Electronic Supporting Information for

Synthesis, structure, and reductive elimination in the series Tp'Rh(PR_3)Ar^FH; Determination of rhodium–carbon bond energies of fluoroaryl substituents†‡

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Part 2:

Structural Parameters of the Complexes 1 (Table S1-S6), 2-d_6 (Table S7-S12), 3a (Table S13-S18), 3b (Table S19-S24), 3d (Table S25-S30), 3g (Table S31-S36), 5 (Table S37-S42), [Tp'$RhCl_2$($PhMe_2$)] (Table S43-S48), 7 (Table S49-S54), 9a (Table S55-S60), 9b (Table S61-S66), 9c (Table S67-S72), 9d (Table S73-S78), 9e (Table S79-S84), 9g (Table S85-S90)

1. Structural Parameters of the Complexes 1, 2-d_6, 3a, 3b, 3d, 3g, 5, [Tp'RhCl$_2$(PhMe$_2$)], 7, 9a, 9b, 9c, 9d, 9e, 9g

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

Identification code	**1**	
Empirical formula	$C_{18}H_{33}BN_6PRh$	
Formula weight	478.19	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.0429(15) Å	α = 62.668(2)°
	b = 11.5505(18) Å	β = 80.643(3)°
	c = 11.6084(18) Å	γ = 66.913(3)°
Volume	1100.2(3) Å^3	
Z	2	
Density (calculated)	1.443 Mg/m^3	
Absorption coefficient	0.864 mm^{-1}	
F(000)	496	
Crystal color, morphology	colorless, plate	
Crystal size	0.34 x 0.26 x 0.08 mm^3	
Theta range for data collection	1.98 to 35.63°	
Index ranges	$-16 \le h \le 16$, $-18 \le k \le 18$, $-19 \le l \le 18$	
Reflections collected	24361	
Independent reflections	9947 [R(int) = 0.0315]	
Observed reflections	8530	
Completeness to theta = 35.63°	98.1%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9341 and 0.7577	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9947 / 0 / 261	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R_1 = 0.0302, wR_2 = 0.0720	
R indices (all data)	R_1 = 0.0385, wR_2 = 0.0762	
Largest diff. peak and hole	1.228 and -0.872 e.Å^{-3}	

Table S2. 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}
Rh1	7953(1)	493(1)	2355(1)	16(1)
P1	10004(1)	-1322(1)	3108(1)	18(1)
N1	8612(1)	2260(1)	1964(1)	18(1)
N2	7739(1)	3174(1)	2458(1)	18(1)
N3	5938(1)	2096(1)	1573(1)	16(1)
N4	5412(1)	3177(1)	1914(1)	17(1)
N5	7039(1)	539(1)	4203(1)	17(1)
N6	6357(1)	1823(1)	4207(1)	18(1)
B1	6230(2)	3152(2)	2952(2)	18(1)
C1	9731(2)	2675(2)	1428(1)	22(1)

C2	9603(2)	3825(2)	1622(2)	23(1)
C3	8329(2)	4118(2)	2272(1)	20(1)
C4	4969(2)	2318(2)	758(1)	18(1)
C5	3800(2)	3559(2)	573(1)	20(1)
C6	4118(2)	4077(2)	1314(1)	18(1)
C7	6835(2)	-399(2)	5377(1)	20(1)
C8	6046(2)	276(2)	6142(1)	24(1)
C9	5753(2)	1680(2)	5372(1)	22(1)
C10	10857(2)	2019(2)	687(2)	34(1)
C11	7634(2)	5252(2)	2705(2)	27(1)
C12	5203(2)	1338(2)	181(2)	24(1)
C13	3236(2)	5369(2)	1484(2)	24(1)
C14	7334(2)	-1924(2)	5732(2)	26(1)
C15	4911(2)	2887(2)	5685(2)	31(1)
C16	9949(2)	-3039(2)	3555(2)	31(1)
C17	10763(2)	-1530(2)	4536(2)	24(1)
C18	11604(2)	-1456(2)	2101(2)	30(1)

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

Rh(1)-N(3)	2.1124(11)	C(7)-C(14)	1.493(2)
Rh(1)-N(5)	2.2076(12)	C(8)-C(9)	1.377(2)
Rh(1)-P(1)	2.2178(5)	C(8)-H(8A)	0.9500
Rh(1)-N(1)	2.2193(13)	C(9)-C(15)	1.494(2)
Rh(1)-H(1)	1.455(19)	C(10)-H(10A)	0.9800
Rh(1)-H(2)	1.51(2)	C(10)-H(10B)	0.9800
P(1)-C(17)	1.8129(15)	C(10)-H(10C)	0.9800
P(1)-C(18)	1.8257(17)	C(11)-H(11A)	0.9800
P(1)-C(16)	1.8280(17)	C(11)-H(11B)	0.9800
N(1)-C(1)	1.3411(19)	C(11)-H(11C)	0.9800
N(1)-N(2)	1.3708(17)	C(12)-H(12A)	0.9800
N(2)-C(3)	1.3544(18)	C(12)-H(12B)	0.9800
N(2)-B(1)	1.537(2)	C(12)-H(12C)	0.9800
N(3)-C(4)	1.3379(17)	C(13)-H(13A)	0.9800
N(3)-N(4)	1.3651(16)	C(13)-H(13B)	0.9800
N(4)-C(6)	1.3511(17)	C(13)-H(13C)	0.9800
N(4)-B(1)	1.5487(19)	C(14)-H(14A)	0.9800
N(5)-C(7)	1.3417(18)	C(14)-H(14B)	0.9800
N(5)-N(6)	1.3699(17)	C(14)-H(14C)	0.9800
N(6)-C(9)	1.3530(18)	C(15)-H(15A)	0.9800
N(6)-B(1)	1.533(2)	C(15)-H(15B)	0.9800
B(1)-H(1B)	1.0000	C(15)-H(15C)	0.9800
C(1)-C(2)	1.402(2)	C(16)-H(16A)	0.9800
C(1)-C(10)	1.484(2)	C(16)-H(16B)	0.9800
C(2)-C(3)	1.379(2)	C(16)-H(16C)	0.9800
C(2)-H(2A)	0.9500	C(17)-H(17A)	0.9800
C(3)-C(11)	1.492(2)	C(17)-H(17B)	0.9800
C(4)-C(5)	1.400(2)	C(17)-H(17C)	0.9800
C(4)-C(12)	1.489(2)	C(18)-H(18A)	0.9800
C(5)-C(6)	1.381(2)	C(18)-H(18B)	0.9800
C(5)-H(5A)	0.9500	C(18)-H(18C)	0.9800
C(6)-C(13)	1.492(2)	N(3)-Rh(1)-N(5)	83.48(4)
C(7)-C(8)	1.396(2)	N(3)-Rh(1)-P(1)	174.03(3)

N(5)-Rh(1)-P(1)	99.21(3)	C(6)-C(5)-C(4)	106.07(12)
N(3)-Rh(1)-N(1)	83.52(5)	C(6)-C(5)-H(5A)	127.0
N(5)-Rh(1)-N(1)	88.77(4)	C(4)-C(5)-H(5A)	127.0
P(1)-Rh(1)-N(1)	101.80(3)	N(4)-C(6)-C(5)	107.64(12)
N(3)-Rh(1)-H(1)	92.2(8)	N(4)-C(6)-C(13)	123.69(13)
N(5)-Rh(1)-H(1)	96.2(8)	C(5)-C(6)-C(13)	128.66(13)
P(1)-Rh(1)-H(1)	82.3(8)	N(5)-C(7)-C(8)	110.09(13)
N(1)-Rh(1)-H(1)	173.1(8)	N(5)-C(7)-C(14)	122.81(14)
N(3)-Rh(1)-H(2)	92.3(8)	C(8)-C(7)-C(14)	127.02(13)
N(5)-Rh(1)-H(2)	174.2(8)	C(9)-C(8)-C(7)	105.78(13)
P(1)-Rh(1)-H(2)	84.6(8)	C(9)-C(8)-H(8A)	127.1
N(1)-Rh(1)-H(2)	94.8(8)	C(7)-C(8)-H(8A)	127.1
H(1)-Rh(1)-H(2)	79.9(11)	N(6)-C(9)-C(8)	107.72(14)
C(17)-P(1)-C(18)	100.04(8)	N(6)-C(9)-C(15)	123.48(14)
C(17)-P(1)-C(16)	104.15(8)	C(8)-C(9)-C(15)	128.80(14)
C(18)-P(1)-C(16)	97.93(9)	C(1)-C(10)-H(10A)	109.5
C(17)-P(1)-Rh(1)	114.62(5)	C(1)-C(10)-H(10B)	109.5
C(18)-P(1)-Rh(1)	120.70(6)	H(10A)-C(10)-H(10B)	109.5
C(16)-P(1)-Rh(1)	116.51(6)	C(1)-C(10)-H(10C)	109.5
C(1)-N(1)-N(2)	106.38(12)	H(10A)-C(10)-H(10C)	109.5
C(1)-N(1)-Rh(1)	137.49(10)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	115.94(9)	C(3)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	110.37(12)	C(3)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	128.86(13)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	120.21(11)	C(3)-C(11)-H(11C)	109.5
C(4)-N(3)-N(4)	107.44(11)	H(11A)-C(11)-H(11C)	109.5
C(4)-N(3)-Rh(1)	133.24(10)	H(11B)-C(11)-H(11C)	109.5
N(4)-N(3)-Rh(1)	119.31(8)	C(4)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.73(11)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	130.22(12)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	119.78(11)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.27(12)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	136.00(10)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	117.36(8)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	110.14(12)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	129.63(13)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	119.86(11)	C(6)-C(13)-H(13C)	109.5
N(6)-B(1)-N(2)	110.44(12)	H(13A)-C(13)-H(13C)	109.5
N(6)-B(1)-N(4)	108.67(12)	H(13B)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	109.32(11)	C(7)-C(14)-H(14A)	109.5
N(6)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14B)	109.5
N(2)-B(1)-H(1B)	109.5	H(14A)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	109.79(14)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	122.81(15)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	127.32(14)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	106.02(13)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2A)	127.0	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2A)	127.0	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	107.40(13)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(11)	123.16(14)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	129.43(14)	P(1)-C(16)-H(16A)	109.5
N(3)-C(4)-C(5)	109.11(12)	P(1)-C(16)-H(16B)	109.5
N(3)-C(4)-C(12)	121.89(13)	H(16A)-C(16)-H(16B)	109.5
C(5)-C(4)-C(12)	128.99(13)	P(1)-C(16)-H(16C)	109.5

H(16A)-C(16)-H(16C)	109.5	H(17B)-C(17)-H(17C)	109.5
H(16B)-C(16)-H(16C)	109.5	P(1)-C(18)-H(18A)	109.5
P(1)-C(17)-H(17A)	109.5	P(1)-C(18)-H(18B)	109.5
P(1)-C(17)-H(17B)	109.5	H(18A)-C(18)-H(18B)	109.5
H(17A)-C(17)-H(17B)	109.5	P(1)-C(18)-H(18C)	109.5
P(1)-C(17)-H(17C)	109.5	H(18A)-C(18)-H(18C)	109.5
H(17A)-C(17)-H(17C)	109.5	H(18B)-C(18)-H(18C)	109.5

Table S4. 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}
Rh1	15(1)	18(1)	13(1)	-6(1)	-1(1)	-7(1)
P1	18(1)	18(1)	17(1)	-8(1)	-1(1)	-6(1)
N1	16(1)	20(1)	18(1)	-7(1)	0(1)	-7(1)
N2	19(1)	20(1)	16(1)	-7(1)	0(1)	-10(1)
N3	15(1)	19(1)	13(1)	-6(1)	-1(1)	-7(1)
N4	16(1)	18(1)	16(1)	-6(1)	0(1)	-7(1)
N5	17(1)	20(1)	14(1)	-5(1)	0(1)	-9(1)
N6	18(1)	23(1)	15(1)	-8(1)	1(1)	-10(1)
B1	17(1)	20(1)	18(1)	-9(1)	2(1)	-8(1)
C1	18(1)	22(1)	20(1)	-3(1)	0(1)	-9(1)
C2	21(1)	23(1)	23(1)	-4(1)	-2(1)	-13(1)
C3	23(1)	22(1)	17(1)	-5(1)	-3(1)	-12(1)
C4	17(1)	23(1)	14(1)	-6(1)	0(1)	-9(1)
C5	16(1)	24(1)	16(1)	-6(1)	-2(1)	-7(1)
C6	16(1)	19(1)	15(1)	-4(1)	0(1)	-7(1)
C7	18(1)	24(1)	15(1)	-3(1)	-1(1)	-11(1)
C8	22(1)	34(1)	15(1)	-7(1)	3(1)	-14(1)
C9	20(1)	32(1)	16(1)	-11(1)	3(1)	-12(1)
C10	25(1)	29(1)	43(1)	-14(1)	13(1)	-14(1)
C11	37(1)	26(1)	25(1)	-12(1)	1(1)	-17(1)
C12	22(1)	31(1)	22(1)	-14(1)	-1(1)	-10(1)
C13	21(1)	21(1)	25(1)	-7(1)	1(1)	-5(1)
C14	24(1)	25(1)	22(1)	-2(1)	0(1)	-13(1)
C15	30(1)	41(1)	26(1)	-20(1)	8(1)	-13(1)
C16	30(1)	22(1)	42(1)	-15(1)	-3(1)	-9(1)
C17	21(1)	28(1)	23(1)	-10(1)	-6(1)	-7(1)
C18	24(1)	30(1)	25(1)	-10(1)	4(1)	-4(1)

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

	x	y	z	U(eq)
H1	7460(20)	-570(20)	2449(19)	24(5)
H2	8430(20)	470(20)	1060(20)	26(5)
H1B	5675	3991	3118	22
H2A	10261	4304	1360	28
H5A	2959	3963	46	24
H8A	5768	-146	7015	29

H10A	10532	1429	494	50
H10B	11759	1445	1204	50
H10C	11025	2750	-126	50
H11A	7480	4839	3641	41
H11B	6701	5878	2248	41
H11C	8265	5784	2509	41
H12A	5763	385	794	35
H12B	5736	1609	-626	35
H12C	4265	1377	-4	35
H13A	3844	5906	1350	36
H13B	2854	5110	2363	36
H13C	2430	5939	850	36
H14A	7343	-2052	4953	39
H14B	6674	-2325	6362	39
H14C	8313	-2395	6115	39
H15A	4091	3525	5073	46
H15B	5539	3385	5618	46
H15C	4553	2543	6570	46
H16A	10882	-3765	3948	46
H16B	9756	-3083	2778	46
H16C	9179	-3190	4179	46
H17A	11627	-2385	4839	36
H17B	10045	-1596	5222	36
H17C	11027	-723	4320	36
H18A	12360	-2375	2539	44
H18B	11961	-724	1957	44
H18C	11350	-1341	1265	44

Table S6. Torsion angles [°] for **1**.

N3-Rh1-P1-C17	-148.8(3)	P1-Rh1-N3-N4	164.5(3)
N5-Rh1-P1-C17	-32.28(7)	N1-Rh1-N3-N4	-42.18(9)
N1-Rh1-P1-C17	58.39(7)	C4-N3-N4-C6	-0.14(15)
N3-Rh1-P1-C18	91.6(3)	Rh1-N3-N4-C6	-179.74(9)
N5-Rh1-P1-C18	-151.96(8)	C4-N3-N4-B1	174.54(12)
N1-Rh1-P1-C18	-61.28(8)	Rh1-N3-N4-B1	-5.07(15)
N3-Rh1-P1-C16	-26.8(3)	N3-Rh1-N5-C7	126.28(14)
N5-Rh1-P1-C16	89.66(8)	P1-Rh1-N5-C7	-48.34(13)
N1-Rh1-P1-C16	-179.67(8)	N1-Rh1-N5-C7	-150.10(13)
N3-Rh1-N1-C1	-133.51(15)	N3-Rh1-N5-N6	-45.55(9)
N5-Rh1-N1-C1	142.91(14)	P1-Rh1-N5-N6	139.83(9)
P1-Rh1-N1-C1	43.75(15)	N1-Rh1-N5-N6	38.07(9)
N3-Rh1-N1-N2	52.39(9)	C7-N5-N6-C9	0.65(15)
N5-Rh1-N1-N2	-31.19(9)	Rh1-N5-N6-C9	174.75(9)
P1-Rh1-N1-N2	-130.35(9)	C7-N5-N6-B1	-172.95(12)
C1-N1-N2-C3	-2.04(15)	Rh1-N5-N6-B1	1.15(15)
Rh1-N1-N2-C3	173.80(9)	C9-N6-B1-N2	126.42(15)
C1-N1-N2-B1	170.14(12)	N5-N6-B1-N2	-61.39(16)
Rh1-N1-N2-B1	-14.01(15)	C9-N6-B1-N4	-113.68(15)
N5-Rh1-N3-C4	-132.17(13)	N5-N6-B1-N4	58.51(16)
P1-Rh1-N3-C4	-15.0(4)	C3-N2-B1-N6	-119.36(15)
N1-Rh1-N3-C4	138.33(13)	N1-N2-B1-N6	70.06(16)
N5-Rh1-N3-N4	47.32(9)	C3-N2-B1-N4	121.13(14)

N1-N2-B1-N4	-49.45(16)	N3-C4-C5-C6	0.29(16)
C6-N4-B1-N6	115.77(15)	C12-C4-C5-C6	-179.33(14)
N3-N4-B1-N6	-57.66(16)	N3-N4-C6-C5	0.32(15)
C6-N4-B1-N2	-123.63(15)	B1-N4-C6-C5	-173.62(13)
N3-N4-B1-N2	62.95(15)	N3-N4-C6-C13	179.38(12)
N2-N1-C1-C2	2.28(16)	B1-N4-C6-C13	5.4(2)
Rh1-N1-C1-C2	-172.19(11)	C4-C5-C6-N4	-0.37(16)
N2-N1-C1-C10	-174.67(14)	C4-C5-C6-C13	-179.36(14)
Rh1-N1-C1-C10	10.9(2)	N6-N5-C7-C8	-1.03(15)
N1-C1-C2-C3	-1.69(17)	Rh1-N5-C7-C8	-173.48(10)
C10-C1-C2-C3	175.08(16)	N6-N5-C7-C14	175.88(13)
N1-N2-C3-C2	1.00(16)	Rh1-N5-C7-C14	3.4(2)
B1-N2-C3-C2	-170.32(13)	N5-C7-C8-C9	1.02(17)
N1-N2-C3-C11	-179.98(13)	C14-C7-C8-C9	-175.73(14)
B1-N2-C3-C11	8.7(2)	N5-N6-C9-C8	-0.02(16)
C1-C2-C3-N2	0.40(16)	B1-N6-C9-C8	172.77(14)
C1-C2-C3-C11	-178.54(15)	N5-N6-C9-C15	-179.15(14)
N4-N3-C4-C5	-0.10(15)	B1-N6-C9-C15	-6.4(2)
Rh1-N3-C4-C5	179.43(10)	C7-C8-C9-N6	-0.59(16)
N4-N3-C4-C12	179.55(12)	C7-C8-C9-C15	178.48(15)
Rh1-N3-C4-C12	-0.9(2)		

Table S7. Crystal data and structure refinement for **2-d_6**.

Identification code	**2-d_6**	
Empirical formula	$C_{24}H_{31}BD_6N_6PRh$	
Formula weight	560.32	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*Cc*	
Unit cell dimensions	a = 12.8303(11) Å	α = 90°
	b = 15.7867(13) Å	β = 111.057(1)°
	c = 14.1339(17) Å	γ = 90°
Volume	2671.6(5) Å^3	
Z	4	
Density (calculated)	1.393 Mg/m^3	
Absorption coefficient	0.722 mm^{-1}	
F(000)	1152	
Crystal color, morphology	colorless, block	
Crystal size	0.24 x 0.20 x 0.16 mm^3	
Theta range for data collection	2.13 to 37.78°	
Index ranges	$-22 \le h \le 21$, $-27 \le k \le 27$, $-24 \le l \le 24$	
Reflections collected	32307	
Independent reflections	14040 [R(int) = 0.0292]	
Observed reflections	13027	
Completeness to theta = 37.78°	99.2%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8932 and 0.8458	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14040 / 2 / 315	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R_1 = 0.0272, wR_2 = 0.0571	

R indices (all data)	R_1 = 0.0311, wR_2 = 0.0592
Absolute structure parameter	-0.024(11)
Largest diff. peak and hole	1.073 and -0.549 e.Å^{-3}

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2-*d*$_6$**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	7279(1)	8774(1)	2275(1)	13(1)
D1	7570(16)	9659(13)	2423(15)	26(5)
P1	6508(1)	9184(1)	644(1)	17(1)
N1	6919(1)	7381(1)	2108(1)	15(1)
N2	6745(1)	7013(1)	2918(1)	15(1)
N3	8072(1)	8584(1)	3850(1)	15(1)
N4	7625(1)	8025(1)	4337(1)	14(1)
N5	5775(1)	8877(1)	2686(1)	16(1)
N6	5612(1)	8216(1)	3250(1)	15(1)
B1	6538(1)	7559(1)	3732(1)	15(1)
C1	7148(1)	6748(1)	1583(1)	16(1)
C2	7145(1)	5975(1)	2065(1)	18(1)
C3	6888(1)	6168(1)	2911(1)	17(1)
C4	8999(1)	8904(1)	4548(1)	16(1)
C5	9158(1)	8536(1)	5493(1)	18(1)
C6	8273(1)	7988(1)	5330(1)	16(1)
C7	4959(1)	9432(1)	2574(1)	18(1)
C8	4241(1)	9131(1)	3046(1)	19(1)
C9	4683(1)	8361(1)	3473(1)	17(1)
C10	7362(1)	6870(1)	627(1)	23(1)
C11	6798(1)	5593(1)	3720(1)	23(1)
C12	9708(1)	9554(1)	4307(1)	23(1)
C13	8003(2)	7447(1)	6076(1)	26(1)
C14	4899(1)	10271(1)	2059(1)	24(1)
C15	4266(1)	7767(1)	4078(1)	24(1)
C16	8781(1)	8630(1)	2140(1)	15(1)
C17	9403(1)	7893(1)	2557(1)	19(1)
C18	10488(1)	7772(1)	2568(1)	24(1)
C19	10989(1)	8379(1)	2163(1)	26(1)
C20	10394(2)	9104(1)	1749(1)	26(1)
C21	9315(1)	9229(1)	1742(1)	20(1)
C22	7103(2)	8892(1)	-312(1)	27(1)
C23	6468(1)	10328(1)	447(1)	24(1)
C24	5069(2)	8839(1)	30(1)	27(1)

Table S9. Bond lengths [Å] and angles [°] for **2-*d*$_6$**.

Rh(1)-D(1)	1.44(2)	N(2)-C(3)	1.3473(17)
Rh(1)-C(16)	2.0171(15)	N(2)-B(1)	1.5344(19)
Rh(1)-N(3)	2.1112(12)	N(3)-C(4)	1.3407(19)
Rh(1)-N(5)	2.2112(13)	N(3)-N(4)	1.3660(16)
Rh(1)-N(1)	2.2421(12)	N(4)-C(6)	1.3511(17)
Rh(1)-P(1)	2.2524(4)	N(4)-B(1)	1.5377(19)
P(1)-C(24)	1.8194(18)	N(5)-C(7)	1.331(2)
P(1)-C(23)	1.8239(16)	N(5)-N(6)	1.3737(17)
P(1)-C(22)	1.8333(17)	N(6)-C(9)	1.3559(17)
N(1)-C(1)	1.3402(18)	N(6)-B(1)	1.5404(19)
N(1)-N(2)	1.3708(16)	B(1)-H(1B)	1.077(19)

C(1)-C(2)	1.399(2)	C(16)-Rh(1)-N(3)	88.19(5)
C(1)-C(10)	1.484(2)	D(1)-Rh(1)-N(5)	95.5(8)
C(2)-C(3)	1.384(2)	C(16)-Rh(1)-N(5)	170.63(5)
C(2)-H(2)	0.9500	N(3)-Rh(1)-N(5)	82.48(5)
C(3)-C(11)	1.497(2)	D(1)-Rh(1)-N(1)	176.8(8)
C(4)-C(5)	1.403(2)	C(16)-Rh(1)-N(1)	92.72(5)
C(4)-C(12)	1.489(2)	N(3)-Rh(1)-N(1)	88.53(4)
C(5)-C(6)	1.379(2)	N(5)-Rh(1)-N(1)	86.15(4)
C(5)-H(5)	0.9500	D(1)-Rh(1)-P(1)	82.3(8)
C(6)-C(13)	1.490(2)	C(16)-Rh(1)-P(1)	91.06(4)
C(7)-C(8)	1.402(2)	N(3)-Rh(1)-P(1)	171.29(3)
C(7)-C(14)	1.499(2)	N(5)-Rh(1)-P(1)	98.30(4)
C(8)-C(9)	1.385(2)	N(1)-Rh(1)-P(1)	100.17(3)
C(8)-H(8)	0.9500	C(24)-P(1)-C(23)	104.82(8)
C(9)-C(15)	1.493(2)	C(24)-P(1)-C(22)	101.16(9)
C(10)-H(10A)	0.9800	C(23)-P(1)-C(22)	97.69(8)
C(10)-H(10B)	0.9800	C(24)-P(1)-Rh(1)	113.49(6)
C(10)-H(10C)	0.9800	C(23)-P(1)-Rh(1)	114.73(5)
C(11)-H(11A)	0.9800	C(22)-P(1)-Rh(1)	122.39(6)
C(11)-H(11B)	0.9800	C(1)-N(1)-N(2)	106.31(11)
C(11)-H(11C)	0.9800	C(1)-N(1)-Rh(1)	135.38(9)
C(12)-H(12A)	0.9800	N(2)-N(1)-Rh(1)	114.66(8)
C(12)-H(12B)	0.9800	C(3)-N(2)-N(1)	110.47(11)
C(12)-H(12C)	0.9800	C(3)-N(2)-B(1)	128.45(12)
C(13)-H(13A)	0.9800	N(1)-N(2)-B(1)	120.80(11)
C(13)-H(13B)	0.9800	C(4)-N(3)-N(4)	107.14(11)
C(13)-H(13C)	0.9800	C(4)-N(3)-Rh(1)	133.35(9)
C(14)-H(14A)	0.9800	N(4)-N(3)-Rh(1)	119.51(8)
C(14)-H(14B)	0.9800	C(6)-N(4)-N(3)	109.80(11)
C(14)-H(14C)	0.9800	C(6)-N(4)-B(1)	130.82(12)
C(15)-H(15A)	0.9800	N(3)-N(4)-B(1)	119.39(11)
C(15)-H(15B)	0.9800	C(7)-N(5)-N(6)	106.93(12)
C(15)-H(15C)	0.9800	C(7)-N(5)-Rh(1)	137.74(10)
C(16)-C(21)	1.397(2)	N(6)-N(5)-Rh(1)	115.27(9)
C(16)-C(17)	1.415(2)	C(9)-N(6)-N(5)	109.73(11)
C(17)-C(18)	1.400(2)	C(9)-N(6)-B(1)	127.80(12)
C(17)-D(17)	0.9500	N(5)-N(6)-B(1)	120.92(11)
C(18)-C(19)	1.387(2)	N(2)-B(1)-N(4)	108.58(11)
C(18)-D(18)	0.9500	N(2)-B(1)-N(6)	111.14(11)
C(19)-C(20)	1.383(3)	N(4)-B(1)-N(6)	108.95(11)
C(19)-D(19)	0.9500	N(2)-B(1)-H(1B)	109.8(11)
C(20)-C(21)	1.396(2)	N(4)-B(1)-H(1B)	109.8(10)
C(20)-D(20)	0.9500	N(6)-B(1)-H(1B)	108.5(11)
C(21)-D(21)	0.9500	N(1)-C(1)-C(2)	109.94(12)
C(22)-H(22A)	0.9800	N(1)-C(1)-C(10)	123.83(13)
C(22)-H(22B)	0.9800	C(2)-C(1)-C(10)	126.23(13)
C(22)-H(22C)	0.9800	C(3)-C(2)-C(1)	105.77(12)
C(23)-H(23A)	0.9800	C(3)-C(2)-H(2)	127.1
C(23)-H(23B)	0.9800	C(1)-C(2)-H(2)	127.1
C(23)-H(23C)	0.9800	N(2)-C(3)-C(2)	107.49(12)
C(24)-H(24A)	0.9800	N(2)-C(3)-C(11)	123.19(13)
C(24)-H(24B)	0.9800	C(2)-C(3)-C(11)	129.30(13)
C(24)-H(24C)	0.9800	N(3)-C(4)-C(5)	109.34(12)
D(1)-Rh(1)-C(16)	85.2(8)	N(3)-C(4)-C(12)	122.99(13)
D(1)-Rh(1)-N(3)	89.0(8)	C(5)-C(4)-C(12)	127.67(13)

C(6)-C(5)-C(4)	105.75(12)	H(14B)-C(14)-H(14C)	109.5
C(6)-C(5)-H(5)	127.1	C(9)-C(15)-H(15A)	109.5
C(4)-C(5)-H(5)	127.1	C(9)-C(15)-H(15B)	109.5
N(4)-C(6)-C(5)	107.96(12)	H(15A)-C(15)-H(15B)	109.5
N(4)-C(6)-C(13)	123.17(13)	C(9)-C(15)-H(15C)	109.5
C(5)-C(6)-C(13)	128.86(13)	H(15A)-C(15)-H(15C)	109.5
N(5)-C(7)-C(8)	110.08(14)	H(15B)-C(15)-H(15C)	109.5
N(5)-C(7)-C(14)	122.74(14)	C(21)-C(16)-C(17)	116.07(13)
C(8)-C(7)-C(14)	127.09(14)	C(21)-C(16)-Rh(1)	125.78(12)
C(9)-C(8)-C(7)	105.57(13)	C(17)-C(16)-Rh(1)	117.93(11)
C(9)-C(8)-H(8)	127.2	C(18)-C(17)-C(16)	121.76(14)
C(7)-C(8)-H(8)	127.2	C(18)-C(17)-D(17)	119.1
N(6)-C(9)-C(8)	107.67(12)	C(16)-C(17)-D(17)	119.1
N(6)-C(9)-C(15)	123.61(13)	C(19)-C(18)-C(17)	120.55(15)
C(8)-C(9)-C(15)	128.72(13)	C(19)-C(18)-D(18)	119.7
C(1)-C(10)-H(10A)	109.5	C(17)-C(18)-D(18)	119.7
C(1)-C(10)-H(10B)	109.5	C(20)-C(19)-C(18)	118.60(14)
H(10A)-C(10)-H(10B)	109.5	C(20)-C(19)-D(19)	120.7
C(1)-C(10)-H(10C)	109.5	C(18)-C(19)-D(19)	120.7
H(10A)-C(10)-H(10C)	109.5	C(19)-C(20)-C(21)	120.98(16)
H(10B)-C(10)-H(10C)	109.5	C(19)-C(20)-D(20)	119.5
C(3)-C(11)-H(11A)	109.5	C(21)-C(20)-D(20)	119.5
C(3)-C(11)-H(11B)	109.5	C(20)-C(21)-C(16)	122.04(16)
H(11A)-C(11)-H(11B)	109.5	C(20)-C(21)-D(21)	119.0
C(3)-C(11)-H(11C)	109.5	C(16)-C(21)-D(21)	119.0
H(11A)-C(11)-H(11C)	109.5	P(1)-C(22)-H(22A)	109.5
H(11B)-C(11)-H(11C)	109.5	P(1)-C(22)-H(22B)	109.5
C(4)-C(12)-H(12A)	109.5	H(22A)-C(22)-H(22B)	109.5
C(4)-C(12)-H(12B)	109.5	P(1)-C(22)-H(22C)	109.5
H(12A)-C(12)-H(12B)	109.5	H(22A)-C(22)-H(22C)	109.5
C(4)-C(12)-H(12C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(12A)-C(12)-H(12C)	109.5	P(1)-C(23)-H(23A)	109.5
H(12B)-C(12)-H(12C)	109.5	P(1)-C(23)-H(23B)	109.5
C(6)-C(13)-H(13A)	109.5	H(23A)-C(23)-H(23B)	109.5
C(6)-C(13)-H(13B)	109.5	P(1)-C(23)-H(23C)	109.5
H(13A)-C(13)-H(13B)	109.5	H(23A)-C(23)-H(23C)	109.5
C(6)-C(13)-H(13C)	109.5	H(23B)-C(23)-H(23C)	109.5
H(13A)-C(13)-H(13C)	109.5	P(1)-C(24)-H(24A)	109.5
H(13B)-C(13)-H(13C)	109.5	P(1)-C(24)-H(24B)	109.5
C(7)-C(14)-H(14A)	109.5	H(24A)-C(24)-H(24B)	109.5
C(7)-C(14)-H(14B)	109.5	P(1)-C(24)-H(24C)	109.5
H(14A)-C(14)-H(14B)	109.5	H(24A)-C(24)-H(24C)	109.5
C(7)-C(14)-H(14C)	109.5	H(24B)-C(24)-H(24C)	109.5
H(14A)-C(14)-H(14C)	109.5		

Table S10. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2-*d*$_6$**. 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}
Rh1	12(1)	13(1)	12(1)	2(1)	4(1)	0(1)
P1	17(1)	18(1)	14(1)	4(1)	3(1)	-1(1)
N1	16(1)	16(1)	14(1)	2(1)	7(1)	-1(1)

N2	16(1)	14(1)	17(1)	1(1)	7(1)	-2(1)
N3	14(1)	18(1)	13(1)	2(1)	5(1)	-2(1)
N4	14(1)	16(1)	12(1)	2(1)	4(1)	0(1)
N5	14(1)	17(1)	16(1)	1(1)	5(1)	1(1)
N6	13(1)	18(1)	15(1)	0(1)	6(1)	-1(1)
B1	16(1)	16(1)	15(1)	2(1)	7(1)	-1(1)
C1	16(1)	16(1)	17(1)	-1(1)	7(1)	-1(1)
C2	17(1)	15(1)	22(1)	0(1)	8(1)	0(1)
C3	15(1)	14(1)	21(1)	2(1)	7(1)	-2(1)
C4	14(1)	20(1)	15(1)	-1(1)	5(1)	-2(1)
C5	16(1)	24(1)	14(1)	1(1)	3(1)	0(1)
C6	17(1)	19(1)	13(1)	3(1)	5(1)	2(1)
C7	15(1)	20(1)	16(1)	-2(1)	3(1)	1(1)
C8	14(1)	25(1)	19(1)	-4(1)	5(1)	2(1)
C9	13(1)	23(1)	15(1)	-4(1)	6(1)	-2(1)
C10	30(1)	23(1)	20(1)	-2(1)	13(1)	0(1)
C11	31(1)	16(1)	26(1)	4(1)	15(1)	-2(1)
C12	21(1)	28(1)	19(1)	-1(1)	5(1)	-10(1)
C13	30(1)	32(1)	16(1)	8(1)	7(1)	-2(1)
C14	21(1)	22(1)	26(1)	3(1)	6(1)	6(1)
C15	20(1)	32(1)	25(1)	2(1)	14(1)	-1(1)
C16	15(1)	18(1)	13(1)	0(1)	5(1)	-1(1)
C17	17(1)	19(1)	20(1)	1(1)	5(1)	0(1)
C18	17(1)	26(1)	29(1)	-3(1)	6(1)	3(1)
C19	17(1)	39(1)	25(1)	-9(1)	10(1)	-3(1)
C20	21(1)	36(1)	22(1)	0(1)	10(1)	-10(1)
C21	19(1)	25(1)	16(1)	3(1)	6(1)	-3(1)
C22	32(1)	32(1)	16(1)	4(1)	9(1)	-1(1)
C23	26(1)	21(1)	24(1)	10(1)	5(1)	1(1)
C24	20(1)	34(1)	21(1)	6(1)	0(1)	-5(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **2-*d*$_6$**.

	x	y	z	U(eq)
H1B	6286(16)	7162(13)	4232(14)	20(5)
H2	7289	5430	1855	21
H5	9752	8642	6117	22
H8	3587	9398	3069	23
H10A	7920	7318	722	35
H10B	6666	7033	84	35
H10C	7640	6341	444	35
H11A	6081	5685	3802	35
H11B	7408	5713	4361	35
H11C	6848	5002	3526	35
H12A	9230	9968	3831	35
H12B	10194	9278	4001	35
H12C	10166	9843	4932	35
H13A	7927	6857	5848	39
H13B	7300	7638	6130	39
H13C	8605	7492	6740	39

H14A	5657	10472	2171	35
H14B	4515	10681	2340	35
H14C	4486	10207	1330	35
H15A	4792	7757	4781	37
H15B	4200	7196	3789	37
H15C	3533	7957	4062	37
D17	9076	7469	2838	23
D18	10885	7271	2856	29
D19	11726	8299	2169	32
D20	10725	9523	1465	31
D21	8931	9736	1459	24
H22A	6770	9244	-917	40
H22B	6945	8294	-493	40
H22C	7913	8981	-36	40
H23A	6080	10452	-274	37
H23B	7232	10549	666	37
H23C	6069	10596	843	37
H24A	4748	9106	-638	40
H24B	4634	9002	447	40
H24C	5049	8221	-49	40

Table S12. Torsion angles [°] for **2-d_6**.

D1-Rh1-P1-C24	-129.6(8)	C16-Rh1-N3-C4	47.52(14)
C16-Rh1-P1-C24	145.39(8)	N5-Rh1-N3-C4	-133.40(14)
N3-Rh1-P1-C24	-129.6(2)	N1-Rh1-N3-C4	140.29(14)
N5-Rh1-P1-C24	-35.11(8)	P1-Rh1-N3-C4	-37.7(3)
N1-Rh1-P1-C24	52.44(8)	D1-Rh1-N3-N4	143.0(8)
D1-Rh1-P1-C23	-9.1(8)	C16-Rh1-N3-N4	-131.73(10)
C16-Rh1-P1-C23	-94.12(7)	N5-Rh1-N3-N4	47.36(10)
N3-Rh1-P1-C23	-9.1(2)	N1-Rh1-N3-N4	-38.96(10)
N5-Rh1-P1-C23	85.37(7)	P1-Rh1-N3-N4	143.06(18)
N1-Rh1-P1-C23	172.92(7)	C4-N3-N4-C6	-0.67(15)
D1-Rh1-P1-C22	108.7(8)	Rh1-N3-N4-C6	178.76(9)
C16-Rh1-P1-C22	23.69(8)	C4-N3-N4-B1	179.27(12)
N3-Rh1-P1-C22	108.7(2)	Rh1-N3-N4-B1	-1.31(15)
N5-Rh1-P1-C22	-156.81(8)	D1-Rh1-N5-C7	36.1(8)
N1-Rh1-P1-C22	-69.26(8)	C16-Rh1-N5-C7	130.0(3)
D1-Rh1-N1-C1	-84(15)	N3-Rh1-N5-C7	124.39(16)
C16-Rh1-N1-C1	-34.49(14)	N1-Rh1-N5-C7	-146.59(16)
N3-Rh1-N1-C1	-122.61(13)	P1-Rh1-N5-C7	-46.85(16)
N5-Rh1-N1-C1	154.83(14)	D1-Rh1-N5-N6	-140.6(8)
P1-Rh1-N1-C1	57.08(13)	C16-Rh1-N5-N6	-46.7(4)
D1-Rh1-N1-N2	71(15)	N3-Rh1-N5-N6	-52.33(10)
C16-Rh1-N1-N2	120.37(9)	N1-Rh1-N5-N6	36.69(10)
N3-Rh1-N1-N2	32.25(9)	P1-Rh1-N5-N6	136.43(10)
N5-Rh1-N1-N2	-50.31(9)	C7-N5-N6-C9	0.91(16)
P1-Rh1-N1-N2	-148.06(8)	Rh1-N5-N6-C9	178.61(9)
C1-N1-N2-C3	1.36(15)	C7-N5-N6-B1	-165.92(12)
Rh1-N1-N2-C3	-160.53(9)	Rh1-N5-N6-B1	11.77(16)
C1-N1-N2-B1	175.82(11)	C3-N2-B1-N4	104.15(15)
Rh1-N1-N2-B1	13.93(14)	N1-N2-B1-N4	-69.21(15)
D1-Rh1-N3-C4	-37.7(8)	C3-N2-B1-N6	-136.02(14)

N1-N2-B1-N6	50.61(16)	C4-C5-C6-C13	-178.18(15)
C6-N4-B1-N2	-118.17(15)	N6-N5-C7-C8	-1.27(17)
N3-N4-B1-N2	61.91(15)	Rh1-N5-C7-C8	-178.17(12)
C6-N4-B1-N6	120.65(15)	N6-N5-C7-C14	175.62(13)
N3-N4-B1-N6	-59.27(15)	Rh1-N5-C7-C14	-1.3(2)
C9-N6-B1-N2	127.67(14)	N5-C7-C8-C9	1.15(18)
N5-N6-B1-N2	-68.07(16)	C14-C7-C8-C9	-175.57(15)
C9-N6-B1-N4	-112.72(14)	N5-N6-C9-C8	-0.20(16)
N5-N6-B1-N4	51.54(16)	B1-N6-C9-C8	165.49(13)
N2-N1-C1-C2	-1.21(15)	N5-N6-C9-C15	-179.94(13)
Rh1-N1-C1-C2	155.07(10)	B1-N6-C9-C15	-14.3(2)
N2-N1-C1-C10	178.33(13)	C7-C8-C9-N6	-0.56(17)
Rh1-N1-C1-C10	-25.4(2)	C7-C8-C9-C15	179.17(14)
N1-C1-C2-C3	0.65(16)	D1-Rh1-C16-C21	-31.9(8)
C10-C1-C2-C3	-178.88(14)	N3-Rh1-C16-C21	-121.03(13)
N1-N2-C3-C2	-0.96(16)	N5-Rh1-C16-C21	-126.6(3)
B1-N2-C3-C2	-174.89(13)	N1-Rh1-C16-C21	150.53(13)
N1-N2-C3-C11	177.59(13)	P1-Rh1-C16-C21	50.29(13)
B1-N2-C3-C11	3.7(2)	D1-Rh1-C16-C17	142.4(8)
C1-C2-C3-N2	0.20(15)	N3-Rh1-C16-C17	53.26(11)
C1-C2-C3-C11	-178.24(15)	N5-Rh1-C16-C17	47.7(4)
N4-N3-C4-C5	0.91(16)	N1-Rh1-C16-C17	-35.18(11)
Rh1-N3-C4-C5	-178.41(10)	P1-Rh1-C16-C17	-135.42(11)
N4-N3-C4-C12	-178.72(14)	C21-C16-C17-C18	-0.1(2)
Rh1-N3-C4-C12	2.0(2)	Rh1-C16-C17-C18	-174.97(12)
N3-C4-C5-C6	-0.81(17)	C16-C17-C18-C19	-0.1(2)
C12-C4-C5-C6	178.80(15)	C17-C18-C19-C20	0.0(2)
N3-N4-C6-C5	0.16(16)	C18-C19-C20-C21	0.4(3)
B1-N4-C6-C5	-179.76(13)	C19-C20-C21-C16	-0.7(3)
N3-N4-C6-C13	178.82(13)	C17-C16-C21-C20	0.5(2)
B1-N4-C6-C13	-1.1(2)	Rh1-C16-C21-C20	174.92(13)
C4-C5-C6-N4	0.38(16)		

Table S13. Crystal data and structure refinement for **3a**.

