
C(5)	13962(5)	4148(4)	8276(3)	40(1)
C(6)	12593(5)	4292(4)	8552(3)	36(1)
C(7)	11565(4)	6682(3)	8309(2)	25(1)
C(8)	10380(4)	6395(3)	8647(2)	23(1)
C(9)	10225(5)	6693(3)	9383(2)	33(1)
C(10)	9092(5)	6465(4)	9673(3)	40(1)
C(11)	8128(5)	5932(4)	9217(3)	39(1)
C(12)	8329(4)	5633(4)	8486(3)	34(1)
C(13)	12069(4)	5072(3)	6144(2)	26(1)
C(14)	10883(4)	4550(3)	5730(2)	24(1)
C(15)	10879(5)	4082(3)	5009(2)	28(1)
C(16)	9787(5)	3568(3)	4670(3)	33(1)
C(17)	8708(5)	3523(3)	5066(3)	32(1)
C(18)	8743(4)	4020(3)	5775(3)	29(1)
C(19)	10821(5)	3404(3)	7665(3)	34(1)
C(20)	9520(5)	3404(3)	7994(3)	34(1)
C(21)	8390(5)	3112(4)	7559(3)	43(1)
C(22)	7222(5)	3086(4)	7892(4)	53(2)
C(23)	7227(5)	3352(4)	8629(4)	54(2)
C(24)	8396(5)	3663(5)	9023(3)	51(2)
Pt(2)	10101(1)	8600(1)	7127(1)	17(1)
Pt(2B)	10214(6)	8913(3)	7164(4)	29(1)
Cl(2)	12090(1)	7913(1)	6915(1)	29(1)

P(2)	8156(1)	9097(1)	7334(1)	20(1)
N(8)	5652(4)	9664(3)	7526(2)	35(1)
N(9)	7498(3)	8641(3)	7965(2)	28(1)
N(10)	7292(3)	8792(3)	6550(2)	25(1)
N(11)	8295(3)	10192(3)	7660(2)	24(1)
N(12)	10435(3)	8780(2)	8208(2)	25(1)
N(13)	9941(3)	8603(2)	6058(2)	22(1)
N(14)	11214(4)	11040(3)	6988(2)	34(1)
C(25)	5281(5)	9101(4)	7999(3)	44(1)
C(26)	6104(4)	8317(4)	7874(3)	41(1)
C(27)	5190(4)	9395(4)	6772(2)	34(1)
C(28)	6368(4)	9356(4)	6313(2)	30(1)
C(29)	6044(5)	10588(4)	7849(3)	40(1)
C(30)	7427(4)	10662(3)	8192(2)	31(1)
C(31)	8291(5)	8066(3)	8280(2)	30(1)
C(32)	9536(4)	8554(3)	8642(2)	28(1)
C(33)	9783(5)	8751(3)	9390(3)	36(1)
C(34)	10974(5)	9159(4)	9688(3)	41(1)
C(35)	11890(5)	9385(3)	9249(3)	37(1)
C(36)	11587(4)	9188(3)	8509(3)	31(1)
C(37)	7700(4)	8027(3)	6004(2)	28(1)
C(38)	8842(4)	8331(3)	5639(2)	25(1)
C(39)	8779(5)	8351(3)	4916(2)	32(1)
C(40)	9858(5)	8684(4)	4626(3)	37(1)
C(41)	10972(5)	8969(3)	5056(3)	33(1)
C(42)	10986(4)	8919(3)	5764(3)	29(1)
C(43)	9015(4)	10703(3)	7230(2)	26(1)
C(44)	10394(4)	10986(3)	7504(2)	26(1)
C(45)	10790(5)	11197(3)	8239(3)	35(1)
C(46)	12069(5)	11482(4)	8446(3)	41(1)
C(47)	12917(5)	11536(4)	7915(3)	42(1)
C(48)	12458(5)	11301(4)	7200(3)	41(1)
P(3)	5211(1)	2085(1)	10037(1)	34(1)
F(1)	4756(3)	2381(3)	9329(2)	61(1)
F(2)	5679(3)	1787(2)	10741(2)	43(1)
F(3)	4281(5)	1209(3)	9785(2)	98(2)
F(4)	6363(4)	1626(3)	9614(2)	88(2)
F(5)	6146(3)	2988(2)	10294(2)	56(1)
F(6)	4104(3)	2588(3)	10486(2)	72(1)
P(4)	5569(1)	11870(1)	5806(1)	29(1)
F(7)	4355(3)	12255(2)	5491(2)	53(1)
F(8)	6123(3)	11637(2)	5026(2)	50(1)
F(9)	6327(3)	12837(2)	5990(2)	50(1)
F(10)	5007(3)	12115(2)	6595(2)	53(1)

F(11)	4804(4)	10915(2)	5643(2)	71(1)
F(12)	6788(3)	11499(3)	6138(2)	62(1)

Table S28. Bond lengths [Å] and angles [°] for **6**

Pt(1)-N(5)	2.034(4)	C(21)-C(22)	1.394(8)
Pt(1)-N(6)	2.041(4)	C(22)-C(23)	1.363(9)
Pt(1)-P(1)	2.2245(11)	C(23)-C(24)	1.392(8)
Pt(1)-Cl(1)	2.4153(13)	Pt(2)-N(12)	2.024(4)
Pt(1B)-N(5)	2.003(6)	Pt(2)-N(13)	2.041(3)
Pt(1B)-N(6)	2.122(5)	Pt(2)-P(2)	2.2339(11)
Pt(1B)-P(1)	2.142(4)	Pt(2)-Cl(2)	2.4011(12)
Pt(1B)-Cl(1)	2.652(4)	Pt(2B)-N(13)	2.047(7)
P(1)-N(4)	1.642(4)	Pt(2B)-N(12)	2.059(7)
P(1)-N(3)	1.649(4)	Pt(2B)-P(2)	2.207(6)
P(1)-N(2)	1.666(4)	Pt(2B)-Cl(2)	2.569(6)
P(1)-N(1)	2.927(4)	P(2)-N(11)	1.647(4)
N(1)-C(5)	1.418(7)	P(2)-N(10)	1.659(4)
N(1)-C(1)	1.432(7)	P(2)-N(9)	1.682(4)
N(1)-C(3)	1.445(6)	P(2)-N(8)	2.821(4)
N(2)-C(7)	1.474(5)	N(8)-C(29)	1.430(7)
N(2)-C(2)	1.482(6)	N(8)-C(25)	1.446(7)
N(3)-C(13)	1.464(6)	N(8)-C(27)	1.447(6)
N(3)-C(4)	1.464(5)	N(9)-C(31)	1.476(6)
N(4)-C(6)	1.466(5)	N(9)-C(26)	1.488(6)
N(4)-C(19)	1.467(6)	N(10)-C(37)	1.471(6)
N(5)-C(12)	1.344(6)	N(10)-C(28)	1.478(5)
N(5)-C(8)	1.353(6)	N(11)-C(43)	1.461(6)
N(6)-C(18)	1.350(6)	N(11)-C(30)	1.474(5)
N(6)-C(14)	1.354(5)	N(12)-C(36)	1.349(6)
N(7)-C(24)	1.339(7)	N(12)-C(32)	1.354(6)
N(7)-C(20)	1.343(7)	N(13)-C(38)	1.348(5)
C(1)-C(2)	1.520(7)	N(13)-C(42)	1.355(5)
C(3)-C(4)	1.521(6)	N(14)-C(44)	1.340(6)
C(5)-C(6)	1.550(7)	N(14)-C(48)	1.343(6)
C(7)-C(8)	1.500(6)	C(25)-C(26)	1.514(8)
C(8)-C(9)	1.383(6)	C(27)-C(28)	1.528(6)
C(9)-C(10)	1.378(7)	C(29)-C(30)	1.543(6)
C(10)-C(11)	1.377(8)	C(31)-C(32)	1.500(7)
C(11)-C(12)	1.384(7)	C(32)-C(33)	1.392(6)
C(13)-C(14)	1.503(6)	C(33)-C(34)	1.381(7)
C(14)-C(15)	1.385(6)	C(34)-C(35)	1.373(8)
C(15)-C(16)	1.376(7)	C(35)-C(36)	1.385(7)
C(16)-C(17)	1.382(7)	C(37)-C(38)	1.501(6)
C(17)-C(18)	1.378(6)	C(38)-C(39)	1.387(6)
C(19)-C(20)	1.513(7)	C(39)-C(40)	1.389(7)
C(20)-C(21)	1.392(7)	C(40)-C(41)	1.373(7)