Identification code	**3a**	
Empirical formula	$C_{27}H_{39}BF_5N_6PRh$	
Formula weight	687.33	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.6504(13) Å	α = 90°
	b = 33.930(5) Å	β = 100.671(2)°
	c = 20.878(3) Å	γ = 90°
Volume	6021.8(15) Å^3	
Z	8	
Density (calculated)	1.516 Mg/m^3	
Absorption coefficient	0.680 mm^{-1}	
F(000)	2824	
Crystal color, morphology	colorless, block	
Crystal size	0.20 x 0.16 x 0.06 mm^3	
Theta range for data collection	1.99 to 26.37°	

Index ranges	$-10 \le h \le 10$, $-42 \le k \le 42$, $-26 \le l \le 26$
Reflections collected	74170
Independent reflections	12307 [R(int) = 0.1197]
Observed reflections	7797
Completeness to theta = 26.37°	100.0%
Absorption correction	Multi-scan
Max. and min. transmission	0.9604 and 0.8760
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12307 / 43 / 787
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R_1 = 0.0802, wR_2 = 0.1734
R indices (all data)	R_1 = 0.1300, wR_2 = 0.1985
Largest diff. peak and hole	3.058 and -1.204 e.Å^{-3}

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	8588(1)	3982(1)	1634(1)	36(1)
N1	10274(7)	4462(2)	1922(3)	40(2)
N2	11182(7)	4424(2)	2533(3)	42(2)
N3	7897(7)	4055(2)	2539(3)	38(1)
N4	9077(7)	4115(2)	3062(3)	40(2)
N5	10108(7)	3554(2)	2172(3)	39(2)
N6	11112(7)	3689(2)	2720(3)	39(1)
B1	10819(11)	4099(3)	2993(5)	45(2)
C1	10704(10)	4802(2)	1682(4)	44(2)
C2	11932(10)	4973(3)	2118(5)	55(2)
C3	12171(9)	4733(2)	2654(4)	47(2)
C4	6523(10)	4058(2)	2751(4)	44(2)
C5	6844(10)	4119(2)	3420(4)	45(2)
C6	8427(10)	4155(2)	3602(4)	45(2)
C7	10365(10)	3168(2)	2133(4)	45(2)
C8	11557(9)	3059(2)	2654(4)	47(2)
C9	11982(9)	3384(2)	3012(4)	44(2)
C10	9861(11)	4983(3)	1064(4)	58(2)
C11	13304(12)	4783(3)	3278(5)	68(3)
C12	5010(9)	3996(3)	2297(4)	50(2)
C13	9402(11)	4214(3)	4260(4)	57(2)
C14	9439(12)	2896(3)	1643(4)	63(3)
C15	13149(10)	3433(3)	3632(4)	55(2)
C16	6884(9)	4372(2)	1225(4)	38(2)
C17	5787(9)	4309(2)	673(4)	45(2)
F1	5886(6)	3979(1)	311(2)	58(1)
C18	4573(10)	4556(3)	437(4)	54(2)
F2	3556(6)	4466(2)	-119(3)	72(2)
C19	4389(10)	4897(3)	763(5)	53(2)
F3	3187(6)	5148(2)	528(3)	73(2)
C20	5423(10)	4978(2)	1305(4)	46(2)
F4	5233(6)	5318(1)	1644(3)	67(2)
C21	6637(9)	4726(2)	1547(4)	45(2)
F5	7555(5)	4838(1)	2097(2)	51(1)

P1	9542(3)	3853(1)	716(1)	43(1)
C22	11660(11)	3771(3)	926(5)	72(3)
C23	8829(13)	3437(3)	224(4)	68(3)
C24	9507(12)	4214(3)	82(4)	58(2)
Rh2	3818(1)	1927(1)	2725(1)	41(1)
N7	5056(7)	2463(2)	2742(3)	42(2)
N8	6056(7)	2559(2)	3312(3)	43(2)
N9	5944(7)	1671(2)	3384(3)	41(2)
N10	6575(7)	1909(2)	3896(3)	42(2)
N11	3105(7)	2167(2)	3569(3)	43(2)
N12	4280(8)	2325(2)	4044(3)	44(2)
B2	5999(11)	2331(3)	3943(5)	45(2)
C25	5234(10)	2729(2)	2305(4)	46(2)
C26	6381(11)	3003(2)	2574(4)	53(2)
C27	6851(10)	2887(2)	3213(4)	48(2)
C28	6756(9)	1339(2)	3459(4)	43(2)
C29	7892(9)	1357(2)	4024(4)	44(2)
C30	7757(9)	1716(2)	4287(4)	43(2)
C31	1756(10)	2278(2)	3736(4)	46(2)
C32	2032(10)	2486(2)	4319(4)	46(2)
C33	3646(10)	2513(2)	4494(4)	46(2)
C34	4309(11)	2736(3)	1624(4)	57(2)
C35	8034(10)	3084(3)	3735(4)	56(2)
C36	6521(10)	1008(3)	2981(4)	56(2)
C37	8690(9)	1902(3)	4888(4)	52(2)
C38	204(10)	2187(3)	3319(4)	57(2)
C39	4605(11)	2713(3)	5065(4)	55(2)
C40	4533(10)	1796(2)	1860(4)	47(2)
C41	3467(11)	1723(3)	1292(4)	53(2)
F6	1861(6)	1706(2)	1278(2)	60(1)
C42	3918(12)	1677(3)	700(4)	59(2)
F7	2818(7)	1594(2)	155(3)	89(2)
C43	5455(12)	1700(3)	654(4)	61(2)
F8	5914(8)	1661(2)	77(3)	88(2)
C44	6515(12)	1781(3)	1212(5)	63(3)
F9	8054(7)	1816(2)	1177(3)	79(2)
C45	5990(11)	1823(2)	1781(4)	46(2)
F10	7189(6)	1908(2)	2306(2)	60(1)
P2	2377(3)	1364(1)	2683(1)	50(1)
C46	2614(13)	1136(3)	3469(5)	69(3)
C47	265(11)	1367(3)	2436(5)	71(3)
C48	2763(11)	974(3)	2124(5)	65(3)
C49	9310(80)	5280(30)	3460(40)	138(9)
C50	8050(50)	5498(12)	3588(18)	145(9)
C51	7520(50)	5375(12)	4185(18)	168(10)
C52	6280(60)	5708(14)	4250(30)	169(10)
C53	5690(50)	5510(13)	4789(17)	173(10)
C54	4180(50)	5600(30)	4830(30)	230(40)
C49'	9470(80)	5240(30)	3560(40)	138(9)
C50'	8060(50)	5268(9)	3770(20)	145(9)
C51'	7780(50)	5661(11)	4050(20)	168(10)
C52'	6290(60)	5543(13)	4340(30)	169(10)
C53'	5990(50)	5911(11)	4654(19)	173(10)
C54'	4700(50)	5890(30)	4950(30)	230(40)

Table S15. Bond lengths [Å] and angles [°] for **3a**.

Rh(1)-C(16)	2.046(7)	C(15)-H(15C)	0.9800
Rh(1)-N(3)	2.099(6)	C(16)-C(17)	1.368(10)
Rh(1)-N(5)	2.134(6)	C(16)-C(21)	1.413(11)
Rh(1)-N(1)	2.196(6)	C(17)-F(1)	1.359(9)
Rh(1)-P(1)	2.266(2)	C(17)-C(18)	1.363(11)
Rh(1)-H(1)	1.87(9)	C(18)-F(2)	1.357(10)
N(1)-C(1)	1.336(9)	C(18)-C(19)	1.365(13)
N(1)-N(2)	1.374(8)	C(19)-C(20)	1.335(12)
N(2)-C(3)	1.347(10)	C(19)-F(3)	1.364(9)
N(2)-B(1)	1.533(11)	C(20)-C(21)	1.374(11)
N(3)-C(4)	1.343(10)	C(20)-F(4)	1.379(9)
N(3)-N(4)	1.365(8)	C(21)-F(5)	1.324(9)
N(4)-C(6)	1.356(10)	P(1)-C(23)	1.788(9)
N(4)-B(1)	1.540(11)	P(1)-C(24)	1.798(8)
N(5)-C(7)	1.332(9)	P(1)-C(22)	1.824(9)
N(5)-N(6)	1.382(8)	C(22)-H(22A)	0.9800
N(6)-C(9)	1.357(9)	C(22)-H(22B)	0.9800
N(6)-B(1)	1.541(11)	C(22)-H(22C)	0.9800
B(1)-H(1B)	1.10(8)	C(23)-H(23A)	0.9800
C(1)-C(2)	1.391(12)	C(23)-H(23B)	0.9800
C(1)-C(10)	1.492(11)	C(23)-H(23C)	0.9800
C(2)-C(3)	1.368(12)	C(24)-H(24A)	0.9800
C(2)-H(2A)	0.9500	C(24)-H(24B)	0.9800
C(3)-C(11)	1.488(12)	C(24)-H(24C)	0.9800
C(4)-C(5)	1.389(11)	Rh(2)-C(40)	2.062(9)
C(4)-C(12)	1.481(11)	Rh(2)-N(7)	2.107(6)
C(5)-C(6)	1.357(11)	Rh(2)-N(11)	2.133(7)
C(5)-H(5A)	0.9500	Rh(2)-N(9)	2.256(6)
C(6)-C(13)	1.486(11)	Rh(2)-P(2)	2.273(2)
C(7)-C(8)	1.402(11)	Rh(2)-H(2)	1.61(9)
C(7)-C(14)	1.497(12)	N(7)-C(25)	1.314(10)
C(8)-C(9)	1.343(11)	N(7)-N(8)	1.375(8)
C(8)-H(8A)	0.9500	N(8)-C(27)	1.343(10)
C(9)-C(15)	1.497(11)	N(8)-B(2)	1.536(11)
C(10)-H(10A)	0.9800	N(9)-C(28)	1.320(9)
C(10)-H(10B)	0.9800	N(9)-N(10)	1.371(8)
C(10)-H(10C)	0.9800	N(10)-C(30)	1.353(9)
C(11)-H(11A)	0.9800	N(10)-B(2)	1.524(11)
C(11)-H(11B)	0.9800	N(11)-C(31)	1.333(10)
C(11)-H(11C)	0.9800	N(11)-N(12)	1.390(8)
C(12)-H(12A)	0.9800	N(12)-C(33)	1.335(10)
C(12)-H(12B)	0.9800	N(12)-B(2)	1.541(12)
C(12)-H(12C)	0.9800	B(2)-H(2B)	1.14(8)
C(13)-H(13A)	0.9800	C(25)-C(26)	1.398(12)
C(13)-H(13B)	0.9800	C(25)-C(34)	1.496(11)
C(13)-H(13C)	0.9800	C(26)-C(27)	1.378(11)
C(14)-H(14A)	0.9800	C(26)-H(26A)	0.9500
C(14)-H(14B)	0.9800	C(27)-C(35)	1.506(12)
C(14)-H(14C)	0.9800	C(28)-C(29)	1.390(10)
C(15)-H(15A)	0.9800	C(28)-C(36)	1.492(11)
C(15)-H(15B)	0.9800	C(29)-C(30)	1.350(11)

C(29)-H(29A)	0.9500	C(51)-C(52)	1.58(4)
C(30)-C(37)	1.498(11)	C(51)-H(51A)	0.9900
C(31)-C(32)	1.389(11)	C(51)-H(51B)	0.9900
C(31)-C(38)	1.492(11)	C(52)-C(53)	1.48(3)
C(32)-C(33)	1.379(11)	C(52)-H(52A)	0.9900
C(32)-H(32A)	0.9500	C(52)-H(52B)	0.9900
C(33)-C(39)	1.484(11)	C(53)-C(54)	1.36(3)
C(34)-H(34A)	0.9800	C(53)-H(53A)	0.9900
C(34)-H(34B)	0.9800	C(53)-H(53B)	0.9900
C(34)-H(34C)	0.9800	C(54)-H(54A)	0.9800
C(35)-H(35A)	0.9800	C(54)-H(54B)	0.9800
C(35)-H(35B)	0.9800	C(54)-H(54C)	0.9800
C(35)-H(35C)	0.9800	C(49')-C(50')	1.38(3)
C(36)-H(36A)	0.9800	C(49')-H(49D)	0.9800
C(36)-H(36B)	0.9800	C(49')-H(49E)	0.9800
C(36)-H(36C)	0.9800	C(49')-H(49F)	0.9800
C(37)-H(37A)	0.9800	C(50')-C(51')	1.49(3)
C(37)-H(37B)	0.9800	C(50')-H(50C)	0.9900
C(37)-H(37C)	0.9800	C(50')-H(50D)	0.9900
C(38)-H(38A)	0.9800	C(51')-C(52')	1.57(4)
C(38)-H(38B)	0.9800	C(51')-H(51C)	0.9900
C(38)-H(38C)	0.9800	C(51')-H(51D)	0.9900
C(39)-H(39A)	0.9800	C(52')-C(53')	1.46(3)
C(39)-H(39B)	0.9800	C(52')-H(52C)	0.9900
C(39)-H(39C)	0.9800	C(52')-H(52D)	0.9900
C(40)-C(45)	1.305(12)	C(53')-C(54')	1.37(3)
C(40)-C(41)	1.384(11)	C(53')-H(53C)	0.9900
C(41)-C(42)	1.372(12)	C(53')-H(53D)	0.9900
C(41)-F(6)	1.385(10)	C(54')-H(54D)	0.9800
C(42)-C(43)	1.353(13)	C(54')-H(54E)	0.9800
C(42)-F(7)	1.370(9)	C(54')-H(54F)	0.9800
C(43)-F(8)	1.342(10)	C(16)-Rh(1)-N(3)	89.8(3)
C(43)-C(44)	1.371(13)	C(16)-Rh(1)-N(5)	170.4(3)
C(44)-F(9)	1.352(11)	N(3)-Rh(1)-N(5)	81.8(2)
C(44)-C(45)	1.355(12)	C(16)-Rh(1)-N(1)	91.4(3)
C(45)-F(10)	1.392(9)	N(3)-Rh(1)-N(1)	87.2(2)
P(2)-C(46)	1.791(9)	N(5)-Rh(1)-N(1)	92.7(2)
P(2)-C(47)	1.804(10)	C(16)-Rh(1)-P(1)	96.8(2)
P(2)-C(48)	1.837(10)	N(3)-Rh(1)-P(1)	173.40(17)
C(46)-H(46A)	0.9800	N(5)-Rh(1)-P(1)	91.59(17)
C(46)-H(46B)	0.9800	N(1)-Rh(1)-P(1)	92.73(17)
C(46)-H(46C)	0.9800	C(16)-Rh(1)-H(1)	90(3)
C(47)-H(47A)	0.9800	N(3)-Rh(1)-H(1)	91(3)
C(47)-H(47B)	0.9800	N(5)-Rh(1)-H(1)	86(3)
C(47)-H(47C)	0.9800	N(1)-Rh(1)-H(1)	178(3)
C(48)-H(48A)	0.9800	P(1)-Rh(1)-H(1)	89(3)
C(48)-H(48B)	0.9800	C(1)-N(1)-N(2)	106.2(6)
C(48)-H(48C)	0.9800	C(1)-N(1)-Rh(1)	138.9(6)
C(49)-C(50)	1.38(3)	N(2)-N(1)-Rh(1)	114.9(4)
C(49)-H(49A)	0.9800	C(3)-N(2)-N(1)	109.5(6)
C(49)-H(49B)	0.9800	C(3)-N(2)-B(1)	129.7(7)
C(49)-H(49C)	0.9800	N(1)-N(2)-B(1)	120.1(6)
C(50)-C(51)	1.47(3)	C(4)-N(3)-N(4)	108.2(6)
C(50)-H(50A)	0.9900	C(4)-N(3)-Rh(1)	135.5(5)
C(50)-H(50B)	0.9900	N(4)-N(3)-Rh(1)	116.3(5)

C(6)-N(4)-N(3)	108.4(6)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	130.1(7)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	121.3(6)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.9(6)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	136.9(5)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	116.2(4)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	109.2(6)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	129.7(7)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	119.0(6)	C(6)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	110.6(7)	H(13A)-C(13)-H(13C)	109.5
N(2)-B(1)-N(6)	110.5(7)	H(13B)-C(13)-H(13C)	109.5
N(4)-B(1)-N(6)	107.3(7)	C(7)-C(14)-H(14A)	109.5
N(2)-B(1)-H(1B)	113(4)	C(7)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	112(4)	H(14A)-C(14)-H(14B)	109.5
N(6)-B(1)-H(1B)	104(4)	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	110.2(8)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	123.7(8)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	125.8(8)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	105.6(8)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2A)	127.2	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2A)	127.2	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	108.3(8)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(11)	123.0(8)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	128.7(8)	C(17)-C(16)-C(21)	113.1(7)
N(3)-C(4)-C(5)	108.0(7)	C(17)-C(16)-Rh(1)	125.7(6)
N(3)-C(4)-C(12)	121.3(7)	C(21)-C(16)-Rh(1)	120.8(6)
C(5)-C(4)-C(12)	130.7(8)	F(1)-C(17)-C(18)	115.5(7)
C(6)-C(5)-C(4)	107.3(8)	F(1)-C(17)-C(16)	119.5(7)
C(6)-C(5)-H(5A)	126.3	C(18)-C(17)-C(16)	125.0(8)
C(4)-C(5)-H(5A)	126.3	F(2)-C(18)-C(17)	120.2(8)
N(4)-C(6)-C(5)	108.1(7)	F(2)-C(18)-C(19)	120.0(8)
N(4)-C(6)-C(13)	122.0(7)	C(17)-C(18)-C(19)	119.7(8)
C(5)-C(6)-C(13)	129.9(8)	C(20)-C(19)-F(3)	121.5(8)
N(5)-C(7)-C(8)	108.6(7)	C(20)-C(19)-C(18)	118.3(8)
N(5)-C(7)-C(14)	124.9(7)	F(3)-C(19)-C(18)	120.1(8)
C(8)-C(7)-C(14)	126.3(7)	C(19)-C(20)-C(21)	122.0(8)
C(9)-C(8)-C(7)	107.6(7)	C(19)-C(20)-F(4)	118.8(7)
C(9)-C(8)-H(8A)	126.2	C(21)-C(20)-F(4)	119.1(8)
C(7)-C(8)-H(8A)	126.2	F(5)-C(21)-C(20)	115.8(7)
C(8)-C(9)-N(6)	107.7(7)	F(5)-C(21)-C(16)	122.4(7)
C(8)-C(9)-C(15)	130.1(7)	C(20)-C(21)-C(16)	121.7(8)
N(6)-C(9)-C(15)	122.2(7)	C(23)-P(1)-C(24)	99.1(4)
C(1)-C(10)-H(10A)	109.5	C(23)-P(1)-C(22)	104.0(5)
C(1)-C(10)-H(10B)	109.5	C(24)-P(1)-C(22)	99.2(5)
H(10A)-C(10)-H(10B)	109.5	C(23)-P(1)-Rh(1)	119.8(3)
C(1)-C(10)-H(10C)	109.5	C(24)-P(1)-Rh(1)	122.1(3)
H(10A)-C(10)-H(10C)	109.5	C(22)-P(1)-Rh(1)	109.5(3)
H(10B)-C(10)-H(10C)	109.5	P(1)-C(22)-H(22A)	109.5
C(3)-C(11)-H(11A)	109.5	P(1)-C(22)-H(22B)	109.5
C(3)-C(11)-H(11B)	109.5	H(22A)-C(22)-H(22B)	109.5
H(11A)-C(11)-H(11B)	109.5	P(1)-C(22)-H(22C)	109.5
C(3)-C(11)-H(11C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(11B)-C(11)-H(11C)	109.5	P(1)-C(23)-H(23A)	109.5
C(4)-C(12)-H(12A)	109.5	P(1)-C(23)-H(23B)	109.5

H(23A)-C(23)-H(23B)	109.5	N(8)-C(27)-C(26)	108.5(7)
P(1)-C(23)-H(23C)	109.5	N(8)-C(27)-C(35)	123.8(7)
H(23A)-C(23)-H(23C)	109.5	C(26)-C(27)-C(35)	127.7(8)
H(23B)-C(23)-H(23C)	109.5	N(9)-C(28)-C(29)	110.0(7)
P(1)-C(24)-H(24A)	109.5	N(9)-C(28)-C(36)	123.9(7)
P(1)-C(24)-H(24B)	109.5	C(29)-C(28)-C(36)	126.0(7)
H(24A)-C(24)-H(24B)	109.5	C(30)-C(29)-C(28)	106.5(7)
P(1)-C(24)-H(24C)	109.5	C(30)-C(29)-H(29A)	126.8
H(24A)-C(24)-H(24C)	109.5	C(28)-C(29)-H(29A)	126.8
H(24B)-C(24)-H(24C)	109.5	C(29)-C(30)-N(10)	107.7(7)
C(40)-Rh(2)-N(7)	88.1(3)	C(29)-C(30)-C(37)	130.2(7)
C(40)-Rh(2)-N(11)	170.0(3)	N(10)-C(30)-C(37)	122.1(7)
N(7)-Rh(2)-N(11)	83.1(2)	N(11)-C(31)-C(32)	110.9(7)
C(40)-Rh(2)-N(9)	96.2(3)	N(11)-C(31)-C(38)	121.7(8)
N(7)-Rh(2)-N(9)	88.1(2)	C(32)-C(31)-C(38)	127.4(8)
N(11)-Rh(2)-N(9)	88.3(2)	C(33)-C(32)-C(31)	105.5(8)
C(40)-Rh(2)-P(2)	92.1(2)	C(33)-C(32)-H(32A)	127.2
N(7)-Rh(2)-P(2)	177.23(18)	C(31)-C(32)-H(32A)	127.2
N(11)-Rh(2)-P(2)	96.44(18)	N(12)-C(33)-C(32)	108.0(7)
N(9)-Rh(2)-P(2)	94.59(17)	N(12)-C(33)-C(39)	122.9(8)
C(40)-Rh(2)-H(2)	88(3)	C(32)-C(33)-C(39)	129.1(8)
N(7)-Rh(2)-H(2)	98(3)	C(25)-C(34)-H(34A)	109.5
N(11)-Rh(2)-H(2)	88(3)	C(25)-C(34)-H(34B)	109.5
N(9)-Rh(2)-H(2)	173(3)	H(34A)-C(34)-H(34B)	109.5
P(2)-Rh(2)-H(2)	80(3)	C(25)-C(34)-H(34C)	109.5
C(25)-N(7)-N(8)	107.6(6)	H(34A)-C(34)-H(34C)	109.5
C(25)-N(7)-Rh(2)	134.9(5)	H(34B)-C(34)-H(34C)	109.5
N(8)-N(7)-Rh(2)	117.1(5)	C(27)-C(35)-H(35A)	109.5
C(27)-N(8)-N(7)	108.8(6)	C(27)-C(35)-H(35B)	109.5
C(27)-N(8)-B(2)	130.3(7)	H(35A)-C(35)-H(35B)	109.5
N(7)-N(8)-B(2)	120.5(6)	C(27)-C(35)-H(35C)	109.5
C(28)-N(9)-N(10)	106.5(6)	H(35A)-C(35)-H(35C)	109.5
C(28)-N(9)-Rh(2)	139.1(5)	H(35B)-C(35)-H(35C)	109.5
N(10)-N(9)-Rh(2)	114.3(4)	C(28)-C(36)-H(36A)	109.5
C(30)-N(10)-N(9)	109.4(6)	C(28)-C(36)-H(36B)	109.5
C(30)-N(10)-B(2)	129.4(7)	H(36A)-C(36)-H(36B)	109.5
N(9)-N(10)-B(2)	121.1(6)	C(28)-C(36)-H(36C)	109.5
C(31)-N(11)-N(12)	105.3(6)	H(36A)-C(36)-H(36C)	109.5
C(31)-N(11)-Rh(2)	136.5(5)	H(36B)-C(36)-H(36C)	109.5
N(12)-N(11)-Rh(2)	116.9(5)	C(30)-C(37)-H(37A)	109.5
C(33)-N(12)-N(11)	110.3(7)	C(30)-C(37)-H(37B)	109.5
C(33)-N(12)-B(2)	128.5(7)	H(37A)-C(37)-H(37B)	109.5
N(11)-N(12)-B(2)	120.2(7)	C(30)-C(37)-H(37C)	109.5
N(10)-B(2)-N(8)	110.8(7)	H(37A)-C(37)-H(37C)	109.5
N(10)-B(2)-N(12)	109.4(7)	H(37B)-C(37)-H(37C)	109.5
N(8)-B(2)-N(12)	108.0(7)	C(31)-C(38)-H(38A)	109.5
N(10)-B(2)-H(2B)	107(4)	C(31)-C(38)-H(38B)	109.5
N(8)-B(2)-H(2B)	112(4)	H(38A)-C(38)-H(38B)	109.5
N(12)-B(2)-H(2B)	110(4)	C(31)-C(38)-H(38C)	109.5
N(7)-C(25)-C(26)	110.0(7)	H(38A)-C(38)-H(38C)	109.5
N(7)-C(25)-C(34)	124.0(8)	H(38B)-C(38)-H(38C)	109.5
C(26)-C(25)-C(34)	125.9(8)	C(33)-C(39)-H(39A)	109.5
C(27)-C(26)-C(25)	105.1(7)	C(33)-C(39)-H(39B)	109.5
C(27)-C(26)-H(26A)	127.4	H(39A)-C(39)-H(39B)	109.5
C(25)-C(26)-H(26A)	127.4	C(33)-C(39)-H(39C)	109.5

H(39A)-C(39)-H(39C)	109.5	H(50A)-C(50)-H(50B)	107.7
H(39B)-C(39)-H(39C)	109.5	C(50)-C(51)-C(52)	101(3)
C(45)-C(40)-C(41)	114.2(9)	C(50)-C(51)-H(51A)	111.5
C(45)-C(40)-Rh(2)	123.3(6)	C(52)-C(51)-H(51A)	111.5
C(41)-C(40)-Rh(2)	122.0(7)	C(50)-C(51)-H(51B)	111.5
C(42)-C(41)-C(40)	122.5(9)	C(52)-C(51)-H(51B)	111.5
C(42)-C(41)-F(6)	115.4(7)	H(51A)-C(51)-H(51B)	109.3
C(40)-C(41)-F(6)	122.1(8)	C(53)-C(52)-C(51)	94(3)
C(43)-C(42)-F(7)	119.5(8)	C(53)-C(52)-H(52A)	112.8
C(43)-C(42)-C(41)	120.3(8)	C(51)-C(52)-H(52A)	112.8
F(7)-C(42)-C(41)	120.1(9)	C(53)-C(52)-H(52B)	112.8
F(8)-C(43)-C(42)	121.1(8)	C(51)-C(52)-H(52B)	112.8
F(8)-C(43)-C(44)	121.3(9)	H(52A)-C(52)-H(52B)	110.3
C(42)-C(43)-C(44)	117.5(9)	C(54)-C(53)-C(52)	115(4)
F(9)-C(44)-C(45)	122.2(9)	C(54)-C(53)-H(53A)	108.6
F(9)-C(44)-C(43)	118.7(9)	C(52)-C(53)-H(53A)	108.6
C(45)-C(44)-C(43)	119.1(9)	C(54)-C(53)-H(53B)	108.6
C(40)-C(45)-C(44)	126.3(9)	C(52)-C(53)-H(53B)	108.6
C(40)-C(45)-F(10)	120.8(7)	H(53A)-C(53)-H(53B)	107.6
C(44)-C(45)-F(10)	112.9(8)	C(53)-C(54)-H(54A)	109.5
C(46)-P(2)-C(47)	101.7(5)	C(53)-C(54)-H(54B)	109.5
C(46)-P(2)-C(48)	105.5(5)	H(54A)-C(54)-H(54B)	109.5
C(47)-P(2)-C(48)	96.6(5)	C(53)-C(54)-H(54C)	109.5
C(46)-P(2)-Rh(2)	111.0(3)	H(54A)-C(54)-H(54C)	109.5
C(47)-P(2)-Rh(2)	121.7(3)	H(54B)-C(54)-H(54C)	109.5
C(48)-P(2)-Rh(2)	117.9(3)	C(50')-C(49')-H(49D)	109.5
P(2)-C(46)-H(46A)	109.5	C(50')-C(49')-H(49E)	109.5
P(2)-C(46)-H(46B)	109.5	H(49D)-C(49')-H(49E)	109.5
H(46A)-C(46)-H(46B)	109.5	C(50')-C(49')-H(49F)	109.5
P(2)-C(46)-H(46C)	109.5	H(49D)-C(49')-H(49F)	109.5
H(46A)-C(46)-H(46C)	109.5	H(49E)-C(49')-H(49F)	109.5
H(46B)-C(46)-H(46C)	109.5	C(49')-C(50')-C(51')	113(4)
P(2)-C(47)-H(47A)	109.5	C(49')-C(50')-H(50C)	108.9
P(2)-C(47)-H(47B)	109.5	C(51')-C(50')-H(50C)	108.9
H(47A)-C(47)-H(47B)	109.5	C(49')-C(50')-H(50D)	108.9
P(2)-C(47)-H(47C)	109.5	C(51')-C(50')-H(50D)	108.9
H(47A)-C(47)-H(47C)	109.5	H(50C)-C(50')-H(50D)	107.7
H(47B)-C(47)-H(47C)	109.5	C(50')-C(51')-C(52')	97(3)
P(2)-C(48)-H(48A)	109.5	C(50')-C(51')-H(51C)	112.4
P(2)-C(48)-H(48B)	109.5	C(52')-C(51')-H(51C)	112.4
H(48A)-C(48)-H(48B)	109.5	C(50')-C(51')-H(51D)	112.4
P(2)-C(48)-H(48C)	109.5	C(52')-C(51')-H(51D)	112.4
H(48A)-C(48)-H(48C)	109.5	H(51C)-C(51')-H(51D)	109.9
H(48B)-C(48)-H(48C)	109.5	C(53')-C(52')-C(51')	101(3)
C(50)-C(49)-H(49A)	109.5	C(53')-C(52')-H(52C)	111.6
C(50)-C(49)-H(49B)	109.5	C(51')-C(52')-H(52C)	111.6
H(49A)-C(49)-H(49B)	109.5	C(53')-C(52')-H(52D)	111.6
C(50)-C(49)-H(49C)	109.5	C(51')-C(52')-H(52D)	111.6
H(49A)-C(49)-H(49C)	109.5	H(52C)-C(52')-H(52D)	109.4
H(49B)-C(49)-H(49C)	109.5	C(54')-C(53')-C(52')	113(4)
C(49)-C(50)-C(51)	113(4)	C(54')-C(53')-H(53C)	109.1
C(49)-C(50)-H(50A)	108.9	C(52')-C(53')-H(53C)	109.1
C(51)-C(50)-H(50A)	108.9	C(54')-C(53')-H(53D)	109.1
C(49)-C(50)-H(50B)	108.9	C(52')-C(53')-H(53D)	109.1
C(51)-C(50)-H(50B)	108.9	H(53C)-C(53')-H(53D)	107.8

C(53')-C(54')-H(54D)	109.5	C(53')-C(54')-H(54F)	109.5
C(53')-C(54')-H(54E)	109.5	H(54D)-C(54')-H(54F)	109.5
H(54D)-C(54')-H(54E)	109.5	H(54E)-C(54')-H(54F)	109.5

Table S16. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3a**. 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}
Rh1	39(1)	32(1)	36(1)	4(1)	4(1)	4(1)
N1	43(4)	34(3)	47(4)	2(3)	15(3)	1(3)
N2	39(4)	39(4)	47(4)	5(3)	3(3)	-3(3)
N3	37(4)	36(3)	39(3)	5(3)	-1(3)	1(3)
N4	41(4)	41(4)	39(4)	4(3)	4(3)	-1(3)
N5	47(4)	35(3)	34(3)	6(3)	7(3)	8(3)
N6	32(3)	42(4)	44(4)	4(3)	9(3)	6(3)
B1	35(5)	52(6)	44(5)	2(4)	0(4)	5(4)
C1	52(5)	34(4)	52(5)	1(4)	19(4)	-1(4)
C2	45(5)	46(5)	78(7)	-8(5)	20(5)	-9(4)
C3	42(5)	38(4)	61(5)	0(4)	9(4)	8(4)
C4	49(5)	34(4)	48(5)	-1(3)	7(4)	7(3)
C5	52(5)	45(5)	39(4)	6(4)	7(4)	5(4)
C6	48(5)	40(4)	46(5)	7(4)	5(4)	7(4)
C7	53(5)	40(4)	42(5)	7(4)	10(4)	13(4)
C8	49(5)	43(5)	52(5)	11(4)	17(4)	11(4)
C9	43(5)	44(5)	44(5)	16(4)	8(4)	9(4)
C10	82(7)	44(5)	51(5)	11(4)	18(5)	-7(5)
C11	67(6)	49(5)	85(7)	-15(5)	5(5)	-14(5)
C12	39(5)	54(5)	54(5)	14(4)	6(4)	3(4)
C13	70(6)	62(6)	36(5)	3(4)	1(4)	2(5)
C14	82(7)	45(5)	58(6)	-4(4)	1(5)	13(5)
C15	50(5)	52(5)	59(6)	20(4)	1(4)	2(4)
C16	42(4)	31(4)	40(4)	6(3)	7(3)	6(3)
C17	44(5)	43(5)	45(5)	6(4)	2(4)	1(4)
F1	58(3)	55(3)	53(3)	0(2)	-11(2)	-3(2)
C18	49(5)	59(6)	52(5)	14(4)	-1(4)	-9(4)
F2	60(3)	74(4)	69(4)	15(3)	-18(3)	-2(3)
C19	40(5)	53(5)	68(6)	15(5)	9(4)	9(4)
F3	50(3)	73(4)	93(4)	31(3)	4(3)	17(3)
C20	47(5)	30(4)	62(5)	5(4)	13(4)	-5(3)
F4	61(3)	43(3)	97(4)	4(3)	15(3)	16(2)
C21	38(4)	42(5)	55(5)	14(4)	7(4)	2(3)
F5	51(3)	39(2)	58(3)	-5(2)	2(2)	8(2)
P1	50(1)	40(1)	37(1)	3(1)	5(1)	8(1)
C22	63(6)	101(8)	53(6)	8(5)	12(5)	35(6)
C23	113(9)	45(5)	47(5)	-3(4)	19(5)	0(5)
C24	80(7)	54(5)	42(5)	4(4)	11(5)	10(5)
Rh2	40(1)	40(1)	40(1)	2(1)	-5(1)	1(1)
N7	36(4)	44(4)	40(4)	2(3)	-5(3)	0(3)
N8	45(4)	36(3)	44(4)	3(3)	0(3)	-2(3)
N9	40(4)	39(4)	42(4)	-1(3)	0(3)	1(3)
N10	38(4)	42(4)	38(4)	6(3)	-9(3)	-4(3)
N11	39(4)	43(4)	42(4)	4(3)	-5(3)	-8(3)

N12	48(4)	35(3)	45(4)	6(3)	-1(3)	-2(3)
B2	47(6)	44(5)	39(5)	-1(4)	-2(4)	0(4)
C25	52(5)	43(5)	44(5)	5(4)	10(4)	5(4)
C26	65(6)	37(5)	58(5)	14(4)	12(4)	0(4)
C27	49(5)	47(5)	49(5)	9(4)	10(4)	5(4)
C28	43(5)	37(4)	48(5)	9(4)	7(4)	4(3)
C29	43(5)	41(4)	44(5)	9(4)	-1(4)	3(3)
C30	35(4)	51(5)	39(4)	12(4)	-3(3)	-2(3)
C31	43(5)	32(4)	60(5)	7(4)	2(4)	1(3)
C32	43(5)	40(4)	56(5)	6(4)	8(4)	-2(4)
C33	51(5)	31(4)	53(5)	3(4)	7(4)	0(4)
C34	71(6)	59(6)	42(5)	15(4)	8(4)	14(5)
C35	61(6)	43(5)	62(6)	3(4)	5(4)	-6(4)
C36	54(5)	47(5)	61(6)	1(4)	-4(4)	4(4)
C37	38(5)	66(6)	46(5)	2(4)	-5(4)	-5(4)
C38	57(6)	61(6)	49(5)	-1(4)	2(4)	-7(4)
C39	63(6)	53(5)	45(5)	-6(4)	-1(4)	4(4)
C40	51(5)	36(4)	45(5)	12(4)	-17(4)	-6(4)
C41	56(6)	55(5)	45(5)	3(4)	0(4)	0(4)
F6	50(3)	80(4)	44(3)	4(2)	-10(2)	-4(3)
C42	65(6)	81(7)	27(4)	-3(4)	-5(4)	0(5)
F7	93(5)	123(5)	43(3)	-10(3)	-5(3)	3(4)
C43	70(7)	74(7)	40(5)	-2(4)	10(5)	6(5)
F8	102(5)	114(5)	50(3)	-2(3)	20(3)	7(4)
C44	61(6)	70(6)	61(6)	3(5)	15(5)	0(5)
F9	61(4)	109(5)	72(4)	10(3)	24(3)	6(3)
C45	62(6)	42(5)	37(4)	4(3)	13(4)	2(4)
F10	47(3)	72(3)	59(3)	3(3)	0(2)	-3(2)
P2	50(1)	45(1)	52(1)	0(1)	1(1)	-6(1)
C46	87(8)	56(6)	64(6)	9(5)	10(5)	-22(5)
C47	61(6)	66(6)	82(7)	-10(5)	7(5)	-14(5)
C48	64(6)	52(5)	72(6)	-5(5)	-5(5)	-9(5)
C49	176(19)	111(18)	130(20)	35(16)	36(16)	16(13)
C50	170(20)	130(20)	130(20)	32(17)	37(17)	24(19)
C51	198(19)	210(30)	95(14)	-32(18)	24(12)	0(20)
C52	204(18)	210(30)	91(13)	-33(17)	22(11)	-6(19)
C53	202(19)	210(30)	101(14)	-20(18)	21(13)	-10(20)
C54	170(30)	430(130)	90(20)	-60(40)	10(30)	20(40)
C49'	176(19)	111(18)	130(20)	35(16)	36(16)	16(13)
C50'	170(20)	130(20)	130(20)	32(17)	37(17)	24(19)
C51'	198(19)	210(30)	95(14)	-32(18)	24(12)	0(20)
C52'	204(18)	210(30)	91(13)	-33(17)	22(11)	-6(19)
C53'	202(19)	210(30)	101(14)	-20(18)	21(13)	-10(20)
C54'	170(30)	430(130)	90(20)	-60(40)	10(30)	20(40)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **3a**.

	x	y	z	U(eq)
H1	7170(100)	3570(30)	1430(40)	72
H1B	11610(90)	4110(20)	3470(40)	54
H2A	12489	5207	2056	66

H5A	6093	4132	3699	54
H8A	11987	2803	2738	57
H10A	9061	4800	844	88
H10B	10614	5041	779	88
H10C	9353	5228	1164	88
H11A	13896	4537	3384	102
H11B	12728	4845	3628	102
H11C	14034	4997	3234	102
H12A	5199	3854	1911	74
H12B	4528	4252	2166	74
H12C	4302	3842	2515	74
H13A	10176	4001	4352	86
H13B	8724	4212	4587	86
H13C	9949	4467	4274	86
H14A	8429	3019	1458	95
H14B	9251	2648	1855	95
H14C	10029	2844	1294	95
H15A	13798	3195	3714	82
H15B	12590	3475	3994	82
H15C	13823	3660	3594	82
H22A	12087	3738	526	108
H22B	11868	3533	1194	108
H22C	12162	3998	1170	108
H23A	9525	3385	-87	102
H23B	7764	3492	-14	102
H23C	8805	3206	504	102
H24A	9977	4101	-269	87
H24B	10108	4446	261	87
H24C	8416	4290	-90	87
H2	2170(110)	2080(30)	2300(40)	83
H2B	6780(90)	2470(20)	4380(40)	53
H26A	6755	3221	2363	64
H29A	8620	1156	4192	52
H32A	1270	2588	4549	56
H34A	3274	2617	1618	86
H34B	4871	2587	1337	86
H34C	4176	3010	1472	86
H35A	8602	2884	4025	84
H35B	7488	3263	3987	84
H35C	8781	3235	3531	84
H36A	6261	1115	2538	84
H36B	5658	840	3064	84
H36C	7488	853	3026	84
H37A	7980	1982	5179	77
H37B	9244	2134	4765	77
H37C	9457	1711	5111	77
H38A	350	2132	2873	85
H38B	-503	2413	3316	85
H38C	-255	1955	3493	85
H39A	5363	2526	5304	83
H39B	3914	2810	5354	83
H39C	5170	2935	4916	83
H46A	1890	912	3449	104
H46B	2381	1328	3788	104
H46C	3699	1043	3598	104

H47A	-117	1096	2365	106
H47B	-25	1517	2030	106
H47C	-211	1490	2778	106
H48A	2214	733	2211	98
H48B	3896	923	2189	98
H48C	2384	1058	1673	98
H49A	9635	5385	3069	207
H49B	8996	5005	3391	207
H49C	10181	5302	3832	207
H50A	7160	5471	3215	174
H50B	8345	5780	3626	174
H51A	8395	5373	4563	202
H51B	7019	5111	4136	202
H52A	6778	5965	4380	203
H52B	5464	5737	3853	203
H53A	5755	5221	4731	207
H53B	6380	5579	5206	207
H54A	3899	5475	5217	349
H54B	3462	5512	4440	349
H54C	4080	5890	4872	349
H49D	9525	4991	3336	207
H49E	10337	5261	3933	207
H49F	9547	5460	3257	207
H50C	8036	5065	4110	174
H50D	7193	5211	3403	174
H51C	7544	5866	3705	202
H51D	8671	5747	4387	202
H52C	5399	5468	3988	203
H52D	6527	5324	4652	203
H53C	6920	5980	4985	207
H53D	5816	6125	4326	207
H54D	4415	6150	5080	349
H54E	4942	5717	5335	349
H54F	3810	5774	4643	349

Table S18. Torsion angles [°] for **3a**.