C(41)-C(42)	1.371(6)
C(43)-C(44)	1.504(6)
C(44)-C(45)	1.396(6)
C(45)-C(46)	1.381(7)
C(46)-C(47)	1.381(8)
C(47)-C(48)	1.377(8)
P(3)-F(3)	1.565(4)
P(3)-F(4)	1.584(4)
P(3)-F(6)	1.595(4)
P(3)-F(2)	1.596(3)
P(3)-F(1)	1.597(3)
P(3)-F(5)	1.598(4)
P(4)-F(11)	1.578(4)
P(4)-F(8)	1.583(3)
P(4)-F(9)	1.589(3)
P(4)-F(7)	1.597(3)
P(4)-F(10)	1.600(3)
P(4)-F(12)	1.604(3)

N(5)-Pt(1)-N(6)	171.84(15)
N(5)-Pt(1)-P(1)	87.62(10)
N(6)-Pt(1)-P(1)	93.00(10)
N(5)-Pt(1)-Cl(1)	90.48(10)
N(6)-Pt(1)-Cl(1)	90.09(11)
P(1)-Pt(1)-Cl(1)	171.28(5)
N(5)-Pt(1B)-N(6)	160.4(2)
N(5)-Pt(1B)-P(1)	90.8(2)
N(6)-Pt(1B)-P(1)	93.15(19)
N(5)-Pt(1B)-Cl(1)	84.66(17)
N(6)-Pt(1B)-Cl(1)	82.24(15)
P(1)-Pt(1B)-Cl(1)	149.51(15)
N(4)-P(1)-N(3)	110.10(19)
N(4)-P(1)-N(2)	107.4(2)
N(3)-P(1)-N(2)	110.05(19)
N(4)-P(1)-Pt(1B)	101.99(15)
N(3)-P(1)-Pt(1B)	111.38(17)
N(2)-P(1)-Pt(1B)	115.49(17)
N(4)-P(1)-Pt(1)	114.43(14)
N(3)-P(1)-Pt(1)	107.03(13)
N(2)-P(1)-Pt(1)	107.77(13)
N(4)-P(1)-N(1)	71.14(16)
N(3)-P(1)-N(1)	68.96(15)
N(2)-P(1)-N(1)	70.70(15)
Pt(1B)-P(1)-N(1)	172.30(13)
Pt(1)-P(1)-N(1)	174.29(10)
C(5)-N(1)-C(1)	119.1(4)
C(5)-N(1)-C(3)	120.4(4)
C(1)-N(1)-C(3)	119.5(4)
C(5)-N(1)-P(1)	93.3(3)
C(1)-N(1)-P(1)	92.7(3)
C(3)-N(1)-P(1)	94.3(3)
C(7)-N(2)-C(2)	114.5(4)
C(7)-N(2)-P(1)	118.2(3)
C(2)-N(2)-P(1)	120.3(3)
C(13)-N(3)-C(4)	119.4(3)
C(13)-N(3)-P(1)	115.8(3)
C(4)-N(3)-P(1)	124.6(3)
C(6)-N(4)-C(19)	119.0(4)
C(6)-N(4)-P(1)	122.7(3)
C(19)-N(4)-P(1)	117.5(3)
C(12)-N(5)-C(8)	119.6(4)
C(12)-N(5)-Pt(1B)	110.2(3)
C(8)-N(5)-Pt(1B)	127.4(3)
C(12)-N(5)-Pt(1)	117.9(3)
C(8)-N(5)-Pt(1)	122.3(3)
C(18)-N(6)-C(14)	118.7(4)
C(18)-N(6)-Pt(1)	117.8(3)
C(14)-N(6)-Pt(1)	123.4(3)
C(18)-N(6)-Pt(1B)	111.7(3)
C(14)-N(6)-Pt(1B)	128.2(3)
C(24)-N(7)-C(20)	116.8(5)
N(1)-C(1)-C(2)	111.8(4)
N(2)-C(2)-C(1)	110.0(4)
N(1)-C(3)-C(4)	110.0(4)
N(3)-C(4)-C(3)	110.5(4)
N(1)-C(5)-C(6)	111.5(4)
N(4)-C(6)-C(5)	111.0(4)
N(2)-C(7)-C(8)	113.7(4)
N(5)-C(8)-C(9)	120.4(4)
N(5)-C(8)-C(7)	118.0(4)
C(9)-C(8)-C(7)	121.5(4)
C(10)-C(9)-C(8)	120.4(5)
C(11)-C(10)-C(9)	118.7(4)
C(10)-C(11)-C(12)	119.2(5)
N(5)-C(12)-C(11)	121.7(5)
N(3)-C(13)-C(14)	109.5(4)
N(6)-C(14)-C(15)	120.8(4)
N(6)-C(14)-C(13)	116.5(4)

C(15)-C(14)-C(13)	122.7(4)	C(27)-N(8)-P(2)	97.5(3)
C(16)-C(15)-C(14)	120.2(4)	C(31)-N(9)-C(26)	112.8(4)
C(15)-C(16)-C(17)	118.7(4)	C(31)-N(9)-P(2)	117.2(3)
C(18)-C(17)-C(16)	119.0(4)	C(26)-N(9)-P(2)	119.0(3)
N(6)-C(18)-C(17)	122.3(4)	C(37)-N(10)-C(28)	118.2(3)
N(4)-C(19)-C(20)	113.6(4)	C(37)-N(10)-P(2)	116.6(3)
N(7)-C(20)-C(21)	123.1(5)	C(28)-N(10)-P(2)	123.6(3)
N(7)-C(20)-C(19)	116.0(4)	C(43)-N(11)-C(30)	118.4(4)
C(21)-C(20)-C(19)	120.9(5)	C(43)-N(11)-P(2)	115.7(3)
C(20)-C(21)-C(22)	118.6(6)	C(30)-N(11)-P(2)	122.8(3)
C(23)-C(22)-C(21)	118.9(5)	C(36)-N(12)-C(32)	119.1(4)
C(22)-C(23)-C(24)	118.8(5)	C(36)-N(12)-Pt(2)	117.8(3)
N(7)-C(24)-C(23)	123.8(6)	C(32)-N(12)-Pt(2)	123.0(3)
N(12)-Pt(2)-N(13)	170.95(15)	C(36)-N(12)-Pt(2B)	109.4(3)
N(12)-Pt(2)-P(2)	89.16(10)	C(32)-N(12)-Pt(2B)	129.4(3)
N(13)-Pt(2)-P(2)	92.61(10)	C(38)-N(13)-C(42)	118.8(4)
N(12)-Pt(2)-Cl(2)	90.00(10)	C(38)-N(13)-Pt(2)	123.2(3)
N(13)-Pt(2)-Cl(2)	89.16(10)	C(42)-N(13)-Pt(2)	117.9(3)
P(2)-Pt(2)-Cl(2)	173.90(4)	C(38)-N(13)-Pt(2B)	129.3(3)
N(13)-Pt(2B)-N(12)	161.4(3)	C(42)-N(13)-Pt(2B)	110.1(3)
N(13)-Pt(2B)-P(2)	93.2(3)	C(44)-N(14)-C(48)	117.5(4)
N(12)-Pt(2B)-P(2)	89.0(3)	N(8)-C(25)-C(26)	109.3(4)
N(13)-Pt(2B)-Cl(2)	84.5(2)	N(9)-C(26)-C(25)	110.4(4)
N(12)-Pt(2B)-Cl(2)	84.7(2)	N(8)-C(27)-C(28)	107.5(4)
P(2)-Pt(2B)-Cl(2)	151.36(19)	N(10)-C(28)-C(27)	109.4(4)
N(11)-P(2)-N(10)	111.63(19)	N(8)-C(29)-C(30)	108.5(4)
N(11)-P(2)-N(9)	107.66(19)	N(11)-C(30)-C(29)	110.8(4)
N(10)-P(2)-N(9)	111.94(19)	N(9)-C(31)-C(32)	112.4(4)
N(11)-P(2)-Pt(2B)	98.16(17)	N(12)-C(32)-C(33)	120.7(4)
N(10)-P(2)-Pt(2B)	110.6(2)	N(12)-C(32)-C(31)	117.2(4)
N(9)-P(2)-Pt(2B)	116.0(2)	C(33)-C(32)-C(31)	122.1(4)
N(11)-P(2)-Pt(2)	110.18(13)	C(34)-C(33)-C(32)	119.4(5)
N(10)-P(2)-Pt(2)	107.03(13)	C(35)-C(34)-C(33)	120.0(5)
N(9)-P(2)-Pt(2)	108.36(13)	C(34)-C(35)-C(36)	118.3(5)
N(11)-P(2)-N(8)	72.04(16)	N(12)-C(36)-C(35)	122.5(5)
N(10)-P(2)-N(8)	70.14(15)	N(10)-C(37)-C(38)	109.5(4)
N(9)-P(2)-N(8)	72.38(15)	N(13)-C(38)-C(39)	121.0(4)
Pt(2B)-P(2)-N(8)	169.15(15)	N(13)-C(38)-C(37)	116.4(4)
Pt(2)-P(2)-N(8)	177.04(10)	C(39)-C(38)-C(37)	122.6(4)
C(29)-N(8)-C(25)	118.0(4)	C(38)-C(39)-C(40)	119.3(4)
C(29)-N(8)-C(27)	119.1(4)	C(41)-C(40)-C(39)	119.4(4)
C(25)-N(8)-C(27)	119.0(4)	C(42)-C(41)-C(40)	118.9(4)
C(29)-N(8)-P(2)	96.6(3)	N(13)-C(42)-C(41)	122.5(4)
C(25)-N(8)-P(2)	95.6(3)	N(11)-C(43)-C(44)	114.1(3)

N(14)-C(44)-C(45)	122.3(4)	F(6)-P(3)-F(5)	88.9(2)
N(14)-C(44)-C(43)	114.7(4)	F(2)-P(3)-F(5)	89.97(18)
C(45)-C(44)-C(43)	122.9(4)	F(1)-P(3)-F(5)	89.92(19)
C(46)-C(45)-C(44)	119.2(5)	F(11)-P(4)-F(8)	90.7(2)
C(47)-C(46)-C(45)	118.6(5)	F(11)-P(4)-F(9)	178.6(2)
C(48)-C(47)-C(46)	118.9(5)	F(8)-P(4)-F(9)	90.70(19)
N(14)-C(48)-C(47)	123.5(5)	F(11)-P(4)-F(7)	90.0(2)
F(3)-P(3)-F(4)	92.3(3)	F(8)-P(4)-F(7)	89.99(18)
F(3)-P(3)-F(6)	90.5(3)	F(9)-P(4)-F(7)	90.07(19)
F(4)-P(3)-F(6)	177.1(3)	F(11)-P(4)-F(10)	89.69(19)
F(3)-P(3)-F(2)	90.5(2)	F(8)-P(4)-F(10)	179.5(2)
F(4)-P(3)-F(2)	89.98(19)	F(9)-P(4)-F(10)	88.92(18)
F(6)-P(3)-F(2)	89.14(19)	F(7)-P(4)-F(10)	89.70(19)
F(3)-P(3)-F(1)	89.6(2)	F(11)-P(4)-F(12)	90.6(2)
F(4)-P(3)-F(1)	89.4(2)	F(8)-P(4)-F(12)	90.91(18)
F(6)-P(3)-F(1)	91.4(2)	F(9)-P(4)-F(12)	89.3(2)
F(2)-P(3)-F(1)	179.4(2)	F(7)-P(4)-F(12)	178.9(2)
F(3)-P(3)-F(5)	179.3(3)	F(10)-P(4)-F(12)	89.39(19)
F(4)-P(3)-F(5)	88.2(2)		

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	14(1)	25(1)	16(1)	6(1)	0(1)	3(1)
Pt(1B)	23(1)	29(2)	22(1)	17(1)	4(1)	9(1)
Cl(1)	33(1)	45(1)	33(1)	13(1)	0(1)	1(1)
P(1)	16(1)	28(1)	19(1)	2(1)	1(1)	4(1)
N(1)	32(2)	43(3)	31(2)	3(2)	3(2)	14(2)
N(2)	17(2)	27(2)	28(2)	-3(2)	2(1)	5(2)
N(3)	21(2)	29(2)	21(2)	0(2)	3(1)	6(2)
N(4)	23(2)	36(2)	23(2)	7(2)	-2(2)	8(2)
N(5)	21(2)	32(2)	21(2)	6(2)	5(1)	10(2)
N(6)	26(2)	26(2)	22(2)	6(2)	-2(2)	1(2)
N(7)	27(2)	74(3)	39(2)	29(2)	0(2)	13(2)
C(1)	19(2)	53(3)	41(3)	-6(2)	-4(2)	5(2)
C(2)	19(2)	34(3)	36(3)	-7(2)	1(2)	-2(2)
C(3)	26(2)	40(3)	37(3)	-2(2)	4(2)	11(2)
C(4)	25(2)	29(2)	29(2)	-2(2)	5(2)	9(2)
C(5)	29(3)	51(3)	39(3)	6(2)	-6(2)	18(2)
C(6)	32(3)	50(3)	30(3)	15(2)	-3(2)	14(2)
C(7)	25(2)	24(2)	23(2)	2(2)	0(2)	5(2)
C(8)	25(2)	24(2)	22(2)	6(2)	0(2)	12(2)
C(9)	36(3)	41(3)	23(2)	8(2)	2(2)	14(2)
C(10)	46(3)	57(3)	22(2)	15(2)	11(2)	20(3)
C(11)	30(3)	63(4)	32(3)	21(3)	14(2)	16(2)
C(12)	23(2)	50(3)	31(3)	13(2)	6(2)	10(2)
C(13)	26(2)	31(2)	21(2)	3(2)	8(2)	2(2)
C(14)	29(2)	22(2)	20(2)	5(2)	1(2)	5(2)
C(15)	40(3)	23(2)	23(2)	6(2)	3(2)	5(2)
C(16)	51(3)	25(2)	22(2)	2(2)	-8(2)	10(2)
C(17)	41(3)	23(2)	29(2)	5(2)	-14(2)	-2(2)
C(18)	25(2)	30(3)	32(2)	8(2)	-5(2)	0(2)
C(19)	41(3)	29(3)	34(3)	11(2)	4(2)	5(2)
C(20)	32(3)	38(3)	40(3)	22(2)	1(2)	7(2)
C(21)	40(3)	42(3)	52(3)	23(3)	-10(2)	-2(2)
C(22)	35(3)	47(4)	83(5)	32(3)	-13(3)	0(3)
C(23)	24(3)	72(4)	88(5)	60(4)	8(3)	8(3)
C(24)	38(3)	83(5)	49(3)	43(3)	8(3)	19(3)
Pt(2)	13(1)	21(1)	15(1)	3(1)	1(1)	3(1)
Pt(2B)	23(2)	26(3)	38(2)	10(2)	0(1)	4(2)
Cl(2)	26(1)	33(1)	27(1)	7(1)	2(1)	3(1)