C16-Rh1-N1-C1	-39.9(8)	C16-Rh1-N3-N4	-133.2(5)
N3-Rh1-N1-C1	-129.6(8)	N5-Rh1-N3-N4	51.3(5)
N5-Rh1-N1-C1	148.7(8)	N1-Rh1-N3-N4	-41.8(5)
P1-Rh1-N1-C1	57.0(8)	P1-Rh1-N3-N4	47.4(18)
C16-Rh1-N1-N2	138.8(5)	C4-N3-N4-C6	-0.1(8)
N3-Rh1-N1-N2	49.0(5)	Rh1-N3-N4-C6	-179.9(5)
N5-Rh1-N1-N2	-32.6(5)	C4-N3-N4-B1	175.6(7)
P1-Rh1-N1-N2	-124.4(5)	Rh1-N3-N4-B1	-4.1(8)
C1-N1-N2-C3	-1.2(8)	C16-Rh1-N5-C7	92.6(18)
Rh1-N1-N2-C3	179.7(5)	N3-Rh1-N5-C7	121.5(8)
C1-N1-N2-B1	170.3(7)	N1-Rh1-N5-C7	-151.8(8)
Rh1-N1-N2-B1	-8.7(8)	P1-Rh1-N5-C7	-59.0(8)
C16-Rh1-N3-C4	47.1(7)	C16-Rh1-N5-N6	-85.9(17)
N5-Rh1-N3-C4	-128.3(7)	N3-Rh1-N5-N6	-57.0(5)
N1-Rh1-N3-C4	138.5(7)	N1-Rh1-N5-N6	29.7(5)
P1-Rh1-N3-C4	-132.3(13)	P1-Rh1-N5-N6	122.5(5)

C7-N5-N6-C9	0.3(8)	P1-Rh1-C16-C17	51.0(7)
Rh1-N5-N6-C9	179.2(5)	N3-Rh1-C16-C21	43.7(6)
C7-N5-N6-B1	-165.0(7)	N5-Rh1-C16-C21	72.2(18)
Rh1-N5-N6-B1	14.0(8)	N1-Rh1-C16-C21	-43.5(6)
C3-N2-B1-N4	117.2(9)	P1-Rh1-C16-C21	-136.4(6)
N1-N2-B1-N4	-52.5(9)	C21-C16-C17-F1	179.7(7)
C3-N2-B1-N6	-124.3(8)	Rh1-C16-C17-F1	-7.2(11)
N1-N2-B1-N6	66.1(9)	C21-C16-C17-C18	0.7(12)
C6-N4-B1-N2	-122.7(8)	Rh1-C16-C17-C18	173.9(7)
N3-N4-B1-N2	62.6(9)	F1-C17-C18-F2	0.5(12)
C6-N4-B1-N6	116.8(8)	C16-C17-C18-F2	179.5(8)
N3-N4-B1-N6	-57.9(9)	F1-C17-C18-C19	-179.2(7)
C9-N6-B1-N2	128.2(8)	C16-C17-C18-C19	-0.2(14)
N5-N6-B1-N2	-70.0(8)	F2-C18-C19-C20	-179.3(8)
C9-N6-B1-N4	-111.2(8)	C17-C18-C19-C20	0.4(13)
N5-N6-B1-N4	50.6(9)	F2-C18-C19-F3	-0.3(13)
N2-N1-C1-C2	2.9(9)	C17-C18-C19-F3	179.4(8)
Rh1-N1-C1-C2	-178.3(6)	F3-C19-C20-C21	179.9(7)
N2-N1-C1-C10	-171.5(7)	C18-C19-C20-C21	-1.2(13)
Rh1-N1-C1-C10	7.2(13)	F3-C19-C20-F4	2.2(12)
N1-C1-C2-C3	-3.5(9)	C18-C19-C20-F4	-178.9(7)
C10-C1-C2-C3	170.8(8)	C19-C20-C21-F5	-178.5(7)
N1-N2-C3-C2	-1.0(9)	F4-C20-C21-F5	-0.8(11)
B1-N2-C3-C2	-171.5(8)	C19-C20-C21-C16	1.8(13)
N1-N2-C3-C11	179.3(8)	F4-C20-C21-C16	179.5(7)
B1-N2-C3-C11	8.9(13)	C17-C16-C21-F5	178.8(7)
C1-C2-C3-N2	2.7(9)	Rh1-C16-C21-F5	5.3(10)
C1-C2-C3-C11	-177.7(9)	C17-C16-C21-C20	-1.4(11)
N4-N3-C4-C5	-0.2(8)	Rh1-C16-C21-C20	-175.0(6)
Rh1-N3-C4-C5	179.5(5)	C16-Rh1-P1-C23	-94.5(5)
N4-N3-C4-C12	-179.3(7)	N3-Rh1-P1-C23	84.9(16)
Rh1-N3-C4-C12	0.4(11)	N5-Rh1-P1-C23	81.0(4)
N3-C4-C5-C6	0.5(9)	N1-Rh1-P1-C23	173.8(4)
C12-C4-C5-C6	179.5(8)	C16-Rh1-P1-C24	30.7(4)
N3-N4-C6-C5	0.4(8)	N3-Rh1-P1-C24	-150.0(16)
B1-N4-C6-C5	-174.8(7)	N5-Rh1-P1-C24	-153.9(4)
N3-N4-C6-C13	178.4(7)	N1-Rh1-P1-C24	-61.1(4)
B1-N4-C6-C13	3.2(13)	C16-Rh1-P1-C22	145.7(5)
C4-C5-C6-N4	-0.5(9)	N3-Rh1-P1-C22	-35.0(16)
C4-C5-C6-C13	-178.4(8)	N5-Rh1-P1-C22	-38.9(4)
N6-N5-C7-C8	-1.1(9)	N1-Rh1-P1-C22	53.9(4)
Rh1-N5-C7-C8	-179.6(6)	C40-Rh2-N7-C25	41.5(8)
N6-N5-C7-C14	174.7(8)	N11-Rh2-N7-C25	-133.6(8)
Rh1-N5-C7-C14	-3.9(14)	N9-Rh2-N7-C25	137.8(8)
N5-C7-C8-C9	1.4(10)	P2-Rh2-N7-C25	-53(4)
C14-C7-C8-C9	-174.3(8)	C40-Rh2-N7-N8	-130.8(5)
C7-C8-C9-N6	-1.2(9)	N11-Rh2-N7-N8	54.0(5)
C7-C8-C9-C15	177.3(8)	N9-Rh2-N7-N8	-34.5(5)
N5-N6-C9-C8	0.6(9)	P2-Rh2-N7-N8	135(4)
B1-N6-C9-C8	163.8(8)	C25-N7-N8-C27	-0.3(9)
N5-N6-C9-C15	-178.1(7)	Rh2-N7-N8-C27	174.0(5)
B1-N6-C9-C15	-14.9(12)	C25-N7-N8-B2	173.1(7)
N3-Rh1-C16-C17	-129.0(7)	Rh2-N7-N8-B2	-12.6(9)
N5-Rh1-C16-C17	-100.4(17)	C40-Rh2-N9-C28	-52.1(9)
N1-Rh1-C16-C17	143.9(7)	N7-Rh2-N9-C28	-140.0(8)

N11-Rh2-N9-C28	136.8(8)	B2-N10-C30-C29	-175.9(8)
P2-Rh2-N9-C28	40.5(8)	N9-N10-C30-C37	179.4(7)
C40-Rh2-N9-N10	133.6(5)	B2-N10-C30-C37	3.0(13)
N7-Rh2-N9-N10	45.7(5)	N12-N11-C31-C32	-2.9(8)
N11-Rh2-N9-N10	-37.5(5)	Rh2-N11-C31-C32	-168.5(6)
P2-Rh2-N9-N10	-133.8(5)	N12-N11-C31-C38	176.1(7)
C28-N9-N10-C30	-1.0(8)	Rh2-N11-C31-C38	10.5(12)
Rh2-N9-N10-C30	175.1(5)	N11-C31-C32-C33	2.6(9)
C28-N9-N10-B2	175.7(7)	C38-C31-C32-C33	-176.4(8)
Rh2-N9-N10-B2	-8.2(9)	N11-N12-C33-C32	-0.6(8)
C40-Rh2-N11-C31	87.5(17)	B2-N12-C33-C32	168.0(7)
N7-Rh2-N11-C31	116.5(8)	N11-N12-C33-C39	180.0(7)
N9-Rh2-N11-C31	-155.2(8)	B2-N12-C33-C39	-11.5(12)
P2-Rh2-N11-C31	-60.8(7)	C31-C32-C33-N12	-1.1(9)
C40-Rh2-N11-N12	-77.0(17)	C31-C32-C33-C39	178.2(8)
N7-Rh2-N11-N12	-48.0(5)	N7-Rh2-C40-C45	49.6(7)
N9-Rh2-N11-N12	40.3(5)	N11-Rh2-C40-C45	78.4(18)
P2-Rh2-N11-N12	134.8(5)	N9-Rh2-C40-C45	-38.3(7)
C31-N11-N12-C33	2.2(8)	P2-Rh2-C40-C45	-133.1(7)
Rh2-N11-N12-C33	171.1(5)	N7-Rh2-C40-C41	-121.4(7)
C31-N11-N12-B2	-167.5(7)	N11-Rh2-C40-C41	-92.6(17)
Rh2-N11-N12-B2	1.5(8)	N9-Rh2-C40-C41	150.7(7)
C30-N10-B2-N8	123.2(8)	P2-Rh2-C40-C41	55.8(7)
N9-N10-B2-N8	-52.8(10)	C45-C40-C41-C42	1.1(13)
C30-N10-B2-N12	-117.8(8)	Rh2-C40-C41-C42	172.9(7)
N9-N10-B2-N12	66.1(9)	C45-C40-C41-F6	-176.5(7)
C27-N8-B2-N10	-119.9(9)	Rh2-C40-C41-F6	-4.7(11)
N7-N8-B2-N10	68.3(9)	C40-C41-C42-C43	0.3(15)
C27-N8-B2-N12	120.3(9)	F6-C41-C42-C43	178.0(9)
N7-N8-B2-N12	-51.5(9)	C40-C41-C42-F7	178.2(8)
C33-N12-B2-N10	129.5(8)	F6-C41-C42-F7	-4.1(13)
N11-N12-B2-N10	-62.9(9)	F7-C42-C43-F8	2.9(15)
C33-N12-B2-N8	-109.9(8)	C41-C42-C43-F8	-179.1(9)
N11-N12-B2-N8	57.7(9)	F7-C42-C43-C44	-179.5(9)
N8-N7-C25-C26	1.2(9)	C41-C42-C43-C44	-1.6(15)
Rh2-N7-C25-C26	-171.7(6)	F8-C43-C44-F9	-0.8(15)
N8-N7-C25-C34	-177.8(7)	C42-C43-C44-F9	-178.4(9)
Rh2-N7-C25-C34	9.4(13)	F8-C43-C44-C45	179.0(9)
N7-C25-C26-C27	-1.5(10)	C42-C43-C44-C45	1.5(15)
C34-C25-C26-C27	177.4(8)	C41-C40-C45-C44	-1.2(13)
N7-N8-C27-C26	-0.6(9)	Rh2-C40-C45-C44	-172.9(7)
B2-N8-C27-C26	-173.2(8)	C41-C40-C45-F10	178.1(7)
N7-N8-C27-C35	178.8(7)	Rh2-C40-C45-F10	6.4(11)
B2-N8-C27-C35	6.2(14)	F9-C44-C45-C40	179.8(8)
C25-C26-C27-N8	1.3(10)	C43-C44-C45-C40	-0.1(15)
C25-C26-C27-C35	-178.1(8)	F9-C44-C45-F10	0.4(13)
N10-N9-C28-C29	1.1(9)	C43-C44-C45-F10	-179.4(8)
Rh2-N9-C28-C29	-173.4(6)	C40-Rh2-P2-C46	138.0(5)
N10-N9-C28-C36	-175.7(7)	N7-Rh2-P2-C46	-128(4)
Rh2-N9-C28-C36	9.7(13)	N11-Rh2-P2-C46	-47.2(4)
N9-C28-C29-C30	-0.8(9)	N9-Rh2-P2-C46	41.6(4)
C36-C28-C29-C30	175.9(8)	C40-Rh2-P2-C47	-102.4(5)
C28-C29-C30-N10	0.2(9)	N7-Rh2-P2-C47	-8(4)
C28-C29-C30-C37	-178.6(8)	N11-Rh2-P2-C47	72.3(5)
N9-N10-C30-C29	0.5(9)	N9-Rh2-P2-C47	161.1(5)

C40-Rh2-P2-C48	16.3(4)	C50-C51-C52-C53	171(4)
N7-Rh2-P2-C48	111(4)	C51-C52-C53-C54	-154(5)
N11-Rh2-P2-C48	-169.0(4)	C49'-C50'-C51'-C52'	-170(5)
N9-Rh2-P2-C48	-80.1(4)	C50'-C51'-C52'-C53'	177(4)
C49-C50-C51-C52	172(6)	C51'-C52'-C53'-C54'	179(5)

Table S19. Crystal data and structure refinement for **3b**.

Identification code	**3b**	
Empirical formula	$C_{24}H_{33}BF_4N_6PRh$	
Formula weight	626.25	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 29.063(3) Å	α = 90°
	b = 10.5847(12) Å	β = 90°
	c = 17.7982(19) Å	γ = 90°
Volume	5475.0(10) Å^3	
Z	8	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	0.735 mm^{-1}	
F(000)	2560	
Crystal color, morphology	colorless, block	
Crystal size	0.22 x 0.16 x 0.12 mm^3	
Theta range for data collection	1.81 to 36.32°	
Index ranges	$-48 \le h \le 48$, $-17 \le k \le 17$, $-29 \le l \le 29$	
Reflections collected	117833	
Independent reflections	26396 [R(int) = 0.1168]	
Observed reflections	16014	
Completeness to theta = 36.32°	99.5%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9170 and 0.8551	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26396 / 329 / 906	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R_1 = 0.0646, wR_2 = 0.1235	
R indices (all data)	R_1 = 0.1239, wR_2 = 0.1464	
Absolute structure parameter	0.0(9)	
Largest diff. peak and hole	1.091 and -1.167 e.Å^{-3}	

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	4680(1)	5034(1)	6118(1)	16(1)
N1	4497(1)	3616(4)	5210(2)	17(1)
N2	4168(1)	4019(4)	4711(2)	17(1)
N3	4655(2)	6434(5)	5269(3)	20(1)

N4	4324(2)	6352(4)	4726(3)	18(1)
N5	3962(1)	5498(4)	6202(3)	18(1)
N6	3708(1)	5482(4)	5546(2)	19(1)
B1	3953(2)	5327(4)	4786(3)	20(1)
C1	4665(2)	2536(5)	4940(3)	24(1)
C2	4445(2)	2227(5)	4270(3)	25(1)
C3	4140(2)	3181(5)	4132(3)	23(1)
C4	4916(2)	7438(5)	5103(3)	24(1)
C5	4741(2)	8016(5)	4452(3)	26(1)
C6	4372(2)	7320(5)	4233(3)	22(1)
C7	3675(2)	5947(4)	6734(3)	23(1)
C8	3244(2)	6177(5)	6430(3)	25(1)
C9	3278(2)	5889(5)	5683(3)	21(1)
C10	5037(2)	1777(5)	5299(3)	28(1)
C11	3807(2)	3371(6)	3502(3)	29(1)
C12	5309(2)	7857(5)	5582(3)	28(1)
C13	4037(2)	7490(6)	3601(3)	34(1)
C14	3830(2)	6182(6)	7520(3)	30(1)
C15	2921(2)	6019(6)	5085(3)	34(1)
C16	5366(2)	4850(4)	5934(3)	15(1)
C17	5712(3)	4992(6)	6432(4)	23(1)
F1	5613(4)	5130(6)	7182(4)	34(1)
C18	6174(2)	4989(6)	6263(4)	26(1)
F2	6497(2)	5148(4)	6799(4)	33(1)
C19	6307(2)	4868(6)	5525(4)	23(1)
F3	6760(2)	4898(6)	5337(6)	30(1)
C20	5972(2)	4741(5)	4991(3)	20(1)
F4	6104(1)	4657(3)	4265(2)	29(1)
C21	5513(2)	4722(5)	5183(3)	21(1)
P1	4681(1)	3722(1)	7116(1)	20(1)
C22	4145(2)	2853(5)	7198(3)	26(1)
C23	5094(2)	2410(5)	7149(4)	28(1)
C24	4764(2)	4411(6)	8051(3)	27(1)
B1'	3982(7)	4795(17)	4770(14)	20(1)
N1'	4605(10)	6430(20)	5163(12)	20(1)
N2'	4264(10)	6010(20)	4684(16)	18(1)
C3'	4182(7)	6970(20)	4197(11)	22(1)
C2'	4456(8)	7960(20)	4358(13)	26(1)
C1'	4721(6)	7590(20)	4976(12)	24(1)
N3'	4685(6)	3658(16)	5251(9)	17(1)
N4'	4354(6)	3773(18)	4707(11)	17(1)
C6'	4405(7)	2800(20)	4204(10)	23(1)
C5'	4765(8)	2076(19)	4428(12)	25(1)
C4'	4941(6)	2628(18)	5092(11)	24(1)
N5'	3965(2)	4554(16)	6197(11)	18(1)
N6'	3728(6)	4573(17)	5514(10)	19(1)
C9'	3302(6)	4166(16)	5628(11)	21(1)
C8'	3259(7)	3886(19)	6376(12)	25(1)
C7'	3670(6)	4129(14)	6714(11)	23(1)
C10'	5080(8)	8340(30)	5375(18)	28(1)
C11'	3834(9)	6910(40)	3579(15)	34(1)
C12'	5332(8)	2250(30)	5586(16)	28(1)
C13'	4064(9)	2810(30)	3576(14)	29(1)
C14'	3829(11)	4000(30)	7508(12)	30(1)
C15'	2964(10)	4080(30)	5000(16)	34(1)

C16'	5387(10)	5240(20)	5957(15)	15(1)
C17'	5728(12)	5070(20)	6463(16)	23(1)
F1'	5620(20)	5010(30)	7213(18)	34(1)
C18'	6188(12)	4950(20)	6296(17)	26(1)
F2'	6505(13)	4790(30)	6840(20)	33(1)
C19'	6327(10)	5000(20)	5559(17)	23(1)
F3'	6779(11)	4880(30)	5380(40)	30(1)
C20'	5998(9)	5168(15)	5019(13)	20(1)
F4'	6132(9)	5218(19)	4296(13)	29(1)
C21'	5542(8)	5287(18)	5210(14)	21(1)
P1'	4715(3)	6283(7)	7143(4)	20(1)
C22'	4193(7)	7200(30)	7217(18)	26(1)
C23'	5136(8)	7560(20)	7200(20)	28(1)
C24'	4796(10)	5570(30)	8087(13)	27(1)
Rh2	2781(1)	232(1)	6780(1)	17(1)
N7	2934(1)	1651(4)	7685(3)	16(1)
N8	3274(1)	1309(4)	8192(3)	18(1)
N9	2781(1)	-1132(4)	7638(3)	18(1)
N10	3106(1)	-1021(4)	8203(3)	20(1)
N11	3504(1)	-209(4)	6723(3)	21(1)
N12	3743(1)	-193(4)	7401(3)	18(1)
B2	3482(2)	-10(5)	8139(4)	22(1)
C25	2803(2)	2806(4)	7895(3)	18(1)
C26	3044(2)	3203(5)	8527(3)	24(1)
C27	3331(2)	2228(5)	8704(3)	19(1)
C28	2530(2)	-2168(5)	7792(3)	27(1)
C29	2679(2)	-2686(5)	8454(4)	30(1)
C30	3043(2)	-1961(5)	8706(3)	28(1)
C31	3799(2)	-641(5)	6219(3)	21(1)
C32	4224(2)	-883(5)	6551(3)	30(1)
C33	4176(2)	-600(5)	7296(3)	24(1)
C34	2435(2)	3546(5)	7499(3)	27(1)
C35	3675(2)	2108(6)	9328(3)	30(1)
C36	2143(2)	-2599(5)	7299(4)	31(1)
C37	3348(2)	-2087(6)	9385(3)	42(2)
C38	3660(2)	-912(6)	5425(3)	33(1)
C39	4525(2)	-728(6)	7914(4)	36(1)
C40	2093(2)	368(5)	6949(3)	21(1)
C41	1749(2)	170(6)	6416(4)	24(1)
F5	1847(3)	4(6)	5677(3)	36(1)
C42	1284(2)	89(6)	6595(4)	27(1)
F6	970(2)	-145(6)	6051(5)	38(1)
C43	1148(2)	217(5)	7325(4)	26(1)
F7	696(2)	156(4)	7506(5)	35(1)
C44	1477(2)	409(5)	7869(3)	22(1)
F8	1339(1)	490(3)	8601(2)	30(1)
C45	1937(2)	488(5)	7696(3)	19(1)
P2	2772(1)	1509(1)	5758(1)	20(1)
C46	3292(2)	2451(6)	5657(4)	32(1)
C47	2715(2)	766(6)	4832(3)	28(1)
C48	2334(2)	2728(6)	5668(3)	30(1)
Rh2'	2800(2)	-91(3)	6801(4)	17(1)
B2'	3561(9)	121(19)	8167(15)	22(1)
N7'	2977(6)	-1611(14)	7792(8)	18(1)
N8'	3312(6)	-1145(18)	8241(12)	20(1)

C27'	3362(7)	-2050(20)	8769(10)	28(1)
C26'	3062(8)	-3029(19)	8625(13)	30(1)
C25'	2814(6)	-2709(17)	7984(12)	27(1)
N9'	2839(6)	1130(15)	7559(9)	16(1)
N10'	3166(7)	1070(20)	8172(13)	18(1)
C30'	3124(7)	1972(19)	8712(10)	19(1)
C29'	2756(7)	2699(18)	8484(12)	24(1)
C28'	2595(5)	2196(16)	7816(10)	18(1)
N11'	3490(3)	334(17)	6740(14)	21(1)
N12'	3767(7)	277(17)	7383(12)	18(1)
C33'	4196(7)	656(16)	7285(12)	24(1)
C32'	4212(7)	988(19)	6541(14)	30(1)
C31'	3779(7)	779(15)	6235(11)	21(1)
C34'	2443(8)	-3390(30)	7561(18)	31(1)
C35'	3712(10)	-1870(30)	9380(14)	42(2)
C36'	2191(7)	2790(30)	7422(17)	27(1)
C37'	3355(10)	2340(30)	9434(12)	30(1)
C38'	3655(12)	1030(30)	5430(12)	33(1)
C39'	4571(9)	710(30)	7866(18)	36(1)
C40'	2142(8)	-190(20)	7013(14)	21(1)
C41'	1799(10)	-70(20)	6467(15)	24(1)
F5'	1890(20)	30(30)	5719(16)	36(1)
C42'	1331(10)	-40(20)	6635(16)	27(1)
F6'	1022(15)	90(40)	6070(20)	38(1)
C43'	1185(9)	-124(19)	7363(15)	26(1)
F7'	730(9)	-90(30)	7510(30)	35(1)
C44'	1499(7)	-248(13)	7933(12)	22(1)
F8'	1360(7)	-335(18)	8664(11)	30(1)
C45'	1956(7)	-278(16)	7746(14)	19(1)
P2'	2797(3)	-1409(7)	5800(4)	20(1)
C46'	3308(7)	-2330(30)	5680(20)	32(1)
C47'	2732(11)	-700(30)	4863(13)	28(1)
C48'	2344(8)	-2600(30)	5700(19)	30(1)

Table S21. Bond lengths [Å] and angles [°] for **3b**.

Rh(1)-C(16)	2.030(5)	N(4)-B(1)	1.534(6)
Rh(1)-C(16')	2.09(3)	N(5)-C(7)	1.349(6)
Rh(1)-N(3)	2.117(5)	N(5)-N(6)	1.380(6)
Rh(1)-N(3')	2.121(7)	N(6)-C(9)	1.344(6)
Rh(1)-N(5')	2.145(6)	N(6)-B(1)	1.538(5)
Rh(1)-N(5)	2.149(4)	B(1)-H(1)	1.0000
Rh(1)-P(1)	2.2552(16)	C(1)-C(2)	1.391(7)
Rh(1)-P(1')	2.256(5)	C(1)-C(10)	1.493(6)
Rh(1)-N(1')	2.265(6)	C(2)-C(3)	1.365(7)
Rh(1)-N(1)	2.268(4)	C(2)-H(2)	0.9500
N(1)-C(1)	1.333(6)	C(3)-C(11)	1.496(5)
N(1)-N(2)	1.374(5)	C(4)-C(5)	1.405(8)
N(2)-C(3)	1.361(6)	C(4)-C(12)	1.494(6)
N(2)-B(1)	1.525(5)	C(5)-C(6)	1.358(7)
N(3)-C(4)	1.338(7)	C(5)-H(5)	0.9500
N(3)-N(4)	1.365(6)	C(6)-C(13)	1.499(6)
N(4)-C(6)	1.356(7)	C(7)-C(8)	1.386(7)

C(7)-C(14)	1.491(6)	C(2')-H(2')	0.9500
C(8)-C(9)	1.368(7)	C(1')-C(10')	1.491(8)
C(8)-H(8)	0.9500	N(3')-C(4')	1.350(18)
C(9)-C(15)	1.493(5)	N(3')-N(4')	1.371(17)
C(10)-H(10A)	0.9800	N(4')-C(6')	1.370(18)
C(10)-H(10B)	0.9800	C(6')-C(5')	1.360(19)
C(10)-H(10C)	0.9800	C(6')-C(13')	1.494(8)
C(11)-H(11A)	0.9800	C(5')-C(4')	1.413(19)
C(11)-H(11B)	0.9800	C(5')-H(5')	0.9500
C(11)-H(11C)	0.9800	C(4')-C(12')	1.492(8)
C(12)-H(12A)	0.9800	N(5')-C(7')	1.336(17)
C(12)-H(12B)	0.9800	N(5')-N(6')	1.397(17)
C(12)-H(12C)	0.9800	N(6')-C(9')	1.328(17)
C(13)-H(13A)	0.9800	C(9')-C(8')	1.370(18)
C(13)-H(13B)	0.9800	C(9')-C(15')	1.491(8)
C(13)-H(13C)	0.9800	C(8')-C(7')	1.361(18)
C(14)-H(14A)	0.9800	C(8')-H(8')	0.9500
C(14)-H(14B)	0.9800	C(7')-C(14')	1.494(8)
C(14)-H(14C)	0.9800	C(10')-H(10D)	0.9800
C(15)-H(15A)	0.9800	C(10')-H(10E)	0.9800
C(15)-H(15B)	0.9800	C(10')-H(10F)	0.9800
C(15)-H(15C)	0.9800	C(11')-H(11D)	0.9800
C(16)-C(17)	1.351(8)	C(11')-H(11E)	0.9800
C(16)-C(21)	1.408(7)	C(11')-H(11F)	0.9800
C(17)-F(1)	1.373(7)	C(12')-H(12D)	0.9800
C(17)-C(18)	1.376(7)	C(12')-H(12E)	0.9800
C(18)-F(2)	1.349(7)	C(12')-H(12F)	0.9800
C(18)-C(19)	1.374(9)	C(13')-H(13D)	0.9800
C(19)-F(3)	1.357(6)	C(13')-H(13E)	0.9800
C(19)-C(20)	1.369(8)	C(13')-H(13F)	0.9800
C(20)-F(4)	1.350(6)	C(14')-H(14D)	0.9800
C(20)-C(21)	1.377(7)	C(14')-H(14E)	0.9800
C(21)-H(21)	0.9500	C(14')-H(14F)	0.9800
P(1)-C(22)	1.813(5)	C(15')-H(15D)	0.9800
P(1)-C(24)	1.833(6)	C(15')-H(15E)	0.9800
P(1)-C(23)	1.837(5)	C(15')-H(15F)	0.9800
C(22)-H(22A)	0.9800	C(16')-C(17')	1.351(17)
C(22)-H(22B)	0.9800	C(16')-C(21')	1.404(18)
C(22)-H(22C)	0.9800	C(17')-F(1')	1.373(17)
C(23)-H(23A)	0.9800	C(17')-C(18')	1.375(16)
C(23)-H(23B)	0.9800	C(18')-F(2')	1.348(17)
C(23)-H(23C)	0.9800	C(18')-C(19')	1.375(17)
C(24)-H(24A)	0.9800	C(19')-F(3')	1.356(16)
C(24)-H(24B)	0.9800	C(19')-C(20')	1.369(17)
C(24)-H(24C)	0.9800	C(20')-F(4')	1.345(17)
B(1')-N(2')	1.531(9)	C(20')-C(21')	1.374(17)
B(1')-N(4')	1.531(9)	C(21')-H(21')	0.9500
B(1')-N(6')	1.534(9)	P(1')-C(22')	1.808(17)
B(1')-H(1')	1.0000	P(1')-C(23')	1.821(17)
N(1')-C(1')	1.312(18)	P(1')-C(24')	1.856(17)
N(1')-N(2')	1.381(19)	C(22')-H(22D)	0.9800
N(2')-C(3')	1.359(19)	C(22')-H(22E)	0.9800
C(3')-C(2')	1.352(19)	C(22')-H(22F)	0.9800
C(3')-C(11')	1.494(8)	C(23')-H(23D)	0.9800
C(2')-C(1')	1.400(19)	C(23')-H(23E)	0.9800

C(23')-H(23F)	0.9800	C(40)-C(41)	1.395(7)
C(24')-H(24D)	0.9800	C(40)-C(45)	1.409(7)
C(24')-H(24E)	0.9800	C(41)-F(5)	1.358(7)
C(24')-H(24F)	0.9800	C(41)-C(42)	1.392(8)
Rh(2)-C(40)	2.026(5)	C(42)-F(6)	1.352(7)
Rh(2)-N(9)	2.102(4)	C(42)-C(43)	1.365(9)
Rh(2)-N(11)	2.156(4)	C(43)-F(7)	1.356(6)
Rh(2)-N(7)	2.247(4)	C(43)-C(44)	1.374(8)
Rh(2)-P(2)	2.2658(16)	C(44)-F(8)	1.365(6)
N(7)-C(25)	1.333(6)	C(44)-C(45)	1.376(6)
N(7)-N(8)	1.387(6)	C(45)-H(45)	0.9500
N(8)-C(27)	1.344(6)	P(2)-C(46)	1.819(6)
N(8)-B(2)	1.524(5)	P(2)-C(48)	1.819(6)
N(9)-C(28)	1.347(6)	P(2)-C(47)	1.834(5)
N(9)-N(10)	1.384(6)	C(46)-H(46A)	0.9800
N(10)-C(30)	1.351(6)	C(46)-H(46B)	0.9800
N(10)-B(2)	1.534(5)	C(46)-H(46C)	0.9800
N(11)-C(31)	1.322(6)	C(47)-H(47A)	0.9800
N(11)-N(12)	1.391(7)	C(47)-H(47B)	0.9800
N(12)-C(33)	1.343(6)	C(47)-H(47C)	0.9800
N(12)-B(2)	1.529(6)	C(48)-H(48A)	0.9800
B(2)-H(2A)	1.0000	C(48)-H(48B)	0.9800
C(25)-C(26)	1.389(7)	C(48)-H(48C)	0.9800
C(25)-C(34)	1.501(5)	Rh(2')-N(9')	1.870(9)
C(26)-C(27)	1.365(7)	Rh(2')-C(40')	1.95(2)
C(26)-H(26)	0.9500	Rh(2')-N(11')	2.058(8)
C(27)-C(35)	1.498(6)	Rh(2')-P(2')	2.263(5)
C(28)-C(29)	1.370(8)	Rh(2')-N(7')	2.442(8)
C(28)-C(36)	1.497(6)	B(2')-N(10')	1.528(8)
C(29)-C(30)	1.381(8)	B(2')-N(8')	1.528(9)
C(29)-H(29)	0.9500	B(2')-N(12')	1.528(8)
C(30)-C(37)	1.504(6)	B(2')-H(2B)	1.0000
C(31)-C(32)	1.394(7)	N(7')-C(25')	1.301(17)
C(31)-C(38)	1.498(6)	N(7')-N(8')	1.353(18)
C(32)-C(33)	1.366(8)	N(8')-C(27')	1.351(18)
C(32)-H(32)	0.9500	C(27')-C(26')	1.378(19)
C(33)-C(39)	1.503(6)	C(27')-C(35')	1.500(8)
C(34)-H(34A)	0.9800	C(26')-C(25')	1.390(19)
C(34)-H(34B)	0.9800	C(26')-H(26')	0.9500
C(34)-H(34C)	0.9800	C(25')-C(34')	1.499(8)
C(35)-H(35A)	0.9800	N(9')-C(28')	1.408(17)
C(35)-H(35B)	0.9800	N(9')-N(10')	1.449(18)
C(35)-H(35C)	0.9800	N(10')-C(30')	1.357(18)
C(36)-H(36A)	0.9800	C(30')-C(29')	1.378(19)
C(36)-H(36B)	0.9800	C(30')-C(37')	1.503(8)
C(36)-H(36C)	0.9800	C(29')-C(28')	1.385(19)
C(37)-H(37A)	0.9800	C(29')-H(29')	0.9500
C(37)-H(37B)	0.9800	C(28')-C(36')	1.503(8)
C(37)-H(37C)	0.9800	N(11')-C(31')	1.317(17)
C(38)-H(38A)	0.9800	N(11')-N(12')	1.401(18)
C(38)-H(38B)	0.9800	N(12')-C(33')	1.321(17)
C(38)-H(38C)	0.9800	C(33')-C(32')	1.370(19)
C(39)-H(39A)	0.9800	C(33')-C(39')	1.503(8)
C(39)-H(39B)	0.9800	C(32')-C(31')	1.387(18)
C(39)-H(39C)	0.9800	C(32')-H(32')	0.9500

C(31')-C(38')	1.502(8)	N(5')-Rh(1)-N(1')	96.3(9)
C(34')-H(34D)	0.9800	P(1')-Rh(1)-N(1')	103.2(8)
C(34')-H(34E)	0.9800	C(16)-Rh(1)-N(1)	92.97(16)
C(34')-H(34F)	0.9800	N(3)-Rh(1)-N(1)	86.9(2)
C(35')-H(35D)	0.9800	N(5)-Rh(1)-N(1)	88.42(15)
C(35')-H(35E)	0.9800	P(1)-Rh(1)-N(1)	98.85(12)
C(35')-H(35F)	0.9800	C(1)-N(1)-N(2)	106.6(4)
C(36')-H(36D)	0.9800	C(1)-N(1)-Rh(1)	137.6(3)
C(36')-H(36E)	0.9800	N(2)-N(1)-Rh(1)	114.8(3)
C(36')-H(36F)	0.9800	C(3)-N(2)-N(1)	109.2(4)
C(37')-H(37D)	0.9800	C(3)-N(2)-B(1)	129.4(4)
C(37')-H(37E)	0.9800	N(1)-N(2)-B(1)	120.6(4)
C(37')-H(37F)	0.9800	C(4)-N(3)-N(4)	107.0(4)
C(38')-H(38D)	0.9800	C(4)-N(3)-Rh(1)	133.9(4)
C(38')-H(38E)	0.9800	N(4)-N(3)-Rh(1)	119.0(4)
C(38')-H(38F)	0.9800	C(6)-N(4)-N(3)	109.8(4)
C(39')-H(39D)	0.9800	C(6)-N(4)-B(1)	130.6(5)
C(39')-H(39E)	0.9800	N(3)-N(4)-B(1)	119.4(5)
C(39')-H(39F)	0.9800	C(7)-N(5)-N(6)	105.5(4)
C(40')-C(41')	1.398(18)	C(7)-N(5)-Rh(1)	136.9(3)
C(40')-C(45')	1.413(18)	N(6)-N(5)-Rh(1)	117.3(3)
C(41')-F(5')	1.361(17)	C(9)-N(6)-N(5)	109.9(4)
C(41')-C(42')	1.393(17)	C(9)-N(6)-B(1)	128.6(4)
C(42')-F(6')	1.356(17)	N(5)-N(6)-B(1)	119.8(4)
C(42')-C(43')	1.366(17)	N(2)-B(1)-N(4)	110.4(4)
C(43')-F(7')	1.352(17)	N(2)-B(1)-N(6)	111.4(4)
C(43')-C(44')	1.372(18)	N(4)-B(1)-N(6)	108.1(4)
C(44')-F(8')	1.366(17)	N(2)-B(1)-H(1)	109.0
C(44')-C(45')	1.370(17)	N(4)-B(1)-H(1)	109.0
C(45')-H(45')	0.9500	N(6)-B(1)-H(1)	109.0
P(2')-C(46')	1.787(17)	N(1)-C(1)-C(2)	110.1(4)
P(2')-C(48')	1.830(17)	N(1)-C(1)-C(10)	124.9(5)
P(2')-C(47')	1.841(17)	C(2)-C(1)-C(10)	125.0(5)
C(46')-H(46D)	0.9800	C(3)-C(2)-C(1)	106.2(5)
C(46')-H(46E)	0.9800	C(3)-C(2)-H(2)	126.9
C(46')-H(46F)	0.9800	C(1)-C(2)-H(2)	126.9
C(47')-H(47D)	0.9800	N(2)-C(3)-C(2)	107.9(4)
C(47')-H(47E)	0.9800	N(2)-C(3)-C(11)	121.2(5)
C(47')-H(47F)	0.9800	C(2)-C(3)-C(11)	130.9(5)
C(48')-H(48D)	0.9800	N(3)-C(4)-C(5)	108.9(5)
C(48')-H(48E)	0.9800	N(3)-C(4)-C(12)	122.9(5)
C(48')-H(48F)	0.9800	C(5)-C(4)-C(12)	128.2(5)
C(16)-Rh(1)-N(3)	89.2(2)	C(6)-C(5)-C(4)	106.6(5)
C(16')-Rh(1)-N(3')	88.1(8)	C(6)-C(5)-H(5)	126.7
C(16')-Rh(1)-N(5')	171.4(8)	C(4)-C(5)-H(5)	126.7
N(3')-Rh(1)-N(5')	83.7(7)	N(4)-C(6)-C(5)	107.7(4)
N(3)-Rh(1)-N(5)	81.7(2)	N(4)-C(6)-C(13)	120.8(5)
C(16)-Rh(1)-P(1)	93.88(14)	C(5)-C(6)-C(13)	131.5(5)
N(3)-Rh(1)-P(1)	173.28(19)	N(5)-C(7)-C(8)	110.3(5)
N(5)-Rh(1)-P(1)	94.99(12)	N(5)-C(7)-C(14)	122.1(4)
C(16')-Rh(1)-P(1')	90.3(7)	C(8)-C(7)-C(14)	127.5(5)
N(3')-Rh(1)-P(1')	172.0(6)	C(9)-C(8)-C(7)	105.9(4)
N(5')-Rh(1)-P(1')	97.5(6)	C(9)-C(8)-H(8)	127.0
C(16')-Rh(1)-N(1')	85.6(11)	C(7)-C(8)-H(8)	127.0
N(3')-Rh(1)-N(1')	84.5(10)	N(6)-C(9)-C(8)	108.3(4)

N(6)-C(9)-C(15)	123.2(5)	N(4')-C(6')-C(13')	115(2)
C(8)-C(9)-C(15)	128.5(5)	C(6')-C(5')-C(4')	106.8(15)
C(17)-C(16)-C(21)	114.1(5)	C(6')-C(5')-H(5')	126.6
C(17)-C(16)-Rh(1)	127.9(4)	C(4')-C(5')-H(5')	126.6
C(21)-C(16)-Rh(1)	117.4(4)	N(3')-C(4')-C(5')	108.1(14)
C(16)-C(17)-F(1)	119.6(6)	N(3')-C(4')-C(12')	121(2)
C(16)-C(17)-C(18)	125.6(6)	C(5')-C(4')-C(12')	131(2)
F(1)-C(17)-C(18)	114.8(6)	C(7')-N(5')-N(6')	106.7(11)
F(2)-C(18)-C(19)	119.5(5)	C(7')-N(5')-Rh(1)	138.4(14)
F(2)-C(18)-C(17)	121.5(6)	N(6')-N(5')-Rh(1)	114.6(12)
C(19)-C(18)-C(17)	119.0(5)	C(9')-N(6')-N(5')	108.8(13)
F(3)-C(19)-C(20)	121.3(6)	C(9')-N(6')-B(1')	129.1(18)
F(3)-C(19)-C(18)	120.5(6)	N(5')-N(6')-B(1')	121.1(18)
C(20)-C(19)-C(18)	118.2(5)	N(6')-C(9')-C(8')	107.7(15)
F(4)-C(20)-C(19)	117.9(5)	N(6')-C(9')-C(15')	121(2)
F(4)-C(20)-C(21)	120.9(5)	C(8')-C(9')-C(15')	131(2)
C(19)-C(20)-C(21)	121.2(5)	C(7')-C(8')-C(9')	107.9(16)
C(20)-C(21)-C(16)	121.9(5)	C(7')-C(8')-H(8')	126.0
C(20)-C(21)-H(21)	119.1	C(9')-C(8')-H(8')	126.0
C(16)-C(21)-H(21)	119.1	N(5')-C(7')-C(8')	108.9(15)
C(22)-P(1)-C(24)	104.0(3)	N(5')-C(7')-C(14')	119(2)
C(22)-P(1)-C(23)	100.1(3)	C(8')-C(7')-C(14')	132(2)
C(24)-P(1)-C(23)	100.7(3)	C(1')-C(10')-H(10D)	109.5
C(22)-P(1)-Rh(1)	112.03(18)	C(1')-C(10')-H(10E)	109.5
C(24)-P(1)-Rh(1)	118.0(2)	H(10D)-C(10')-H(10E)	109.5
C(23)-P(1)-Rh(1)	119.4(2)	C(1')-C(10')-H(10F)	109.5
N(2')-B(1')-N(4')	102.0(18)	H(10D)-C(10')-H(10F)	109.5
N(2')-B(1')-N(6')	118(2)	H(10E)-C(10')-H(10F)	109.5
N(4')-B(1')-N(6')	107.1(16)	C(3')-C(11')-H(11D)	109.5
N(2')-B(1')-H(1')	109.7	C(3')-C(11')-H(11E)	109.5
N(4')-B(1')-H(1')	109.7	H(11D)-C(11')-H(11E)	109.5
N(6')-B(1')-H(1')	109.7	C(3')-C(11')-H(11F)	109.5
C(1')-N(1')-N(2')	109.4(14)	H(11D)-C(11')-H(11F)	109.5
C(1')-N(1')-Rh(1)	141(2)	H(11E)-C(11')-H(11F)	109.5
N(2')-N(1')-Rh(1)	108.6(16)	C(4')-C(12')-H(12D)	109.5
C(3')-N(2')-N(1')	106.1(13)	C(4')-C(12')-H(12E)	109.5
C(3')-N(2')-B(1')	127(2)	H(12D)-C(12')-H(12E)	109.5
N(1')-N(2')-B(1')	127(2)	C(4')-C(12')-H(12F)	109.5
C(2')-C(3')-N(2')	110.1(16)	H(12D)-C(12')-H(12F)	109.5
C(2')-C(3')-C(11')	126(2)	H(12E)-C(12')-H(12F)	109.5
N(2')-C(3')-C(11')	124(3)	C(6')-C(13')-H(13D)	109.5
C(3')-C(2')-C(1')	105.7(16)	C(6')-C(13')-H(13E)	109.5
C(3')-C(2')-H(2')	127.2	H(13D)-C(13')-H(13E)	109.5
C(1')-C(2')-H(2')	127.2	C(6')-C(13')-H(13F)	109.5
N(1')-C(1')-C(2')	108.8(15)	H(13D)-C(13')-H(13F)	109.5
N(1')-C(1')-C(10')	124(3)	H(13E)-C(13')-H(13F)	109.5
C(2')-C(1')-C(10')	127(2)	C(7')-C(14')-H(14D)	109.5
C(4')-N(3')-N(4')	108.0(12)	C(7')-C(14')-H(14E)	109.5
C(4')-N(3')-Rh(1)	135.3(15)	H(14D)-C(14')-H(14E)	109.5
N(4')-N(3')-Rh(1)	116.7(13)	C(7')-C(14')-H(14F)	109.5
C(6')-N(4')-N(3')	108.6(13)	H(14D)-C(14')-H(14F)	109.5
C(6')-N(4')-B(1')	130.7(19)	H(14E)-C(14')-H(14F)	109.5
N(3')-N(4')-B(1')	120.4(19)	C(9')-C(15')-H(15D)	109.5
C(5')-C(6')-N(4')	108.4(15)	C(9')-C(15')-H(15E)	109.5
C(5')-C(6')-C(13')	137(2)	H(15D)-C(15')-H(15E)	109.5

C(9')-C(15')-H(15F)	109.5	C(25)-N(7)-N(8)	105.0(4)
H(15D)-C(15')-H(15F)	109.5	C(25)-N(7)-Rh(2)	139.3(3)
H(15E)-C(15')-H(15F)	109.5	N(8)-N(7)-Rh(2)	115.6(3)
C(17')-C(16')-C(21')	113.5(19)	C(27)-N(8)-N(7)	109.9(4)
C(17')-C(16')-Rh(1)	128.2(18)	C(27)-N(8)-B(2)	130.9(5)
C(21')-C(16')-Rh(1)	116.7(17)	N(7)-N(8)-B(2)	118.9(4)
C(16')-C(17')-F(1')	119(2)	C(28)-N(9)-N(10)	107.0(4)
C(16')-C(17')-C(18')	126(2)	C(28)-N(9)-Rh(2)	135.0(4)
F(1')-C(17')-C(18')	115(2)	N(10)-N(9)-Rh(2)	118.0(3)
F(2')-C(18')-C(19')	119(2)	C(30)-N(10)-N(9)	109.1(4)
F(2')-C(18')-C(17')	122(2)	C(30)-N(10)-B(2)	131.2(5)
C(19')-C(18')-C(17')	119.2(18)	N(9)-N(10)-B(2)	119.5(4)
F(3')-C(19')-C(20')	121(2)	C(31)-N(11)-N(12)	105.7(4)
F(3')-C(19')-C(18')	121(2)	C(31)-N(11)-Rh(2)	137.6(4)
C(20')-C(19')-C(18')	118.0(18)	N(12)-N(11)-Rh(2)	116.3(3)
F(4')-C(20')-C(19')	118(2)	C(33)-N(12)-N(11)	110.0(4)
F(4')-C(20')-C(21')	121(2)	C(33)-N(12)-B(2)	128.6(5)
C(19')-C(20')-C(21')	120.8(19)	N(11)-N(12)-B(2)	120.0(4)
C(20')-C(21')-C(16')	122.8(19)	N(8)-B(2)-N(12)	111.5(4)
C(20')-C(21')-H(21')	118.6	N(8)-B(2)-N(10)	110.5(4)
C(16')-C(21')-H(21')	118.6	N(12)-B(2)-N(10)	109.1(4)
C(22')-P(1')-C(23')	99.4(12)	N(8)-B(2)-H(2A)	108.5
C(22')-P(1')-C(24')	104.9(13)	N(12)-B(2)-H(2A)	108.5
C(23')-P(1')-C(24')	99.5(13)	N(10)-B(2)-H(2A)	108.5
C(22')-P(1')-Rh(1)	109.6(11)	N(7)-C(25)-C(26)	111.2(4)
C(23')-P(1')-Rh(1)	120.5(12)	N(7)-C(25)-C(34)	123.3(4)
C(24')-P(1')-Rh(1)	120.0(11)	C(26)-C(25)-C(34)	125.5(5)
P(1')-C(22')-H(22D)	109.5	C(27)-C(26)-C(25)	105.5(4)
P(1')-C(22')-H(22E)	109.5	C(27)-C(26)-H(26)	127.3
H(22D)-C(22')-H(22E)	109.5	C(25)-C(26)-H(26)	127.3
P(1')-C(22')-H(22F)	109.5	N(8)-C(27)-C(26)	108.3(4)
H(22D)-C(22')-H(22F)	109.5	N(8)-C(27)-C(35)	121.6(5)
H(22E)-C(22')-H(22F)	109.5	C(26)-C(27)-C(35)	130.0(5)
P(1')-C(23')-H(23D)	109.5	N(9)-C(28)-C(29)	109.1(5)
P(1')-C(23')-H(23E)	109.5	N(9)-C(28)-C(36)	122.4(5)
H(23D)-C(23')-H(23E)	109.5	C(29)-C(28)-C(36)	128.4(5)
P(1')-C(23')-H(23F)	109.5	C(28)-C(29)-C(30)	107.5(5)
H(23D)-C(23')-H(23F)	109.5	C(28)-C(29)-H(29)	126.3
H(23E)-C(23')-H(23F)	109.5	C(30)-C(29)-H(29)	126.3
P(1')-C(24')-H(24D)	109.5	N(10)-C(30)-C(29)	107.3(5)
P(1')-C(24')-H(24E)	109.5	N(10)-C(30)-C(37)	121.2(5)
H(24D)-C(24')-H(24E)	109.5	C(29)-C(30)-C(37)	131.4(5)
P(1')-C(24')-H(24F)	109.5	N(11)-C(31)-C(32)	110.5(5)
H(24D)-C(24')-H(24F)	109.5	N(11)-C(31)-C(38)	122.2(5)
H(24E)-C(24')-H(24F)	109.5	C(32)-C(31)-C(38)	127.1(5)
C(40)-Rh(2)-N(9)	86.61(19)	C(33)-C(32)-C(31)	106.3(5)
C(40)-Rh(2)-N(11)	169.75(19)	C(33)-C(32)-H(32)	126.9
N(9)-Rh(2)-N(11)	83.36(17)	C(31)-C(32)-H(32)	126.9
C(40)-Rh(2)-N(7)	92.33(18)	N(12)-C(33)-C(32)	107.5(5)
N(9)-Rh(2)-N(7)	86.43(17)	N(12)-C(33)-C(39)	124.0(5)
N(11)-Rh(2)-N(7)	89.15(17)	C(32)-C(33)-C(39)	128.4(5)
C(40)-Rh(2)-P(2)	93.82(16)	C(41)-C(40)-C(45)	115.1(5)
N(9)-Rh(2)-P(2)	173.24(13)	C(41)-C(40)-Rh(2)	126.5(4)
N(11)-Rh(2)-P(2)	95.90(14)	C(45)-C(40)-Rh(2)	117.7(4)
N(7)-Rh(2)-P(2)	100.28(12)	F(5)-C(41)-C(42)	114.7(6)