P(2)	15(1)	32(1)	15(1)	6(1)	2(1)	4(1)
N(8)	23(2)	54(3)	27(2)	9(2)	4(2)	9(2)
N(9)	18(2)	44(2)	25(2)	15(2)	5(2)	4(2)
N(10)	15(2)	41(2)	18(2)	5(2)	0(1)	5(2)
N(11)	20(2)	35(2)	20(2)	7(2)	4(1)	9(2)
N(12)	24(2)	28(2)	21(2)	1(2)	-2(1)	14(2)
N(13)	17(2)	31(2)	20(2)	9(2)	6(1)	6(2)
N(14)	30(2)	41(2)	33(2)	9(2)	4(2)	8(2)
C(25)	23(2)	83(4)	31(3)	21(3)	10(2)	6(3)
C(26)	22(2)	68(4)	37(3)	24(3)	8(2)	-6(2)
C(27)	19(2)	56(3)	26(2)	10(2)	1(2)	6(2)
C(28)	19(2)	50(3)	23(2)	13(2)	-2(2)	11(2)
C(29)	30(3)	66(4)	27(2)	10(2)	3(2)	28(3)
C(30)	31(2)	42(3)	21(2)	2(2)	6(2)	19(2)
C(31)	36(3)	35(3)	24(2)	14(2)	3(2)	3(2)
C(32)	33(2)	26(2)	27(2)	7(2)	4(2)	16(2)
C(33)	50(3)	34(3)	24(2)	5(2)	4(2)	15(2)
C(34)	55(3)	42(3)	22(2)	-2(2)	-10(2)	18(3)
C(35)	35(3)	38(3)	33(3)	-4(2)	-13(2)	13(2)
C(36)	27(2)	33(3)	30(2)	1(2)	-4(2)	11(2)
C(37)	22(2)	40(3)	18(2)	3(2)	0(2)	1(2)
C(38)	24(2)	29(2)	23(2)	6(2)	4(2)	7(2)
C(39)	32(3)	44(3)	22(2)	7(2)	3(2)	11(2)
C(40)	45(3)	48(3)	25(2)	19(2)	10(2)	15(2)
C(41)	32(2)	42(3)	34(3)	21(2)	15(2)	11(2)
C(42)	20(2)	35(3)	35(3)	11(2)	8(2)	8(2)
C(43)	29(2)	28(2)	24(2)	9(2)	-2(2)	6(2)
C(44)	31(2)	23(2)	24(2)	10(2)	-3(2)	6(2)
C(45)	38(3)	41(3)	26(2)	12(2)	-6(2)	-1(2)
C(46)	42(3)	43(3)	39(3)	17(2)	-16(2)	-1(2)
C(47)	25(2)	38(3)	62(4)	13(3)	-10(2)	6(2)
C(48)	28(3)	44(3)	53(3)	11(3)	11(2)	10(2)
P(3)	32(1)	44(1)	23(1)	5(1)	-1(1)	1(1)
F(1)	55(2)	87(3)	44(2)	32(2)	-19(2)	-16(2)
F(2)	49(2)	54(2)	30(2)	13(1)	3(1)	12(2)
F(3)	132(4)	66(3)	88(3)	35(2)	-60(3)	-53(3)
F(4)	100(3)	131(4)	38(2)	12(2)	28(2)	66(3)
F(5)	58(2)	68(2)	39(2)	15(2)	-6(2)	-20(2)
F(6)	51(2)	96(3)	92(3)	49(2)	34(2)	38(2)
P(4)	25(1)	34(1)	28(1)	6(1)	4(1)	4(1)
F(7)	30(2)	64(2)	57(2)	-1(2)	-7(1)	19(2)
F(8)	41(2)	81(2)	30(2)	10(2)	6(1)	21(2)
F(9)	48(2)	52(2)	49(2)	17(2)	-1(2)	-18(2)
F(10)	48(2)	65(2)	40(2)	3(2)	20(2)	-10(2)

F(11)	102(3)	38(2)	65(2)	5(2)	7(2)	-13(2)
F(12)	67(2)	84(3)	42(2)	16(2)	-1(2)	42(2)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**

	x	y	z	U(eq)
H(1A)	15529	5835	8053	49
H(1B)	14612	5767	8698	49
H(2A)	13920	6875	8168	39
H(2B)	13816	6194	7378	39
H(3A)	15179	3881	7054	43
H(3B)	15053	4842	6897	43
H(4A)	13547	3830	6110	35
H(4B)	12985	3466	6764	35
H(5A)	14593	4258	8697	48
H(5B)	13983	3519	7995	48
H(6A)	12333	3832	8811	43
H(6B)	12606	4887	8900	43
H(7A)	11299	6952	7912	29
H(7B)	12093	7151	8678	29
H(9A)	10902	7056	9690	39
H(10A)	8979	6671	10177	48
H(11A)	7334	5772	9402	47
H(12A)	7667	5260	8173	41
H(13A)	12788	5055	5816	32
H(13B)	11898	5704	6339	32
H(15A)	11633	4115	4748	34
H(16A)	9775	3252	4174	40
H(17A)	7953	3154	4851	38
H(18A)	7994	3997	6043	35
H(19A)	11271	2899	7759	41
H(19B)	10686	3301	7133	41
H(21A)	8414	2936	7046	52
H(22A)	6435	2885	7609	63
H(23A)	6448	3325	8870	64
H(24A)	8384	3874	9535	61
H(25A)	4358	8879	7898	53
H(25B)	5401	9450	8512	53
H(26A)	5902	7956	8224	49
H(26B)	5907	7930	7378	49
H(27A)	4616	9832	6663	41
H(27B)	4696	8800	6664	41
H(28A)	6098	9103	5795	36
H(28B)	6785	9968	6370	36

H(29A)	5449	10836	8227	48
H(29B)	6023	10933	7477	48
H(30A)	7753	11301	8365	38
H(30B)	7416	10398	8614	38
H(31A)	8483	7544	7892	36
H(31B)	7793	7840	8640	36
H(33A)	9139	8607	9693	43
H(34A)	11159	9283	10197	49
H(35A)	12711	9669	9447	45
H(36A)	12214	9347	8203	38
H(37A)	6981	7773	5638	33
H(37B)	7934	7554	6240	33
H(39A)	8008	8140	4622	39
H(40A)	9825	8714	4134	44
H(41A)	11720	9196	4866	40
H(42A)	11759	9115	6061	35
H(43A)	8570	11244	7224	32
H(43B)	9004	10335	6724	32
H(45A)	10188	11145	8592	42
H(46A)	12359	11638	8943	49
H(47A)	13802	11731	8040	50
H(48A)	13053	11326	6838	49

Table S31. **Optimized Coordinates for 1**

Co	4.371075687008	11.960855530715	3.048982070568
Cl	4.634713442546	9.695386084716	3.587945203238
P	3.738984775026	14.022572200466	3.177398006133
N	6.273616426953	12.361825325558	3.495916561202
N	4.952065534771	15.095450696038	3.723405033398
N	3.290682630871	14.592556736451	1.603298717068
N	3.003339093560	17.174173732985	3.062922060984
N	2.437895432826	14.422833797314	4.232200144291
C	1.486728536005	13.034470522625	8.364083788467
H	0.955263198367	13.551050552162	9.162566464228
N	2.800274799624	11.570224399275	1.873753200258
C	6.801790419335	13.463652844559	4.092847751244
C	5.843265644102	14.468171889881	4.699351441080
H	5.234715324823	13.966337309665	5.464159130147
H	6.411449474160	15.250799387243	5.213352249917
C	2.149834874698	15.493617109708	1.400955032421
H	1.284887452616	15.183863901210	2.004815578377
H	1.843242424522	15.432874559297	0.349425202851
C	2.497078236601	16.956247500414	1.727259332162
H	3.254160130979	17.308590926891	1.016782381624
H	1.588843279163	17.561211633978	1.554153699903
C	2.131870960059	16.936649802999	4.195644039218
H	1.103123328453	16.893653403632	3.817515135583
H	2.173634354997	17.791590840110	4.893515840063
C	2.423025481301	15.666445870365	5.016811421084
H	3.377016840274	15.799187493067	5.542640473493
H	1.653991506101	15.560042429694	5.788748622340
C	1.533052715584	13.358168029460	4.705984343495
H	1.573952837974	12.535555234651	3.990171483705
H	0.507318499323	13.746111339029	4.717269719694
C	1.850613698756	12.837964955671	6.100995022459
C	2.764754596444	11.793199862328	6.298633161718
H	3.255326733253	11.318719225908	5.451147405105
C	3.029554630684	11.371641370684	7.600797590524
H	3.727276858030	10.557302442681	7.777319482489
C	2.380020175406	12.005136732564	8.661018116039
H	2.553134558732	11.708152616618	9.691446726738
N	1.216647763369	13.447418214625	7.119087710089
C	4.402076947816	17.476793200098	3.270439668702
H	4.519042889421	17.805876093755	4.310466754472
H	4.711828821696	18.322631423499	2.632163872152
C	5.363660623560	16.295223773277	3.005821531419
H	5.409216578672	16.102345927616	1.926111004805

H	6.377950927859	16.568154541549	3.324432375759
C	3.477271698282	13.545425161549	0.580618093821
H	4.521088315234	13.215424510258	0.604998511665
H	3.291926678090	13.989517979107	-0.403315530927
C	2.583031424049	12.332810950276	0.768220129943
C	1.993750185417	10.505206608229	2.077769523040
H	2.229877286551	9.911161925270	2.951625135808
C	0.961571659498	10.157474208989	1.210987648680
H	0.349675129463	9.289469014964	1.434372165995
C	0.745565041635	10.928445896135	0.072069776587
H	-0.045533668704	10.682373902507	-0.630661162498
C	1.573919185569	12.028978435577	-0.144859193610
H	1.445957632252	12.658028326720	-1.020808997719
C	8.177499453162	13.695335059296	4.134934388166
H	8.545718841048	14.587729854096	4.632892110005
C	9.060169660021	12.790735512434	3.549631175000
H	10.132715899438	12.961328673895	3.576068818384
C	8.522009564285	11.661984637730	2.937110946612
H	9.152146555760	10.913028961072	2.468224369897
C	7.143073832921	11.482540241864	2.939135013291
H	6.691796479408	10.598568674903	2.508942527354

Table S32. Optimized Coordinates for 2

Co	7.188603486027	6.552243987197	10.731733250787
P	7.131874270102	8.072006821056	12.407513779643
N	7.167607304849	9.969609977505	14.457987791084
N	8.652670931652	7.996116901656	13.171923804625
N	8.097988922452	5.237507276670	12.033056914030
N	6.863755534259	9.598840576035	11.755314057291
N	7.336060810928	8.047962685134	9.249766716643
N	5.849981286239	7.700613914186	13.455167841377
N	5.031041776946	6.212754268297	10.945346682264
N	7.295061915420	5.092319837347	9.308079573808
C	7.106065869020	11.166165254834	13.632992591230
H	7.721636348697	11.982890871593	14.036354567093
H	6.071513260794	11.523340323033	13.608060530078
C	7.560304124288	10.812786995971	12.205544409076
H	7.337828533743	11.623015549087	11.504770855600
H	8.644640034089	10.654490033788	12.183776832051
C	6.007516380443	9.632350352832	10.566725355300
H	5.577207444283	10.632556087095	10.470636285354
H	5.167957852170	8.939276166014	10.696906972606
C	6.772962814937	9.278780860342	9.307651966047
C	6.935083980843	10.210073723761	8.281967739859
H	6.450168894150	11.178010588255	8.359674316559
C	7.724270466053	9.897313976994	7.176455018642
H	7.863124499469	10.615098876054	6.373831855945
C	8.341178975880	8.648960919078	7.137182768404
H	8.984655252855	8.358146149582	6.313811129147
C	8.115845082846	7.761526963200	8.183334773845
H	8.572041298011	6.780083419442	8.172711026929
C	8.448114089342	9.598882841099	15.038167343516
H	8.455142574052	9.689900145401	16.134357074646
H	9.215596959476	10.276064187203	14.651193651550
C	8.798226306737	8.161624506335	14.634935599449
H	9.836646535017	7.939337277056	14.899507974021
H	8.163096616438	7.448405703232	15.177428671118
C	9.614463727916	7.092029998796	12.516318673844
H	10.602909608420	7.266629474605	12.948655461484
H	9.692248694809	7.361632638348	11.454946698951
C	9.242011081053	5.623425869326	12.646208847905
C	10.007074000510	4.722359191039	13.386464010194
H	10.925146248054	5.058398181398	13.857805925393
C	9.582739942390	3.399623269124	13.514051506305
H	10.165794226324	2.687125757948	14.089521432616
C	8.393861506158	3.013081341235	12.894633212914

H	8.017751529012	1.998692457761	12.973591187552
C	7.686969173628	3.959430046164	12.161166181659
H	6.761714134578	3.703891633088	11.655861165745
C	5.950857014670	9.527711574116	15.120331762342
H	5.382675685480	10.364599152337	15.553087553843
H	6.222335342084	8.860019071939	15.943993088478
C	5.069611142837	8.764250480258	14.121194774677
H	4.226152101255	8.296449030451	14.637133470897
H	4.649324186956	9.459769073259	13.383768774004
C	5.251308199915	6.358407682072	13.379290477203
H	4.642021405439	6.208337335300	14.273893749233
H	6.044284121014	5.608096556974	13.416991075664
C	4.401221142910	6.135442370900	12.140410573989
C	3.032213708559	5.878430910430	12.230910928852
H	2.560103963156	5.813304495009	13.206273820150
C	2.283193926921	5.709701882677	11.066231130831
H	1.217064696925	5.511209107370	11.119710084931
C	2.930450195558	5.809854797764	9.835595542542
H	2.391579120222	5.697709140788	8.900743177721
C	4.299544109767	6.060026495110	9.824615506834
H	4.841180917187	6.143283232290	8.888084704234
C	7.361222745830	4.213593254398	8.555507202851
C	7.446115596997	3.110513297339	7.605397510488
H	6.656064477041	2.380026268114	7.807977029260
H	8.419262073778	2.616322812076	7.692763309295
H	7.328099820143	3.486024103832	6.583710727502

Table S33. **Optimized Coordinates for 3b**

Ni	3.092092727440	8.976607300487	1.823344947458
P	2.773411852696	10.896272011393	0.554976223733
O	2.934407829855	9.391796238451	4.725641108455
N	2.739165341336	13.677703711092	-1.231178480607
C	2.340267053286	12.900372100782	-2.370073379133
H	3.226758247895	12.732001598835	-2.997417123283
H	1.620984761522	13.459729637931	-2.995610702955
O	1.615321904791	6.535960684506	1.120535984834
N	1.532953872957	12.052767560957	0.940123374738
C	1.717090138635	11.558245082109	-2.000922078467
H	0.766503835853	11.744390692123	-1.481314613428
H	1.458694649723	11.006885044473	-2.916187227633
N	2.565210457143	10.715348892731	-1.184800443904
C	1.748033272697	14.188687668603	-0.323226621358
H	0.763917373876	14.085483534235	-0.799760915199
H	1.895422479606	15.270244535225	-0.149234397727
N	4.263058001145	11.885908673561	0.697375773062
C	1.740140422965	13.482493695685	1.028604441889
H	2.692349659476	13.678869038929	1.540580943330
H	0.951172391793	13.904546876758	1.666477717133
N	-1.512554274930	11.441523459181	2.880272929338
C	4.130505354226	13.804128950551	-0.906530045891
H	4.224400284071	14.537670125641	-0.095350298259
H	4.692412891471	14.216501429202	-1.765004110068
N	3.333851995881	7.308672418325	-2.337863110128
C	4.833354680451	12.517956083374	-0.488071712779
H	4.872812638300	11.829437289085	-1.348691036958
H	5.876784896232	12.772449436016	-0.257058105679
N	5.103053994040	8.903419035708	1.097351642186
C	0.218672019317	11.532385902526	1.220254593301
H	0.176408362243	10.476905329065	0.907687707425
H	-0.553623940097	12.044200768430	0.623430231071
C	-0.204649215734	11.588899189525	2.667973172438
C	0.715613881562	11.737343652210	3.698365746468
H	1.769874867320	11.854591487579	3.463530389263
C	0.258266056943	11.710267526713	5.005169897346
H	0.955751510509	11.803980952268	5.832010720495
C	-1.098514925887	11.549056157521	5.236268909094
H	-1.501823469031	11.520568682314	6.242886147347
C	-1.937871249732	11.422146443697	4.138632290853
H	-3.010793608176	11.298060592768	4.281990363261
C	3.298726650645	9.650228700086	-1.821142260874
H	4.217905509535	9.423243637348	-1.263739763323