F(5)-C(41)-C(40)	121.9(6)	C(30')-N(10')-B(2')	122.3(19)
C(42)-C(41)-C(40)	123.4(6)	N(9')-N(10')-B(2')	121(2)
F(6)-C(42)-C(43)	120.4(6)	N(10')-C(30')-C(29')	104.6(15)
F(6)-C(42)-C(41)	120.1(6)	N(10')-C(30')-C(37')	138(2)
C(43)-C(42)-C(41)	119.4(5)	C(29')-C(30')-C(37')	117(2)
F(7)-C(43)-C(42)	120.0(6)	C(30')-C(29')-C(28')	107.4(15)
F(7)-C(43)-C(44)	120.9(6)	C(30')-C(29')-H(29')	126.3
C(42)-C(43)-C(44)	119.1(5)	C(28')-C(29')-H(29')	126.3
F(8)-C(44)-C(43)	118.6(5)	C(29')-C(28')-N(9')	114.7(14)
F(8)-C(44)-C(45)	119.7(5)	C(29')-C(28')-C(36')	120(2)
C(43)-C(44)-C(45)	121.8(5)	N(9')-C(28')-C(36')	125(2)
C(44)-C(45)-C(40)	121.2(5)	C(31')-N(11')-N(12')	101.8(12)
C(44)-C(45)-H(45)	119.4	C(31')-N(11')-Rh(2')	137.4(17)
C(40)-C(45)-H(45)	119.4	N(12')-N(11')-Rh(2')	120.5(15)
C(46)-P(2)-C(48)	100.6(3)	C(33')-N(12')-N(11')	114.9(15)
C(46)-P(2)-C(47)	102.8(3)	C(33')-N(12')-B(2')	122(2)
C(48)-P(2)-C(47)	99.3(3)	N(11')-N(12')-B(2')	122(2)
C(46)-P(2)-Rh(2)	113.4(2)	N(12')-C(33')-C(32')	103.7(15)
C(48)-P(2)-Rh(2)	120.1(2)	N(12')-C(33')-C(39')	127(2)
C(47)-P(2)-Rh(2)	117.8(2)	C(32')-C(33')-C(39')	129(2)
N(9')-Rh(2')-C(40')	87.6(9)	C(33')-C(32')-C(31')	107.9(16)
N(9')-Rh(2')-N(11')	80.2(9)	C(33')-C(32')-H(32')	126.0
C(40')-Rh(2')-N(11')	167.7(9)	C(31')-C(32')-H(32')	126.0
N(9')-Rh(2')-P(2')	173.4(7)	N(11')-C(31')-C(32')	111.6(15)
C(40')-Rh(2')-P(2')	96.5(7)	N(11')-C(31')-C(38')	124(2)
N(11')-Rh(2')-P(2')	95.5(7)	C(32')-C(31')-C(38')	124(2)
N(9')-Rh(2')-N(7')	85.5(8)	C(25')-C(34')-H(34D)	109.5
C(40')-Rh(2')-N(7')	91.7(8)	C(25')-C(34')-H(34E)	109.5
N(11')-Rh(2')-N(7')	88.7(8)	H(34D)-C(34')-H(34E)	109.5
P(2')-Rh(2')-N(7')	99.4(5)	C(25')-C(34')-H(34F)	109.5
N(10')-B(2')-N(8')	102.9(18)	H(34D)-C(34')-H(34F)	109.5
N(10')-B(2')-N(12')	103.3(19)	H(34E)-C(34')-H(34F)	109.5
N(8')-B(2')-N(12')	111.0(19)	C(27')-C(35')-H(35D)	109.5
N(10')-B(2')-H(2B)	112.9	C(27')-C(35')-H(35E)	109.5
N(8')-B(2')-H(2B)	112.9	H(35D)-C(35')-H(35E)	109.5
N(12')-B(2')-H(2B)	112.9	C(27')-C(35')-H(35F)	109.5
C(25')-N(7')-N(8')	115.6(13)	H(35D)-C(35')-H(35F)	109.5
C(25')-N(7')-Rh(2')	134.6(15)	H(35E)-C(35')-H(35F)	109.5
N(8')-N(7')-Rh(2')	109.7(12)	C(28')-C(36')-H(36D)	109.5
C(27')-N(8')-N(7')	103.3(14)	C(28')-C(36')-H(36E)	109.5
C(27')-N(8')-B(2')	129(2)	H(36D)-C(36')-H(36E)	109.5
N(7')-N(8')-B(2')	128(2)	C(28')-C(36')-H(36F)	109.5
N(8')-C(27')-C(26')	109.6(16)	H(36D)-C(36')-H(36F)	109.5
N(8')-C(27')-C(35')	119(2)	H(36E)-C(36')-H(36F)	109.5
C(26')-C(27')-C(35')	131(2)	C(30')-C(37')-H(37D)	109.5
C(27')-C(26')-C(25')	107.3(16)	C(30')-C(37')-H(37E)	109.5
C(27')-C(26')-H(26')	126.4	H(37D)-C(37')-H(37E)	109.5
C(25')-C(26')-H(26')	126.4	C(30')-C(37')-H(37F)	109.5
N(7')-C(25')-C(26')	104.2(14)	H(37D)-C(37')-H(37F)	109.5
N(7')-C(25')-C(34')	124(2)	H(37E)-C(37')-H(37F)	109.5
C(26')-C(25')-C(34')	132(2)	C(31')-C(38')-H(38D)	109.5
C(28')-N(9')-N(10')	96.7(12)	C(31')-C(38')-H(38E)	109.5
C(28')-N(9')-Rh(2')	139.3(14)	H(38D)-C(38')-H(38E)	109.5
N(10')-N(9')-Rh(2')	123.7(13)	C(31')-C(38')-H(38F)	109.5
C(30')-N(10')-N(9')	116.5(15)	H(38D)-C(38')-H(38F)	109.5

H(38E)-C(38')-H(38F)	109.5	C(46')-P(2')-C(48')	102.2(14)
C(33')-C(39')-H(39D)	109.5	C(46')-P(2')-C(47')	101.4(13)
C(33')-C(39')-H(39E)	109.5	C(48')-P(2')-C(47')	96.8(13)
H(39D)-C(39')-H(39E)	109.5	C(46')-P(2')-Rh(2')	115.4(12)
C(33')-C(39')-H(39F)	109.5	C(48')-P(2')-Rh(2')	120.2(11)
H(39D)-C(39')-H(39F)	109.5	C(47')-P(2')-Rh(2')	117.4(11)
H(39E)-C(39')-H(39F)	109.5	P(2')-C(46')-H(46D)	109.5
C(41')-C(40')-C(45')	112.1(18)	P(2')-C(46')-H(46E)	109.5
C(41')-C(40')-Rh(2')	123.9(17)	H(46D)-C(46')-H(46E)	109.5
C(45')-C(40')-Rh(2')	123.7(17)	P(2')-C(46')-H(46F)	109.5
F(5')-C(41')-C(42')	114(2)	H(46D)-C(46')-H(46F)	109.5
F(5')-C(41')-C(40')	123(2)	H(46E)-C(46')-H(46F)	109.5
C(42')-C(41')-C(40')	123.2(19)	P(2')-C(47')-H(47D)	109.5
F(6')-C(42')-C(43')	120(2)	P(2')-C(47')-H(47E)	109.5
F(6')-C(42')-C(41')	119(2)	H(47D)-C(47')-H(47E)	109.5
C(43')-C(42')-C(41')	120.3(18)	P(2')-C(47')-H(47F)	109.5
F(7')-C(43')-C(42')	119(2)	H(47D)-C(47')-H(47F)	109.5
F(7')-C(43')-C(44')	120(2)	H(47E)-C(47')-H(47F)	109.5
C(42')-C(43')-C(44')	120.1(18)	P(2')-C(48')-H(48D)	109.5
F(8')-C(44')-C(45')	121.2(19)	P(2')-C(48')-H(48E)	109.5
F(8')-C(44')-C(43')	120.9(18)	H(48D)-C(48')-H(48E)	109.5
C(45')-C(44')-C(43')	117.8(18)	P(2')-C(48')-H(48F)	109.5
C(44')-C(45')-C(40')	126.3(19)	H(48D)-C(48')-H(48F)	109.5
C(44')-C(45')-H(45')	116.8	H(48E)-C(48')-H(48F)	109.5
C(40')-C(45')-H(45')	116.8		

Table S22. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3b**. 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}
Rh1	15(1)	18(1)	15(1)	-1(1)	0(1)	-1(1)
N1	12(2)	21(2)	18(2)	-2(1)	-4(2)	-1(2)
N2	13(2)	25(2)	12(2)	-1(1)	-4(2)	0(2)
N3	23(2)	25(2)	14(2)	4(2)	-3(2)	0(2)
N4	24(2)	14(2)	16(2)	-2(2)	-4(2)	2(2)
N5	19(2)	20(2)	14(2)	2(2)	-2(2)	-1(1)
N6	16(2)	22(2)	20(2)	2(2)	-2(1)	3(2)
B1	19(2)	22(3)	18(3)	4(2)	-3(2)	4(2)
C1	26(3)	24(2)	23(3)	-1(2)	-1(2)	4(2)
C2	30(3)	24(3)	21(2)	-5(2)	-3(2)	2(2)
C3	22(2)	27(3)	18(2)	-3(2)	-4(2)	-1(2)
C4	20(2)	17(2)	34(3)	-1(2)	6(2)	0(2)
C5	26(3)	21(2)	31(3)	4(2)	13(2)	3(2)
C6	22(3)	18(2)	25(3)	2(2)	2(2)	3(2)
C7	25(2)	20(2)	24(2)	0(2)	8(2)	5(2)
C8	16(2)	34(3)	25(3)	2(2)	6(2)	7(2)
C9	15(2)	22(2)	27(3)	5(2)	-1(2)	2(2)
C10	30(3)	25(3)	29(3)	-5(2)	-3(2)	7(2)
C11	27(3)	36(3)	24(3)	-4(2)	-6(2)	0(2)
C12	24(3)	22(3)	38(3)	-6(2)	6(2)	-6(2)
C13	38(3)	34(3)	29(3)	10(2)	-4(3)	2(2)
C14	34(3)	35(3)	21(3)	-7(2)	5(2)	8(2)

C15	21(2)	49(4)	32(3)	4(3)	-5(2)	5(2)
C16	19(2)	10(2)	17(2)	0(2)	2(2)	2(2)
C17	26(2)	25(2)	18(2)	-7(2)	4(2)	-2(2)
F1	24(2)	59(3)	20(2)	-6(2)	-4(1)	-2(2)
C18	17(2)	29(2)	32(4)	-3(2)	-5(2)	-6(2)
F2	21(1)	48(3)	31(2)	-3(2)	-5(2)	-2(2)
C19	15(2)	21(2)	33(3)	1(2)	1(2)	1(2)
F3	16(1)	33(2)	41(2)	-5(1)	0(1)	0(1)
C20	23(2)	18(3)	19(2)	-2(2)	1(2)	5(2)
F4	26(2)	42(2)	19(2)	3(2)	8(1)	10(2)
C21	20(2)	17(2)	25(3)	3(2)	-3(2)	2(2)
P1	18(1)	22(1)	20(1)	1(1)	-2(1)	0(1)
C22	28(3)	28(3)	23(3)	8(2)	-2(2)	-6(2)
C23	29(3)	24(3)	32(3)	6(2)	-5(2)	7(2)
C24	24(2)	39(3)	19(3)	0(2)	0(2)	3(2)
B1'	19(2)	22(3)	18(3)	4(2)	-3(2)	4(2)
N1'	23(2)	25(2)	14(2)	4(2)	-3(2)	0(2)
N2'	24(2)	14(2)	16(2)	-2(2)	-4(2)	2(2)
C3'	22(3)	18(2)	25(3)	2(2)	2(2)	3(2)
C2'	26(3)	21(2)	31(3)	4(2)	13(2)	3(2)
C1'	20(2)	17(2)	34(3)	-1(2)	6(2)	0(2)
N3'	12(2)	21(2)	18(2)	-2(1)	-4(2)	-1(2)
N4'	13(2)	25(2)	12(2)	-1(1)	-4(2)	0(2)
C6'	22(2)	27(3)	18(2)	-3(2)	-4(2)	-1(2)
C5'	30(3)	24(3)	21(2)	-5(2)	-3(2)	2(2)
C4'	26(3)	24(2)	23(3)	-1(2)	-1(2)	4(2)
N5'	19(2)	20(2)	14(2)	2(2)	-2(2)	-1(1)
N6'	16(2)	22(2)	20(2)	2(2)	-2(1)	3(2)
C9'	15(2)	22(2)	27(3)	5(2)	-1(2)	2(2)
C8'	16(2)	34(3)	25(3)	2(2)	6(2)	7(2)
C7'	25(2)	20(2)	24(2)	0(2)	8(2)	5(2)
C10'	24(3)	22(3)	38(3)	-6(2)	6(2)	-6(2)
C11'	38(3)	34(3)	29(3)	10(2)	-4(3)	2(2)
C12'	30(3)	25(3)	29(3)	-5(2)	-3(2)	7(2)
C13'	27(3)	36(3)	24(3)	-4(2)	-6(2)	0(2)
C14'	34(3)	35(3)	21(3)	-7(2)	5(2)	8(2)
C15'	21(2)	49(4)	32(3)	4(3)	-5(2)	5(2)
C16'	19(2)	10(2)	17(2)	0(2)	2(2)	2(2)
C17'	26(2)	25(2)	18(2)	-7(2)	4(2)	-2(2)
F1'	24(2)	59(3)	20(2)	-6(2)	-4(1)	-2(2)
C18'	17(2)	29(2)	32(4)	-3(2)	-5(2)	-6(2)
F2'	21(1)	48(3)	31(2)	-3(2)	-5(2)	-2(2)
C19'	15(2)	21(2)	33(3)	1(2)	1(2)	1(2)
F3'	16(1)	33(2)	41(2)	-5(1)	0(1)	0(1)
C20'	23(2)	18(3)	19(2)	-2(2)	1(2)	5(2)
F4'	26(2)	42(2)	19(2)	3(2)	8(1)	10(2)
C21'	20(2)	17(2)	25(3)	3(2)	-3(2)	2(2)
P1'	18(1)	22(1)	20(1)	1(1)	-2(1)	0(1)
C22'	28(3)	28(3)	23(3)	8(2)	-2(2)	-6(2)
C23'	29(3)	24(3)	32(3)	6(2)	-5(2)	7(2)
C24'	24(2)	39(3)	19(3)	0(2)	0(2)	3(2)
Rh2	16(1)	18(1)	16(1)	-2(1)	1(1)	-1(1)
N7	14(2)	18(2)	16(2)	-5(2)	-6(2)	5(1)
N8	13(2)	22(2)	19(2)	-3(2)	-4(2)	-3(2)
N9	16(2)	13(2)	25(2)	-1(1)	6(2)	-1(1)

N10	19(2)	18(2)	22(2)	3(2)	4(2)	-1(2)
N11	24(2)	16(2)	22(2)	-6(2)	8(2)	7(2)
N12	16(2)	16(2)	24(2)	2(2)	1(1)	3(2)
B2	17(3)	29(3)	22(3)	2(2)	-3(2)	0(2)
C25	14(2)	23(2)	17(2)	2(2)	1(2)	0(2)
C26	30(3)	20(2)	20(2)	-6(2)	-2(2)	0(2)
C27	18(2)	23(2)	15(2)	-3(2)	-1(2)	-5(2)
C28	32(3)	20(2)	29(3)	-2(2)	14(2)	0(2)
C29	35(3)	19(2)	37(3)	5(2)	16(2)	5(2)
C30	44(3)	20(2)	19(2)	3(2)	5(2)	10(2)
C31	20(2)	25(2)	19(2)	-1(2)	4(2)	5(2)
C32	18(2)	28(3)	42(3)	-5(2)	8(2)	8(2)
C33	17(2)	28(3)	28(3)	6(2)	5(2)	5(2)
C34	23(3)	30(3)	29(3)	-3(2)	-5(2)	5(2)
C35	29(3)	35(3)	27(3)	-6(2)	-3(2)	-4(2)
C36	24(3)	21(2)	47(4)	-7(2)	12(2)	-6(2)
C37	68(5)	38(3)	18(3)	10(2)	6(3)	14(3)
C38	27(3)	46(3)	28(3)	-6(2)	8(2)	10(2)
C39	19(2)	45(4)	44(4)	8(3)	-6(2)	7(2)
C40	16(2)	18(2)	28(3)	-3(2)	-1(2)	-4(2)
C41	23(2)	26(3)	21(3)	0(2)	-7(2)	-1(2)
F5	30(3)	56(2)	20(2)	-5(1)	-4(2)	-6(2)
C42	22(2)	28(3)	31(3)	2(2)	-10(2)	-6(2)
F6	21(2)	49(3)	45(2)	1(2)	-20(2)	-2(2)
C43	16(2)	26(3)	36(3)	3(2)	0(2)	1(2)
F7	13(1)	34(3)	58(3)	6(2)	6(2)	0(1)
C44	18(2)	21(2)	28(3)	0(2)	8(2)	1(2)
F8	26(2)	36(2)	29(2)	0(2)	12(1)	3(1)
C45	16(2)	22(2)	19(2)	-6(2)	1(2)	1(2)
P2	18(1)	26(1)	15(1)	0(1)	-1(1)	0(1)
C46	28(3)	39(3)	28(3)	9(2)	2(2)	-4(2)
C47	29(3)	39(3)	14(2)	-4(2)	-1(2)	-1(2)
C48	31(3)	37(3)	22(3)	0(2)	-1(2)	6(2)
Rh2'	16(1)	18(1)	16(1)	-2(1)	1(1)	-1(1)
B2'	17(3)	29(3)	22(3)	2(2)	-3(2)	0(2)
N7'	16(2)	13(2)	25(2)	-1(1)	6(2)	-1(1)
N8'	19(2)	18(2)	22(2)	3(2)	4(2)	-1(2)
C27'	44(3)	20(2)	19(2)	3(2)	5(2)	10(2)
C26'	35(3)	19(2)	37(3)	5(2)	16(2)	5(2)
C25'	32(3)	20(2)	29(3)	-2(2)	14(2)	0(2)
N9'	14(2)	18(2)	16(2)	-5(2)	-6(2)	5(1)
N10'	13(2)	22(2)	19(2)	-3(2)	-4(2)	-3(2)
C30'	18(2)	23(2)	15(2)	-3(2)	-1(2)	-5(2)
C29'	30(3)	20(2)	20(2)	-6(2)	-2(2)	0(2)
C28'	14(2)	23(2)	17(2)	2(2)	1(2)	0(2)
N11'	24(2)	16(2)	22(2)	-6(2)	8(2)	7(2)
N12'	16(2)	16(2)	24(2)	2(2)	1(1)	3(2)
C33'	17(2)	28(3)	28(3)	6(2)	5(2)	5(2)
C32'	18(2)	28(3)	42(3)	-5(2)	8(2)	8(2)
C31'	20(2)	25(2)	19(2)	-1(2)	4(2)	5(2)
C34'	24(3)	21(2)	47(4)	-7(2)	12(2)	-6(2)
C35'	68(5)	38(3)	18(3)	10(2)	6(3)	14(3)
C36'	23(3)	30(3)	29(3)	-3(2)	-5(2)	5(2)
C37'	29(3)	35(3)	27(3)	-6(2)	-3(2)	-4(2)
C38'	27(3)	46(3)	28(3)	-6(2)	8(2)	10(2)

C39'	19(2)	45(4)	44(4)	8(3)	-6(2)	7(2)
C40'	16(2)	18(2)	28(3)	-3(2)	-1(2)	-4(2)
C41'	23(2)	26(3)	21(3)	0(2)	-7(2)	-1(2)
F5'	30(3)	56(2)	20(2)	-5(1)	-4(2)	-6(2)
C42'	22(2)	28(3)	31(3)	2(2)	-10(2)	-6(2)
F6'	21(2)	49(3)	45(2)	1(2)	-20(2)	-2(2)
C43'	16(2)	26(3)	36(3)	3(2)	0(2)	1(2)
F7'	13(1)	34(3)	58(3)	6(2)	6(2)	0(1)
C44'	18(2)	21(2)	28(3)	0(2)	8(2)	1(2)
F8'	26(2)	36(2)	29(2)	0(2)	12(1)	3(1)
C45'	16(2)	22(2)	19(2)	-6(2)	1(2)	1(2)
P2'	18(1)	26(1)	15(1)	0(1)	-1(1)	0(1)
C46'	28(3)	39(3)	28(3)	9(2)	2(2)	-4(2)
C47'	29(3)	39(3)	14(2)	-4(2)	-1(2)	-1(2)
C48'	31(3)	37(3)	22(3)	0(2)	-1(2)	6(2)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **3b**.

	x	y	z	U(eq)
H1	3725	5449	4373	24
H2	4496	1499	3970	30
H5	4857	8751	4212	32
H8	2979	6474	6688	30
H10A	5200	2300	5668	42
H10B	5254	1490	4914	42
H10C	4902	1043	5552	42
H11A	3883	2796	3089	43
H11B	3824	4246	3326	43
H11C	3494	3194	3680	43
H12A	5256	7592	6102	42
H12B	5335	8779	5561	42
H12C	5594	7474	5397	42
H13A	3995	6684	3339	51
H13B	4157	8121	3248	51
H13C	3741	7777	3801	51
H14A	3766	5435	7828	45
H14B	3664	6910	7726	45
H14C	4161	6357	7523	45
H15A	3002	6722	4752	51
H15B	2621	6185	5318	51
H15C	2905	5235	4793	51
H21	5289	4619	4799	25
H22A	4152	2333	7653	39
H22B	4107	2307	6758	39
H22C	3888	3448	7227	39
H23A	5100	2051	7657	43
H23B	5402	2723	7019	43
H23C	5002	1757	6789	43
H24A	4541	5094	8128	41
H24B	5077	4748	8091	41
H24C	4718	3758	8434	41

H1'	3762	4716	4341	24
H2'	4467	8754	4105	32
H5'	4878	1339	4185	30
H8'	2989	3577	6617	30
H10D	5176	7890	5830	42
H10E	4954	9166	5512	42
H10F	5346	8457	5044	42
H11D	3660	6118	3619	51
H11E	3992	6937	3092	51
H11F	3623	7626	3620	51
H12D	5357	2844	6006	42
H12E	5618	2256	5296	42
H12F	5277	1396	5782	42
H13D	3857	3531	3630	43
H13E	3884	2023	3589	43
H13F	4227	2864	3095	43
H14D	4151	4270	7545	45
H14E	3801	3121	7668	45
H14F	3638	4538	7833	45
H15D	3107	4379	4535	51
H15E	2694	4599	5116	51
H15F	2868	3196	4937	51
H21'	5322	5404	4821	25
H22D	3926	6636	7192	39
H22E	4178	7809	6803	39
H22F	4190	7655	7697	39
H23D	5446	7209	7135	43
H23E	5113	7969	7691	43
H23F	5075	8175	6802	43
H24D	5077	5061	8090	41
H24E	4531	5037	8208	41
H24F	4822	6246	8463	41
H2A	3703	-123	8565	27
H26	3014	3987	8782	28
H29	2556	-3410	8696	36
H32	4494	-1184	6308	35
H34A	2234	2965	7225	41
H34B	2578	4137	7145	41
H34C	2254	4017	7869	41
H35A	3611	1341	9617	46
H35B	3653	2847	9658	46
H35C	3986	2058	9116	46
H36A	1857	-2187	7456	46
H36B	2109	-3517	7341	46
H36C	2210	-2375	6776	46
H37A	3660	-2319	9225	62
H37B	3225	-2744	9717	62
H37C	3358	-1281	9654	62
H38A	3333	-1131	5409	50
H38B	3842	-1621	5231	50
H38C	3715	-163	5114	50
H39A	4560	84	8172	54
H39B	4821	-985	7700	54
H39C	4421	-1369	8274	54
H45	2154	626	8086	23

H46A	3558	1891	5596	47
H46B	3334	2973	6107	47
H46C	3264	2998	5215	47
H47A	2669	1420	4450	41
H47B	2450	193	4834	41
H47C	2995	288	4717	41
H48A	2300	2961	5138	45
H48B	2426	3473	5959	45
H48C	2040	2407	5858	45
H2B	3789	271	8578	27
H26'	3030	-3782	8911	36
H29'	2635	3414	8740	28
H32'	4472	1306	6280	35
H34D	2353	-2884	7122	46
H34E	2175	-3504	7889	46
H34F	2557	-4211	7395	46
H35D	3876	-1073	9298	62
H35E	3931	-2573	9372	62
H35F	3556	-1844	9868	62
H36D	2117	2294	6972	41
H36E	2269	3654	7277	41
H36F	1925	2795	7761	41
H37D	3608	1757	9540	46
H37E	3131	2314	9845	46
H37F	3477	3204	9388	46
H38D	3330	828	5349	50
H38E	3846	501	5102	50
H38F	3709	1921	5314	50
H39D	4450	417	8350	54
H39E	4682	1576	7915	54
H39F	4826	158	7711	54
H45'	2170	-363	8147	23
H46D	3379	-2775	6144	47
H46E	3565	-1768	5547	47
H46F	3260	-2940	5272	47
H47D	2451	-183	4851	41
H47E	2711	-1365	4484	41
H47F	2999	-160	4755	41
H48D	2043	-2188	5736	45
H48E	2374	-3229	6100	45
H48F	2373	-3012	5210	45

Table S24. Torsion angles [°] for **3b**.

C16-Rh1-N1-C1	36.9(6)	Rh1-N1-N2-C3	170.6(3)
N3-Rh1-N1-C1	125.9(6)	C1-N1-N2-B1	-171.1(4)
N5-Rh1-N1-C1	-152.3(5)	Rh1-N1-N2-B1	-0.1(5)
P1-Rh1-N1-C1	-57.5(5)	C16-Rh1-N3-C4	-45.4(7)
C16-Rh1-N1-N2	-130.3(3)	N5-Rh1-N3-C4	132.8(7)
N3-Rh1-N1-N2	-41.3(4)	P1-Rh1-N3-C4	72.0(17)
N5-Rh1-N1-N2	40.5(3)	N1-Rh1-N3-C4	-138.4(7)
P1-Rh1-N1-N2	135.3(3)	C16-Rh1-N3-N4	131.3(4)
C1-N1-N2-C3	-0.5(5)	N5-Rh1-N3-N4	-50.5(4)

P1-Rh1-N3-N4	-111.3(13)	Rh1-N5-C7-C8	174.0(4)
N1-Rh1-N3-N4	38.3(4)	N6-N5-C7-C14	-176.3(4)
C4-N3-N4-C6	-1.5(6)	Rh1-N5-C7-C14	-4.0(8)
Rh1-N3-N4-C6	-179.0(4)	N5-C7-C8-C9	-1.8(6)
C4-N3-N4-B1	-176.7(5)	C14-C7-C8-C9	176.1(5)
Rh1-N3-N4-B1	5.8(6)	N5-N6-C9-C8	0.0(6)
C16-Rh1-N5-C7	-108.4(11)	B1-N6-C9-C8	-165.0(5)
N3-Rh1-N5-C7	-120.0(5)	N5-N6-C9-C15	178.2(5)
P1-Rh1-N5-C7	54.1(5)	B1-N6-C9-C15	13.2(8)
N1-Rh1-N5-C7	152.9(5)	C7-C8-C9-N6	1.1(6)
C16-Rh1-N5-N6	63.2(12)	C7-C8-C9-C15	-177.0(5)
N3-Rh1-N5-N6	51.6(3)	N3-Rh1-C16-C17	122.6(5)
P1-Rh1-N5-N6	-134.3(3)	N5-Rh1-C16-C17	111.1(11)
N1-Rh1-N5-N6	-35.6(3)	P1-Rh1-C16-C17	-51.4(5)
C7-N5-N6-C9	-1.1(5)	N1-Rh1-C16-C17	-150.5(5)
Rh1-N5-N6-C9	-175.1(3)	N3-Rh1-C16-C21	-48.1(4)
C7-N5-N6-B1	165.4(4)	N5-Rh1-C16-C21	-59.6(12)
Rh1-N5-N6-B1	-8.6(5)	P1-Rh1-C16-C21	137.8(3)
C3-N2-B1-N4	-108.5(6)	N1-Rh1-C16-C21	38.7(4)
N1-N2-B1-N4	60.0(6)	C21-C16-C17-F1	179.8(5)
C3-N2-B1-N6	131.4(5)	Rh1-C16-C17-F1	8.8(8)
N1-N2-B1-N6	-60.1(5)	C21-C16-C17-C18	-1.6(8)
C6-N4-B1-N2	120.4(6)	Rh1-C16-C17-C18	-172.7(4)
N3-N4-B1-N2	-65.5(6)	C16-C17-C18-F2	179.5(6)
C6-N4-B1-N6	-117.5(6)	F1-C17-C18-F2	-1.8(8)
N3-N4-B1-N6	56.6(5)	C16-C17-C18-C19	2.0(9)
C9-N6-B1-N2	-129.2(5)	F1-C17-C18-C19	-179.4(5)
N5-N6-B1-N2	67.1(5)	F2-C18-C19-F3	0.5(8)
C9-N6-B1-N4	109.3(6)	C17-C18-C19-F3	178.1(5)
N5-N6-B1-N4	-54.4(5)	F2-C18-C19-C20	-178.3(5)
N2-N1-C1-C2	-0.5(6)	C17-C18-C19-C20	-0.7(8)
Rh1-N1-C1-C2	-168.4(4)	F3-C19-C20-F4	-0.6(7)
N2-N1-C1-C10	178.9(5)	C18-C19-C20-F4	178.2(5)
Rh1-N1-C1-C10	11.0(9)	F3-C19-C20-C21	-179.4(5)
N1-C1-C2-C3	1.2(7)	C18-C19-C20-C21	-0.7(8)
C10-C1-C2-C3	-178.1(5)	F4-C20-C21-C16	-177.9(4)
N1-N2-C3-C2	1.3(6)	C19-C20-C21-C16	1.0(8)
B1-N2-C3-C2	170.8(5)	C17-C16-C21-C20	0.1(7)
N1-N2-C3-C11	179.5(5)	Rh1-C16-C21-C20	172.2(4)
B1-N2-C3-C11	-10.9(8)	C16-Rh1-P1-C22	-147.7(2)
C1-C2-C3-N2	-1.5(6)	N3-Rh1-P1-C22	95.2(14)
C1-C2-C3-C11	-179.5(6)	N5-Rh1-P1-C22	35.1(2)
N4-N3-C4-C5	1.3(6)	N1-Rh1-P1-C22	-54.1(2)
Rh1-N3-C4-C5	178.3(5)	C16-Rh1-P1-C24	91.6(2)
N4-N3-C4-C12	178.4(5)	N3-Rh1-P1-C24	-25.5(14)
Rh1-N3-C4-C12	-4.7(10)	N5-Rh1-P1-C24	-85.7(2)
N3-C4-C5-C6	-0.6(6)	N1-Rh1-P1-C24	-174.8(2)
C12-C4-C5-C6	-177.5(5)	C16-Rh1-P1-C23	-31.2(3)
N3-N4-C6-C5	1.1(6)	N5-Rh1-P1-C23	151.6(3)
B1-N4-C6-C5	175.7(5)	N1-Rh1-P1-C23	62.4(3)
N3-N4-C6-C13	-177.0(5)	C16'-Rh1-N1'-C1'	-59(3)
B1-N4-C6-C13	-2.5(9)	N3'-Rh1-N1'-C1'	-147(3)
C4-C5-C6-N4	-0.3(6)	N5'-Rh1-N1'-C1'	130(3)
C4-C5-C6-C13	177.5(6)	P1'-Rh1-N1'-C1'	31(3)
N6-N5-C7-C8	1.7(6)	C16'-Rh1-N1'-N2'	136.0(10)

N3'-Rh1-N1'-N2'	47.5(9)	C16'-Rh1-N5'-N6'	-69(6)
N5'-Rh1-N1'-N2'	-35.5(9)	N3'-Rh1-N5'-N6'	-50.5(8)
P1'-Rh1-N1'-N2'	-134.8(7)	P1'-Rh1-N5'-N6'	137.4(6)
C1'-N1'-N2'-C3'	0.0(3)	N1'-Rh1-N5'-N6'	33.2(11)
Rh1-N1'-N2'-C3'	170(2)	C7'-N5'-N6'-C9'	0.0(3)
C1'-N1'-N2'-B1'	-171(3)	Rh1-N5'-N6'-C9'	175.2(13)
Rh1-N1'-N2'-B1'	-0.3(15)	C7'-N5'-N6'-B1'	-169.5(17)
N4'-B1'-N2'-C3'	128(2)	Rh1-N5'-N6'-B1'	5.7(13)
N6'-B1'-N2'-C3'	-115(3)	N2'-B1'-N6'-C9'	136(2)
N4'-B1'-N2'-N1'	-63(2)	N4'-B1'-N6'-C9'	-110(2)
N6'-B1'-N2'-N1'	54(2)	N2'-B1'-N6'-N5'	-57(2)
N1'-N2'-C3'-C2'	-0.1(5)	N4'-B1'-N6'-N5'	57(2)
B1'-N2'-C3'-C2'	171(3)	N5'-N6'-C9'-C8'	0.1(5)
N1'-N2'-C3'-C11'	-180.0(5)	B1'-N6'-C9'-C8'	168.5(19)
B1'-N2'-C3'-C11'	-9(3)	N5'-N6'-C9'-C15'	-179.9(4)
N2'-C3'-C2'-C1'	0.2(6)	B1'-N6'-C9'-C15'	-12(2)
C11'-C3'-C2'-C1'	-180.0(5)	N6'-C9'-C8'-C7'	-0.2(6)
N2'-N1'-C1'-C2'	0.1(3)	C15'-C9'-C8'-C7'	179.9(5)
Rh1-N1'-C1'-C2'	-165(3)	N6'-N5'-C7'-C8'	-0.1(3)
N2'-N1'-C1'-C10'	180.0(3)	Rh1-N5'-C7'-C8'	-173.5(17)
Rh1-N1'-C1'-C10'	15(3)	N6'-N5'-C7'-C14'	179.9(2)
C3'-C2'-C1'-N1'	-0.1(5)	Rh1-N5'-C7'-C14'	6.5(18)
C3'-C2'-C1'-C10'	179.9(4)	C9'-C8'-C7'-N5'	0.2(5)
C16'-Rh1-N3'-C4'	48.9(18)	C9'-C8'-C7'-C14'	-179.8(4)
N5'-Rh1-N3'-C4'	-128.3(18)	N3'-Rh1-C16'-C17'	-121.4(13)
P1'-Rh1-N3'-C4'	-29(5)	N5'-Rh1-C16'-C17'	-103(6)
N1'-Rh1-N3'-C4'	134.7(18)	P1'-Rh1-C16'-C17'	50.7(12)
C16'-Rh1-N3'-N4'	-132.2(10)	N1'-Rh1-C16'-C17'	154.0(14)
N5'-Rh1-N3'-N4'	50.6(9)	N3'-Rh1-C16'-C21'	43.1(11)
P1'-Rh1-N3'-N4'	150(4)	N5'-Rh1-C16'-C21'	62(7)
N1'-Rh1-N3'-N4'	-46.4(10)	P1'-Rh1-C16'-C21'	-144.7(10)
C4'-N3'-N4'-C6'	0.0(3)	N1'-Rh1-C16'-C21'	-41.5(12)
Rh1-N3'-N4'-C6'	-179.2(15)	C21'-C16'-C17'-F1'	180.0(4)
C4'-N3'-N4'-B1'	174.8(19)	Rh1-C16'-C17'-F1'	-15.1(16)
Rh1-N3'-N4'-B1'	-4.3(13)	C21'-C16'-C17'-C18'	0.0(3)
N2'-B1'-N4'-C6'	-120(2)	Rh1-C16'-C17'-C18'	164.9(16)
N6'-B1'-N4'-C6'	115(2)	C16'-C17'-C18'-F2'	180.0(3)
N2'-B1'-N4'-N3'	66.5(19)	F1'-C17'-C18'-F2'	0.0(5)
N6'-B1'-N4'-N3'	-58(2)	C16'-C17'-C18'-C19'	0.0(3)
N3'-N4'-C6'-C5'	0.1(5)	F1'-C17'-C18'-C19'	-180.0(4)
B1'-N4'-C6'-C5'	-174(2)	F2'-C18'-C19'-F3'	0.0(8)
N3'-N4'-C6'-C13'	179.9(4)	C17'-C18'-C19'-F3'	180.0(5)
B1'-N4'-C6'-C13'	6(2)	F2'-C18'-C19'-C20'	180.0(6)
N4'-C6'-C5'-C4'	-0.1(6)	C17'-C18'-C19'-C20'	0.0(7)
C13'-C6'-C5'-C4'	-179.9(6)	F3'-C19'-C20'-F4'	-0.1(10)
N4'-N3'-C4'-C5'	0.0(2)	C18'-C19'-C20'-F4'	179.9(6)
Rh1-N3'-C4'-C5'	178.9(19)	F3'-C19'-C20'-C21'	-180.0(7)
N4'-N3'-C4'-C12'	-179.9(3)	C18'-C19'-C20'-C21'	0.1(10)
Rh1-N3'-C4'-C12'	-1.0(19)	F4'-C20'-C21'-C16'	-179.9(6)
C6'-C5'-C4'-N3'	0.1(5)	C19'-C20'-C21'-C16'	-0.1(10)
C6'-C5'-C4'-C12'	180.0(4)	C17'-C16'-C21'-C20'	0.1(7)
C16'-Rh1-N5'-C7'	104(6)	Rh1-C16'-C21'-C20'	-166.7(15)
N3'-Rh1-N5'-C7'	122.5(17)	C16'-Rh1-P1'-C22'	145.8(12)
P1'-Rh1-N5'-C7'	-49.5(16)	N3'-Rh1-P1'-C22'	-136(4)
N1'-Rh1-N5'-C7'	-153.8(17)	N5'-Rh1-P1'-C22'	-38.0(11)

N1'-Rh1-P1'-C22'	60.3(13)	C30-N10-B2-N12	117.3(6)
C16'-Rh1-P1'-C23'	31.6(13)	N9-N10-B2-N12	-56.1(6)
N3'-Rh1-P1'-C23'	110(4)	N8-N7-C25-C26	-1.0(6)
N5'-Rh1-P1'-C23'	-152.3(12)	Rh2-N7-C25-C26	-178.7(4)
N1'-Rh1-P1'-C23'	-54.0(14)	N8-N7-C25-C34	-179.6(5)
C16'-Rh1-P1'-C24'	-92.7(14)	Rh2-N7-C25-C34	2.7(8)
N3'-Rh1-P1'-C24'	-15(4)	N7-C25-C26-C27	-0.2(6)
N5'-Rh1-P1'-C24'	83.4(13)	C34-C25-C26-C27	178.3(5)
N1'-Rh1-P1'-C24'	-178.3(14)	N7-N8-C27-C26	-2.1(6)
C40-Rh2-N7-C25	-50.2(6)	B2-N8-C27-C26	-176.0(5)
N9-Rh2-N7-C25	-136.6(5)	N7-N8-C27-C35	179.4(5)
N11-Rh2-N7-C25	140.0(5)	B2-N8-C27-C35	5.5(8)
P2-Rh2-N7-C25	44.1(5)	C25-C26-C27-N8	1.4(6)
C40-Rh2-N7-N8	132.3(4)	C25-C26-C27-C35	179.7(5)
N9-Rh2-N7-N8	45.9(4)	N10-N9-C28-C29	2.0(6)
N11-Rh2-N7-N8	-37.5(4)	Rh2-N9-C28-C29	-178.3(4)
P2-Rh2-N7-N8	-133.4(3)	N10-N9-C28-C36	-179.7(5)
C25-N7-N8-C27	1.9(6)	Rh2-N9-C28-C36	0.0(8)
Rh2-N7-N8-C27	-179.8(3)	N9-C28-C29-C30	-1.6(6)
C25-N7-N8-B2	176.6(4)	C36-C28-C29-C30	-179.8(5)
Rh2-N7-N8-B2	-5.0(6)	N9-N10-C30-C29	0.7(6)
C40-Rh2-N9-C28	48.6(5)	B2-N10-C30-C29	-173.3(5)
N11-Rh2-N9-C28	-129.2(5)	N9-N10-C30-C37	179.9(5)
N7-Rh2-N9-C28	141.2(5)	B2-N10-C30-C37	5.9(8)
P2-Rh2-N9-C28	-45.2(13)	C28-C29-C30-N10	0.5(6)
C40-Rh2-N9-N10	-131.7(4)	C28-C29-C30-C37	-178.5(6)
N11-Rh2-N9-N10	50.4(3)	N12-N11-C31-C32	-1.1(6)
N7-Rh2-N9-N10	-39.2(3)	Rh2-N11-C31-C32	-172.4(4)
P2-Rh2-N9-N10	134.5(9)	N12-N11-C31-C38	174.3(5)
C28-N9-N10-C30	-1.7(5)	Rh2-N11-C31-C38	3.0(8)
Rh2-N9-N10-C30	178.6(3)	N11-C31-C32-C33	1.1(7)
C28-N9-N10-B2	173.1(4)	C38-C31-C32-C33	-174.0(6)
Rh2-N9-N10-B2	-6.6(5)	N11-N12-C33-C32	0.0(6)
C40-Rh2-N11-C31	108.6(12)	B2-N12-C33-C32	166.5(5)
N9-Rh2-N11-C31	120.6(5)	N11-N12-C33-C39	-178.6(5)
N7-Rh2-N11-C31	-152.9(5)	B2-N12-C33-C39	-12.1(9)
P2-Rh2-N11-C31	-52.7(5)	C31-C32-C33-N12	-0.7(6)
C40-Rh2-N11-N12	-62.0(12)	C31-C32-C33-C39	177.9(5)
N9-Rh2-N11-N12	-50.1(3)	N9-Rh2-C40-C41	-122.2(5)
N7-Rh2-N11-N12	36.4(3)	N11-Rh2-C40-C41	-110.3(12)
P2-Rh2-N11-N12	136.7(3)	N7-Rh2-C40-C41	151.5(5)
C31-N11-N12-C33	0.7(5)	P2-Rh2-C40-C41	51.0(5)
Rh2-N11-N12-C33	174.1(3)	N9-Rh2-C40-C45	47.7(4)
C31-N11-N12-B2	-167.2(4)	N11-Rh2-C40-C45	59.5(13)
Rh2-N11-N12-B2	6.3(5)	N7-Rh2-C40-C45	-38.6(4)
C27-N8-B2-N12	-122.0(6)	P2-Rh2-C40-C45	-139.1(4)
N7-N8-B2-N12	64.5(6)	C45-C40-C41-F5	-178.3(5)
C27-N8-B2-N10	116.4(6)	Rh2-C40-C41-F5	-8.2(8)
N7-N8-B2-N10	-57.0(6)	C45-C40-C41-C42	-0.2(8)
C33-N12-B2-N8	127.8(5)	Rh2-C40-C41-C42	169.8(4)
N11-N12-B2-N8	-66.8(5)	F5-C41-C42-F6	0.3(8)
C33-N12-B2-N10	-109.8(6)	C40-C41-C42-F6	-177.8(5)
N11-N12-B2-N10	55.5(6)	F5-C41-C42-C43	178.7(5)
C30-N10-B2-N8	-119.7(6)	C40-C41-C42-C43	0.6(9)
N9-N10-B2-N8	66.8(6)	F6-C42-C43-F7	-2.4(8)