H	3.651565240874	9.983431265432	-2.811441617560
C	2.561656160905	8.344409702929	-2.002304135416
C	1.184927720291	8.234931557693	-1.843878053741
H	0.603862176433	9.101224541807	-1.543964730412
C	0.588112518789	7.001968473450	-2.046746401081
H	-0.483761050682	6.883087746091	-1.921062339626
C	1.381914288332	5.921453049799	-2.393638716227
H	0.959465084590	4.935038891708	-2.550831713480
C	2.747110639817	6.130553711319	-2.521577650763
H	3.403695691583	5.301871151562	-2.785445101198
C	5.254619605183	11.275878968045	1.584209579189
H	4.774274527667	11.043709733674	2.541259666071
H	6.039887578506	12.015853869761	1.780053822268
C	5.864392209980	10.009842541012	1.039106705315
C	7.119035080906	9.999757648659	0.443186242974
H	7.707132418381	10.912694071313	0.420493136504
C	7.599040900196	8.827131735407	-0.117075276191
H	8.573048581791	8.802361945308	-0.595634746548
C	6.811845844835	7.689412323974	-0.054902883945
H	7.138227879458	6.748912074256	-0.483437023234
C	5.577206135029	7.774127771471	0.564593634200
H	4.926520298037	6.906870650178	0.632043361471
C	3.023314946651	9.275837216355	3.589396131157
C	2.202434338598	7.500287530795	1.307549283405

Table S34. **Optimized Coordinates for 4**

Ni	3.125730684072	2.083130086723	2.981539824812
P	1.841404721093	3.078432592631	1.419727162616
N	0.176766262113	4.293538894561	-0.325453038752
N	2.617779474989	2.913867045240	-0.136814498496
N	1.748417572387	4.758839574322	1.839609365719
N	0.368357379571	2.213703124330	1.458417688801
N	3.606900933220	0.752830486431	1.657112178955
N	2.574327922453	3.361174521022	4.348481731340
N	0.985151960079	0.472596385156	3.888743999588
N	4.492985253087	1.354604180472	4.209765188062
C	1.006895590067	4.162008331871	-1.504988278082
H	0.892793573625	5.013390080072	-2.191695660130
H	0.700144353743	3.265371462907	-2.053772214675
C	2.458213353443	4.018182583185	-1.097584106031
H	3.063255947582	3.773401659827	-1.976151625472
H	2.847786048447	4.963066044332	-0.684979212566
C	0.088103561686	5.603435705079	0.285075056932
H	-0.916747176345	6.038619043695	0.191665358475
H	0.781137840335	6.278032734745	-0.228786087994
C	0.495169627054	5.503591737992	1.749011373983
H	0.658498118025	6.500685736990	2.172869982618
H	-0.306022351168	5.039044905358	2.345476845345
C	-0.961321125851	3.406230377341	-0.213990979195
H	-1.515788741863	3.307798530248	-1.158601655277
H	-1.659348849327	3.818643778926	0.524594500286
C	-0.446622651394	2.053366731314	0.261180697776
H	-1.257973310684	1.356291629218	0.495734355881
H	0.158518773254	1.579367345004	-0.519263203433
C	4.011137786514	2.459459389560	-0.015384388206
H	4.609315443413	3.086599625918	0.667036827219
H	4.471480329442	2.541404919235	-1.002648054869
C	4.039678271610	1.030846351214	0.415113108330
C	4.432100179190	0.024689565229	-0.452789809643
H	4.779627890776	0.287387595281	-1.445839129467
C	4.366048291733	-1.296889442038	-0.047496532279
H	4.669988306395	-2.094594523616	-0.716747004220
C	3.895569939143	-1.578522269319	1.225291990637
H	3.813881209557	-2.596097608768	1.587965533608
C	3.530051409113	-0.530664274840	2.043943636355
H	3.164361454118	-0.707149430754	3.047424881363
C	2.766898381403	5.196212035219	2.779436031529
H	3.751573170898	4.843254648207	2.446458092089
H	2.810014364524	6.289230913839	2.772091596881

C	2.490471938214	4.690035164009	4.165338358138
C	2.085811899324	5.536185777734	5.184288251016
H	2.035742634687	6.604273586627	4.998725135725
C	1.752984572733	5.007440478404	6.420865945854
H	1.432207537547	5.655130757262	7.229760465742
C	1.835747098175	3.635982007958	6.602430899601
H	1.581163689218	3.173416899805	7.548514907290
C	2.251926399591	2.848784502290	5.547775108248
H	2.316520687752	1.771115543088	5.641722238151
C	-0.316433577873	2.160676604448	2.751749093427
H	-1.369085241301	2.434992755357	2.606626138841
H	0.099996413212	2.913640872234	3.434159804675
C	-0.219122729400	0.814750553205	3.416171053590
C	-1.334240684675	0.000167403292	3.554501378546
H	-2.294151995103	0.317987355713	3.158442948928
C	-1.206709330774	-1.212182387566	4.216329843713
H	-2.063265165499	-1.866545613607	4.339026704261
C	0.031300267157	-1.562839017300	4.728116264141
H	0.177115934342	-2.490533652189	5.269397391558
C	1.088493887078	-0.687469844124	4.535529579365
H	2.074278165444	-0.928629990257	4.938979216872
C	5.389449422597	1.026161626852	4.849271062889
C	6.516254994649	0.619996486085	5.648555603380
H	7.367603367881	1.275445732760	5.448233994819
H	6.798554336364	-0.407729317933	5.408105334456
H	6.267184307140	0.680842912491	6.710651746362

Table S35. **Optimized Coordinates For 5**

Pd	15.306692659287	10.600074854391	9.569444379304
P	13.793220133832	9.061853287116	8.620605271103
N	12.038983959002	7.303046465038	7.709805192916
N	14.342135687983	7.500152956934	9.122703129194
N	13.852694412908	9.242438439405	6.888243118087
N	12.280283460978	9.564791005500	9.228867435190
N	15.715226449677	9.265993235293	11.154892713548
N	14.775881208167	11.921196188966	8.023819984532
N	13.230697508324	11.760078896131	11.253864299040
N	16.822157227076	11.995579367985	10.317961934223
C	12.538614865647	6.091033115646	8.329061485722
C	12.281066952905	7.470775248921	6.289197791771
C	13.390041448626	6.470284530086	9.531202253531
C	10.818617044759	7.876389524596	8.241516841640
C	13.675227632478	8.022433424954	6.083003364832
C	15.717691887244	7.414515247803	9.588897774190
C	16.128911695005	7.112838021674	12.065615268984
C	11.065836563331	9.365681260887	8.449165868645
C	15.881121349937	7.945317575008	10.986858032763
C	16.197957805744	7.650895603723	13.341641524150
C	14.933496851672	10.118450119565	6.404458790822
C	12.143474479539	9.678988550937	10.685462815195
C	16.007621753657	9.013928588320	13.504594933030
C	14.662810570609	11.551088311656	6.737671755039
C	15.767008983927	9.790158820115	12.387163289214
C	12.068099457813	11.106613967404	11.157112322899
C	14.283240506725	12.463295074786	5.765738772062
C	10.853718887523	11.693327305413	11.486266811702
C	14.010544128283	13.773361550925	6.123376511148
C	14.500504399603	13.184742065151	8.375774812456
C	10.839802227850	13.008255473428	11.928138482237
C	13.205026305995	13.017128518785	11.690322049013
C	14.118104355381	14.139422918130	7.455300662378
C	17.734426334845	12.640440941396	10.588400152978
C	12.041916058706	13.687708664206	12.037349001391
C	18.881158335382	13.445064013251	10.925569760398
H	11.727506816829	5.410677877295	8.623220183667
H	13.163812041215	5.557112843316	7.606006867230
H	12.153848127591	6.532195451366	5.731403653522
H	13.956688381377	5.606284876718	9.893958927936
H	14.439860303661	7.267309122730	6.323296375753
H	9.952868608888	7.704910137783	7.586203445175
H	10.595067731834	7.398374404407	9.202968053038