C41-C42-C43-F7	179.2(5)	C40'-Rh2'-N9'-N10'	128.6(11)
F6-C42-C43-C44	177.6(5)	N11'-Rh2'-N9'-N10'	-52.8(10)
C41-C42-C43-C44	-0.8(8)	P2'-Rh2'-N9'-N10'	-102(6)
F7-C43-C44-F8	2.4(8)	N7'-Rh2'-N9'-N10'	36.6(9)
C42-C43-C44-F8	-177.6(5)	C28'-N9'-N10'-C30'	-0.1(2)
F7-C43-C44-C45	-179.2(5)	Rh2'-N9'-N10'-C30'	-174.4(16)
C42-C43-C44-C45	0.7(8)	C28'-N9'-N10'-B2'	-174.9(19)
F8-C44-C45-C40	177.9(5)	Rh2'-N9'-N10'-B2'	10.7(14)
C43-C44-C45-C40	-0.4(8)	N8'-B2'-N10'-C30'	118(2)
C41-C40-C45-C44	0.2(8)	N12'-B2'-N10'-C30'	-126.0(19)
Rh2-C40-C45-C44	-170.9(4)	N8'-B2'-N10'-N9'	-67.1(19)
C40-Rh2-P2-C46	147.1(3)	N12'-B2'-N10'-N9'	48.5(19)
N9-Rh2-P2-C46	-119.5(10)	N9'-N10'-C30'-C29'	0.0(4)
N11-Rh2-P2-C46	-36.2(3)	B2'-N10'-C30'-C29'	174.8(19)
N7-Rh2-P2-C46	54.0(3)	N9'-N10'-C30'-C37'	179.8(5)
C40-Rh2-P2-C48	28.2(3)	B2'-N10'-C30'-C37'	-5(2)
N9-Rh2-P2-C48	121.6(10)	N10'-C30'-C29'-C28'	0.0(5)
N11-Rh2-P2-C48	-155.0(3)	C37'-C30'-C29'-C28'	-179.8(4)
N7-Rh2-P2-C48	-64.8(3)	C30'-C29'-C28'-N9'	-0.1(4)
C40-Rh2-P2-C47	-92.9(3)	C30'-C29'-C28'-C36'	-180.0(3)
N9-Rh2-P2-C47	0.5(10)	N10'-N9'-C28'-C29'	0.1(2)
N11-Rh2-P2-C47	83.9(2)	Rh2'-N9'-C28'-C29'	173(2)
N7-Rh2-P2-C47	174.1(2)	N10'-N9'-C28'-C36'	180.0(2)
N9'-Rh2'-N7'-C25'	135.2(15)	Rh2'-N9'-C28'-C36'	-7(2)
C40'-Rh2'-N7'-C25'	47.7(16)	N9'-Rh2'-N11'-C31'	-119.8(17)
N11'-Rh2'-N7'-C25'	-144.6(15)	C40'-Rh2'-N11'-C31'	-113(5)
P2'-Rh2'-N7'-C25'	-49.2(15)	P2'-Rh2'-N11'-C31'	55.2(16)
N9'-Rh2'-N7'-N8'	-42.3(8)	N7'-Rh2'-N11'-C31'	154.5(17)
C40'-Rh2'-N7'-N8'	-129.7(9)	N9'-Rh2'-N11'-N12'	53.3(10)
N11'-Rh2'-N7'-N8'	38.0(8)	C40'-Rh2'-N11'-N12'	60(5)
P2'-Rh2'-N7'-N8'	133.4(6)	P2'-Rh2'-N11'-N12'	-131.6(8)
C25'-N7'-N8'-C27'	-0.1(3)	N7'-Rh2'-N11'-N12'	-32.4(9)
Rh2'-N7'-N8'-C27'	177.9(12)	C31'-N11'-N12'-C33'	-0.1(3)
C25'-N7'-N8'-B2'	-179(2)	Rh2'-N11'-N12'-C33'	-175.4(14)
Rh2'-N7'-N8'-B2'	-0.7(15)	C31'-N11'-N12'-B2'	164.8(18)
N10'-B2'-N8'-C27'	-122(2)	Rh2'-N11'-N12'-B2'	-10.4(14)
N12'-B2'-N8'-C27'	128(2)	N10'-B2'-N12'-C33'	117.9(19)
N10'-B2'-N8'-N7'	56(2)	N8'-B2'-N12'-C33'	-132.4(18)
N12'-B2'-N8'-N7'	-54(2)	N10'-B2'-N12'-N11'	-46(2)
N7'-N8'-C27'-C26'	0.3(5)	N8'-B2'-N12'-N11'	64(2)
B2'-N8'-C27'-C26'	179(2)	N11'-N12'-C33'-C32'	0.1(5)
N7'-N8'-C27'-C35'	179.9(5)	B2'-N12'-C33'-C32'	-164.8(18)
B2'-N8'-C27'-C35'	-2(2)	N11'-N12'-C33'-C39'	179.8(4)
N8'-C27'-C26'-C25'	-0.4(6)	B2'-N12'-C33'-C39'	14.9(19)
C35'-C27'-C26'-C25'	-179.9(6)	N12'-C33'-C32'-C31'	0.0(5)
N8'-N7'-C25'-C26'	-0.2(3)	C39'-C33'-C32'-C31'	-179.8(5)
Rh2'-N7'-C25'-C26'	-177.5(16)	N12'-N11'-C31'-C32'	0.1(2)
N8'-N7'-C25'-C34'	180.0(3)	Rh2'-N11'-C31'-C32'	174.0(17)
Rh2'-N7'-C25'-C34'	2.7(16)	N12'-N11'-C31'-C38'	-179.9(3)
C27'-C26'-C25'-N7'	0.3(5)	Rh2'-N11'-C31'-C38'	-5.9(18)
C27'-C26'-C25'-C34'	-179.9(4)	C33'-C32'-C31'-N11'	0.0(5)
C40'-Rh2'-N9'-C28'	-43(2)	C33'-C32'-C31'-C38'	179.9(4)
N11'-Rh2'-N9'-C28'	136(2)	N9'-Rh2'-C40'-C41'	127.3(12)
P2'-Rh2'-N9'-C28'	87(6)	N11'-Rh2'-C40'-C41'	121(5)
N7'-Rh2'-N9'-C28'	-135(2)	P2'-Rh2'-C40'-C41'	-47.6(11)

N7'-Rh2'-C40'-C41'	-147.2(11)	F7'-C43'-C44'-C45'	179.9(6)
N9'-Rh2'-C40'-C45'	-46.2(11)	C42'-C43'-C44'-C45'	0.1(9)
N11'-Rh2'-C40'-C45'	-52(5)	F8'-C44'-C45'-C40'	-179.9(5)
P2'-Rh2'-C40'-C45'	138.9(9)	C43'-C44'-C45'-C40'	-0.1(9)
N7'-Rh2'-C40'-C45'	39.3(11)	C41'-C40'-C45'-C44'	0.0(7)
C45'-C40'-C41'-F5'	-180.0(4)	Rh2'-C40'-C45'-C44'	174.2(14)
Rh2'-C40'-C41'-F5'	5.8(14)	N9'-Rh2'-P2'-C46'	83(6)
C45'-C40'-C41'-C42'	0.0(3)	C40'-Rh2'-P2'-C46'	-147.6(13)
Rh2'-C40'-C41'-C42'	-174.2(13)	N11'-Rh2'-P2'-C46'	34.8(13)
F5'-C41'-C42'-F6'	-0.1(4)	N7'-Rh2'-P2'-C46'	-54.8(12)
C40'-C41'-C42'-F6'	179.9(3)	N9'-Rh2'-P2'-C48'	-153(6)
F5'-C41'-C42'-C43'	-180.0(4)	C40'-Rh2'-P2'-C48'	-24.4(14)
C40'-C41'-C42'-C43'	0.0(3)	N11'-Rh2'-P2'-C48'	158.1(13)
F6'-C42'-C43'-F7'	0.2(7)	N7'-Rh2'-P2'-C48'	68.5(13)
C41'-C42'-C43'-F7'	-179.9(4)	N9'-Rh2'-P2'-C47'	-36(6)
F6'-C42'-C43'-C44'	-180.0(5)	C40'-Rh2'-P2'-C47'	92.9(13)
C41'-C42'-C43'-C44'	-0.1(7)	N11'-Rh2'-P2'-C47'	-84.7(13)
F7'-C43'-C44'-F8'	-0.2(10)	N7'-Rh2'-P2'-C47'	-174.3(12)
C42'-C43'-C44'-F8'	179.9(5)		

Table S25. Crystal data and structure refinement for **3d·0.5Et$_2$O**.

Identification code	**3d**	
Empirical formula	$C_{26}H_{39}BF_3N_6O_{0.5}PRh$	
Formula weight	645.32	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.612(10) Å	α = 90°
	b = 33.54(4) Å	β = 99.62(2)°
	c = 20.40(2) Å	γ = 90°
Volume	5809(12) Å^3	
Z	8	
Density (calculated)	1.476 Mg/m^3	
Absorption coefficient	0.691 mm^{-1}	
F(000)	2664	
Crystal color, morphology	colorless, needle	
Crystal size	0.40 x 0.06 x 0.02 mm^3	
Theta range for data collection	1.58 to 18.00°	
Index ranges	$-7 \le h \le 7$, $-29 \le k \le 29$, $-17 \le l \le 17$	
Reflections collected	21541	
Independent reflections	3999 [R(int) = 0.3773]	
Observed reflections	1935	
Completeness to theta = 18.00°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9863 and 0.7695	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3999 / 0 / 323	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R_1 = 0.1059, wR_2 = 0.2330	
R indices (all data)	R_1 = 0.2150, wR_2 = 0.2957	
Largest diff. peak and hole	1.306 and -0.847 e.Å^{-3}	

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3d·0.5Et$_2$O**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	1542(3)	1008(1)	3327(1)	28(1)
F1	4085(18)	1062(5)	4697(8)	47(5)
F2	7060(20)	-80(6)	4594(10)	83(7)
F3	2758(19)	155(5)	2952(9)	53(5)
N1	-90(30)	511(7)	3039(11)	26(7)
N2	-960(20)	541(7)	2395(10)	19(6)
N3	10(20)	1439(6)	2751(10)	14(6)
N4	-960(20)	1275(7)	2215(11)	23(6)
N5	2340(30)	920(6)	2417(11)	24(7)
N6	1120(30)	866(7)	1861(12)	30(7)
B1	-660(40)	868(10)	1927(17)	21(10)
C1	-580(40)	154(10)	3266(16)	42(10)
C2	-1700(30)	-23(10)	2804(15)	37(9)
C3	-1900(30)	227(9)	2293(14)	22(8)
C4	-330(30)	1823(9)	2780(13)	21(8)
C5	-1480(30)	1937(9)	2275(12)	16(8)
C6	-1800(30)	1592(10)	1948(15)	36(9)
C7	3670(30)	899(8)	2223(14)	28(9)
C8	3390(30)	846(7)	1522(12)	5(7)
C9	1890(30)	814(9)	1332(15)	29(9)
C10	300(30)	-4(8)	3910(13)	27(8)
C11	-3000(40)	162(11)	1632(17)	67(12)
C12	640(40)	2096(9)	3279(15)	45(10)
C13	-3000(40)	1534(10)	1306(16)	51(10)
C14	5220(30)	969(9)	2647(14)	30(8)
C15	920(40)	728(10)	659(16)	55(11)
C16	3302(19)	620(6)	3781(10)	29(9)
C17	4280(20)	743(5)	4358(10)	32(9)
C18	5550(20)	508(6)	4635(8)	52(10)
C19	5840(20)	150(6)	4335(10)	42(10)
C20	4870(20)	27(5)	3757(10)	45(10)
C21	3600(20)	262(6)	3480(8)	39(10)
P1	518(10)	1147(3)	4248(4)	35(3)
C22	510(30)	790(8)	4889(13)	28(9)
C23	1130(40)	1566(9)	4762(16)	52(10)
C24	-1540(30)	1217(9)	4023(15)	41(10)
Rh2	6229(3)	3046(1)	2266(1)	32(1)
F4	8160(20)	3230(5)	3739(9)	60(6)
F5	3980(20)	3364(6)	4923(10)	78(7)
F6	2839(19)	3086(5)	2667(8)	54(5)
N7	4140(30)	3323(7)	1602(11)	30(7)
N8	3500(30)	3082(7)	1065(11)	25(7)
N9	5040(20)	2524(7)	2240(11)	22(6)
N10	3930(20)	2419(7)	1637(11)	21(6)
N11	6970(30)	2816(6)	1380(11)	21(6)
N12	5810(30)	2654(7)	910(11)	27(7)
B2	4120(40)	2656(11)	1023(18)	30(11)

C25	3310(30)	3653(9)	1551(14)	24(8)
C26	2190(30)	3618(9)	945(13)	23(8)
C27	2390(30)	3256(8)	674(14)	18(8)
C28	4730(30)	2239(9)	2625(14)	25(8)
C29	3670(30)	1946(9)	2354(14)	27(8)
C30	3180(40)	2079(10)	1698(17)	46(10)
C31	8360(30)	2727(8)	1208(14)	23(8)
C32	8010(30)	2507(8)	605(14)	28(9)
C33	6470(30)	2470(9)	450(14)	25(8)
C34	3510(30)	3993(8)	1996(14)	29(8)
C35	1460(30)	3090(9)	79(13)	28(8)
C36	5630(30)	2222(9)	3346(14)	44(10)
C37	2080(30)	1870(9)	1160(14)	40(9)
C38	9880(30)	2820(9)	1639(15)	42(10)
C39	5560(30)	2261(8)	-144(12)	20(8)
C40	5510(20)	3179(6)	3151(8)	16(8)
C41	6594(18)	3236(7)	3731(11)	48(10)
C42	6070(20)	3287(7)	4334(8)	50(10)
C43	4470(30)	3282(7)	4357(9)	54(11)
C44	3386(19)	3225(7)	3777(12)	82(13)
C45	3910(20)	3173(7)	3174(9)	61(11)
P2	7708(11)	3598(3)	2341(4)	48(3)
C46	7270(40)	3984(10)	2900(17)	69(12)
C47	9770(30)	3597(10)	2620(16)	52(11)
C48	7650(40)	3843(10)	1582(17)	66(12)
C49	10(90)	4220(20)	4770(40)	230(40)
C50	1010(90)	4200(20)	4480(40)	190(30)
O1	1900(60)	4484(15)	4200(30)	192(18)
C51	3060(130)	4500(30)	3840(60)	330(60)
C52	3810(60)	4689(17)	3570(30)	140(20)

Table S27. Bond lengths [Å] and angles [°] for **3d·0.5Et$_2$O**.

Rh(1)-C(16)	2.090(14)	C(15)-H(15C)	0.9800
Rh(1)-N(5)	2.10(2)	C(16)-C(17)	1.3900
Rh(1)-N(3)	2.17(2)	C(16)-C(21)	1.3900
Rh(1)-N(1)	2.19(2)	C(17)-C(18)	1.3900
Rh(1)-P(1)	2.252(9)	C(18)-C(19)	1.3900
F(1)-C(17)	1.30(2)	C(18)-H(18A)	0.9500
F(2)-C(19)	1.34(2)	C(19)-C(20)	1.3900
F(3)-C(21)	1.25(2)	C(20)-C(21)	1.3900
N(1)-C(1)	1.37(3)	C(20)-H(20A)	0.9500
N(1)-N(2)	1.40(3)	P(1)-C(24)	1.77(3)
N(2)-C(3)	1.32(3)	P(1)-C(22)	1.77(3)
N(2)-B(1)	1.51(4)	P(1)-C(23)	1.78(3)
N(3)-C(4)	1.32(3)	C(22)-H(22A)	0.9800
N(3)-N(4)	1.37(3)	C(22)-H(22B)	0.9800
N(4)-C(6)	1.35(3)	C(22)-H(22C)	0.9800
N(4)-B(1)	1.52(4)	C(23)-H(23A)	0.9800
N(5)-C(7)	1.28(3)	C(23)-H(23B)	0.9800
N(5)-N(6)	1.42(3)	C(23)-H(23C)	0.9800
N(6)-C(9)	1.37(3)	C(24)-H(24A)	0.9800
N(6)-B(1)	1.57(4)	C(24)-H(24B)	0.9800
B(1)-H(1B)	1.0000	C(24)-H(24C)	0.9800
C(1)-C(2)	1.37(4)	Rh(2)-N(9)	2.02(2)
C(1)-C(10)	1.50(4)	Rh(2)-C(40)	2.051(16)
C(2)-C(3)	1.33(4)	Rh(2)-N(11)	2.16(2)
C(2)-H(2A)	0.9500	Rh(2)-P(2)	2.239(11)
C(3)-C(11)	1.53(4)	Rh(2)-N(7)	2.26(2)
C(4)-C(5)	1.36(3)	F(4)-C(41)	1.35(2)
C(4)-C(12)	1.52(4)	F(5)-C(43)	1.32(2)
C(5)-C(6)	1.34(4)	F(6)-C(45)	1.30(2)
C(5)-H(5A)	0.9500	N(7)-C(25)	1.31(3)
C(6)-C(13)	1.54(4)	N(7)-N(8)	1.40(3)
C(7)-C(8)	1.42(3)	N(8)-C(27)	1.28(3)
C(7)-C(14)	1.48(4)	N(8)-B(2)	1.53(4)
C(8)-C(9)	1.29(3)	N(9)-C(28)	1.29(3)
C(8)-H(8A)	0.9500	N(9)-N(10)	1.47(3)
C(9)-C(15)	1.51(4)	N(10)-C(30)	1.33(3)
C(10)-H(10A)	0.9800	N(10)-B(2)	1.52(4)
C(10)-H(10B)	0.9800	N(11)-C(31)	1.34(3)
C(10)-H(10C)	0.9800	N(11)-N(12)	1.38(3)
C(11)-H(11A)	0.9800	N(12)-C(33)	1.33(3)
C(11)-H(11B)	0.9800	N(12)-B(2)	1.51(4)
C(11)-H(11C)	0.9800	B(2)-H(2B)	1.0000
C(12)-H(12A)	0.9800	C(25)-C(26)	1.44(4)
C(12)-H(12B)	0.9800	C(25)-C(34)	1.45(4)
C(12)-H(12C)	0.9800	C(26)-C(27)	1.36(3)
C(13)-H(13A)	0.9800	C(26)-H(26A)	0.9500
C(13)-H(13B)	0.9800	C(27)-C(35)	1.45(3)
C(13)-H(13C)	0.9800	C(28)-C(29)	1.39(4)
C(14)-H(14A)	0.9800	C(28)-C(36)	1.54(4)
C(14)-H(14B)	0.9800	C(29)-C(30)	1.41(4)
C(14)-H(14C)	0.9800	C(29)-H(29A)	0.9500
C(15)-H(15A)	0.9800	C(30)-C(37)	1.50(4)
C(15)-H(15B)	0.9800	C(31)-C(32)	1.42(4)

C(31)-C(38)	1.48(4)	C(52)-H(52C)	0.9800
C(32)-C(33)	1.32(3)	C(16)-Rh(1)-N(5)	89.1(8)
C(32)-H(32A)	0.9500	C(16)-Rh(1)-N(3)	170.2(8)
C(33)-C(39)	1.50(3)	N(5)-Rh(1)-N(3)	82.8(8)
C(34)-H(34A)	0.9800	C(16)-Rh(1)-N(1)	91.8(8)
C(34)-H(34B)	0.9800	N(5)-Rh(1)-N(1)	86.9(8)
C(34)-H(34C)	0.9800	N(3)-Rh(1)-N(1)	93.3(8)
C(35)-H(35A)	0.9800	C(16)-Rh(1)-P(1)	96.6(6)
C(35)-H(35B)	0.9800	N(5)-Rh(1)-P(1)	174.2(7)
C(35)-H(35C)	0.9800	N(3)-Rh(1)-P(1)	91.5(6)
C(36)-H(36A)	0.9800	N(1)-Rh(1)-P(1)	93.4(6)
C(36)-H(36B)	0.9800	C(1)-N(1)-N(2)	103(2)
C(36)-H(36C)	0.9800	C(1)-N(1)-Rh(1)	142(2)
C(37)-H(37A)	0.9800	N(2)-N(1)-Rh(1)	114.5(17)
C(37)-H(37B)	0.9800	C(3)-N(2)-N(1)	108(2)
C(37)-H(37C)	0.9800	C(3)-N(2)-B(1)	130(2)
C(38)-H(38A)	0.9800	N(1)-N(2)-B(1)	122(2)
C(38)-H(38B)	0.9800	C(4)-N(3)-N(4)	109(2)
C(38)-H(38C)	0.9800	C(4)-N(3)-Rh(1)	138.0(18)
C(39)-H(39A)	0.9800	N(4)-N(3)-Rh(1)	113.3(16)
C(39)-H(39B)	0.9800	C(6)-N(4)-N(3)	103(2)
C(39)-H(39C)	0.9800	C(6)-N(4)-B(1)	131(2)
C(40)-C(41)	1.3900	N(3)-N(4)-B(1)	123(2)
C(40)-C(45)	1.3900	C(7)-N(5)-N(6)	109(2)
C(41)-C(42)	1.3900	C(7)-N(5)-Rh(1)	136(2)
C(42)-C(43)	1.3900	N(6)-N(5)-Rh(1)	114.7(16)
C(42)-H(42A)	0.9500	C(9)-N(6)-N(5)	105(2)
C(43)-C(44)	1.3900	C(9)-N(6)-B(1)	133(2)
C(44)-C(45)	1.3900	N(5)-N(6)-B(1)	122(2)
C(44)-H(44A)	0.9500	N(2)-B(1)-N(4)	111(2)
P(2)-C(48)	1.75(3)	N(2)-B(1)-N(6)	109(2)
P(2)-C(47)	1.77(3)	N(4)-B(1)-N(6)	105(2)
P(2)-C(46)	1.81(3)	N(2)-B(1)-H(1B)	110.6
C(46)-H(46A)	0.9800	N(4)-B(1)-H(1B)	110.6
C(46)-H(46B)	0.9800	N(6)-B(1)-H(1B)	110.6
C(46)-H(46C)	0.9800	C(2)-C(1)-N(1)	112(3)
C(47)-H(47A)	0.9800	C(2)-C(1)-C(10)	130(3)
C(47)-H(47B)	0.9800	N(1)-C(1)-C(10)	118(3)
C(47)-H(47C)	0.9800	C(3)-C(2)-C(1)	105(3)
C(48)-H(48A)	0.9800	C(3)-C(2)-H(2A)	127.7
C(48)-H(48B)	0.9800	C(1)-C(2)-H(2A)	127.7
C(48)-H(48C)	0.9800	N(2)-C(3)-C(2)	112(3)
C(49)-C(50)	1.12(8)	N(2)-C(3)-C(11)	122(3)
C(49)-H(49A)	0.9800	C(2)-C(3)-C(11)	126(3)
C(49)-H(49B)	0.9800	N(3)-C(4)-C(5)	112(3)
C(49)-H(49C)	0.9800	N(3)-C(4)-C(12)	121(2)
C(50)-O(1)	1.40(7)	C(5)-C(4)-C(12)	126(3)
C(50)-H(50A)	0.9900	C(6)-C(5)-C(4)	102(3)
C(50)-H(50B)	0.9900	C(6)-C(5)-H(5A)	129.2
O(1)-C(51)	1.33(10)	C(4)-C(5)-H(5A)	129.2
C(51)-C(52)	1.12(11)	C(5)-C(6)-N(4)	115(3)
C(51)-H(51A)	0.9900	C(5)-C(6)-C(13)	126(3)
C(51)-H(51B)	0.9900	N(4)-C(6)-C(13)	119(3)
C(52)-H(52A)	0.9800	N(5)-C(7)-C(8)	108(2)
C(52)-H(52B)	0.9800	N(5)-C(7)-C(14)	125(3)

C(8)-C(7)-C(14)	126(3)	C(19)-C(20)-C(21)	120.0
C(9)-C(8)-C(7)	108(2)	C(19)-C(20)-H(20A)	120.0
C(9)-C(8)-H(8A)	126.0	C(21)-C(20)-H(20A)	120.0
C(7)-C(8)-H(8A)	126.0	F(3)-C(21)-C(20)	119.3(17)
C(8)-C(9)-N(6)	110(3)	F(3)-C(21)-C(16)	120.7(18)
C(8)-C(9)-C(15)	132(3)	C(20)-C(21)-C(16)	120.0
N(6)-C(9)-C(15)	118(3)	C(24)-P(1)-C(22)	98.8(14)
C(1)-C(10)-H(10A)	109.5	C(24)-P(1)-C(23)	103.3(15)
C(1)-C(10)-H(10B)	109.5	C(22)-P(1)-C(23)	97.9(15)
H(10A)-C(10)-H(10B)	109.5	C(24)-P(1)-Rh(1)	109.0(11)
C(1)-C(10)-H(10C)	109.5	C(22)-P(1)-Rh(1)	121.7(10)
H(10A)-C(10)-H(10C)	109.5	C(23)-P(1)-Rh(1)	122.4(11)
H(10B)-C(10)-H(10C)	109.5	P(1)-C(22)-H(22A)	109.5
C(3)-C(11)-H(11A)	109.5	P(1)-C(22)-H(22B)	109.5
C(3)-C(11)-H(11B)	109.5	H(22A)-C(22)-H(22B)	109.5
H(11A)-C(11)-H(11B)	109.5	P(1)-C(22)-H(22C)	109.5
C(3)-C(11)-H(11C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(11B)-C(11)-H(11C)	109.5	P(1)-C(23)-H(23A)	109.5
C(4)-C(12)-H(12A)	109.5	P(1)-C(23)-H(23B)	109.5
C(4)-C(12)-H(12B)	109.5	H(23A)-C(23)-H(23B)	109.5
H(12A)-C(12)-H(12B)	109.5	P(1)-C(23)-H(23C)	109.5
C(4)-C(12)-H(12C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(23B)-C(23)-H(23C)	109.5
H(12B)-C(12)-H(12C)	109.5	P(1)-C(24)-H(24A)	109.5
C(6)-C(13)-H(13A)	109.5	P(1)-C(24)-H(24B)	109.5
C(6)-C(13)-H(13B)	109.5	H(24A)-C(24)-H(24B)	109.5
H(13A)-C(13)-H(13B)	109.5	P(1)-C(24)-H(24C)	109.5
C(6)-C(13)-H(13C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(24B)-C(24)-H(24C)	109.5
H(13B)-C(13)-H(13C)	109.5	N(9)-Rh(2)-C(40)	89.3(9)
C(7)-C(14)-H(14A)	109.5	N(9)-Rh(2)-N(11)	83.6(9)
C(7)-C(14)-H(14B)	109.5	C(40)-Rh(2)-N(11)	171.7(8)
H(14A)-C(14)-H(14B)	109.5	N(9)-Rh(2)-P(2)	175.4(7)
C(7)-C(14)-H(14C)	109.5	C(40)-Rh(2)-P(2)	90.6(6)
H(14A)-C(14)-H(14C)	109.5	N(11)-Rh(2)-P(2)	96.1(6)
H(14B)-C(14)-H(14C)	109.5	N(9)-Rh(2)-N(7)	89.6(9)
C(9)-C(15)-H(15A)	109.5	C(40)-Rh(2)-N(7)	96.5(8)
C(9)-C(15)-H(15B)	109.5	N(11)-Rh(2)-N(7)	87.8(8)
H(15A)-C(15)-H(15B)	109.5	P(2)-Rh(2)-N(7)	95.0(6)
C(9)-C(15)-H(15C)	109.5	C(25)-N(7)-N(8)	107(2)
H(15A)-C(15)-H(15C)	109.5	C(25)-N(7)-Rh(2)	139.6(19)
H(15B)-C(15)-H(15C)	109.5	N(8)-N(7)-Rh(2)	113.7(17)
C(17)-C(16)-C(21)	120.0	C(27)-N(8)-N(7)	112(2)
C(17)-C(16)-Rh(1)	118.8(11)	C(27)-N(8)-B(2)	128(3)
C(21)-C(16)-Rh(1)	120.9(11)	N(7)-N(8)-B(2)	119(2)
F(1)-C(17)-C(18)	114.4(17)	C(28)-N(9)-N(10)	99(2)
F(1)-C(17)-C(16)	125.6(17)	C(28)-N(9)-Rh(2)	141(2)
C(18)-C(17)-C(16)	120.0	N(10)-N(9)-Rh(2)	119.1(16)
C(17)-C(18)-C(19)	120.0	C(30)-N(10)-N(9)	113(2)
C(17)-C(18)-H(18A)	120.0	C(30)-N(10)-B(2)	131(3)
C(19)-C(18)-H(18A)	120.0	N(9)-N(10)-B(2)	115(2)
F(2)-C(19)-C(20)	119.3(18)	C(31)-N(11)-N(12)	108(2)
F(2)-C(19)-C(18)	120.7(18)	C(31)-N(11)-Rh(2)	134.6(18)
C(20)-C(19)-C(18)	120.0	N(12)-N(11)-Rh(2)	116.2(16)

C(33)-N(12)-N(11)	109(2)	C(30)-C(37)-H(37B)	109.5
C(33)-N(12)-B(2)	130(3)	H(37A)-C(37)-H(37B)	109.5
N(11)-N(12)-B(2)	120(2)	C(30)-C(37)-H(37C)	109.5
N(12)-B(2)-N(10)	112(3)	H(37A)-C(37)-H(37C)	109.5
N(12)-B(2)-N(8)	111(3)	H(37B)-C(37)-H(37C)	109.5
N(10)-B(2)-N(8)	111(2)	C(31)-C(38)-H(38A)	109.5
N(12)-B(2)-H(2B)	107.7	C(31)-C(38)-H(38B)	109.5
N(10)-B(2)-H(2B)	107.7	H(38A)-C(38)-H(38B)	109.5
N(8)-B(2)-H(2B)	107.7	C(31)-C(38)-H(38C)	109.5
N(7)-C(25)-C(26)	106(2)	H(38A)-C(38)-H(38C)	109.5
N(7)-C(25)-C(34)	127(3)	H(38B)-C(38)-H(38C)	109.5
C(26)-C(25)-C(34)	126(3)	C(33)-C(39)-H(39A)	109.5
C(27)-C(26)-C(25)	108(3)	C(33)-C(39)-H(39B)	109.5
C(27)-C(26)-H(26A)	126.0	H(39A)-C(39)-H(39B)	109.5
C(25)-C(26)-H(26A)	126.0	C(33)-C(39)-H(39C)	109.5
N(8)-C(27)-C(26)	107(3)	H(39A)-C(39)-H(39C)	109.5
N(8)-C(27)-C(35)	127(3)	H(39B)-C(39)-H(39C)	109.5
C(26)-C(27)-C(35)	127(3)	C(41)-C(40)-C(45)	120.0
N(9)-C(28)-C(29)	118(3)	C(41)-C(40)-Rh(2)	121.5(12)
N(9)-C(28)-C(36)	119(3)	C(45)-C(40)-Rh(2)	118.2(12)
C(29)-C(28)-C(36)	123(3)	F(4)-C(41)-C(40)	122.3(17)
C(28)-C(29)-C(30)	103(3)	F(4)-C(41)-C(42)	117.7(17)
C(28)-C(29)-H(29A)	128.5	C(40)-C(41)-C(42)	120.0
C(30)-C(29)-H(29A)	128.5	C(43)-C(42)-C(41)	120.0
N(10)-C(30)-C(29)	107(3)	C(43)-C(42)-H(42A)	120.0
N(10)-C(30)-C(37)	126(3)	C(41)-C(42)-H(42A)	120.0
C(29)-C(30)-C(37)	127(3)	F(5)-C(43)-C(44)	120.5(19)
N(11)-C(31)-C(32)	106(2)	F(5)-C(43)-C(42)	119.3(19)
N(11)-C(31)-C(38)	123(3)	C(44)-C(43)-C(42)	120.0
C(32)-C(31)-C(38)	131(3)	C(43)-C(44)-C(45)	120.0
C(33)-C(32)-C(31)	108(3)	C(43)-C(44)-H(44A)	120.0
C(33)-C(32)-H(32A)	126.0	C(45)-C(44)-H(44A)	120.0
C(31)-C(32)-H(32A)	126.0	F(6)-C(45)-C(44)	116.1(18)
C(32)-C(33)-N(12)	109(3)	F(6)-C(45)-C(40)	123.6(18)
C(32)-C(33)-C(39)	127(3)	C(44)-C(45)-C(40)	120.0
N(12)-C(33)-C(39)	124(2)	C(48)-P(2)-C(47)	99.6(16)
C(25)-C(34)-H(34A)	109.5	C(48)-P(2)-C(46)	104.1(17)
C(25)-C(34)-H(34B)	109.5	C(47)-P(2)-C(46)	95.8(16)
H(34A)-C(34)-H(34B)	109.5	C(48)-P(2)-Rh(2)	113.4(12)
C(25)-C(34)-H(34C)	109.5	C(47)-P(2)-Rh(2)	123.3(12)
H(34A)-C(34)-H(34C)	109.5	C(46)-P(2)-Rh(2)	117.4(12)
H(34B)-C(34)-H(34C)	109.5	P(2)-C(46)-H(46A)	109.5
C(27)-C(35)-H(35A)	109.5	P(2)-C(46)-H(46B)	109.5
C(27)-C(35)-H(35B)	109.5	H(46A)-C(46)-H(46B)	109.5
H(35A)-C(35)-H(35B)	109.5	P(2)-C(46)-H(46C)	109.5
C(27)-C(35)-H(35C)	109.5	H(46A)-C(46)-H(46C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(46B)-C(46)-H(46C)	109.5
H(35B)-C(35)-H(35C)	109.5	P(2)-C(47)-H(47A)	109.5
C(28)-C(36)-H(36A)	109.5	P(2)-C(47)-H(47B)	109.5
C(28)-C(36)-H(36B)	109.5	H(47A)-C(47)-H(47B)	109.5
H(36A)-C(36)-H(36B)	109.5	P(2)-C(47)-H(47C)	109.5
C(28)-C(36)-H(36C)	109.5	H(47A)-C(47)-H(47C)	109.5
H(36A)-C(36)-H(36C)	109.5	H(47B)-C(47)-H(47C)	109.5
H(36B)-C(36)-H(36C)	109.5	P(2)-C(48)-H(48A)	109.5
C(30)-C(37)-H(37A)	109.5	P(2)-C(48)-H(48B)	109.5

H(48A)-C(48)-H(48B)	109.5	H(50A)-C(50)-H(50B)	105.3
P(2)-C(48)-H(48C)	109.5	C(51)-O(1)-C(50)	140(8)
H(48A)-C(48)-H(48C)	109.5	C(52)-C(51)-O(1)	148(10)
H(48B)-C(48)-H(48C)	109.5	C(52)-C(51)-H(51A)	99.7
C(50)-C(49)-H(49A)	109.5	O(1)-C(51)-H(51A)	99.7
C(50)-C(49)-H(49B)	109.5	C(52)-C(51)-H(51B)	99.7
H(49A)-C(49)-H(49B)	109.5	O(1)-C(51)-H(51B)	99.7
C(50)-C(49)-H(49C)	109.5	H(51A)-C(51)-H(51B)	104.1
H(49A)-C(49)-H(49C)	109.5	C(51)-C(52)-H(52A)	109.5
H(49B)-C(49)-H(49C)	109.5	C(51)-C(52)-H(52B)	109.5
C(49)-C(50)-O(1)	134(9)	H(52A)-C(52)-H(52B)	109.5
C(49)-C(50)-H(50A)	103.7	C(51)-C(52)-H(52C)	109.5
O(1)-C(50)-H(50A)	103.7	H(52A)-C(52)-H(52C)	109.5
C(49)-C(50)-H(50B)	103.7	H(52B)-C(52)-H(52C)	109.5
O(1)-C(50)-H(50B)	103.7		

Table S28. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3d·0.5Et$_2$O**. 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_{11}	U_{33}	U_{23}	U_{13}	U_{12}
Rh1	39(2)	36(2)	9(2)	2(1)	4(1)	2(2)
P1	50(6)	45(7)	10(5)	0(4)	7(5)	0(5)
Rh2	43(2)	39(2)	11(2)	-1(1)	-7(1)	3(2)
P2	50(7)	72(8)	23(6)	-4(5)	10(5)	4(6)

Table S29. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2\ x\ 10^3$) for **3d·0.5Et$_2$O**.

	x	y	z	U(eq)
H1B	-1339	832	1482	25
H2A	-2212	-271	2841	45
H5A	-1936	2192	2180	19
H8A	4166	836	1243	6
H10A	1329	127	4012	40
H10B	443	-292	3873	40
H10C	-305	52	4267	40
H11A	-3694	394	1533	101
H11B	-3636	-77	1661	101
H11C	-2372	128	1277	101
H12A	1561	1951	3511	67
H12B	2	2189	3603	67
H12C	999	2326	3048	67
H13A	-3697	1310	1362	77
H13B	-2445	1480	935	77
H13C	-3635	1777	1213	77
H14A	5066	1051	3092	45
H14B	5788	1179	2449	45
H14C	5842	722	2680	45
H15A	1613	652	346	82

H15B	319	966	494	82
H15C	183	509	699	82
H18A	6215	591	5030	62
H20A	5067	-217	3552	54
H22A	28	907	5247	43
H22B	1589	709	5064	43
H22C	-105	556	4709	43
H23A	566	1568	5141	78
H23B	893	1812	4504	78
H23C	2265	1550	4923	78
H24A	-2007	1258	4424	62
H24B	-2013	981	3784	62
H24C	-1745	1452	3735	62
H2B	3467	2524	631	36
H26A	1435	3814	768	28
H29A	3353	1712	2561	32
H32A	8765	2404	356	33
H34A	3740	3900	2458	44
H34B	2546	4153	1931	44
H34C	4391	4157	1901	44
H35A	2168	3000	-221	41
H35B	749	3295	-143	41
H35C	848	2864	199	41
H36A	6715	2316	3356	66
H36B	5649	1947	3508	66
H36C	5105	2393	3630	66
H37A	1401	2066	895	60
H37B	1426	1681	1360	60
H37C	2691	1725	872	60
H38A	9738	2823	2105	63
H38B	10251	3083	1519	63
H38C	10663	2617	1577	63
H39A	4753	2440	-375	30
H39B	5065	2022	2	30
H39C	6286	2185	-446	30
H42A	6807	3326	4730	60
H44A	2290	3221	3793	99
H46A	7786	4233	2802	103
H46B	7662	3904	3360	103
H46C	6130	4025	2841	103
H47A	10044	3814	2940	77
H47B	10313	3635	2241	77
H47C	10082	3342	2835	77
H48A	8030	4117	1662	99
H48B	6561	3848	1343	99
H48C	8316	3702	1314	99
H49A	419	4317	5225	338
H49B	-470	3961	4794	338
H49C	-776	4413	4555	338
H50A	586	4027	4105	234
H50B	1806	4040	4772	234
H51A	3893	4357	4143	399
H51B	2664	4305	3494	399
H52A	4920	4631	3727	213
H52B	3601	4972	3638	213

H52C	3553	4628	3090	213

Table S30. Torsion angles [°] for **3d·0.5Et$_2$O**.