H	11.553778323283	8.185632543476	5.890688394847
H	16.036231063469	6.368726006343	9.540966897208
H	12.757574938363	6.802477664030	10.369102205522
H	13.811854267250	8.298326687698	5.033478299506
H	16.268699777915	6.049627869420	11.897660420002
H	16.371382163817	7.975007127210	8.908524083945
H	11.170165320989	9.874188054670	7.484491688561
H	16.392281890059	7.013693421082	14.197811102876
H	10.240469792825	9.856684019321	8.974100229088
H	14.965971816461	10.014067593436	5.317563551713
H	11.247288895769	9.126592990308	10.996770529456
H	15.923972790556	9.821319925560	6.786278801909
H	12.992691375818	9.194698562269	11.182629215436
H	14.203865390948	12.138946850062	4.733867241628
H	16.041699708170	9.477495369196	14.483266147031
H	9.931984191524	11.123475316702	11.412075021433
H	15.596675797420	10.859080050299	12.462206897307
H	13.716259183275	14.498036145092	5.371849007036
H	14.597647225311	13.422713473961	9.429013017597
H	9.905239488882	13.490162339526	12.195484093572
H	14.173206107077	13.512938711070	11.781069123297
H	13.911660528181	15.151073098656	7.783580308269
H	19.683786453128	13.267450721816	10.205654470646
H	19.240533274170	13.187713225797	11.924681796743
H	12.081184488519	14.710247856943	12.395150565958
H	18.618030145007	14.505216528920	10.906310797768

Table S36. Optimized Coordinates For 6

Pt	9.133310647764	10.003969537026	13.130973184868
Cl	11.447258675812	9.380148362969	12.706918712896
P	6.890398381546	10.591526690249	13.538034189185
N	4.183609347932	11.312274020319	13.820176070621
N	6.247617446589	9.634150426210	14.865005608878
N	6.020998677703	10.228980310792	12.069630149212
N	6.783850535656	12.238035584700	13.975545012614
N	9.383370125499	9.618693843756	15.156430696500
N	8.931939163303	10.516380904373	11.121057769728
N	10.028918009502	13.465513914241	12.970195595011
C	3.872485953722	10.298595301981	14.798314132842
H	2.851271465905	9.903703818698	14.676627528118
H	3.921076256457	10.750956060933	15.795387014948
C	4.864452418900	9.153376151321	14.732429538976
H	4.675537342902	8.466409516306	15.564114325332
H	4.733133149271	8.579140707188	13.800195551326
C	3.782299964565	11.102760006975	12.450693453432
H	3.039342138862	11.843766030190	12.117630129743
H	3.312831107401	10.115577489393	12.369163828531
C	5.006226310501	11.138425711324	11.549345529826
H	4.744990104013	10.811271019168	10.536533523085
H	5.384739799947	12.169631775143	11.455809296737
C	4.391589888435	12.663326351564	14.281080926906
H	3.624551489184	12.987470218857	15.002440080330
H	4.331766645948	13.341209348913	13.420575947130
C	5.781030366929	12.752148655608	14.893386799125
H	6.047636740301	13.784639162695	15.143150846428
H	5.814720316335	12.179118440045	15.829887922891
C	7.174578411605	8.554539206155	15.245161740669
H	7.449884595632	7.913212649280	14.391135838169
H	6.644982260569	7.921454280209	15.961831809737
C	8.418694545515	9.056762844457	15.913466289406
C	8.581978610916	8.926771540606	17.281993662254
H	7.790273838944	8.470382011921	17.865847621975
C	9.748663913451	9.366458790746	17.885909319732
H	9.886440374894	9.261857049480	18.956788628296
C	10.735138125819	9.926994097190	17.095610633837
H	11.673087837718	10.272930517882	17.513661575692
C	10.519361653284	10.040596375760	15.736445139513
H	11.266802817955	10.457116269058	15.070627666546
C	6.756135945492	9.417262654441	11.106035635200
H	6.042762277457	9.025543014958	10.374004172711
H	7.193892948360	8.550094770971	11.614567619480

C	7.842770877249	10.179189081753	10.400418571274
C	7.718308138907	10.567360505997	9.079342244932
H	6.835344311590	10.270284859477	8.522450237916
C	8.721349914279	11.318301981975	8.484558340758
H	8.636052567159	11.627055872145	7.448072579337
C	9.829089092012	11.663519915372	9.235658977806
H	10.639056010800	12.249583303286	8.819393163829
C	9.905162071236	11.244585844469	10.550502940463
H	10.756183709242	11.483115340098	11.175574636014
C	7.657628029013	13.147937739660	13.249133188367
H	7.164176662348	14.129185500717	13.211605803291
H	7.774993962550	12.843623505343	12.200115045673
C	9.038580380346	13.290253377262	13.843957204415
C	9.241877240764	13.264076085774	15.219876864764
H	8.408286746141	13.101117843084	15.897588440483
C	10.527199569725	13.446981867540	15.702542964494
H	10.718367513120	13.448909487206	16.771806942391
C	11.564763915466	13.626607874033	14.800182397218
H	12.587104663206	13.767948379998	15.132580953459
C	11.261867176166	13.622204859604	13.446725700255
H	12.052246819990	13.749191341252	12.708902084524

Table S37. Representative Calculation Input for Geometry Optimization and Vibrational Frequency Analysis

```
%mem=50GB
%nproc=12
%Chk=pt2tpap_m06.chk
# M06/GenECP Opt Freq

pt2tpap/m06/opt and freq

1 1
Pt      9.0901005673     9.9232684074    13.2120358793
Cl     11.1864682092     8.9660080671    12.7817823928
P       6.9075304391    10.4626836050    13.5059769692
N       4.1769351761    11.3062161791    13.8794455613
N       6.2096242266     9.4229826191    14.7085820071
N       5.9240368543    10.3526394893    12.0886117499
N       6.9619925669    12.1017586994    14.0896875417
N       9.3054973047     9.5634060628    15.1342491953
N       8.9538821289    10.3445607035    11.2040724837
N       9.9014253526    13.6702235122    12.8855776391
C       3.8727947899    10.1870594364    14.7455465338
H       2.8434250131     9.8640511238    14.5518826557
H       3.9278766605    10.5029489649    15.7965615825
C       4.8298384694     9.0356367706    14.4986249776
H       4.5688760258     8.2537701518    15.2161837558
H       4.6983838539     8.6395809085    13.4931704776
C       3.8188473369    11.2560092542    12.4760418117
H       3.1068338790    12.0441797286    12.2463623479
H       3.3508809522    10.2850361256    12.2492547467
C       5.0597157973    11.4130515581    11.6536294987
H       4.8186348715    11.2705294237    10.5902435744
H       5.4974117778    12.4100251959    11.7587360776
C       4.5214525147    12.5773162162    14.4674860461
H       3.7677655683    12.8110730635    15.2368196868
H       4.4721994042    13.3657673511    13.7109392480
C       5.9206631242    12.5171110539    15.0577524505
H       6.1639943075    13.5071481140    15.4644656518
H       5.9085863381    11.8362442725    15.9297822925
C       7.0942597925     8.4428560026    15.2644566860
H       7.4269129476     7.7633437185    14.4781043812
H       6.5426483152     7.8762411909    16.0152186644
C       8.2668128616     9.0560745197    15.9310194465
C       8.4322890055     8.9765361971    17.2551539559
```

H	7.7132588108	8.5497209957	17.9122672312
C	9.6621738501	9.4670679345	17.8798826973
H	9.8308259842	9.4159339060	18.9506384903
C	10.6726153974	10.0345023643	16.9953020775
H	11.5450548897	10.4430889778	17.4363153383
C	10.4870039237	10.0471808557	15.6923701635
H	11.1799009590	10.5297830179	15.0525317297
C	6.5975459975	9.5173524334	11.0715194320
H	5.8686736221	9.2520024043	10.3114552420
H	6.9495376892	8.5771297042	11.5284645064
C	7.7819497192	10.1342652105	10.4312862820
C	7.7594249548	10.4797565189	9.1251312143
H	6.9193478447	10.3227876328	8.4837976515
C	8.9059176012	11.1521808162	8.5055071509
H	8.9041072770	11.5015559364	7.4728513253
C	10.0508711760	11.4063642325	9.3679738198
H	10.8846260810	11.9159127625	8.9476254853
C	10.0506591388	11.0092269667	10.6307680636
H	10.8848335248	11.2023938818	11.2416457731
C	7.6199380666	13.0744363312	13.3005961014
H	7.0417354316	13.9944116651	13.3029899277
H	7.6935920784	12.7085679728	12.2779504587
C	8.9743183608	13.3380886587	13.8017127976
C	9.3147098824	13.3176123373	15.1637085636
H	8.6097043106	13.0528228944	15.9191732618
C	10.6024060402	13.6540145499	15.5433948087
H	10.8899344116	13.6551296470	16.5779730282
C	11.5256056699	13.9941584406	14.5782994960
H	12.5226240776	14.2581000463	14.8529615092
C	11.1564587914	13.9873004815	13.2473801893
H	11.8660880051	14.2360227362	12.5038782148

C H N 0
6-311G**++
****
P Cl 0
6-311G++(3df,3pd)
****
Pt 0
LANL2DZ
****

Table S38. Representative Calculation for NBO Analyses

```
%mem=50GB
%nproc=12
%Chk=pt2tpap_m06.chk
# M06/GenECP Geom=Checkpoint Guess=Read Pop=(nbo,savenbo,regular)

pt2tpap/m06/NBO and pop

1 1

C H N 0
6-311G**++
****
P Cl 0
6-311G++(3df,3pd)
****
Pt 0
LANL2DZ
****

Pt 0
LANL2DZ
```

Effect of Complex Charges on Calculated Distances. Compounds $[Ni(TPAP)(CH_3CN)]^{2+}$ (**4**) and $[Pd(TPAP)(CH_3CN)]^{2+}$ (**5**) were isolated with axial CH_3CN ligands, while $[Pt(TPAP)Cl]^{+}$ (**6**) was isolated with an anionic chloride ligand in the axial position. As a result, **6** is mono-cationic while **4** and **5** are di-cationic. To probe whether the overall complex charge significantly impacts the M–P and P---N_{ax} distances, the compounds $[Pd(TPAP)Cl]^{+}$ and $[Pt(TPAP)(CH_3CN)]^{2+}$ were investigated computationally and compared to their di-cationic and mono-cationic analogues, respectively.

Table S39 shows that the M–P distances are not particularly sensitive to changes in the overall complex charges, as increasing the charge changes the M–P distances at most by ca. 0.01 Å. For both Pt and Pd compounds, the angles θ and P---N_{ax} distances increase by 5.1° and 0.15 Å, respectively, when going from mono-cationic to di-cationic. Because the differences in changes of θ and P---N_{ax} are identical for each compound, the complex charge does not account for any non-monotonic trends observed. All angles and distances in Figure 1 were calculated from X-ray structures.

Table S39. Calculated Geometrical Parameters for Selected Mono-Cationic and Di-Cationic Comparison

parameter	$[Pt(TPAP)(CH_3CN)]^{2+}$	$[Pt(TPAP)Cl]^{+}$	$[Pd(TPAP)(CH_3CN)]^{2+}$	$[Pd(TPAP)Cl]^{+}$
M–P (Å)	2.35025	2.35406	2.35733	2.37091
P---N_{ax} (Å)	2.65028	2.81528	2.64581	2.81892
θ (º)	18.8896	13.78628	18.61757	13.4973

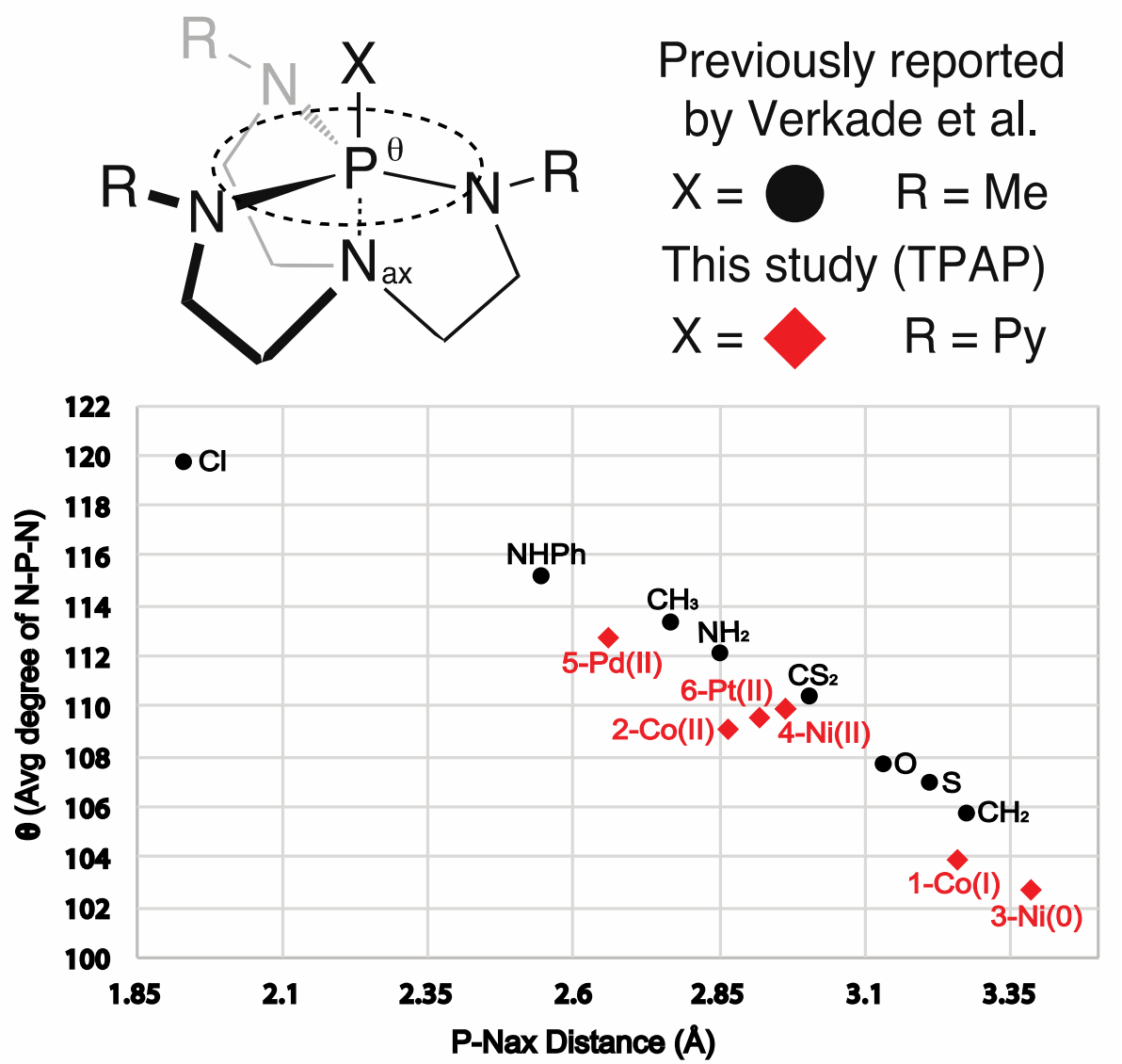

Figure S9. (top) Depiction of the angle of the Neq-P-Neq, θ, and the P-Nax transannular distance. (bottom) Plot of the transannular distance versus the average angle of the Neq-P-Neq, θ, for Verkade's Superbase with various main groups (denoted in black circles •) and TPAP with various transition metals (denoted in red diamonds ◆). Values used in this figure are from structural data.