C16-Rh1-N1-C1	39(3)	Rh1-N1-C1-C2	-179(2)
N5-Rh1-N1-C1	128(3)	N2-N1-C1-C10	171(2)
N3-Rh1-N1-C1	-149(3)	Rh1-N1-C1-C10	-7(5)
P1-Rh1-N1-C1	-57(3)	N1-C1-C2-C3	0(3)
C16-Rh1-N1-N2	-138.5(17)	C10-C1-C2-C3	-171(3)
N5-Rh1-N1-N2	-49.5(17)	N1-N2-C3-C2	-3(3)
N3-Rh1-N1-N2	33.1(17)	B1-N2-C3-C2	172(3)
P1-Rh1-N1-N2	124.7(16)	N1-N2-C3-C11	-179(2)
C1-N1-N2-C3	2(3)	B1-N2-C3-C11	-4(4)
Rh1-N1-N2-C3	-179.1(16)	C1-C2-C3-N2	2(3)
C1-N1-N2-B1	-173(2)	C1-C2-C3-C11	178(3)
Rh1-N1-N2-B1	6(3)	N4-N3-C4-C5	-1(3)
C16-Rh1-N3-C4	-90(5)	Rh1-N3-C4-C5	-177.6(18)
N5-Rh1-N3-C4	-124(3)	N4-N3-C4-C12	-174(2)
N1-Rh1-N3-C4	149(3)	Rh1-N3-C4-C12	9(4)
P1-Rh1-N3-C4	56(3)	N3-C4-C5-C6	0(3)
C16-Rh1-N3-N4	94(5)	C12-C4-C5-C6	173(3)
N5-Rh1-N3-N4	59.2(16)	C4-C5-C6-N4	1(3)
N1-Rh1-N3-N4	-27.2(16)	C4-C5-C6-C13	-178(3)
P1-Rh1-N3-N4	-120.7(15)	N3-N4-C6-C5	-1(3)
C4-N3-N4-C6	1(3)	B1-N4-C6-C5	-163(3)
Rh1-N3-N4-C6	178.9(17)	N3-N4-C6-C13	178(2)
C4-N3-N4-B1	165(2)	B1-N4-C6-C13	16(4)
Rh1-N3-N4-B1	-17(3)	N6-N5-C7-C8	2(3)
C16-Rh1-N5-C7	-43(3)	Rh1-N5-C7-C8	-178.1(19)
N3-Rh1-N5-C7	132(3)	N6-N5-C7-C14	175(3)
N1-Rh1-N5-C7	-134(3)	Rh1-N5-C7-C14	-5(5)
P1-Rh1-N5-C7	133(6)	N5-C7-C8-C9	-4(3)
C16-Rh1-N5-N6	136.9(17)	C14-C7-C8-C9	-177(3)
N3-Rh1-N5-N6	-48.6(17)	C7-C8-C9-N6	4(3)
N1-Rh1-N5-N6	45.1(17)	C7-C8-C9-C15	-175(3)
P1-Rh1-N5-N6	-47(8)	N5-N6-C9-C8	-2(3)
C7-N5-N6-C9	0(3)	B1-N6-C9-C8	179(3)
Rh1-N5-N6-C9	-179.9(17)	N5-N6-C9-C15	177(3)
C7-N5-N6-B1	179(2)	B1-N6-C9-C15	-2(5)
Rh1-N5-N6-B1	-1(3)	N5-Rh1-C16-C17	129.5(11)
C3-N2-B1-N4	125(3)	N3-Rh1-C16-C17	95(5)
N1-N2-B1-N4	-61(3)	N1-Rh1-C16-C17	-143.7(11)
C3-N2-B1-N6	-120(3)	P1-Rh1-C16-C17	-50.1(10)
N1-N2-B1-N6	54(3)	N5-Rh1-C16-C21	-44.5(11)
C6-N4-B1-N2	-131(3)	N3-Rh1-C16-C21	-79(5)
N3-N4-B1-N2	71(3)	N1-Rh1-C16-C21	42.3(11)
C6-N4-B1-N6	111(3)	P1-Rh1-C16-C21	135.9(10)
N3-N4-B1-N6	-47(3)	C21-C16-C17-F1	-177(2)
C9-N6-B1-N2	120(3)	Rh1-C16-C17-F1	9.0(19)
N5-N6-B1-N2	-59(3)	C21-C16-C17-C18	0.0
C9-N6-B1-N4	-122(3)	Rh1-C16-C17-C18	-174.0(13)
N5-N6-B1-N4	59(3)	F1-C17-C18-C19	177.3(19)
N2-N1-C1-C2	-1(3)	C16-C17-C18-C19	0.0

C17-C18-C19-F2	180(2)	Rh2-N11-N12-C33	-170.0(18)
C17-C18-C19-C20	0.0	C31-N11-N12-B2	171(2)
F2-C19-C20-C21	-180(2)	Rh2-N11-N12-B2	2(3)
C18-C19-C20-C21	0.0	C33-N12-B2-N10	108(3)
C19-C20-C21-F3	178(2)	N11-N12-B2-N10	-62(3)
C19-C20-C21-C16	0.0	C33-N12-B2-N8	-127(3)
C17-C16-C21-F3	-178(2)	N11-N12-B2-N8	63(3)
Rh1-C16-C21-F3	-4.0(19)	C30-N10-B2-N12	-112(3)
C17-C16-C21-C20	0.0	N9-N10-B2-N12	51(3)
Rh1-C16-C21-C20	173.9(14)	C30-N10-B2-N8	123(3)
C16-Rh1-P1-C24	-146.2(12)	N9-N10-B2-N8	-74(3)
N5-Rh1-P1-C24	38(7)	C27-N8-B2-N12	116(3)
N3-Rh1-P1-C24	39.3(13)	N7-N8-B2-N12	-67(3)
N1-Rh1-P1-C24	-54.0(13)	C27-N8-B2-N10	-119(3)
C16-Rh1-P1-C22	-32.5(13)	N7-N8-B2-N10	58(3)
N5-Rh1-P1-C22	152(7)	N8-N7-C25-C26	-3(3)
N3-Rh1-P1-C22	153.1(13)	Rh2-N7-C25-C26	176(2)
N1-Rh1-P1-C22	59.7(13)	N8-N7-C25-C34	179(3)
C16-Rh1-P1-C23	93.2(14)	Rh2-N7-C25-C34	-2(5)
N5-Rh1-P1-C23	-83(7)	N7-C25-C26-C27	2(3)
N3-Rh1-P1-C23	-81.2(14)	C34-C25-C26-C27	180(3)
N1-Rh1-P1-C23	-174.6(14)	N7-N8-C27-C26	-2(3)
N9-Rh2-N7-C25	136(3)	B2-N8-C27-C26	175(3)
C40-Rh2-N7-C25	47(3)	N7-N8-C27-C35	-179(3)
N11-Rh2-N7-C25	-140(3)	B2-N8-C27-C35	-2(5)
P2-Rh2-N7-C25	-44(3)	C25-C26-C27-N8	0(3)
N9-Rh2-N7-N8	-45.0(17)	C25-C26-C27-C35	177(3)
C40-Rh2-N7-N8	-134.2(17)	N10-N9-C28-C29	5(3)
N11-Rh2-N7-N8	38.6(17)	Rh2-N9-C28-C29	174(2)
P2-Rh2-N7-N8	134.6(16)	N10-N9-C28-C36	-179(2)
C25-N7-N8-C27	3(3)	Rh2-N9-C28-C36	-10(5)
Rh2-N7-N8-C27	-176.0(17)	N9-C28-C29-C30	-3(4)
C25-N7-N8-B2	-174(2)	C36-C28-C29-C30	-179(3)
Rh2-N7-N8-B2	7(3)	N9-N10-C30-C29	3(3)
C40-Rh2-N9-C28	-39(3)	B2-N10-C30-C29	167(3)
N11-Rh2-N9-C28	137(3)	N9-N10-C30-C37	-174(3)
P2-Rh2-N9-C28	50(10)	B2-N10-C30-C37	-11(5)
N7-Rh2-N9-C28	-136(3)	C28-C29-C30-N10	0(3)
C40-Rh2-N9-N10	128.4(17)	C28-C29-C30-C37	177(3)
N11-Rh2-N9-N10	-55.9(16)	N12-N11-C31-C32	1(3)
P2-Rh2-N9-N10	-143(8)	Rh2-N11-C31-C32	167.4(19)
N7-Rh2-N9-N10	31.9(17)	N12-N11-C31-C38	-174(3)
C28-N9-N10-C30	-5(3)	Rh2-N11-C31-C38	-7(4)
Rh2-N9-N10-C30	-177(2)	N11-C31-C32-C33	-1(3)
C28-N9-N10-B2	-171(2)	C38-C31-C32-C33	173(3)
Rh2-N9-N10-B2	17(3)	C31-C32-C33-N12	0(3)
N9-Rh2-N11-C31	-119(3)	C31-C32-C33-C39	-180(3)
C40-Rh2-N11-C31	-88(6)	N11-N12-C33-C32	0(3)
P2-Rh2-N11-C31	56(3)	B2-N12-C33-C32	-171(3)
N7-Rh2-N11-C31	151(3)	N11-N12-C33-C39	-180(2)
N9-Rh2-N11-N12	46.3(18)	B2-N12-C33-C39	10(5)
C40-Rh2-N11-N12	77(6)	N9-Rh2-C40-C41	118.8(12)
P2-Rh2-N11-N12	-138.3(17)	N11-Rh2-C40-C41	88(6)
N7-Rh2-N11-N12	-43.5(18)	P2-Rh2-C40-C41	-56.6(11)
C31-N11-N12-C33	-1(3)	N7-Rh2-C40-C41	-151.7(12)

N9-Rh2-C40-C45	-55.1(12)	Rh2-C40-C45-F6	0(2)
N11-Rh2-C40-C45	-86(6)	C41-C40-C45-C44	0.0
P2-Rh2-C40-C45	129.5(11)	Rh2-C40-C45-C44	174.0(14)
N7-Rh2-C40-C45	34.4(13)	N9-Rh2-P2-C48	131(9)
C45-C40-C41-F4	178(2)	C40-Rh2-P2-C48	-140.1(14)
Rh2-C40-C41-F4	4(2)	N11-Rh2-P2-C48	44.7(14)
C45-C40-C41-C42	0.0	N7-Rh2-P2-C48	-43.6(15)
Rh2-C40-C41-C42	-173.8(14)	N9-Rh2-P2-C47	11(9)
F4-C41-C42-C43	-178(2)	C40-Rh2-P2-C47	99.8(15)
C40-C41-C42-C43	0.0	N11-Rh2-P2-C47	-75.4(15)
C41-C42-C43-F5	-174(2)	N7-Rh2-P2-C47	-163.6(15)
C41-C42-C43-C44	0.0	N9-Rh2-P2-C46	-107(9)
F5-C43-C44-C45	174(2)	C40-Rh2-P2-C46	-18.6(15)
C42-C43-C44-C45	0.0	N11-Rh2-P2-C46	166.2(15)
C43-C44-C45-F6	174(2)	N7-Rh2-P2-C46	77.9(15)
C43-C44-C45-C40	0.0	C49-C50-O1-C51	-178(12)
C41-C40-C45-F6	-174(2)	C50-O1-C51-C52	174(16)

Table S31. Crystal data and structure refinement for **3g**.

Identification code	**3g**	
Empirical formula	$C_{24}H_{35}BF_2N_6PRh$	
Formula weight	590.27	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.4449(16) Å	α = 90°
	b = 14.597(2) Å	β = 92.021(3)°
	c = 17.499(3) Å	γ = 90°
Volume	2666.4(7) Å^3	
Z	4	
Density (calculated)	1.470 Mg/m^3	
Absorption coefficient	0.739 mm^{-1}	
F(000)	1216	
Crystal color, morphology	colorless, block	
Crystal size	0.18 x 0.14 x 0.08 mm^3	
Theta range for data collection	1.82 to 30.51°	
Index ranges	$-14 \le h \le 14$, $-20 \le k \le 20$, $-24 \le l \le 24$	
Reflections collected	42567	
Independent reflections	8144 [R(int) = 0.1125]	
Observed reflections	4948	
Completeness to theta = 30.51°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9433 and 0.8785	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8144 / 0 / 332	
Goodness-of-fit on F^2	0.995	
Final R indices [I>2sigma(I)]	R_1 = 0.0488, wR_2 = 0.0954	
R indices (all data)	R_1 = 0.1055, wR_2 = 0.1167	
Largest diff. peak and hole	1.270 and -0.632 e.Å^{-3}	

Table S32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3g**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	7599(1)	3055(1)	9757(1)	22(1)
N1	8920(3)	3378(2)	8799(2)	25(1)
N2	8490(3)	4044(2)	8303(2)	24(1)
N3	6121(3)	3019(2)	8910(2)	24(1)
N4	6166(3)	3620(2)	8316(2)	28(1)
N5	7124(3)	4495(2)	9796(2)	25(1)
N6	6987(3)	4937(2)	9102(2)	26(1)
B1	7127(4)	4413(3)	8348(2)	28(1)
C1	10099(3)	3152(3)	8578(2)	24(1)
C2	10419(4)	3685(3)	7951(2)	29(1)
C3	9381(4)	4235(3)	7785(2)	27(1)
C4	5104(4)	2472(3)	8780(2)	31(1)
C5	4502(4)	2727(3)	8092(2)	34(1)
C6	5187(4)	3446(3)	7809(2)	32(1)
C7	6744(3)	5084(3)	10317(2)	28(1)
C8	6410(4)	5907(3)	9976(2)	32(1)
C9	6557(4)	5796(3)	9215(2)	29(1)
C10	10878(4)	2418(3)	8948(2)	32(1)
C11	9195(4)	4939(3)	7175(2)	34(1)
C12	4723(4)	1737(3)	9317(2)	37(1)
C13	4975(4)	3985(3)	7094(2)	42(1)
C14	6668(4)	4855(3)	11142(2)	33(1)
C15	6319(4)	6465(3)	8576(2)	40(1)
C16	7757(3)	1692(3)	9616(2)	26(1)
C17	7650(4)	1018(3)	10164(2)	31(1)
F1	7536(2)	1285(2)	10918(1)	41(1)
C18	7599(4)	95(3)	10042(2)	39(1)
C19	7646(4)	-225(3)	9297(2)	37(1)
C20	7754(4)	417(3)	8738(2)	31(1)
F2	7769(2)	124(2)	7992(1)	41(1)
C21	7822(3)	1337(3)	8875(2)	26(1)
P1	9044(1)	3074(1)	10747(1)	25(1)
C22	10020(4)	4098(3)	10753(2)	33(1)
C23	8465(4)	3024(3)	11721(2)	34(1)
C24	10265(4)	2190(3)	10829(2)	37(1)

Table S33. Bond lengths [Å] and angles [°] for **3g**.

Rh(1)-C(16)	2.013(4)	N(2)-B(1)	1.527(5)
Rh(1)-N(3)	2.102(3)	N(3)-C(4)	1.342(5)
Rh(1)-N(5)	2.161(3)	N(3)-N(4)	1.363(4)
Rh(1)-P(1)	2.2582(9)	N(4)-C(6)	1.355(5)
Rh(1)-N(1)	2.258(3)	N(4)-B(1)	1.531(5)
Rh(1)-H(1)	1.44(4)	N(5)-C(7)	1.325(5)
N(1)-C(1)	1.345(4)	N(5)-N(6)	1.378(4)
N(1)-N(2)	1.369(4)	N(6)-C(9)	1.349(5)
N(2)-C(3)	1.350(4)	N(6)-B(1)	1.537(5)

B(1)-H(1B)	1.07(4)	C(24)-H(24B)	0.9800
C(1)-C(2)	1.394(5)	C(24)-H(24C)	0.9800
C(1)-C(10)	1.481(5)	C(16)-Rh(1)-N(3)	87.11(13)
C(2)-C(3)	1.372(5)	C(16)-Rh(1)-N(5)	170.15(13)
C(2)-H(2)	0.9500	N(3)-Rh(1)-N(5)	83.29(11)
C(3)-C(11)	1.489(5)	C(16)-Rh(1)-P(1)	92.88(11)
C(4)-C(5)	1.388(5)	N(3)-Rh(1)-P(1)	174.65(8)
C(4)-C(12)	1.490(6)	N(5)-Rh(1)-P(1)	96.47(8)
C(5)-C(6)	1.372(6)	C(16)-Rh(1)-N(1)	93.46(13)
C(5)-H(5)	0.9500	N(3)-Rh(1)-N(1)	86.25(11)
C(6)-C(13)	1.488(5)	N(5)-Rh(1)-N(1)	88.15(11)
C(7)-C(8)	1.381(5)	P(1)-Rh(1)-N(1)	99.09(8)
C(7)-C(14)	1.486(5)	C(16)-Rh(1)-H(1)	85.3(17)
C(8)-C(9)	1.357(5)	N(3)-Rh(1)-H(1)	86.9(17)
C(8)-H(8)	0.9500	N(5)-Rh(1)-H(1)	92.0(16)
C(9)-C(15)	1.498(5)	P(1)-Rh(1)-H(1)	87.8(17)
C(10)-H(10A)	0.9800	N(1)-Rh(1)-H(1)	173.0(17)
C(10)-H(10B)	0.9800	C(1)-N(1)-N(2)	105.9(3)
C(10)-H(10C)	0.9800	C(1)-N(1)-Rh(1)	138.8(2)
C(11)-H(11A)	0.9800	N(2)-N(1)-Rh(1)	115.1(2)
C(11)-H(11B)	0.9800	C(3)-N(2)-N(1)	110.7(3)
C(11)-H(11C)	0.9800	C(3)-N(2)-B(1)	128.9(3)
C(12)-H(12A)	0.9800	N(1)-N(2)-B(1)	120.2(3)
C(12)-H(12B)	0.9800	C(4)-N(3)-N(4)	107.6(3)
C(12)-H(12C)	0.9800	C(4)-N(3)-Rh(1)	133.8(3)
C(13)-H(13A)	0.9800	N(4)-N(3)-Rh(1)	118.5(2)
C(13)-H(13B)	0.9800	C(6)-N(4)-N(3)	109.5(3)
C(13)-H(13C)	0.9800	C(6)-N(4)-B(1)	130.1(3)
C(14)-H(14A)	0.9800	N(3)-N(4)-B(1)	120.0(3)
C(14)-H(14B)	0.9800	C(7)-N(5)-N(6)	106.2(3)
C(14)-H(14C)	0.9800	C(7)-N(5)-Rh(1)	136.6(3)
C(15)-H(15A)	0.9800	N(6)-N(5)-Rh(1)	116.4(2)
C(15)-H(15B)	0.9800	C(9)-N(6)-N(5)	109.3(3)
C(15)-H(15C)	0.9800	C(9)-N(6)-B(1)	129.1(3)
C(16)-C(17)	1.381(5)	N(5)-N(6)-B(1)	120.9(3)
C(16)-C(21)	1.400(5)	N(2)-B(1)-N(4)	110.1(3)
C(17)-C(18)	1.365(6)	N(2)-B(1)-N(6)	109.7(3)
C(17)-F(1)	1.387(4)	N(4)-B(1)-N(6)	109.0(3)
C(18)-C(19)	1.386(6)	N(2)-B(1)-H(1B)	111(2)
C(18)-H(18)	0.9500	N(4)-B(1)-H(1B)	110(2)
C(19)-C(20)	1.363(6)	N(6)-B(1)-H(1B)	107(2)
C(19)-H(19)	0.9500	N(1)-C(1)-C(2)	109.7(3)
C(20)-C(21)	1.365(5)	N(1)-C(1)-C(10)	123.1(3)
C(20)-F(2)	1.374(4)	C(2)-C(1)-C(10)	127.2(3)
C(21)-H(21)	0.9500	C(3)-C(2)-C(1)	106.4(3)
P(1)-C(22)	1.809(4)	C(3)-C(2)-H(2)	126.8
P(1)-C(24)	1.816(4)	C(1)-C(2)-H(2)	126.8
P(1)-C(23)	1.830(4)	N(2)-C(3)-C(2)	107.2(3)
C(22)-H(22A)	0.9800	N(2)-C(3)-C(11)	123.2(3)
C(22)-H(22B)	0.9800	C(2)-C(3)-C(11)	129.6(3)
C(22)-H(22C)	0.9800	N(3)-C(4)-C(5)	108.6(4)
C(23)-H(23A)	0.9800	N(3)-C(4)-C(12)	123.2(4)
C(23)-H(23B)	0.9800	C(5)-C(4)-C(12)	128.1(4)
C(23)-H(23C)	0.9800	C(6)-C(5)-C(4)	107.0(3)
C(24)-H(24A)	0.9800	C(6)-C(5)-H(5)	126.5

C(4)-C(5)-H(5)	126.5	C(9)-C(15)-H(15C)	109.5
N(4)-C(6)-C(5)	107.3(3)	H(15A)-C(15)-H(15C)	109.5
N(4)-C(6)-C(13)	122.6(4)	H(15B)-C(15)-H(15C)	109.5
C(5)-C(6)-C(13)	130.1(4)	C(17)-C(16)-C(21)	112.8(3)
N(5)-C(7)-C(8)	110.1(3)	C(17)-C(16)-Rh(1)	127.6(3)
N(5)-C(7)-C(14)	123.5(3)	C(21)-C(16)-Rh(1)	119.1(3)
C(8)-C(7)-C(14)	126.4(4)	C(18)-C(17)-C(16)	126.8(4)
C(9)-C(8)-C(7)	106.6(3)	C(18)-C(17)-F(1)	115.0(3)
C(9)-C(8)-H(8)	126.7	C(16)-C(17)-F(1)	118.2(3)
C(7)-C(8)-H(8)	126.7	C(17)-C(18)-C(19)	118.5(4)
N(6)-C(9)-C(8)	107.7(3)	C(17)-C(18)-H(18)	120.8
N(6)-C(9)-C(15)	122.9(3)	C(19)-C(18)-H(18)	120.8
C(8)-C(9)-C(15)	129.4(4)	C(20)-C(19)-C(18)	116.7(4)
C(1)-C(10)-H(10A)	109.5	C(20)-C(19)-H(19)	121.6
C(1)-C(10)-H(10B)	109.5	C(18)-C(19)-H(19)	121.6
H(10A)-C(10)-H(10B)	109.5	C(19)-C(20)-C(21)	123.8(4)
C(1)-C(10)-H(10C)	109.5	C(19)-C(20)-F(2)	118.1(3)
H(10A)-C(10)-H(10C)	109.5	C(21)-C(20)-F(2)	118.1(4)
H(10B)-C(10)-H(10C)	109.5	C(20)-C(21)-C(16)	121.5(4)
C(3)-C(11)-H(11A)	109.5	C(20)-C(21)-H(21)	119.3
C(3)-C(11)-H(11B)	109.5	C(16)-C(21)-H(21)	119.3
H(11A)-C(11)-H(11B)	109.5	C(22)-P(1)-C(24)	101.1(2)
C(3)-C(11)-H(11C)	109.5	C(22)-P(1)-C(23)	103.40(19)
H(11A)-C(11)-H(11C)	109.5	C(24)-P(1)-C(23)	98.83(19)
H(11B)-C(11)-H(11C)	109.5	C(22)-P(1)-Rh(1)	112.05(13)
C(4)-C(12)-H(12A)	109.5	C(24)-P(1)-Rh(1)	120.05(14)
C(4)-C(12)-H(12B)	109.5	C(23)-P(1)-Rh(1)	118.67(13)
H(12A)-C(12)-H(12B)	109.5	P(1)-C(22)-H(22A)	109.5
C(4)-C(12)-H(12C)	109.5	P(1)-C(22)-H(22B)	109.5
H(12A)-C(12)-H(12C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(12B)-C(12)-H(12C)	109.5	P(1)-C(22)-H(22C)	109.5
C(6)-C(13)-H(13A)	109.5	H(22A)-C(22)-H(22C)	109.5
C(6)-C(13)-H(13B)	109.5	H(22B)-C(22)-H(22C)	109.5
H(13A)-C(13)-H(13B)	109.5	P(1)-C(23)-H(23A)	109.5
C(6)-C(13)-H(13C)	109.5	P(1)-C(23)-H(23B)	109.5
H(13A)-C(13)-H(13C)	109.5	H(23A)-C(23)-H(23B)	109.5
H(13B)-C(13)-H(13C)	109.5	P(1)-C(23)-H(23C)	109.5
C(7)-C(14)-H(14A)	109.5	H(23A)-C(23)-H(23C)	109.5
C(7)-C(14)-H(14B)	109.5	H(23B)-C(23)-H(23C)	109.5
H(14A)-C(14)-H(14B)	109.5	P(1)-C(24)-H(24A)	109.5
C(7)-C(14)-H(14C)	109.5	P(1)-C(24)-H(24B)	109.5
H(14A)-C(14)-H(14C)	109.5	H(24A)-C(24)-H(24B)	109.5
H(14B)-C(14)-H(14C)	109.5	P(1)-C(24)-H(24C)	109.5
C(9)-C(15)-H(15A)	109.5	H(24A)-C(24)-H(24C)	109.5
C(9)-C(15)-H(15B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(15A)-C(15)-H(15B)	109.5		

Table S34. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3g**. 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}
Rh1	24(1)	25(1)	18(1)	-1(1)	0(1)	0(1)

N1	26(2)	28(2)	20(1)	1(1)	-3(1)	2(1)
N2	26(2)	31(2)	16(1)	1(1)	-1(1)	-2(1)
N3	24(1)	24(2)	24(1)	-4(1)	-2(1)	-1(1)
N4	22(2)	37(2)	22(2)	-2(1)	-5(1)	5(1)
N5	26(2)	29(2)	19(1)	-1(1)	-4(1)	2(1)
N6	28(2)	26(2)	22(1)	1(1)	-2(1)	2(1)
B1	31(2)	32(2)	20(2)	1(2)	-1(2)	3(2)
C1	21(2)	28(2)	23(2)	-8(2)	-2(1)	-1(2)
C2	29(2)	37(2)	22(2)	-4(2)	3(2)	-7(2)
C3	30(2)	32(2)	19(2)	-2(2)	-2(1)	-6(2)
C4	26(2)	34(2)	34(2)	-12(2)	-1(2)	2(2)
C5	25(2)	42(2)	33(2)	-14(2)	-4(2)	-1(2)
C6	26(2)	43(2)	25(2)	-9(2)	-6(2)	9(2)
C7	24(2)	31(2)	30(2)	-5(2)	-1(2)	2(2)
C8	32(2)	29(2)	35(2)	-8(2)	0(2)	7(2)
C9	26(2)	31(2)	30(2)	3(2)	-2(2)	2(2)
C10	30(2)	37(2)	31(2)	3(2)	3(2)	7(2)
C11	39(2)	42(2)	20(2)	5(2)	-1(2)	-6(2)
C12	28(2)	31(2)	52(3)	-5(2)	1(2)	-3(2)
C13	39(2)	59(3)	26(2)	-8(2)	-6(2)	11(2)
C14	32(2)	37(2)	29(2)	-6(2)	1(2)	7(2)
C15	46(3)	34(2)	41(2)	6(2)	-2(2)	10(2)
C16	22(2)	28(2)	28(2)	1(1)	-1(1)	-3(1)
C17	36(2)	31(2)	27(2)	0(2)	-2(2)	-1(2)
F1	59(2)	38(1)	26(1)	4(1)	1(1)	-8(1)
C18	49(3)	31(2)	35(2)	7(2)	-11(2)	-3(2)
C19	40(2)	25(2)	44(2)	-6(2)	-8(2)	-3(2)
C20	27(2)	34(2)	31(2)	-12(2)	-1(2)	0(2)
F2	45(1)	42(1)	36(1)	-18(1)	2(1)	-2(1)
C21	21(2)	27(2)	31(2)	-1(2)	0(2)	-2(2)
P1	27(1)	27(1)	20(1)	0(1)	-2(1)	1(1)
C22	32(2)	38(2)	29(2)	-1(2)	-5(2)	-6(2)
C23	41(2)	41(2)	20(2)	2(2)	-3(2)	4(2)
C24	39(2)	44(3)	28(2)	1(2)	-3(2)	8(2)

Table S35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3g**.

	x	y	z	U(eq)
H1	6640(40)	2830(30)	10290(20)	45(13)
H1B	6910(40)	4880(30)	7890(20)	33
H2	11202	3670	7691	35
H5	3757	2456	7862	40
H8	6133	6446	10226	39
H10A	10319	2008	9229	49
H10B	11516	2691	9303	49
H10C	11314	2067	8556	49
H11A	8385	4824	6892	51
H11B	9904	4907	6824	51
H11C	9173	5549	7408	51
H12A	5040	1888	9836	56
H12B	5091	1152	9160	56

H12C	3787	1687	9310	56
H13A	4834	4630	7223	63
H13B	4221	3747	6809	63
H13C	5729	3933	6779	63
H14A	6433	4209	11197	49
H14B	6018	5241	11373	49
H14C	7502	4965	11400	49
H15A	5684	6210	8209	61
H15B	7121	6579	8318	61
H15C	5997	7041	8782	61
H18	7532	-319	10457	47
H19	7605	-861	9182	44
H21	7915	1745	8458	32
H22A	10637	4077	11188	49
H22B	9470	4638	10800	49
H22C	10481	4135	10276	49
H23A	9194	2962	12085	51
H23B	7893	2497	11769	51
H23C	7996	3588	11830	51
H24A	10670	2207	11343	55
H24B	10915	2298	10448	55
H24C	9871	1589	10740	55

Table S36. Torsion angles [°] for **3g**.

C16-Rh1-N1-C1	-52.3(4)	C16-Rh1-N5-N6	-60.1(8)
N3-Rh1-N1-C1	-139.2(4)	N3-Rh1-N5-N6	-46.9(2)
N5-Rh1-N1-C1	137.5(4)	P1-Rh1-N5-N6	138.5(2)
P1-Rh1-N1-C1	41.2(4)	N1-Rh1-N5-N6	39.5(2)
C16-Rh1-N1-N2	133.8(2)	C7-N5-N6-C9	1.6(4)
N3-Rh1-N1-N2	47.0(2)	Rh1-N5-N6-C9	173.4(2)
N5-Rh1-N1-N2	-36.4(2)	C7-N5-N6-B1	-169.9(3)
P1-Rh1-N1-N2	-132.7(2)	Rh1-N5-N6-B1	1.9(4)
C1-N1-N2-C3	-0.2(4)	C3-N2-B1-N4	121.5(4)
Rh1-N1-N2-C3	175.6(2)	N1-N2-B1-N4	-53.1(4)
C1-N1-N2-B1	175.3(3)	C3-N2-B1-N6	-118.6(4)
Rh1-N1-N2-B1	-8.9(4)	N1-N2-B1-N6	66.8(4)
C16-Rh1-N3-C4	45.4(3)	C6-N4-B1-N2	-120.3(4)
N5-Rh1-N3-C4	-132.4(3)	N3-N4-B1-N2	68.2(4)
P1-Rh1-N3-C4	-44.7(12)	C6-N4-B1-N6	119.4(4)
N1-Rh1-N3-C4	139.0(3)	N3-N4-B1-N6	-52.2(4)
C16-Rh1-N3-N4	-129.9(3)	C9-N6-B1-N2	126.9(4)
N5-Rh1-N3-N4	52.3(2)	N5-N6-B1-N2	-63.5(4)
P1-Rh1-N3-N4	140.0(9)	C9-N6-B1-N4	-112.5(4)
N1-Rh1-N3-N4	-36.2(2)	N5-N6-B1-N4	57.1(4)
C4-N3-N4-C6	-0.7(4)	N2-N1-C1-C2	0.9(4)
Rh1-N3-N4-C6	175.7(2)	Rh1-N1-C1-C2	-173.4(3)
C4-N3-N4-B1	172.4(3)	N2-N1-C1-C10	-177.1(3)
Rh1-N3-N4-B1	-11.1(4)	Rh1-N1-C1-C10	8.7(6)
C16-Rh1-N5-C7	108.4(8)	N1-C1-C2-C3	-1.2(4)
N3-Rh1-N5-C7	121.6(4)	C10-C1-C2-C3	176.7(4)
P1-Rh1-N5-C7	-53.0(4)	N1-N2-C3-C2	-0.5(4)
N1-Rh1-N5-C7	-152.0(4)	B1-N2-C3-C2	-175.5(3)

N1-N2-C3-C11	-179.4(3)	N1-Rh1-C16-C17	151.3(3)
B1-N2-C3-C11	5.6(6)	N3-Rh1-C16-C21	48.4(3)
C1-C2-C3-N2	1.0(4)	N5-Rh1-C16-C21	61.5(9)
C1-C2-C3-C11	179.8(4)	P1-Rh1-C16-C21	-136.9(3)
N4-N3-C4-C5	0.4(4)	N1-Rh1-C16-C21	-37.6(3)
Rh1-N3-C4-C5	-175.2(3)	C21-C16-C17-C18	-0.5(6)
N4-N3-C4-C12	-178.5(3)	Rh1-C16-C17-C18	171.1(3)
Rh1-N3-C4-C12	5.9(6)	C21-C16-C17-F1	-177.9(3)
N3-C4-C5-C6	0.1(4)	Rh1-C16-C17-F1	-6.4(5)
C12-C4-C5-C6	178.9(4)	C16-C17-C18-C19	-0.5(7)
N3-N4-C6-C5	0.8(4)	F1-C17-C18-C19	177.0(4)
B1-N4-C6-C5	-171.5(4)	C17-C18-C19-C20	0.6(6)
N3-N4-C6-C13	-179.8(3)	C18-C19-C20-C21	0.3(6)
B1-N4-C6-C13	8.0(6)	C18-C19-C20-F2	-178.3(3)
C4-C5-C6-N4	-0.5(4)	C19-C20-C21-C16	-1.4(6)
C4-C5-C6-C13	-179.9(4)	F2-C20-C21-C16	177.2(3)
N6-N5-C7-C8	-2.2(4)	C17-C16-C21-C20	1.4(5)
Rh1-N5-C7-C8	-171.5(3)	Rh1-C16-C21-C20	-171.0(3)
N6-N5-C7-C14	176.2(3)	C16-Rh1-P1-C22	144.18(18)
Rh1-N5-C7-C14	7.0(6)	N3-Rh1-P1-C22	-126.0(10)
N5-C7-C8-C9	2.0(5)	N5-Rh1-P1-C22	-38.94(17)
C14-C7-C8-C9	-176.4(4)	N1-Rh1-P1-C22	50.21(17)
N5-N6-C9-C8	-0.3(4)	C16-Rh1-P1-C24	25.8(2)
B1-N6-C9-C8	170.2(4)	N3-Rh1-P1-C24	115.7(10)
N5-N6-C9-C15	179.3(3)	N5-Rh1-P1-C24	-157.28(19)
B1-N6-C9-C15	-10.1(6)	N1-Rh1-P1-C24	-68.12(19)
C7-C8-C9-N6	-1.0(4)	C16-Rh1-P1-C23	-95.39(19)
C7-C8-C9-C15	179.4(4)	N3-Rh1-P1-C23	-5.6(10)
N3-Rh1-C16-C17	-122.7(3)	N5-Rh1-P1-C23	81.49(18)
N5-Rh1-C16-C17	-109.6(8)	N1-Rh1-P1-C23	170.64(18)
P1-Rh1-C16-C17	52.0(3)		

Table S37. Crystal data and structure refinement for [Tp'$RhCl_2(PPhMe_2)$].

Identification code	[Tp'$RhCl_2(PPhMe_2)$]	
Empirical formula	$C_{23}H_{33}BCl_2N_6PRh$	
Formula weight	609.14	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.3576(19) Å	α = 90°
	b = 13.122(2) Å	β = 105.373(3)°
	c = 18.725(3) Å	γ = 90°
Volume	2690.8(8) $Å^3$	
Z	4	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	0.916 mm^{-1}	
F(000)	1248	
Crystal color, morphology	colorless, plate	
Crystal size	0.18 x 0.14 x 0.04 mm^3	
Theta range for data collection	1.90 to 36.32°	
Index ranges	$-18 \le h \le 18$, $-21 \le k \le 21$, $-31 \le l \le 31$	

Reflections collected	61181
Independent reflections	12968 [*R*(int) = 0.1263]
Observed reflections	7915
Completeness to theta = 36.32°	99.5%
Absorption correction	Multi-scan
Max. and min. transmission	0.9643 and 0.8524
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12968 / 0 / 315
Goodness-of-fit on F^2	0.994
Final *R* indices [*I*>2sigma(*I*)]	R_1 = 0.0533, wR_2 = 0.0883
R indices (all data)	R_1 = 0.1119, wR_2 = 0.1054
Largest diff. peak and hole	0.743 and -0.878 e.Å^{-3}

Table S38. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for [Tp'RhCl$_2$(PPhMe$_2$)]. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	1610(1)	145(1)	8317(1)	12(1)
Cl1	3468(1)	10(1)	8002(1)	18(1)
Cl2	2656(1)	1184(1)	9292(1)	19(1)
P1	1041(1)	1586(1)	7631(1)	15(1)
N1	48(2)	140(2)	8708(1)	14(1)
N2	-687(2)	-710(2)	8504(1)	14(1)
N3	1996(2)	-1231(2)	8948(1)	14(1)
N4	1069(2)	-1932(2)	8802(1)	13(1)
N5	839(2)	-773(2)	7401(1)	14(1)
N6	37(2)	-1514(2)	7490(1)	14(1)
B1	-167(3)	-1680(2)	8251(2)	15(1)
C1	-504(2)	730(2)	9114(1)	16(1)
C2	-1596(3)	276(2)	9146(2)	20(1)
C3	-1690(2)	-621(2)	8757(2)	19(1)
C4	2932(2)	-1639(2)	9459(1)	16(1)
C5	2608(2)	-2618(2)	9636(1)	16(1)
C6	1433(2)	-2780(2)	9212(1)	15(1)
C7	920(2)	-850(2)	6697(1)	16(1)
C8	173(3)	-1636(2)	6349(2)	19(1)
C9	-369(3)	-2043(2)	6857(2)	18(1)
C10	-29(3)	1685(2)	9524(2)	21(1)
C11	-2680(3)	-1398(2)	8622(2)	28(1)
C12	4106(2)	-1086(2)	9768(2)	19(1)
C13	644(3)	-3697(2)	9168(2)	23(1)
C14	1724(3)	-234(2)	6349(2)	19(1)
C15	-1216(3)	-2935(2)	6778(2)	29(1)
C16	-1242(3)	822(2)	6900(2)	19(1)
C17	-2224(3)	641(2)	6296(2)	24(1)
C18	-2219(3)	1009(2)	5604(2)	25(1)
C19	-1230(3)	1570(2)	5519(2)	24(1)
C20	-239(3)	1738(2)	6125(2)	20(1)
C21	-234(2)	1364(2)	6820(1)	16(1)
C22	455(3)	2639(2)	8063(2)	22(1)
C23	2244(3)	2214(2)	7343(2)	20(1)

Table S39. Bond lengths [Å] and angles [°] for [Tp'$RhCl_2(PPhMe_2)$].

Rh(1)-N(5)	2.088(2)	C(14)-H(14C)	0.9800
Rh(1)-N(1)	2.091(2)	C(15)-H(15A)	0.9800
Rh(1)-N(3)	2.139(2)	C(15)-H(15B)	0.9800
Rh(1)-P(1)	2.2807(8)	C(15)-H(15C)	0.9800
Rh(1)-Cl(2)	2.3365(7)	C(16)-C(17)	1.382(4)
Rh(1)-Cl(1)	2.3439(7)	C(16)-C(21)	1.390(4)
P(1)-C(23)	1.797(3)	C(16)-H(16A)	0.9500
P(1)-C(22)	1.815(3)	C(17)-C(18)	1.385(4)
P(1)-C(21)	1.822(3)	C(17)-H(17A)	0.9500
N(1)-C(1)	1.351(3)	C(18)-C(19)	1.387(4)
N(1)-N(2)	1.384(3)	C(18)-H(18A)	0.9500
N(2)-C(3)	1.350(3)	C(19)-C(20)	1.387(4)
N(2)-B(1)	1.530(4)	C(19)-H(19A)	0.9500
N(3)-C(4)	1.339(3)	C(20)-C(21)	1.389(4)
N(3)-N(4)	1.370(3)	C(20)-H(20A)	0.9500
N(4)-C(6)	1.353(3)	C(22)-H(22A)	0.9800
N(4)-B(1)	1.541(4)	C(22)-H(22B)	0.9800
N(5)-C(7)	1.349(3)	C(22)-H(22C)	0.9800
N(5)-N(6)	1.373(3)	C(23)-H(23A)	0.9800
N(6)-C(9)	1.346(3)	C(23)-H(23B)	0.9800
N(6)-B(1)	1.519(4)	C(23)-H(23C)	0.9800
B(1)-H(1B)	1.0000		
C(1)-C(2)	1.391(4)	N(5)-Rh(1)-N(1)	94.36(8)
C(1)-C(10)	1.494(4)	N(5)-Rh(1)-N(3)	86.99(8)
C(2)-C(3)	1.374(4)	N(1)-Rh(1)-N(3)	82.70(8)
C(2)-H(2A)	0.9500	N(5)-Rh(1)-P(1)	91.22(6)
C(3)-C(11)	1.489(4)	N(1)-Rh(1)-P(1)	93.40(6)
C(4)-C(5)	1.399(4)	N(3)-Rh(1)-P(1)	175.57(6)
C(4)-C(12)	1.493(4)	N(5)-Rh(1)-Cl(2)	173.86(6)
C(5)-C(6)	1.377(4)	N(1)-Rh(1)-Cl(2)	91.77(6)
C(5)-H(5A)	0.9500	N(3)-Rh(1)-Cl(2)	94.21(6)
C(6)-C(13)	1.490(4)	P(1)-Rh(1)-Cl(2)	88.00(3)
C(7)-C(8)	1.384(4)	N(5)-Rh(1)-Cl(1)	87.67(6)
C(7)-C(14)	1.493(4)	N(1)-Rh(1)-Cl(1)	172.81(6)
C(8)-C(9)	1.372(4)	N(3)-Rh(1)-Cl(1)	90.53(6)
C(8)-H(8A)	0.9500	P(1)-Rh(1)-Cl(1)	93.45(3)
C(9)-C(15)	1.497(4)	Cl(2)-Rh(1)-Cl(1)	86.29(3)
C(10)-H(10A)	0.9800	C(23)-P(1)-C(22)	100.51(14)
C(10)-H(10B)	0.9800	C(23)-P(1)-C(21)	108.78(13)
C(10)-H(10C)	0.9800	C(22)-P(1)-C(21)	100.89(13)
C(11)-H(11A)	0.9800	C(23)-P(1)-Rh(1)	115.17(10)
C(11)-H(11B)	0.9800	C(22)-P(1)-Rh(1)	117.59(10)
C(11)-H(11C)	0.9800	C(21)-P(1)-Rh(1)	112.37(9)
C(12)-H(12A)	0.9800	C(1)-N(1)-N(2)	106.3(2)
C(12)-H(12B)	0.9800	C(1)-N(1)-Rh(1)	139.42(18)
C(12)-H(12C)	0.9800	N(2)-N(1)-Rh(1)	114.29(15)
C(13)-H(13A)	0.9800	C(3)-N(2)-N(1)	109.7(2)
C(13)-H(13B)	0.9800	C(3)-N(2)-B(1)	127.7(2)
C(13)-H(13C)	0.9800	N(1)-N(2)-B(1)	120.1(2)
C(14)-H(14A)	0.9800	C(4)-N(3)-N(4)	107.3(2)
C(14)-H(14B)	0.9800	C(4)-N(3)-Rh(1)	137.76(18)

N(4)-N(3)-Rh(1)	114.94(15)	C(4)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.6(2)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	130.1(2)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	120.3(2)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.5(2)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	136.35(18)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	117.11(15)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	110.0(2)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	130.6(2)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	119.2(2)	C(6)-C(13)-H(13C)	109.5
N(6)-B(1)-N(2)	109.7(2)	H(13A)-C(13)-H(13C)	109.5
N(6)-B(1)-N(4)	108.6(2)	H(13B)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	109.3(2)	C(7)-C(14)-H(14A)	109.5
N(6)-B(1)-H(1B)	109.7	C(7)-C(14)-H(14B)	109.5
N(2)-B(1)-H(1B)	109.7	H(14A)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.7	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	109.4(2)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	127.7(2)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	122.8(2)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	106.8(2)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2A)	126.6	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2A)	126.6	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	107.8(2)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(11)	123.5(3)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	128.7(3)	C(17)-C(16)-C(21)	120.6(3)
N(3)-C(4)-C(5)	109.1(2)	C(17)-C(16)-H(16A)	119.7
N(3)-C(4)-C(12)	122.7(2)	C(21)-C(16)-H(16A)	119.7
C(5)-C(4)-C(12)	128.2(2)	C(16)-C(17)-C(18)	120.2(3)
C(6)-C(5)-C(4)	106.3(2)	C(16)-C(17)-H(17A)	119.9
C(6)-C(5)-H(5A)	126.8	C(18)-C(17)-H(17A)	119.9
C(4)-C(5)-H(5A)	126.8	C(17)-C(18)-C(19)	119.8(3)
N(4)-C(6)-C(5)	107.7(2)	C(17)-C(18)-H(18A)	120.1
N(4)-C(6)-C(13)	122.9(2)	C(19)-C(18)-H(18A)	120.1
C(5)-C(6)-C(13)	129.3(2)	C(18)-C(19)-C(20)	119.8(3)
N(5)-C(7)-C(8)	109.0(2)	C(18)-C(19)-H(19A)	120.1
N(5)-C(7)-C(14)	126.4(2)	C(20)-C(19)-H(19A)	120.1
C(8)-C(7)-C(14)	124.6(2)	C(19)-C(20)-C(21)	120.7(3)
C(9)-C(8)-C(7)	107.2(2)	C(19)-C(20)-H(20A)	119.6
C(9)-C(8)-H(8A)	126.4	C(21)-C(20)-H(20A)	119.6
C(7)-C(8)-H(8A)	126.4	C(20)-C(21)-C(16)	118.9(3)
N(6)-C(9)-C(8)	107.4(2)	C(20)-C(21)-P(1)	122.0(2)
N(6)-C(9)-C(15)	123.5(3)	C(16)-C(21)-P(1)	119.1(2)
C(8)-C(9)-C(15)	129.1(3)	P(1)-C(22)-H(22A)	109.5
C(1)-C(10)-H(10A)	109.5	P(1)-C(22)-H(22B)	109.5
C(1)-C(10)-H(10B)	109.5	H(22A)-C(22)-H(22B)	109.5
H(10A)-C(10)-H(10B)	109.5	P(1)-C(22)-H(22C)	109.5
C(1)-C(10)-H(10C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(10B)-C(10)-H(10C)	109.5	P(1)-C(23)-H(23A)	109.5
C(3)-C(11)-H(11A)	109.5	P(1)-C(23)-H(23B)	109.5
C(3)-C(11)-H(11B)	109.5	H(23A)-C(23)-H(23B)	109.5
H(11A)-C(11)-H(11B)	109.5	P(1)-C(23)-H(23C)	109.5
C(3)-C(11)-H(11C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(23B)-C(23)-H(23C)	109.5
H(11B)-C(11)-H(11C)	109.5		

Table S40. Anisotropic displacement parameters ($Å^2$ x 10^3) for [Tp'$RhCl_2$($PPhMe_2$)]. 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}
Rh1	12(1)	11(1)	12(1)	-1(1)	3(1)	-1(1)
Cl1	16(1)	19(1)	22(1)	-1(1)	8(1)	-1(1)
Cl2	18(1)	18(1)	18(1)	-5(1)	1(1)	-2(1)
P1	16(1)	13(1)	15(1)	0(1)	4(1)	-1(1)
N1	16(1)	12(1)	14(1)	0(1)	4(1)	-1(1)
N2	14(1)	14(1)	17(1)	2(1)	4(1)	0(1)
N3	13(1)	14(1)	13(1)	-1(1)	2(1)	-2(1)
N4	14(1)	12(1)	14(1)	0(1)	5(1)	-1(1)
N5	15(1)	13(1)	14(1)	-1(1)	4(1)	-2(1)
N6	14(1)	14(1)	13(1)	-1(1)	2(1)	-2(1)
B1	14(1)	14(1)	17(1)	2(1)	4(1)	-3(1)
C1	18(1)	17(1)	15(1)	2(1)	5(1)	5(1)
C2	19(1)	22(1)	24(1)	4(1)	12(1)	5(1)
C3	15(1)	22(1)	21(1)	7(1)	7(1)	3(1)
C4	17(1)	16(1)	14(1)	-1(1)	4(1)	1(1)
C5	17(1)	16(1)	16(1)	1(1)	4(1)	3(1)
C6	17(1)	13(1)	15(1)	1(1)	5(1)	1(1)
C7	16(1)	17(1)	14(1)	-1(1)	4(1)	2(1)
C8	20(1)	21(1)	14(1)	-5(1)	1(1)	1(1)
C9	19(1)	18(1)	15(1)	-2(1)	0(1)	-2(1)
C10	28(2)	20(1)	17(1)	-3(1)	8(1)	4(1)
C11	18(1)	26(2)	43(2)	4(1)	14(1)	0(1)
C12	17(1)	20(1)	18(1)	-2(1)	1(1)	0(1)
C13	21(1)	15(1)	30(2)	6(1)	3(1)	-1(1)
C14	23(1)	19(1)	17(1)	-1(1)	8(1)	-1(1)
C15	31(2)	30(2)	26(2)	-8(1)	8(1)	-15(1)
C16	20(1)	18(1)	19(1)	3(1)	4(1)	0(1)
C17	18(1)	22(1)	29(2)	1(1)	1(1)	-2(1)
C18	21(2)	27(2)	21(1)	-4(1)	-4(1)	4(1)
C19	26(2)	29(2)	16(1)	1(1)	5(1)	6(1)
C20	19(1)	21(1)	21(1)	2(1)	6(1)	2(1)
C21	16(1)	14(1)	16(1)	1(1)	4(1)	3(1)
C22	27(2)	17(1)	24(1)	0(1)	10(1)	4(1)
C23	17(1)	21(1)	23(1)	3(1)	6(1)	-4(1)

Table S41. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Tp'$RhCl_2$($PPhMe_2$)].

	x	y	z	U(eq)
H1B	-749	-2258	8231	18
H2A	-2166	536	9391	24
H5A	3101	-3079	9980	19
H8A	57	-1852	5851	23

H10A	776	1844	9454	32
H10B	42	1589	10053	32
H10C	-592	2248	9335	32
H11A	-2936	-1567	8094	42
H11B	-3378	-1125	8776	42
H11C	-2378	-2014	8909	42
H12A	4310	-687	9375	29
H12B	4758	-1579	9967	29
H12C	4019	-628	10165	29
H13A	-119	-3504	9282	34
H13B	1071	-4208	9525	34
H13C	462	-3983	8666	34
H14A	1998	377	6648	29
H14B	1267	-33	5848	29
H14C	2435	-641	6323	29
H15A	-1875	-2775	7008	44
H15B	-763	-3531	7022	44
H15C	-1565	-3084	6251	44
H16A	-1256	573	7374	23
H17A	-2905	263	6356	29
H18A	-2890	877	5188	30
H19A	-1231	1838	5048	28
H20A	443	2113	6064	24
H22A	341	3235	7737	34
H22B	1036	2805	8537	34
H22C	-330	2446	8149	34
H23A	1937	2856	7096	30
H23B	2525	1774	6999	30
H23C	2925	2356	7777	30

Table S42. Torsion angles [°] for [Tp'$RhCl_2(PPhMe_2)$].

N5-Rh1-P1-C23	-102.47(12)	N3-Rh1-N1-N2	-59.77(16)
N1-Rh1-P1-C23	163.08(12)	P1-Rh1-N1-N2	118.12(15)
N3-Rh1-P1-C23	-168.6(8)	Cl2-Rh1-N1-N2	-153.78(15)
Cl2-Rh1-P1-C23	71.43(11)	Cl1-Rh1-N1-N2	-79.6(5)
Cl1-Rh1-P1-C23	-14.73(11)	C1-N1-N2-C3	2.4(3)
N5-Rh1-P1-C22	139.30(13)	Rh1-N1-N2-C3	-177.55(16)
N1-Rh1-P1-C22	44.86(13)	C1-N1-N2-B1	-161.0(2)
N3-Rh1-P1-C22	73.2(8)	Rh1-N1-N2-B1	19.1(3)
Cl2-Rh1-P1-C22	-46.79(12)	N5-Rh1-N3-C4	135.1(3)
Cl1-Rh1-P1-C22	-132.96(12)	N1-Rh1-N3-C4	-130.1(3)
N5-Rh1-P1-C21	22.84(11)	P1-Rh1-N3-C4	-158.6(6)
N1-Rh1-P1-C21	-71.60(11)	Cl2-Rh1-N3-C4	-38.8(3)
N3-Rh1-P1-C21	-43.3(8)	Cl1-Rh1-N3-C4	47.5(3)
Cl2-Rh1-P1-C21	-163.25(10)	N5-Rh1-N3-N4	-43.00(17)
Cl1-Rh1-P1-C21	110.58(10)	N1-Rh1-N3-N4	51.79(17)
N5-Rh1-N1-C1	-153.3(3)	P1-Rh1-N3-N4	23.3(9)
N3-Rh1-N1-C1	120.3(3)	Cl2-Rh1-N3-N4	143.04(16)
P1-Rh1-N1-C1	-61.8(3)	Cl1-Rh1-N3-N4	-130.64(16)
Cl2-Rh1-N1-C1	26.3(3)	C4-N3-N4-C6	-0.9(3)
Cl1-Rh1-N1-C1	100.5(5)	Rh1-N3-N4-C6	177.79(16)
N5-Rh1-N1-N2	26.63(17)	C4-N3-N4-B1	177.8(2)

Rh1-N3-N4-B1	-3.5(3)	N4-N3-C4-C5	0.7(3)
N1-Rh1-N5-C7	146.0(3)	Rh1-N3-C4-C5	-177.48(19)
N3-Rh1-N5-C7	-131.6(3)	N4-N3-C4-C12	-179.0(2)
P1-Rh1-N5-C7	52.5(3)	Rh1-N3-C4-C12	2.8(4)
Cl2-Rh1-N5-C7	-30.2(7)	N3-C4-C5-C6	-0.3(3)
Cl1-Rh1-N5-C7	-40.9(3)	C12-C4-C5-C6	179.3(3)
N1-Rh1-N5-N6	-34.50(18)	N3-N4-C6-C5	0.7(3)
N3-Rh1-N5-N6	47.94(17)	B1-N4-C6-C5	-177.9(2)
P1-Rh1-N5-N6	-128.01(17)	N3-N4-C6-C13	-178.5(2)
Cl2-Rh1-N5-N6	149.3(5)	B1-N4-C6-C13	2.9(4)
Cl1-Rh1-N5-N6	138.59(17)	C4-C5-C6-N4	-0.2(3)
C7-N5-N6-C9	0.2(3)	C4-C5-C6-C13	178.9(3)
Rh1-N5-N6-C9	-179.41(17)	N6-N5-C7-C8	0.0(3)
C7-N5-N6-B1	174.9(2)	Rh1-N5-C7-C8	179.50(19)
Rh1-N5-N6-B1	-4.8(3)	N6-N5-C7-C14	-177.2(2)
C9-N6-B1-N2	-125.2(3)	Rh1-N5-C7-C14	2.4(4)
N5-N6-B1-N2	61.4(3)	N5-C7-C8-C9	-0.2(3)
C9-N6-B1-N4	115.4(3)	C14-C7-C8-C9	177.0(3)
N5-N6-B1-N4	-58.0(3)	N5-N6-C9-C8	-0.3(3)
C3-N2-B1-N6	128.4(3)	B1-N6-C9-C8	-174.2(3)
N1-N2-B1-N6	-71.5(3)	N5-N6-C9-C15	177.3(3)
C3-N2-B1-N4	-112.6(3)	B1-N6-C9-C15	3.4(5)
N1-N2-B1-N4	47.5(3)	C7-C8-C9-N6	0.3(3)
C6-N4-B1-N6	-118.5(3)	C7-C8-C9-C15	-177.1(3)
N3-N4-B1-N6	63.1(3)	C21-C16-C17-C18	-0.6(4)
C6-N4-B1-N2	121.8(3)	C16-C17-C18-C19	-0.8(5)
N3-N4-B1-N2	-56.6(3)	C17-C18-C19-C20	1.6(4)
N2-N1-C1-C2	-2.0(3)	C18-C19-C20-C21	-1.1(4)
Rh1-N1-C1-C2	177.9(2)	C19-C20-C21-C16	-0.3(4)
N2-N1-C1-C10	173.8(2)	C19-C20-C21-P1	-179.1(2)
Rh1-N1-C1-C10	-6.3(4)	C17-C16-C21-C20	1.1(4)
N1-C1-C2-C3	1.0(3)	C17-C16-C21-P1	179.9(2)
C10-C1-C2-C3	-175.1(2)	C23-P1-C21-C20	-5.7(3)
N1-N2-C3-C2	-1.8(3)	C22-P1-C21-C20	99.5(2)
B1-N2-C3-C2	159.9(2)	Rh1-P1-C21-C20	-134.4(2)
N1-N2-C3-C11	178.9(2)	C23-P1-C21-C16	175.6(2)
B1-N2-C3-C11	-19.3(4)	C22-P1-C21-C16	-79.2(2)
C1-C2-C3-N2	0.5(3)	Rh1-P1-C21-C16	46.9(2)
C1-C2-C3-C11	179.8(3)		

Table S43. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	$C_{23}H_{35}BN_6PRh$	
Formula weight	540.26	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.4148(12) Å	α = 90°
	b = 15.6111(16) Å	β = 107.784(2)°
	c = 14.8282(15) Å	γ = 90°
Volume	2516.1(4) Å^3	

Z	4
Density (calculated)	1.426 Mg/m^3
Absorption coefficient	0.765 mm^{-1}
F(000)	1120
Crystal color, morphology	colorless, block
Crystal size	0.18 x 0.12 x 0.06 mm^3
Theta range for data collection	1.87 to 37.78°
Index ranges	$-19 \le h \le 19$, $-26 \le k \le 26$, $-25 \le l \le 25$
Reflections collected	60723
Independent reflections	13296 [*R*(int) = 0.0989]
Observed reflections	8337
Completeness to theta = 37.78°	98.5%
Absorption correction	Multi-scan
Max. and min. transmission	0.9555 and 0.8746
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13296 / 0 / 305
Goodness-of-fit on F^2	0.993
Final *R* indices [*I*>2sigma(*I*)]	R_1 = 0.0499, wR_2 = 0.0890
R indices (all data)	R_1 = 0.1023, wR_2 = 0.1064
Largest diff. peak and hole	1.210 and -0.655 e.$Å^{-3}$

Table S44. 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}
Rh1	8716(1)	2281(1)	6780(1)	15(1)
P1	6735(1)	2606(1)	6454(1)	20(1)
N1	9302(2)	1780(1)	8263(1)	18(1)
N2	10482(2)	1966(1)	8809(1)	18(1)
N3	10451(2)	1849(1)	6754(1)	17(1)
N4	11471(2)	1956(1)	7522(1)	18(1)
N5	9687(2)	3448(1)	7406(1)	18(1)
N6	10821(2)	3353(1)	8062(1)	18(1)
B1	11349(2)	2456(2)	8385(2)	20(1)
C1	8819(2)	1277(2)	8792(2)	22(1)
C2	9682(2)	1143(2)	9677(2)	25(1)
C3	10725(2)	1587(1)	9666(2)	22(1)
C4	10795(2)	1380(1)	6123(2)	19(1)
C5	12041(2)	1170(2)	6495(2)	23(1)
C6	12443(2)	1549(2)	7377(2)	22(1)
C7	9512(2)	4290(1)	7259(2)	21(1)
C8	10533(2)	4740(2)	7814(2)	25(1)
C9	11344(2)	4131(2)	8311(2)	22(1)
C10	7556(2)	927(2)	8430(2)	30(1)
C11	11926(2)	1644(2)	10424(2)	30(1)
C12	9906(2)	1154(2)	5189(2)	24(1)
C13	13688(2)	1527(2)	8090(2)	30(1)
C14	8370(2)	4654(2)	6586(2)	28(1)
C15	12575(2)	4250(2)	9031(2)	31(1)
C16	7040(2)	3360(2)	8212(2)	23(1)
C17	6700(2)	3853(2)	8873(2)	28(1)
C18	5578(2)	4264(2)	8621(2)	29(1)
C19	4791(3)	4172(2)	7713(2)	45(1)
C20	5123(3)	3671(2)	7062(2)	42(1)

C21	6256(2)	3263(2)	7300(2)	22(1)
C22	6050(2)	3156(2)	5326(2)	32(1)
C23	5633(2)	1717(2)	6243(2)	33(1)

Table S45. Bond lengths [Å] and angles [°] for **5**.

Rh(1)-N(3)	2.1036(18)	C(13)-H(13B)	0.9800
Rh(1)-N(5)	2.1863(18)	C(13)-H(13C)	0.9800
Rh(1)-P(1)	2.2218(6)	C(14)-H(14A)	0.9800
Rh(1)-N(1)	2.2341(18)	C(14)-H(14B)	0.9800
Rh(1)-H(1)	1.49(3)	C(14)-H(14C)	0.9800
Rh(1)-H(2)	1.50(3)	C(15)-H(15A)	0.9800
P(1)-C(21)	1.829(2)	C(15)-H(15B)	0.9800
P(1)-C(22)	1.830(2)	C(15)-H(15C)	0.9800
P(1)-C(23)	1.835(3)	C(16)-C(21)	1.383(3)
N(1)-C(1)	1.342(3)	C(16)-C(17)	1.391(3)
N(1)-N(2)	1.375(2)	C(16)-H(16A)	0.9500
N(2)-C(3)	1.352(3)	C(17)-C(18)	1.378(3)
N(2)-B(1)	1.529(3)	C(17)-H(17A)	0.9500
N(3)-C(4)	1.338(3)	C(18)-C(19)	1.378(4)
N(3)-N(4)	1.368(2)	C(18)-H(18A)	0.9500
N(4)-C(6)	1.352(3)	C(19)-C(20)	1.383(4)
N(4)-B(1)	1.541(3)	C(19)-H(19A)	0.9500
N(5)-C(7)	1.338(3)	C(20)-C(21)	1.387(3)
N(5)-N(6)	1.369(3)	C(20)-H(20A)	0.9500
N(6)-C(9)	1.354(3)	C(22)-H(22A)	0.9800
N(6)-B(1)	1.541(3)	C(22)-H(22B)	0.9800
B(1)-H(1B)	1.0000	C(22)-H(22C)	0.9800
C(1)-C(2)	1.395(3)	C(23)-H(23A)	0.9800
C(1)-C(10)	1.481(3)	C(23)-H(23B)	0.9800
C(2)-C(3)	1.382(3)	C(23)-H(23C)	0.9800
C(2)-H(2A)	0.9500	N(3)-Rh(1)-N(5)	85.23(7)
C(3)-C(11)	1.486(3)	N(3)-Rh(1)-P(1)	166.04(5)
C(4)-C(5)	1.398(3)	N(5)-Rh(1)-P(1)	104.60(5)
C(4)-C(12)	1.488(3)	N(3)-Rh(1)-N(1)	84.62(7)
C(5)-C(6)	1.379(3)	N(5)-Rh(1)-N(1)	85.01(7)
C(5)-H(5A)	0.9500	P(1)-Rh(1)-N(1)	105.82(5)
C(6)-C(13)	1.490(3)	N(3)-Rh(1)-H(1)	89.7(11)
C(7)-C(8)	1.394(3)	N(5)-Rh(1)-H(1)	94.5(11)
C(7)-C(14)	1.491(3)	P(1)-Rh(1)-H(1)	79.8(11)
C(8)-C(9)	1.373(3)	N(1)-Rh(1)-H(1)	174.3(11)
C(8)-H(8A)	0.9500	N(3)-Rh(1)-H(2)	90.1(11)
C(9)-C(15)	1.494(3)	N(5)-Rh(1)-H(2)	174.5(11)
C(10)-H(10A)	0.9800	P(1)-Rh(1)-H(2)	79.6(11)
C(10)-H(10B)	0.9800	N(1)-Rh(1)-H(2)	97.5(11)
C(10)-H(10C)	0.9800	H(1)-Rh(1)-H(2)	82.5(15)
C(11)-H(11A)	0.9800	C(21)-P(1)-C(22)	103.28(11)
C(11)-H(11B)	0.9800	C(21)-P(1)-C(23)	102.03(12)
C(11)-H(11C)	0.9800	C(22)-P(1)-C(23)	96.86(13)
C(12)-H(12A)	0.9800	C(21)-P(1)-Rh(1)	118.48(8)
C(12)-H(12B)	0.9800	C(22)-P(1)-Rh(1)	115.38(9)
C(12)-H(12C)	0.9800	C(23)-P(1)-Rh(1)	117.62(9)
C(13)-H(13A)	0.9800	C(1)-N(1)-N(2)	106.42(18)

C(1)-N(1)-Rh(1)	136.68(15)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	116.77(13)	C(3)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	110.11(18)	C(3)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	129.24(19)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	120.32(17)	C(3)-C(11)-H(11C)	109.5
C(4)-N(3)-N(4)	106.99(17)	H(11A)-C(11)-H(11C)	109.5
C(4)-N(3)-Rh(1)	131.89(15)	H(11B)-C(11)-H(11C)	109.5
N(4)-N(3)-Rh(1)	120.77(13)	C(4)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.92(18)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	131.08(19)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	118.95(17)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.47(17)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	135.96(16)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	117.26(13)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	109.81(18)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	129.2(2)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	120.95(17)	C(6)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	108.78(18)	H(13A)-C(13)-H(13C)	109.5
N(2)-B(1)-N(6)	109.94(18)	H(13B)-C(13)-H(13C)	109.5
N(4)-B(1)-N(6)	109.12(18)	C(7)-C(14)-H(14A)	109.5
N(2)-B(1)-H(1B)	109.7	C(7)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.7	H(14A)-C(14)-H(14B)	109.5
N(6)-B(1)-H(1B)	109.7	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	109.9(2)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	122.1(2)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	128.0(2)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	106.1(2)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2A)	126.9	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2A)	126.9	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	107.5(2)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(11)	124.2(2)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	128.3(2)	C(21)-C(16)-C(17)	120.8(2)
N(3)-C(4)-C(5)	109.43(19)	C(21)-C(16)-H(16A)	119.6
N(3)-C(4)-C(12)	121.16(19)	C(17)-C(16)-H(16A)	119.6
C(5)-C(4)-C(12)	129.4(2)	C(18)-C(17)-C(16)	120.2(2)
C(6)-C(5)-C(4)	106.1(2)	C(18)-C(17)-H(17A)	119.9
C(6)-C(5)-H(5A)	126.9	C(16)-C(17)-H(17A)	119.9
C(4)-C(5)-H(5A)	126.9	C(19)-C(18)-C(17)	119.4(2)
N(4)-C(6)-C(5)	107.5(2)	C(19)-C(18)-H(18A)	120.3
N(4)-C(6)-C(13)	123.3(2)	C(17)-C(18)-H(18A)	120.3
C(5)-C(6)-C(13)	129.2(2)	C(18)-C(19)-C(20)	120.4(2)
N(5)-C(7)-C(8)	110.0(2)	C(18)-C(19)-H(19A)	119.8
N(5)-C(7)-C(14)	122.7(2)	C(20)-C(19)-H(19A)	119.8
C(8)-C(7)-C(14)	127.3(2)	C(19)-C(20)-C(21)	121.0(2)
C(9)-C(8)-C(7)	105.9(2)	C(19)-C(20)-H(20A)	119.5
C(9)-C(8)-H(8A)	127.1	C(21)-C(20)-H(20A)	119.5
C(7)-C(8)-H(8A)	127.1	C(16)-C(21)-C(20)	118.3(2)
N(6)-C(9)-C(8)	107.8(2)	C(16)-C(21)-P(1)	119.47(17)
N(6)-C(9)-C(15)	123.1(2)	C(20)-C(21)-P(1)	122.24(19)
C(8)-C(9)-C(15)	129.0(2)	P(1)-C(22)-H(22A)	109.5
C(1)-C(10)-H(10A)	109.5	P(1)-C(22)-H(22B)	109.5
C(1)-C(10)-H(10B)	109.5	H(22A)-C(22)-H(22B)	109.5
H(10A)-C(10)-H(10B)	109.5	P(1)-C(22)-H(22C)	109.5
C(1)-C(10)-H(10C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(22B)-C(22)-H(22C)	109.5

P(1)-C(23)-H(23A)	109.5	P(1)-C(23)-H(23C)	109.5
P(1)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(23B)-C(23)-H(23C)	109.5

Table S46. 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}
Rh1	15(1)	14(1)	15(1)	0(1)	5(1)	1(1)
P1	16(1)	26(1)	17(1)	-1(1)	3(1)	3(1)
N1	18(1)	16(1)	18(1)	-1(1)	6(1)	-1(1)
N2	17(1)	18(1)	18(1)	0(1)	5(1)	1(1)
N3	17(1)	17(1)	17(1)	0(1)	5(1)	0(1)
N4	16(1)	20(1)	18(1)	-1(1)	5(1)	1(1)
N5	20(1)	17(1)	18(1)	0(1)	7(1)	0(1)
N6	19(1)	18(1)	19(1)	-2(1)	7(1)	-2(1)
B1	19(1)	19(1)	20(1)	-3(1)	5(1)	0(1)
C1	26(1)	21(1)	21(1)	0(1)	11(1)	-2(1)
C2	33(1)	24(1)	19(1)	4(1)	11(1)	3(1)
C3	29(1)	20(1)	18(1)	0(1)	6(1)	6(1)
C4	22(1)	18(1)	17(1)	2(1)	8(1)	2(1)
C5	25(1)	25(1)	23(1)	1(1)	11(1)	7(1)
C6	18(1)	24(1)	25(1)	3(1)	8(1)	3(1)
C7	28(1)	17(1)	23(1)	1(1)	15(1)	0(1)
C8	35(1)	18(1)	28(1)	-4(1)	18(1)	-6(1)
C9	25(1)	23(1)	24(1)	-6(1)	13(1)	-8(1)
C10	31(1)	32(1)	31(1)	1(1)	14(1)	-9(1)
C11	32(1)	31(1)	20(1)	2(1)	-2(1)	6(1)
C12	24(1)	27(1)	21(1)	-4(1)	8(1)	2(1)
C13	20(1)	43(2)	28(1)	-1(1)	6(1)	6(1)
C14	34(1)	19(1)	32(1)	1(1)	13(1)	5(1)
C15	31(1)	32(1)	32(1)	-11(1)	13(1)	-15(1)
C16	17(1)	29(1)	23(1)	-3(1)	5(1)	5(1)
C17	21(1)	36(1)	25(1)	-6(1)	6(1)	1(1)
C18	31(1)	31(1)	30(1)	0(1)	15(1)	8(1)
C19	38(2)	68(2)	29(1)	4(1)	8(1)	35(2)
C20	31(1)	69(2)	21(1)	-3(1)	0(1)	28(1)
C21	19(1)	25(1)	21(1)	2(1)	7(1)	6(1)
C22	29(1)	46(2)	18(1)	2(1)	1(1)	11(1)
C23	21(1)	41(2)	35(1)	-5(1)	5(1)	-6(1)

Table S47. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **5**.

	x	y	z	U(eq)
H1	8450(30)	2586(18)	5780(20)	35(8)
H2	8140(30)	1470(18)	6300(20)	36(8)
H1B	12176	2513	8869	24
H2A	9575	814	10185	30

H5A	12515	835	6200	28
H8A	10645	5343	7843	30
H10A	7432	679	7800	45
H10B	6959	1389	8387	45
H10C	7442	483	8862	45
H11A	12163	2246	10542	45
H11B	12555	1339	10223	45
H11C	11852	1383	11005	45
H12A	9471	1672	4891	35
H12B	9311	737	5280	35
H12C	10351	907	4781	35
H13A	14015	2110	8209	45
H13B	14239	1176	7848	45
H13C	13629	1278	8681	45
H14A	8130	4312	6004	42
H14B	8522	5247	6434	42
H14C	7707	4643	6878	42
H15A	13187	3903	8857	46
H15B	12534	4071	9654	46
H15C	12810	4856	9054	46
H16A	7821	3087	8389	28
H17A	7242	3905	9500	33
H18A	5349	4608	9068	35
H19A	4017	4454	7534	54
H20A	4566	3604	6442	50
H22A	5162	3218	5214	49
H22B	6197	2821	4812	49
H22C	6424	3724	5349	49
H23A	4794	1946	6063	49
H23B	5785	1375	6822	49
H23C	5731	1355	5731	49

Table S48. Torsion angles [°] for **5**.

N3-Rh1-P1-C21	-172.9(2)	N5-Rh1-N3-C4	-142.6(2)
N5-Rh1-P1-C21	-39.12(10)	P1-Rh1-N3-C4	-7.1(4)
N1-Rh1-P1-C21	49.75(10)	N1-Rh1-N3-C4	132.0(2)
N3-Rh1-P1-C22	-49.8(2)	N5-Rh1-N3-N4	45.04(15)
N5-Rh1-P1-C22	84.01(12)	P1-Rh1-N3-N4	-179.49(14)
N1-Rh1-P1-C22	172.88(11)	N1-Rh1-N3-N4	-40.39(15)
N3-Rh1-P1-C23	63.6(2)	C4-N3-N4-C6	-0.6(2)
N5-Rh1-P1-C23	-162.58(11)	Rh1-N3-N4-C6	173.44(14)
N1-Rh1-P1-C23	-73.71(11)	C4-N3-N4-B1	-178.36(19)
N3-Rh1-N1-C1	-131.0(2)	Rh1-N3-N4-B1	-4.3(2)
N5-Rh1-N1-C1	143.3(2)	N3-Rh1-N5-C7	132.2(2)
P1-Rh1-N1-C1	39.5(2)	P1-Rh1-N5-C7	-37.7(2)
N3-Rh1-N1-N2	44.09(14)	N1-Rh1-N5-C7	-142.8(2)
N5-Rh1-N1-N2	-41.57(14)	N3-Rh1-N5-N6	-40.38(14)
P1-Rh1-N1-N2	-145.36(13)	P1-Rh1-N5-N6	149.69(13)
C1-N1-N2-C3	-0.3(2)	N1-Rh1-N5-N6	44.62(14)
Rh1-N1-N2-C3	-176.83(14)	C7-N5-N6-C9	-0.4(2)
C1-N1-N2-B1	173.67(19)	Rh1-N5-N6-C9	174.24(14)
Rh1-N1-N2-B1	-2.8(2)	C7-N5-N6-B1	-178.29(19)

Rh1-N5-N6-B1	-3.6(2)	B1-N4-C6-C5	177.3(2)
C3-N2-B1-N4	115.1(2)	N3-N4-C6-C13	-178.6(2)
N1-N2-B1-N4	-57.6(2)	B1-N4-C6-C13	-1.2(4)
C3-N2-B1-N6	-125.5(2)	C4-C5-C6-N4	0.7(3)
N1-N2-B1-N6	61.8(2)	C4-C5-C6-C13	179.1(2)
C6-N4-B1-N2	-113.6(3)	N6-N5-C7-C8	0.3(2)
N3-N4-B1-N2	63.7(2)	Rh1-N5-C7-C8	-172.87(16)
C6-N4-B1-N6	126.5(2)	N6-N5-C7-C14	-179.9(2)
N3-N4-B1-N6	-56.3(2)	Rh1-N5-C7-C14	7.0(3)
C9-N6-B1-N2	124.0(2)	N5-C7-C8-C9	-0.1(3)
N5-N6-B1-N2	-58.6(2)	C14-C7-C8-C9	-179.9(2)
C9-N6-B1-N4	-116.8(2)	N5-N6-C9-C8	0.4(2)
N5-N6-B1-N4	60.6(2)	B1-N6-C9-C8	178.0(2)
N2-N1-C1-C2	0.3(2)	N5-N6-C9-C15	178.6(2)
Rh1-N1-C1-C2	175.80(16)	B1-N6-C9-C15	-3.8(4)
N2-N1-C1-C10	-178.5(2)	C7-C8-C9-N6	-0.2(3)
Rh1-N1-C1-C10	-3.1(4)	C7-C8-C9-C15	-178.2(2)
N1-C1-C2-C3	-0.2(3)	C21-C16-C17-C18	-1.1(4)
C10-C1-C2-C3	178.5(2)	C16-C17-C18-C19	1.0(4)
N1-N2-C3-C2	0.2(2)	C17-C18-C19-C20	0.1(5)
B1-N2-C3-C2	-173.1(2)	C18-C19-C20-C21	-1.1(5)
N1-N2-C3-C11	178.9(2)	C17-C16-C21-C20	0.1(4)
B1-N2-C3-C11	5.6(4)	C17-C16-C21-P1	-179.7(2)
C1-C2-C3-N2	0.0(3)	C19-C20-C21-C16	1.0(5)
C1-C2-C3-C11	-178.6(2)	C19-C20-C21-P1	-179.2(3)
N4-N3-C4-C5	1.0(2)	C22-P1-C21-C16	-145.4(2)
Rh1-N3-C4-C5	-172.08(16)	C23-P1-C21-C16	114.5(2)
N4-N3-C4-C12	-178.93(19)	Rh1-P1-C21-C16	-16.4(2)
Rh1-N3-C4-C12	7.9(3)	C22-P1-C21-C20	34.8(3)
N3-C4-C5-C6	-1.1(3)	C23-P1-C21-C20	-65.3(3)
C12-C4-C5-C6	178.9(2)	Rh1-P1-C21-C20	163.8(2)
N3-N4-C6-C5	-0.1(3)		

Table S49. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	$C_{23}H_{33}BN_6PRh$	
Formula weight	538.24	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.600(4) Å	α = 90°
	b = 12.888(4) Å	β = 103.895(4)°
	c = 14.424(4) Å	γ = 90°
Volume	2454.0(12) $Å^3$	
Z	4	
Density (calculated)	1.457 Mg/m^3	
Absorption coefficient	0.784 mm^{-1}	
F(000)	1112	
Crystal color, morphology	colorless, block	
Crystal size	0.20 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.85 to 32.57°	

Index ranges	$-20 \le h \le 20$, $-19 \le k \le 19$, $-21 \le l \le 21$
Reflections collected	42160
Independent reflections	8821 [R(int) = 0.1047]
Observed reflections	5887
Completeness to theta = 32.57°	98.7%
Absorption correction	Multi-scan
Max. and min. transmission	0.9399 and 0.8590
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8821 / 0 / 301
Goodness-of-fit on F^2	1.127
Final R indices [I>2sigma(I)]	R_1 = 0.0776, wR_2 = 0.1730
R indices (all data)	R_1 = 0.1209, wR_2 = 0.1888
Largest diff. peak and hole	2.200 and -1.330 e.Å^{-3}

Table S50. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **7**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	7392(1)	3928(1)	10130(1)	17(1)
P1	6405(1)	3624(1)	11145(1)	18(1)
N1	6291(3)	3825(3)	8711(3)	19(1)
N2	6435(3)	4531(3)	8040(3)	20(1)
N3	8506(3)	3939(3)	9343(3)	19(1)
N4	8355(3)	4562(3)	8539(3)	20(1)
N5	7359(3)	5585(3)	9935(3)	18(1)
N6	7360(3)	5984(3)	9059(3)	20(1)
B1	7389(4)	5228(4)	8238(4)	20(1)
C1	5438(4)	3308(4)	8311(4)	21(1)
C2	5012(4)	3706(4)	7398(4)	23(1)
C3	5660(4)	4477(4)	7251(4)	21(1)
C4	9447(4)	3577(4)	9496(4)	23(1)
C5	9925(4)	3978(5)	8813(4)	27(1)
C6	9218(4)	4605(4)	8233(4)	23(1)
C7	7341(4)	6389(4)	10522(4)	21(1)
C8	7339(4)	7318(4)	10015(4)	25(1)
C9	7343(4)	7039(4)	9086(4)	22(1)
C10	5024(4)	2420(4)	8779(4)	24(1)
C11	5579(5)	5153(5)	6391(4)	30(1)
C12	9894(5)	2906(5)	10339(5)	30(1)
C13	9338(5)	5254(5)	7406(4)	29(1)
C14	7328(5)	6229(4)	11539(4)	26(1)
C15	7354(5)	7702(4)	8234(5)	30(1)
C16	7286(4)	2387(4)	10349(4)	20(1)
C17	7619(4)	1486(4)	9972(4)	25(1)
C18	7240(5)	523(4)	10158(4)	28(1)
C19	6520(5)	438(4)	10707(4)	29(1)
C20	6185(5)	1320(4)	11100(4)	25(1)
C21	6585(4)	2272(4)	10920(4)	20(1)
C22	6837(5)	3831(4)	12433(4)	26(1)
C23	5084(4)	3966(5)	10943(4)	28(1)

Table S51. Bond lengths [Å] and angles [°] for **7**.

Rh(1)-C(16)	2.022(5)	C(15)-H(15A)	0.9800
Rh(1)-N(3)	2.099(4)	C(15)-H(15B)	0.9800
Rh(1)-N(5)	2.152(4)	C(15)-H(15C)	0.9800
Rh(1)-N(1)	2.231(4)	C(16)-C(17)	1.403(7)
Rh(1)-P(1)	2.2468(15)	C(16)-C(21)	1.409(8)
Rh(1)-H(1)	1.59(7)	C(17)-C(18)	1.394(8)
P(1)-C(21)	1.799(5)	C(17)-H(17)	0.9500
P(1)-C(23)	1.804(6)	C(18)-C(19)	1.403(9)
P(1)-C(22)	1.828(6)	C(18)-H(18)	0.9500
N(1)-C(1)	1.342(7)	C(19)-C(20)	1.395(8)
N(1)-N(2)	1.376(6)	C(19)-H(19)	0.9500
N(2)-C(3)	1.354(7)	C(20)-C(21)	1.393(7)
N(2)-B(1)	1.548(7)	C(20)-H(20)	0.9500
N(3)-C(4)	1.330(7)	C(22)-H(22A)	0.9800
N(3)-N(4)	1.385(6)	C(22)-H(22B)	0.9800
N(4)-C(6)	1.351(7)	C(22)-H(22C)	0.9800
N(4)-B(1)	1.542(7)	C(23)-H(23A)	0.9800
N(5)-C(7)	1.342(7)	C(23)-H(23B)	0.9800
N(5)-N(6)	1.365(6)	C(23)-H(23C)	0.9800
N(6)-C(9)	1.360(6)	C(16)-Rh(1)-N(3)	100.3(2)
N(6)-B(1)	1.542(7)	C(16)-Rh(1)-N(5)	174.12(19)
B(1)-H(1B)	1.0000	N(3)-Rh(1)-N(5)	85.33(17)
C(1)-C(2)	1.403(7)	C(16)-Rh(1)-N(1)	91.54(18)
C(1)-C(10)	1.505(8)	N(3)-Rh(1)-N(1)	85.23(16)
C(2)-C(3)	1.378(8)	N(5)-Rh(1)-N(1)	87.22(16)
C(2)-H(2)	0.9500	C(16)-Rh(1)-P(1)	69.52(16)
C(3)-C(11)	1.498(8)	N(3)-Rh(1)-P(1)	167.24(12)
C(4)-C(5)	1.404(8)	N(5)-Rh(1)-P(1)	105.13(12)
C(4)-C(12)	1.497(8)	N(1)-Rh(1)-P(1)	102.30(12)
C(5)-C(6)	1.375(8)	C(16)-Rh(1)-H(1)	88(2)
C(5)-H(5)	0.9500	N(3)-Rh(1)-H(1)	93(2)
C(6)-C(13)	1.498(8)	N(5)-Rh(1)-H(1)	94(2)
C(7)-C(8)	1.403(8)	N(1)-Rh(1)-H(1)	178(2)
C(7)-C(14)	1.485(8)	P(1)-Rh(1)-H(1)	79(2)
C(8)-C(9)	1.389(8)	C(21)-P(1)-C(23)	112.4(3)
C(8)-H(8)	0.9500	C(21)-P(1)-C(22)	107.5(2)
C(9)-C(15)	1.500(8)	C(23)-P(1)-C(22)	101.1(3)
C(10)-H(10A)	0.9800	C(21)-P(1)-Rh(1)	85.55(18)
C(10)-H(10B)	0.9800	C(23)-P(1)-Rh(1)	125.4(2)
C(10)-H(10C)	0.9800	C(22)-P(1)-Rh(1)	122.7(2)
C(11)-H(11A)	0.9800	C(1)-N(1)-N(2)	106.3(4)
C(11)-H(11B)	0.9800	C(1)-N(1)-Rh(1)	138.1(4)
C(11)-H(11C)	0.9800	N(2)-N(1)-Rh(1)	115.4(3)
C(12)-H(12A)	0.9800	C(3)-N(2)-N(1)	110.1(4)
C(12)-H(12B)	0.9800	C(3)-N(2)-B(1)	129.3(5)
C(12)-H(12C)	0.9800	N(1)-N(2)-B(1)	120.6(4)
C(13)-H(13A)	0.9800	C(4)-N(3)-N(4)	106.6(4)
C(13)-H(13B)	0.9800	C(4)-N(3)-Rh(1)	134.3(4)
C(13)-H(13C)	0.9800	N(4)-N(3)-Rh(1)	118.4(3)
C(14)-H(14A)	0.9800	C(6)-N(4)-N(3)	109.4(4)
C(14)-H(14B)	0.9800	C(6)-N(4)-B(1)	129.3(5)
C(14)-H(14C)	0.9800	N(3)-N(4)-B(1)	120.2(4)

C(7)-N(5)-N(6)	107.3(4)	H(12A)-C(12)-H(12B)	109.5
C(7)-N(5)-Rh(1)	133.4(4)	C(4)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	119.3(3)	H(12A)-C(12)-H(12C)	109.5
C(9)-N(6)-N(5)	110.3(4)	H(12B)-C(12)-H(12C)	109.5
C(9)-N(6)-B(1)	131.1(5)	C(6)-C(13)-H(13A)	109.5
N(5)-N(6)-B(1)	118.7(4)	C(6)-C(13)-H(13B)	109.5
N(6)-B(1)-N(4)	108.2(4)	H(13A)-C(13)-H(13B)	109.5
N(6)-B(1)-N(2)	109.5(4)	C(6)-C(13)-H(13C)	109.5
N(4)-B(1)-N(2)	110.4(4)	H(13A)-C(13)-H(13C)	109.5
N(6)-B(1)-H(1B)	109.6	H(13B)-C(13)-H(13C)	109.5
N(4)-B(1)-H(1B)	109.6	C(7)-C(14)-H(14A)	109.5
N(2)-B(1)-H(1B)	109.6	C(7)-C(14)-H(14B)	109.5
N(1)-C(1)-C(2)	110.0(5)	H(14A)-C(14)-H(14B)	109.5
N(1)-C(1)-C(10)	124.3(5)	C(7)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	125.8(5)	H(14A)-C(14)-H(14C)	109.5
C(3)-C(2)-C(1)	105.8(5)	H(14B)-C(14)-H(14C)	109.5
C(3)-C(2)-H(2)	127.1	C(9)-C(15)-H(15A)	109.5
C(1)-C(2)-H(2)	127.1	C(9)-C(15)-H(15B)	109.5
N(2)-C(3)-C(2)	107.7(5)	H(15A)-C(15)-H(15B)	109.5
N(2)-C(3)-C(11)	123.6(5)	C(9)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	128.6(5)	H(15A)-C(15)-H(15C)	109.5
N(3)-C(4)-C(5)	110.1(5)	H(15B)-C(15)-H(15C)	109.5
N(3)-C(4)-C(12)	121.6(5)	C(17)-C(16)-C(21)	117.8(5)
C(5)-C(4)-C(12)	128.1(5)	C(17)-C(16)-Rh(1)	135.3(4)
C(6)-C(5)-C(4)	105.6(5)	C(21)-C(16)-Rh(1)	106.1(3)
C(6)-C(5)-H(5)	127.2	C(18)-C(17)-C(16)	119.5(5)
C(4)-C(5)-H(5)	127.2	C(18)-C(17)-H(17)	120.3
N(4)-C(6)-C(5)	108.2(5)	C(16)-C(17)-H(17)	120.3
N(4)-C(6)-C(13)	123.6(5)	C(17)-C(18)-C(19)	121.3(5)
C(5)-C(6)-C(13)	128.2(5)	C(17)-C(18)-H(18)	119.3
N(5)-C(7)-C(8)	109.2(5)	C(19)-C(18)-H(18)	119.3
N(5)-C(7)-C(14)	121.4(5)	C(20)-C(19)-C(18)	120.4(5)
C(8)-C(7)-C(14)	129.4(5)	C(20)-C(19)-H(19)	119.8
C(9)-C(8)-C(7)	106.4(5)	C(18)-C(19)-H(19)	119.8
C(9)-C(8)-H(8)	126.8	C(21)-C(20)-C(19)	117.5(5)
C(7)-C(8)-H(8)	126.8	C(21)-C(20)-H(20)	121.3
N(6)-C(9)-C(8)	106.9(5)	C(19)-C(20)-H(20)	121.3
N(6)-C(9)-C(15)	122.9(5)	C(20)-C(21)-C(16)	123.5(5)
C(8)-C(9)-C(15)	130.2(5)	C(20)-C(21)-P(1)	138.0(4)
C(1)-C(10)-H(10A)	109.5	C(16)-C(21)-P(1)	98.3(3)
C(1)-C(10)-H(10B)	109.5	P(1)-C(22)-H(22A)	109.5
H(10A)-C(10)-H(10B)	109.5	P(1)-C(22)-H(22B)	109.5
C(1)-C(10)-H(10C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(10A)-C(10)-H(10C)	109.5	P(1)-C(22)-H(22C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(22A)-C(22)-H(22C)	109.5
C(3)-C(11)-H(11A)	109.5	H(22B)-C(22)-H(22C)	109.5
C(3)-C(11)-H(11B)	109.5	P(1)-C(23)-H(23A)	109.5
H(11A)-C(11)-H(11B)	109.5	P(1)-C(23)-H(23B)	109.5
C(3)-C(11)-H(11C)	109.5	H(23A)-C(23)-H(23B)	109.5
H(11A)-C(11)-H(11C)	109.5	P(1)-C(23)-H(23C)	109.5
H(11B)-C(11)-H(11C)	109.5	H(23A)-C(23)-H(23C)	109.5
C(4)-C(12)-H(12A)	109.5	H(23B)-C(23)-H(23C)	109.5
C(4)-C(12)-H(12B)	109.5		

Table S52. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7**. 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}
Rh1	18(1)	14(1)	20(1)	1(1)	4(1)	1(1)
P1	21(1)	14(1)	20(1)	0(1)	5(1)	2(1)
N1	22(2)	14(2)	21(2)	2(2)	7(2)	2(2)
N2	22(2)	16(2)	20(2)	1(2)	3(2)	-1(2)
N3	18(2)	18(2)	18(2)	2(2)	-1(2)	-1(2)
N4	22(2)	17(2)	22(2)	2(2)	6(2)	3(2)
N5	19(2)	15(2)	21(2)	2(2)	6(2)	1(2)
N6	22(2)	15(2)	22(2)	0(2)	4(2)	0(2)
B1	22(3)	17(2)	20(3)	3(2)	6(2)	1(2)
C1	22(2)	19(2)	23(2)	-4(2)	6(2)	3(2)
C2	23(2)	23(3)	21(2)	-4(2)	3(2)	-2(2)
C3	22(2)	23(2)	19(2)	0(2)	5(2)	2(2)
C4	19(2)	25(2)	25(3)	0(2)	5(2)	1(2)
C5	19(2)	29(3)	33(3)	4(2)	7(2)	1(2)
C6	25(3)	16(2)	29(3)	-2(2)	10(2)	1(2)
C7	19(2)	19(2)	25(3)	-2(2)	3(2)	0(2)
C8	28(3)	17(2)	29(3)	-1(2)	6(2)	-1(2)
C9	21(2)	16(2)	28(3)	1(2)	5(2)	0(2)
C10	24(3)	17(2)	29(3)	-3(2)	4(2)	-1(2)
C11	30(3)	35(3)	21(3)	7(2)	-1(2)	-2(2)
C12	25(3)	30(3)	34(3)	6(2)	5(2)	6(2)
C13	30(3)	27(3)	32(3)	6(2)	14(2)	0(2)
C14	33(3)	18(3)	27(3)	-4(2)	6(2)	-2(2)
C15	37(3)	15(2)	39(3)	8(2)	9(3)	3(2)
C16	23(2)	14(2)	22(2)	3(2)	2(2)	4(2)
C17	26(3)	17(2)	33(3)	5(2)	9(2)	6(2)
C18	35(3)	16(2)	31(3)	-1(2)	7(2)	2(2)
C19	40(3)	15(2)	29(3)	3(2)	2(2)	-2(2)
C20	32(3)	18(2)	26(3)	3(2)	7(2)	-4(2)
C21	23(2)	15(2)	20(2)	2(2)	3(2)	1(2)
C22	36(3)	19(2)	22(2)	2(2)	4(2)	3(2)
C23	24(3)	24(3)	34(3)	-2(2)	6(2)	2(2)

Table S53. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **7**.

	x	y	z	U(eq)
H1	8200(50)	3980(50)	11130(50)	33(18)
H1B	7407	5630	7649	29
H2	4402	3488	6969	27
H5	10597	3845	8761	32
H8	7337	8003	10259	30
H10A	5576	1943	9064	36
H10B	4512	2049	8300	36
H10C	4716	2688	9279	36
H11A	4936	5015	5929	45

H11B	6142	5002	6097	45
H11C	5606	5884	6584	45
H12A	9394	2800	10719	45
H12B	10496	3245	10733	45
H12C	10085	2234	10118	45
H13A	10046	5234	7362	43
H13B	9145	5972	7499	43
H13C	8902	4980	6814	43
H14A	7774	5648	11800	39
H14B	6636	6074	11584	39
H14C	7567	6860	11903	39
H15A	7421	8433	8427	45
H15B	6720	7604	7747	45
H15C	7927	7503	7971	45
H17	8100	1531	9592	30
H18	7473	-87	9909	33
H19	6260	-225	10811	35
H20	5701	1273	11477	31
H22A	6446	3389	12766	39
H22B	6740	4560	12580	39
H22C	7557	3654	12643	39
H23A	4754	3508	11319	41
H23B	4756	3889	10264	41
H23C	5025	4688	11138	41

Table S54. Torsion angles [°] for **7**.

C16-Rh1-P1-C21	-3.9(2)	N1-Rh1-N3-C4	-146.7(5)
N3-Rh1-P1-C21	-42.2(6)	P1-Rh1-N3-C4	-19.9(10)
N5-Rh1-P1-C21	173.5(2)	C16-Rh1-N3-N4	135.1(4)
N1-Rh1-P1-C21	83.1(2)	N5-Rh1-N3-N4	-43.2(4)
C16-Rh1-P1-C23	-118.4(3)	N1-Rh1-N3-N4	44.4(4)
N3-Rh1-P1-C23	-156.6(6)	P1-Rh1-N3-N4	171.3(4)
N5-Rh1-P1-C23	59.1(3)	C4-N3-N4-C6	-2.4(6)
N1-Rh1-P1-C23	-31.4(3)	Rh1-N3-N4-C6	169.3(3)
C16-Rh1-P1-C22	104.0(3)	C4-N3-N4-B1	-171.7(5)
N3-Rh1-P1-C22	65.8(6)	Rh1-N3-N4-B1	0.0(6)
N5-Rh1-P1-C22	-78.5(2)	C16-Rh1-N5-C7	61(2)
N1-Rh1-P1-C22	-168.9(2)	N3-Rh1-N5-C7	-135.5(5)
C16-Rh1-N1-C1	37.8(5)	N1-Rh1-N5-C7	139.1(5)
N3-Rh1-N1-C1	138.0(5)	P1-Rh1-N5-C7	37.1(5)
N5-Rh1-N1-C1	-136.4(5)	C16-Rh1-N5-N6	-119.4(19)
P1-Rh1-N1-C1	-31.5(5)	N3-Rh1-N5-N6	44.0(4)
C16-Rh1-N1-N2	-149.2(4)	N1-Rh1-N5-N6	-41.4(4)
N3-Rh1-N1-N2	-48.9(3)	P1-Rh1-N5-N6	-143.4(3)
N5-Rh1-N1-N2	36.6(3)	C7-N5-N6-C9	0.0(6)
P1-Rh1-N1-N2	141.5(3)	Rh1-N5-N6-C9	-179.6(3)
C1-N1-N2-C3	2.3(6)	C7-N5-N6-B1	179.5(4)
Rh1-N1-N2-C3	-172.9(3)	Rh1-N5-N6-B1	-0.2(6)
C1-N1-N2-B1	-176.6(4)	C9-N6-B1-N4	120.3(6)
Rh1-N1-N2-B1	8.2(6)	N5-N6-B1-N4	-59.0(6)
C16-Rh1-N3-C4	-56.0(6)	C9-N6-B1-N2	-119.3(6)
N5-Rh1-N3-C4	125.7(5)	N5-N6-B1-N2	61.4(6)

C6-N4-B1-N6	-106.8(6)	Rh1-N5-C7-C14	-0.8(8)
N3-N4-B1-N6	60.2(6)	N5-C7-C8-C9	0.8(6)
C6-N4-B1-N2	133.4(5)	C14-C7-C8-C9	-179.4(6)
N3-N4-B1-N2	-59.6(6)	N5-N6-C9-C8	0.5(6)
C3-N2-B1-N6	115.0(6)	B1-N6-C9-C8	-178.9(5)
N1-N2-B1-N6	-66.3(6)	N5-N6-C9-C15	179.2(5)
C3-N2-B1-N4	-126.0(5)	B1-N6-C9-C15	-0.2(9)
N1-N2-B1-N4	52.7(6)	C7-C8-C9-N6	-0.8(6)
N2-N1-C1-C2	-2.1(6)	C7-C8-C9-C15	-179.3(6)
Rh1-N1-C1-C2	171.3(4)	N3-Rh1-C16-C17	-13.4(6)
N2-N1-C1-C10	176.7(5)	N5-Rh1-C16-C17	149.8(17)
Rh1-N1-C1-C10	-9.9(8)	N1-Rh1-C16-C17	72.1(6)
N1-C1-C2-C3	1.2(6)	P1-Rh1-C16-C17	174.6(6)
C10-C1-C2-C3	-177.5(5)	N3-Rh1-C16-C21	177.2(3)
N1-N2-C3-C2	-1.5(6)	N5-Rh1-C16-C21	-20(2)
B1-N2-C3-C2	177.3(5)	N1-Rh1-C16-C21	-97.4(4)
N1-N2-C3-C11	179.2(5)	P1-Rh1-C16-C21	5.2(3)
B1-N2-C3-C11	-2.0(9)	C21-C16-C17-C18	1.0(8)
C1-C2-C3-N2	0.2(6)	Rh1-C16-C17-C18	-167.5(5)
C1-C2-C3-C11	179.4(6)	C16-C17-C18-C19	0.8(9)
N4-N3-C4-C5	1.5(6)	C17-C18-C19-C20	-1.6(9)
Rh1-N3-C4-C5	-168.3(4)	C18-C19-C20-C21	0.4(9)
N4-N3-C4-C12	177.3(5)	C19-C20-C21-C16	1.5(8)
Rh1-N3-C4-C12	7.5(9)	C19-C20-C21-P1	174.9(5)
N3-C4-C5-C6	-0.2(7)	C17-C16-C21-C20	-2.2(8)
C12-C4-C5-C6	-175.6(6)	Rh1-C16-C21-C20	169.4(5)
N3-N4-C6-C5	2.3(6)	C17-C16-C21-P1	-177.8(4)
B1-N4-C6-C5	170.3(5)	Rh1-C16-C21-P1	-6.1(4)
N3-N4-C6-C13	-176.8(5)	C23-P1-C21-C20	-42.5(7)
B1-N4-C6-C13	-8.8(9)	C22-P1-C21-C20	68.0(7)
C4-C5-C6-N4	-1.3(6)	Rh1-P1-C21-C20	-169.1(6)
C4-C5-C6-C13	177.8(6)	C23-P1-C21-C16	132.0(4)
N6-N5-C7-C8	-0.5(6)	C22-P1-C21-C16	-117.6(4)
Rh1-N5-C7-C8	179.0(4)	Rh1-P1-C21-C16	5.3(3)
N6-N5-C7-C14	179.6(5)		

Table S55. Crystal data and structure refinement for **9a**.

Identification code	**9a**	
Empirical formula	$C_{35}H_{48}BF_5N_6PRh$	
Formula weight	792.48	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.2069(10) Å	α = 105.613(2)°
	b = 13.0730(13) Å	β = 108.235(2)°
	c = 15.3042(15) Å	γ = 101.547(2)°
Volume	1775.4(3) Å^3	
Z	2	
Density (calculated)	1.482 Mg/m^3	
Absorption coefficient	0.587 mm^{-1}	
F(000)	820	

Crystal color, morphology	colorless, block
Crystal size	0.28 x 0.12 x 0.10 mm^3
Theta range for data collection	1.50 to 36.32°
Index ranges	$-17 \le h \le 17$, $-21 \le k \le 21$, $-25 \le l \le 25$
Reflections collected	41158
Independent reflections	16867 [R(int) = 0.0277]
Observed reflections	14559
Completeness to theta = 36.32°	98.0%
Absorption correction	Multi-scan
Max. and min. transmission	0.9436 and 0.8528
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16867 / 0 / 400
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R_1 = 0.0286, wR_2 = 0.0722
R indices (all data)	R_1 = 0.0341, wR_2 = 0.0742
Largest diff. peak and hole	1.104 and -0.351 e.Å^{-3}

Table S56. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **9a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	6772(1)	2473(1)	3698(1)	13(1)
P1	6247(1)	3030(1)	5058(1)	15(1)
N1	4423(1)	1549(1)	2669(1)	18(1)
N2	3963(1)	1804(1)	1836(1)	18(1)
N3	7278(1)	1994(1)	2449(1)	16(1)
N4	6299(1)	1943(1)	1575(1)	18(1)
N5	6556(1)	3896(1)	3280(1)	16(1)
N6	5752(1)	3680(1)	2304(1)	19(1)
B1	5080(1)	2477(1)	1559(1)	19(1)
C1	3261(1)	827(1)	2637(1)	20(1)
C2	2046(1)	634(1)	1792(1)	22(1)
C3	2530(1)	1270(1)	1304(1)	20(1)
C4	8298(1)	1589(1)	2256(1)	19(1)
C5	7964(1)	1255(1)	1244(1)	23(1)
C6	6698(1)	1487(1)	833(1)	21(1)
C7	7194(1)	5008(1)	3695(1)	16(1)
C8	6772(1)	5505(1)	2994(1)	21(1)
C9	5870(1)	4646(1)	2125(1)	22(1)
C10	3296(1)	305(1)	3393(1)	28(1)
C11	1711(1)	1415(1)	369(1)	26(1)
C12	9583(1)	1555(1)	3040(1)	24(1)
C13	5843(2)	1274(1)	-222(1)	30(1)
C14	8239(1)	5596(1)	4734(1)	19(1)
C15	5126(2)	4696(1)	1135(1)	35(1)
C16	7200(1)	1121(1)	4004(1)	16(1)
C17	8214(1)	1176(1)	4886(1)	17(1)
F1	9012(1)	2176(1)	5615(1)	21(1)
C18	8499(1)	267(1)	5107(1)	20(1)
F2	9480(1)	408(1)	5992(1)	26(1)
C19	7774(1)	-791(1)	4417(1)	23(1)
F3	8028(1)	-1689(1)	4615(1)	34(1)

C20	6791(1)	-905(1)	3514(1)	23(1)
F4	6067(1)	-1932(1)	2826(1)	35(1)
C21	6547(1)	29(1)	3322(1)	19(1)
F5	5588(1)	-184(1)	2409(1)	26(1)
C22	7457(1)	4268(1)	6138(1)	17(1)
C23	6877(1)	4922(1)	6698(1)	23(1)
C24	7789(2)	5852(1)	7535(1)	29(1)
C25	9276(2)	6125(1)	7823(1)	29(1)
C26	9866(1)	5469(1)	7282(1)	26(1)
C27	8968(1)	4543(1)	6447(1)	21(1)
C28	5975(1)	2074(1)	5711(1)	21(1)
C29	4527(1)	3327(1)	4706(1)	23(1)

Table S57. Bond lengths [Å] and angles [°] for **9a**.

Rh(1)-C(16)	2.0400(10)	C(10)-H(10B)	0.9800
Rh(1)-N(3)	2.1013(9)	C(10)-H(10C)	0.9800
Rh(1)-N(5)	2.1527(9)	C(11)-H(11A)	0.9800
Rh(1)-N(1)	2.2667(9)	C(11)-H(11B)	0.9800
Rh(1)-P(1)	2.2777(3)	C(11)-H(11C)	0.9800
Rh(1)-H(1)	1.472(16)	C(12)-H(12A)	0.9800
P(1)-C(29)	1.8210(11)	C(12)-H(12B)	0.9800
P(1)-C(28)	1.8290(11)	C(12)-H(12C)	0.9800
P(1)-C(22)	1.8329(11)	C(13)-H(13A)	0.9800
N(1)-C(1)	1.3380(14)	C(13)-H(13B)	0.9800
N(1)-N(2)	1.3691(12)	C(13)-H(13C)	0.9800
N(2)-C(3)	1.3523(14)	C(14)-H(14A)	0.9800
N(2)-B(1)	1.5351(15)	C(14)-H(14B)	0.9800
N(3)-C(4)	1.3341(14)	C(14)-H(14C)	0.9800
N(3)-N(4)	1.3720(12)	C(15)-H(15A)	0.9800
N(4)-C(6)	1.3534(14)	C(15)-H(15B)	0.9800
N(4)-B(1)	1.5406(16)	C(15)-H(15C)	0.9800
N(5)-C(7)	1.3438(13)	C(16)-C(17)	1.3941(14)
N(5)-N(6)	1.3777(12)	C(16)-C(21)	1.3973(14)
N(6)-C(9)	1.3526(14)	C(17)-F(1)	1.3549(12)
N(6)-B(1)	1.5349(15)	C(17)-C(18)	1.3810(15)
B(1)-H(1B)	1.0000	C(18)-F(2)	1.3470(13)
C(1)-C(2)	1.4033(16)	C(18)-C(19)	1.3749(17)
C(1)-C(10)	1.4885(16)	C(19)-F(3)	1.3418(13)
C(2)-C(3)	1.3757(16)	C(19)-C(20)	1.3787(17)
C(2)-H(2)	0.9500	C(20)-F(4)	1.3468(13)
C(3)-C(11)	1.4978(15)	C(20)-C(21)	1.3808(15)
C(4)-C(5)	1.3971(15)	C(21)-F(5)	1.3476(13)
C(4)-C(12)	1.4929(17)	C(22)-C(23)	1.3941(15)
C(5)-C(6)	1.3814(18)	C(22)-C(27)	1.4008(16)
C(5)-H(5)	0.9500	C(23)-C(24)	1.3950(17)
C(6)-C(13)	1.4924(16)	C(23)-H(23)	0.9500
C(7)-C(8)	1.3972(15)	C(24)-C(25)	1.380(2)
C(7)-C(14)	1.4863(15)	C(24)-H(24)	0.9500
C(8)-C(9)	1.3758(16)	C(25)-C(26)	1.3860(19)
C(8)-H(8)	0.9500	C(25)-H(25)	0.9500
C(9)-C(15)	1.4936(16)	C(26)-C(27)	1.3888(16)
C(10)-H(10A)	0.9800	C(26)-H(26)	0.9500

C(27)-H(27)	0.9500	C(3)-C(2)-C(1)	105.70(10)
C(28)-H(28A)	0.9800	C(3)-C(2)-H(2)	127.1
C(28)-H(28B)	0.9800	C(1)-C(2)-H(2)	127.1
C(28)-H(28C)	0.9800	N(2)-C(3)-C(2)	107.42(9)
C(29)-H(29A)	0.9800	N(2)-C(3)-C(11)	122.85(10)
C(29)-H(29B)	0.9800	C(2)-C(3)-C(11)	129.72(10)
C(29)-H(29C)	0.9800	N(3)-C(4)-C(5)	108.98(10)
C(16)-Rh(1)-N(3)	89.58(4)	N(3)-C(4)-C(12)	122.86(10)
C(16)-Rh(1)-N(5)	171.51(4)	C(5)-C(4)-C(12)	128.13(10)
N(3)-Rh(1)-N(5)	83.09(3)	C(6)-C(5)-C(4)	106.51(10)
C(16)-Rh(1)-N(1)	95.23(4)	C(6)-C(5)-H(5)	126.7
N(3)-Rh(1)-N(1)	86.58(3)	C(4)-C(5)-H(5)	126.7
N(5)-Rh(1)-N(1)	88.63(3)	N(4)-C(6)-C(5)	107.43(10)
C(16)-Rh(1)-P(1)	91.31(3)	N(4)-C(6)-C(13)	123.48(11)
N(3)-Rh(1)-P(1)	178.82(2)	C(5)-C(6)-C(13)	129.07(11)
N(5)-Rh(1)-P(1)	95.96(2)	N(5)-C(7)-C(8)	109.79(9)
N(1)-Rh(1)-P(1)	94.10(3)	N(5)-C(7)-C(14)	124.14(9)
C(16)-Rh(1)-H(1)	87.5(6)	C(8)-C(7)-C(14)	126.02(10)
N(3)-Rh(1)-H(1)	89.1(6)	C(9)-C(8)-C(7)	106.21(9)
N(5)-Rh(1)-H(1)	88.1(6)	C(9)-C(8)-H(8)	126.9
N(1)-Rh(1)-H(1)	174.8(6)	C(7)-C(8)-H(8)	126.9
P(1)-Rh(1)-H(1)	90.2(6)	N(6)-C(9)-C(8)	107.69(9)
C(29)-P(1)-C(28)	102.80(6)	N(6)-C(9)-C(15)	123.24(10)
C(29)-P(1)-C(22)	103.51(5)	C(8)-C(9)-C(15)	129.07(10)
C(28)-P(1)-C(22)	97.43(5)	C(1)-C(10)-H(10A)	109.5
C(29)-P(1)-Rh(1)	108.85(4)	C(1)-C(10)-H(10B)	109.5
C(28)-P(1)-Rh(1)	119.96(4)	H(10A)-C(10)-H(10B)	109.5
C(22)-P(1)-Rh(1)	121.70(4)	C(1)-C(10)-H(10C)	109.5
C(1)-N(1)-N(2)	105.95(9)	H(10A)-C(10)-H(10C)	109.5
C(1)-N(1)-Rh(1)	138.89(7)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	115.08(6)	C(3)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	110.71(9)	C(3)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	129.11(9)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	119.61(8)	C(3)-C(11)-H(11C)	109.5
C(4)-N(3)-N(4)	107.64(8)	H(11A)-C(11)-H(11C)	109.5
C(4)-N(3)-Rh(1)	134.57(7)	H(11B)-C(11)-H(11C)	109.5
N(4)-N(3)-Rh(1)	117.30(7)	C(4)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.42(9)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	129.64(9)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	120.58(8)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.27(8)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	136.07(7)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	116.74(6)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	110.03(9)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	128.41(9)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	120.77(8)	C(6)-C(13)-H(13C)	109.5
N(6)-B(1)-N(2)	109.73(9)	H(13A)-C(13)-H(13C)	109.5
N(6)-B(1)-N(4)	108.67(9)	H(13B)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	109.89(9)	C(7)-C(14)-H(14A)	109.5
N(6)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14B)	109.5
N(2)-B(1)-H(1B)	109.5	H(14A)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	110.20(10)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	123.66(10)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	126.14(10)	C(9)-C(15)-H(15A)	109.5

C(9)-C(15)-H(15B)	109.5	C(22)-C(23)-H(23)	119.8
H(15A)-C(15)-H(15B)	109.5	C(24)-C(23)-H(23)	119.8
C(9)-C(15)-H(15C)	109.5	C(25)-C(24)-C(23)	120.35(12)
H(15A)-C(15)-H(15C)	109.5	C(25)-C(24)-H(24)	119.8
H(15B)-C(15)-H(15C)	109.5	C(23)-C(24)-H(24)	119.8
C(17)-C(16)-C(21)	112.23(9)	C(24)-C(25)-C(26)	119.82(11)
C(17)-C(16)-Rh(1)	124.58(7)	C(24)-C(25)-H(25)	120.1
C(21)-C(16)-Rh(1)	123.12(8)	C(26)-C(25)-H(25)	120.1
F(1)-C(17)-C(18)	114.35(9)	C(25)-C(26)-C(27)	120.32(12)
F(1)-C(17)-C(16)	120.53(9)	C(25)-C(26)-H(26)	119.8
C(18)-C(17)-C(16)	125.12(10)	C(27)-C(26)-H(26)	119.8
F(2)-C(18)-C(19)	119.85(10)	C(26)-C(27)-C(22)	120.37(11)
F(2)-C(18)-C(17)	120.54(10)	C(26)-C(27)-H(27)	119.8
C(19)-C(18)-C(17)	119.61(10)	C(22)-C(27)-H(27)	119.8
F(3)-C(19)-C(18)	120.78(11)	P(1)-C(28)-H(28A)	109.5
F(3)-C(19)-C(20)	120.86(11)	P(1)-C(28)-H(28B)	109.5
C(18)-C(19)-C(20)	118.36(10)	H(28A)-C(28)-H(28B)	109.5
F(4)-C(20)-C(19)	119.43(10)	P(1)-C(28)-H(28C)	109.5
F(4)-C(20)-C(21)	120.50(11)	H(28A)-C(28)-H(28C)	109.5
C(19)-C(20)-C(21)	120.06(10)	H(28B)-C(28)-H(28C)	109.5
F(5)-C(21)-C(20)	114.73(9)	P(1)-C(29)-H(29A)	109.5
F(5)-C(21)-C(16)	120.79(9)	P(1)-C(29)-H(29B)	109.5
C(20)-C(21)-C(16)	124.48(10)	H(29A)-C(29)-H(29B)	109.5
C(23)-C(22)-C(27)	118.76(10)	P(1)-C(29)-H(29C)	109.5
C(23)-C(22)-P(1)	119.87(8)	H(29A)-C(29)-H(29C)	109.5
C(27)-C(22)-P(1)	121.29(8)	H(29B)-C(29)-H(29C)	109.5
C(22)-C(23)-C(24)	120.35(11)		

Table S58. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9a**. 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}
Rh1	15(1)	12(1)	12(1)	5(1)	4(1)	4(1)
P1	16(1)	15(1)	13(1)	5(1)	5(1)	5(1)
N1	19(1)	18(1)	16(1)	7(1)	5(1)	3(1)
N2	19(1)	16(1)	14(1)	5(1)	3(1)	4(1)
N3	19(1)	15(1)	14(1)	6(1)	6(1)	5(1)
N4	22(1)	16(1)	13(1)	5(1)	6(1)	3(1)
N5	17(1)	13(1)	15(1)	6(1)	4(1)	4(1)
N6	23(1)	16(1)	16(1)	8(1)	3(1)	5(1)
B1	22(1)	17(1)	15(1)	7(1)	4(1)	4(1)
C1	19(1)	21(1)	18(1)	7(1)	6(1)	2(1)
C2	18(1)	23(1)	19(1)	4(1)	4(1)	2(1)
C3	19(1)	18(1)	15(1)	2(1)	2(1)	4(1)
C4	23(1)	15(1)	21(1)	6(1)	11(1)	6(1)
C5	28(1)	19(1)	20(1)	2(1)	13(1)	4(1)
C6	27(1)	18(1)	16(1)	3(1)	9(1)	1(1)
C7	18(1)	14(1)	18(1)	7(1)	8(1)	6(1)
C8	26(1)	15(1)	22(1)	10(1)	8(1)	7(1)
C9	26(1)	18(1)	22(1)	12(1)	6(1)	6(1)
C10	23(1)	31(1)	23(1)	13(1)	6(1)	-3(1)
C11	24(1)	25(1)	18(1)	6(1)	-1(1)	5(1)

C12	26(1)	26(1)	25(1)	10(1)	12(1)	13(1)
C13	35(1)	32(1)	15(1)	4(1)	9(1)	2(1)
C14	20(1)	15(1)	19(1)	4(1)	7(1)	4(1)
C15	45(1)	26(1)	25(1)	16(1)	1(1)	5(1)
C16	20(1)	14(1)	15(1)	6(1)	7(1)	6(1)
C17	18(1)	16(1)	18(1)	7(1)	7(1)	6(1)
F1	22(1)	18(1)	18(1)	6(1)	2(1)	5(1)
C18	20(1)	22(1)	23(1)	14(1)	10(1)	10(1)
F2	24(1)	31(1)	29(1)	19(1)	8(1)	13(1)
C19	28(1)	18(1)	32(1)	14(1)	15(1)	11(1)
F3	42(1)	21(1)	47(1)	21(1)	18(1)	17(1)
C20	31(1)	13(1)	26(1)	6(1)	12(1)	7(1)
F4	49(1)	13(1)	35(1)	3(1)	12(1)	6(1)
C21	24(1)	15(1)	18(1)	6(1)	7(1)	6(1)
F5	35(1)	18(1)	16(1)	3(1)	3(1)	4(1)
C22	22(1)	15(1)	14(1)	5(1)	7(1)	5(1)
C23	26(1)	21(1)	20(1)	5(1)	11(1)	6(1)
C24	38(1)	22(1)	23(1)	0(1)	14(1)	7(1)
C25	36(1)	20(1)	21(1)	1(1)	8(1)	0(1)
C26	25(1)	23(1)	21(1)	5(1)	5(1)	-1(1)
C27	22(1)	19(1)	18(1)	5(1)	6(1)	4(1)
C28	24(1)	20(1)	19(1)	9(1)	9(1)	4(1)
C29	20(1)	26(1)	22(1)	7(1)	8(1)	11(1)

Table S59. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **9a**.

	x	y	z	U(eq)
H1	8316(18)	3098(13)	4291(12)	30(4)
H1B	4591	2486	884	23
H2	1088	163	1597	27
H5	8503	933	905	28
H8	7051	6279	3097	25
H10A	2591	-446	3082	41
H10B	3049	762	3902	41
H10C	4271	256	3693	41
H11A	1841	2211	490	39
H11B	677	1011	138	39
H11C	2079	1118	-133	39
H12A	9724	2081	3679	36
H12B	10449	1765	2897	36
H12C	9420	798	3058	36
H13A	4866	767	-427	45
H13B	6327	933	-629	45
H13C	5776	1982	-305	45
H14A	8903	5168	4905	28
H14B	7707	5665	5169	28
H14C	8795	6342	4812	28
H15A	5338	5477	1179	52
H15B	4076	4358	911	52
H15C	5475	4286	666	52
H23	5855	4735	6510	27

H24	7385	6299	7908	35
H25	9894	6761	8392	35
H26	10890	5654	7482	31
H27	9381	4093	6084	25
H28A	5519	2357	6161	31
H28B	6915	2021	6088	31
H28C	5346	1333	5235	31
H29A	4192	3418	5248	34
H29B	3804	2706	4120	34
H29C	4658	4016	4559	34

Table S60. Torsion angles [°] for **9a**.

C16-Rh1-P1-C29	-131.04(5)	C16-Rh1-N5-N6	78.1(3)
N3-Rh1-P1-C29	89.5(12)	N3-Rh1-N5-N6	47.60(7)
N5-Rh1-P1-C29	53.34(5)	N1-Rh1-N5-N6	-39.13(7)
N1-Rh1-P1-C29	-35.70(5)	P1-Rh1-N5-N6	-133.10(7)
C16-Rh1-P1-C28	-13.21(5)	C7-N5-N6-C9	-1.18(12)
N3-Rh1-P1-C28	-152.7(12)	Rh1-N5-N6-C9	-171.96(7)
N5-Rh1-P1-C28	171.17(5)	C7-N5-N6-B1	169.47(9)
N1-Rh1-P1-C28	82.13(5)	Rh1-N5-N6-B1	-1.30(12)
C16-Rh1-P1-C22	108.89(5)	C9-N6-B1-N2	-127.95(12)
N3-Rh1-P1-C22	-30.6(12)	N5-N6-B1-N2	63.28(13)
N5-Rh1-P1-C22	-66.73(5)	C9-N6-B1-N4	111.87(12)
N1-Rh1-P1-C22	-155.77(5)	N5-N6-B1-N4	-56.91(12)
C16-Rh1-N1-C1	45.48(12)	C3-N2-B1-N6	120.76(11)
N3-Rh1-N1-C1	134.75(12)	N1-N2-B1-N6	-68.80(12)
N5-Rh1-N1-C1	-142.10(12)	C3-N2-B1-N4	-119.79(11)
P1-Rh1-N1-C1	-46.22(12)	N1-N2-B1-N4	50.64(12)
C16-Rh1-N1-N2	-138.43(7)	C6-N4-B1-N6	-122.42(11)
N3-Rh1-N1-N2	-49.16(7)	N3-N4-B1-N6	49.95(12)
N5-Rh1-N1-N2	34.00(7)	C6-N4-B1-N2	117.49(11)
P1-Rh1-N1-N2	129.87(7)	N3-N4-B1-N2	-70.14(12)
C1-N1-N2-C3	1.40(12)	N2-N1-C1-C2	-1.18(13)
Rh1-N1-N2-C3	-175.94(7)	Rh1-N1-C1-C2	175.14(9)
C1-N1-N2-B1	-170.68(10)	N2-N1-C1-C10	177.99(11)
Rh1-N1-N2-B1	11.99(12)	Rh1-N1-C1-C10	-5.7(2)
C16-Rh1-N3-C4	-40.77(10)	N1-C1-C2-C3	0.56(14)
N5-Rh1-N3-C4	134.94(10)	C10-C1-C2-C3	-178.58(12)
N1-Rh1-N3-C4	-136.03(10)	N1-N2-C3-C2	-1.06(13)
P1-Rh1-N3-C4	98.7(12)	B1-N2-C3-C2	170.05(11)
C16-Rh1-N3-N4	130.07(7)	N1-N2-C3-C11	178.04(10)
N5-Rh1-N3-N4	-54.22(7)	B1-N2-C3-C11	-10.84(18)
N1-Rh1-N3-N4	34.81(7)	C1-C2-C3-N2	0.31(13)
P1-Rh1-N3-N4	-90.4(12)	C1-C2-C3-C11	-178.71(12)
C4-N3-N4-C6	1.01(12)	N4-N3-C4-C5	-0.89(12)
Rh1-N3-N4-C6	-172.16(7)	Rh1-N3-C4-C5	170.58(8)
C4-N3-N4-B1	-172.76(9)	N4-N3-C4-C12	177.46(10)
Rh1-N3-N4-B1	14.07(12)	Rh1-N3-C4-C12	-11.08(17)
C16-Rh1-N5-C7	-89.1(3)	N3-C4-C5-C6	0.45(13)
N3-Rh1-N5-C7	-119.58(10)	C12-C4-C5-C6	-177.78(11)
N1-Rh1-N5-C7	153.69(10)	N3-N4-C6-C5	-0.72(12)
P1-Rh1-N5-C7	59.72(10)	B1-N4-C6-C5	172.32(10)

N3-N4-C6-C13	177.95(10)	C16-C17-C18-C19	1.54(17)
B1-N4-C6-C13	-9.01(18)	F2-C18-C19-F3	0.27(17)
C4-C5-C6-N4	0.17(12)	C17-C18-C19-F3	-179.80(10)
C4-C5-C6-C13	-178.41(12)	F2-C18-C19-C20	-179.18(10)
N6-N5-C7-C8	1.45(12)	C17-C18-C19-C20	0.75(17)
Rh1-N5-C7-C8	169.54(8)	F3-C19-C20-F4	0.58(18)
N6-N5-C7-C14	-176.02(10)	C18-C19-C20-F4	-179.97(11)
Rh1-N5-C7-C14	-7.94(16)	F3-C19-C20-C21	-179.77(11)
N5-C7-C8-C9	-1.20(13)	C18-C19-C20-C21	-0.32(18)
C14-C7-C8-C9	176.22(11)	F4-C20-C21-F5	-1.82(16)
N5-N6-C9-C8	0.45(13)	C19-C20-C21-F5	178.53(11)
B1-N6-C9-C8	-169.29(11)	F4-C20-C21-C16	177.20(11)
N5-N6-C9-C15	179.97(12)	C19-C20-C21-C16	-2.45(18)
B1-N6-C9-C15	10.2(2)	C17-C16-C21-F5	-176.74(10)
C7-C8-C9-N6	0.44(13)	Rh1-C16-C21-F5	0.41(15)
C7-C8-C9-C15	-179.04(13)	C17-C16-C21-C20	4.30(16)
N3-Rh1-C16-C17	123.06(9)	Rh1-C16-C21-C20	-178.55(9)
N5-Rh1-C16-C17	92.8(2)	C29-P1-C22-C23	23.89(10)
N1-Rh1-C16-C17	-150.41(9)	C28-P1-C22-C23	-81.24(10)
P1-Rh1-C16-C17	-56.17(9)	Rh1-P1-C22-C23	146.50(8)
N3-Rh1-C16-C21	-53.74(9)	C29-P1-C22-C27	-159.42(9)
N5-Rh1-C16-C21	-84.0(3)	C28-P1-C22-C27	95.44(10)
N1-Rh1-C16-C21	32.79(9)	Rh1-P1-C22-C27	-36.81(10)
P1-Rh1-C16-C21	127.02(9)	C27-C22-C23-C24	1.78(17)
C21-C16-C17-F1	176.50(9)	P1-C22-C23-C24	178.54(10)
Rh1-C16-C17-F1	-0.61(14)	C22-C23-C24-C25	-0.8(2)
C21-C16-C17-C18	-3.86(16)	C23-C24-C25-C26	-0.3(2)
Rh1-C16-C17-C18	179.03(8)	C24-C25-C26-C27	0.4(2)
F1-C17-C18-F2	1.14(15)	C25-C26-C27-C22	0.65(18)
C16-C17-C18-F2	-178.52(10)	C23-C22-C27-C26	-1.71(17)
F1-C17-C18-C19	-178.80(10)	P1-C22-C27-C26	-178.43(9)

Table S61. Crystal data and structure refinement for **9b**.

Identification code	**9b**	
Empirical formula	$C_{35}H_{49}BF_4N_6PRh$	
Formula weight	774.49	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.2654(11) Å	α = 106.173(2)°
	b = 13.2828(14) Å	β = 107.854(2)°
	c = 15.0471(16) Å	γ = 101.522(2)°
Volume	1782.1(3) Å^3	
Z	2	
Density (calculated)	1.443 Mg/m^3	
Absorption coefficient	0.579 mm^{-1}	
F(000)	804	
Crystal color, morphology	colorless, block	
Crystal size	0.24 x 0.16 x 0.10 mm^3	
Theta range for data collection	1.53 to 37.41°	
Index ranges	$-17 \le h \le 17$, $-22 \le k \le 22$, $-25 \le l \le 25$	

Reflections collected	64752
Independent reflections	18391 [R(int) = 0.0362]
Observed reflections	15601
Completeness to theta = 37.41°	98.6%
Absorption correction	Multi-scan
Max. and min. transmission	0.9443 and 0.8734
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18391 / 0 / 447
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R_1 = 0.0326, wR_2 = 0.0795
R indices (all data)	R_1 = 0.0424, wR_2 = 0.0849
Largest diff. peak and hole	1.183 and -0.642 e.Å^{-3}

Table S62. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **9b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	1724(1)	7464(1)	8659(1)	12(1)
P1	1258(1)	8032(1)	10061(1)	13(1)
N1	-615(1)	6537(1)	7619(1)	16(1)
N2	-1074(1)	6775(1)	6769(1)	16(1)
N3	2200(1)	6957(1)	7369(1)	15(1)
N4	1232(1)	6903(1)	6482(1)	16(1)
N5	1511(1)	8862(1)	8227(1)	14(1)
N6	690(1)	8629(1)	7235(1)	16(1)
B1	27(2)	7434(1)	6477(1)	17(1)
C1	-1787(1)	5869(1)	7618(1)	17(1)
C2	-2998(1)	5692(1)	6771(1)	19(1)
C3	-2506(1)	6283(1)	6253(1)	18(1)
C4	3209(1)	6546(1)	7171(1)	18(1)
C5	2877(2)	6206(1)	6137(1)	21(1)
C6	1627(1)	6441(1)	5725(1)	19(1)
C7	2121(1)	9962(1)	8642(1)	15(1)
C8	1665(1)	10437(1)	7929(1)	19(1)
C9	770(1)	9572(1)	7049(1)	19(1)
C10	-1771(1)	5403(1)	8414(1)	22(1)
C11	-3331(2)	6424(1)	5312(1)	23(1)
C12	4471(2)	6510(1)	7969(1)	24(1)
C13	774(2)	6212(1)	4647(1)	26(1)
C14	3179(1)	10560(1)	9694(1)	18(1)
C15	1(2)	9603(1)	6045(1)	30(1)
C16	2070(1)	6110(1)	8925(1)	15(1)
C17	3118(1)	6106(1)	9766(1)	16(1)
F1	4036(1)	7060(1)	10518(1)	20(1)
C18	3312(1)	5154(1)	9913(1)	17(1)
F2	4338(1)	5213(1)	10753(1)	22(1)
C19	2460(1)	4136(1)	9191(1)	20(1)
F3	2637(1)	3208(1)	9332(1)	28(1)
C20	1433(1)	4105(1)	8329(1)	20(1)
F4	588(1)	3107(1)	7619(1)	27(1)
C21	1252(1)	5058(1)	8191(1)	17(1)
C22	3992(1)	9482(1)	11434(1)	20(1)

C23	4933(2)	10408(1)	12264(1)	24(1)
C24	4396(2)	11122(1)	12810(1)	27(1)
C25	2922(2)	10898(1)	12537(1)	28(1)
C26	1976(2)	9970(1)	11712(1)	22(1)
C27	2500(1)	9262(1)	11141(1)	16(1)
C28	1036(1)	7106(1)	10739(1)	18(1)
C29	-438(1)	8342(1)	9748(1)	21(1)
C30	2963(2)	2629(2)	6826(2)	44(1)
C31	3820(2)	1939(2)	6450(1)	36(1)
C32	5400(2)	2578(2)	6892(1)	39(1)
C33	6360(2)	1918(2)	6558(2)	44(1)
C34	6190(2)	1676(2)	5493(1)	38(1)
C35	7192(2)	1074(2)	5225(2)	50(1)

Table S63. Bond lengths [Å] and angles [°] for **9b**.

Rh(1)-C(16)	2.0228(11)	C(10)-H(10A)	0.9800
Rh(1)-N(3)	2.1078(10)	C(10)-H(10B)	0.9800
Rh(1)-N(5)	2.1592(10)	C(10)-H(10C)	0.9800
Rh(1)-P(1)	2.2649(4)	C(11)-H(11A)	0.9800
Rh(1)-N(1)	2.2744(10)	C(11)-H(11B)	0.9800
Rh(1)-H(1)	1.486(19)	C(11)-H(11C)	0.9800
P(1)-C(29)	1.8199(13)	C(12)-H(12A)	0.9800
P(1)-C(28)	1.8267(12)	C(12)-H(12B)	0.9800
P(1)-C(27)	1.8311(12)	C(12)-H(12C)	0.9800
N(1)-C(1)	1.3444(15)	C(13)-H(13A)	0.9800
N(1)-N(2)	1.3689(14)	C(13)-H(13B)	0.9800
N(2)-C(3)	1.3504(15)	C(13)-H(13C)	0.9800
N(2)-B(1)	1.5368(17)	C(14)-H(14A)	0.9800
N(3)-C(4)	1.3353(16)	C(14)-H(14B)	0.9800
N(3)-N(4)	1.3702(14)	C(14)-H(14C)	0.9800
N(4)-C(6)	1.3538(16)	C(15)-H(15A)	0.9800
N(4)-B(1)	1.5411(18)	C(15)-H(15B)	0.9800
N(5)-C(7)	1.3428(15)	C(15)-H(15C)	0.9800
N(5)-N(6)	1.3786(14)	C(16)-C(17)	1.3896(16)
N(6)-C(9)	1.3500(15)	C(16)-C(21)	1.4074(16)
N(6)-B(1)	1.5382(17)	C(17)-F(1)	1.3577(14)
B(1)-H(1B)	1.0000	C(17)-C(18)	1.3842(17)
C(1)-C(2)	1.4031(17)	C(18)-F(2)	1.3452(14)
C(1)-C(10)	1.4908(17)	C(18)-C(19)	1.3783(18)
C(2)-C(3)	1.3801(18)	C(19)-F(3)	1.3454(14)
C(2)-H(2)	0.9500	C(19)-C(20)	1.3826(19)
C(3)-C(11)	1.4942(17)	C(20)-F(4)	1.3546(15)
C(4)-C(5)	1.4010(18)	C(20)-C(21)	1.3768(17)
C(4)-C(12)	1.4913(19)	C(21)-H(21)	0.9500
C(5)-C(6)	1.381(2)	C(22)-C(23)	1.3915(18)
C(5)-H(5)	0.9500	C(22)-C(27)	1.3997(17)
C(6)-C(13)	1.4963(18)	C(22)-H(22)	0.9500
C(7)-C(8)	1.3978(16)	C(23)-C(24)	1.389(2)
C(7)-C(14)	1.4899(17)	C(23)-H(23)	0.9500
C(8)-C(9)	1.3793(18)	C(24)-C(25)	1.385(2)
C(8)-H(8)	0.9500	C(24)-H(24)	0.9500
C(9)-C(15)	1.4919(18)	C(25)-C(26)	1.391(2)

C(25)-H(25)	0.9500	C(4)-N(3)-N(4)	107.88(10)
C(26)-C(27)	1.3958(18)	C(4)-N(3)-Rh(1)	133.97(8)
C(26)-H(26)	0.9500	N(4)-N(3)-Rh(1)	117.75(7)
C(28)-H(28A)	0.9800	C(6)-N(4)-N(3)	109.34(10)
C(28)-H(28B)	0.9800	C(6)-N(4)-B(1)	130.04(10)
C(28)-H(28C)	0.9800	N(3)-N(4)-B(1)	120.30(9)
C(29)-H(29A)	0.9800	C(7)-N(5)-N(6)	106.22(9)
C(29)-H(29B)	0.9800	C(7)-N(5)-Rh(1)	136.67(8)
C(29)-H(29C)	0.9800	N(6)-N(5)-Rh(1)	116.48(7)
C(30)-C(31)	1.508(3)	C(9)-N(6)-N(5)	110.06(10)
C(30)-H(30A)	0.9800	C(9)-N(6)-B(1)	128.19(10)
C(30)-H(30B)	0.9800	N(5)-N(6)-B(1)	121.03(9)
C(30)-H(30C)	0.9800	N(2)-B(1)-N(6)	109.61(10)
C(31)-C(32)	1.506(3)	N(2)-B(1)-N(4)	109.62(10)
C(31)-H(31A)	0.9900	N(6)-B(1)-N(4)	109.19(10)
C(31)-H(31B)	0.9900	N(2)-B(1)-H(1B)	109.5
C(32)-C(33)	1.549(3)	N(6)-B(1)-H(1B)	109.5
C(32)-H(32A)	0.9900	N(4)-B(1)-H(1B)	109.5
C(32)-H(32B)	0.9900	N(1)-C(1)-C(2)	109.96(10)
C(33)-C(34)	1.490(3)	N(1)-C(1)-C(10)	123.94(11)
C(33)-H(33A)	0.9900	C(2)-C(1)-C(10)	126.09(11)
C(33)-H(33B)	0.9900	C(3)-C(2)-C(1)	105.80(11)
C(34)-C(35)	1.505(3)	C(3)-C(2)-H(2)	127.1
C(34)-H(34A)	0.9900	C(1)-C(2)-H(2)	127.1
C(34)-H(34B)	0.9900	N(2)-C(3)-C(2)	107.41(10)
C(35)-H(35A)	0.9800	N(2)-C(3)-C(11)	123.33(11)
C(35)-H(35B)	0.9800	C(2)-C(3)-C(11)	129.24(12)
C(35)-H(35C)	0.9800	N(3)-C(4)-C(5)	108.77(11)
C(16)-Rh(1)-N(3)	88.84(4)	N(3)-C(4)-C(12)	122.74(11)
C(16)-Rh(1)-N(5)	171.73(4)	C(5)-C(4)-C(12)	128.47(12)
N(3)-Rh(1)-N(5)	83.18(4)	C(6)-C(5)-C(4)	106.43(11)
C(16)-Rh(1)-P(1)	91.32(3)	C(6)-C(5)-H(5)	126.8
N(3)-Rh(1)-P(1)	178.89(3)	C(4)-C(5)-H(5)	126.8
N(5)-Rh(1)-P(1)	96.61(3)	N(4)-C(6)-C(5)	107.58(11)
C(16)-Rh(1)-N(1)	92.74(4)	N(4)-C(6)-C(13)	123.59(13)
N(3)-Rh(1)-N(1)	85.96(4)	C(5)-C(6)-C(13)	128.80(12)
N(5)-Rh(1)-N(1)	88.89(4)	N(5)-C(7)-C(8)	109.94(10)
P(1)-Rh(1)-N(1)	95.13(3)	N(5)-C(7)-C(14)	124.00(10)
C(16)-Rh(1)-H(1)	88.1(7)	C(8)-C(7)-C(14)	126.00(11)
N(3)-Rh(1)-H(1)	89.4(7)	C(9)-C(8)-C(7)	105.95(11)
N(5)-Rh(1)-H(1)	89.6(7)	C(9)-C(8)-H(8)	127.0
P(1)-Rh(1)-H(1)	89.5(7)	C(7)-C(8)-H(8)	127.0
N(1)-Rh(1)-H(1)	175.3(7)	N(6)-C(9)-C(8)	107.79(10)
C(29)-P(1)-C(28)	103.33(6)	N(6)-C(9)-C(15)	123.33(12)
C(29)-P(1)-C(27)	103.41(6)	C(8)-C(9)-C(15)	128.88(12)
C(28)-P(1)-C(27)	97.71(6)	C(1)-C(10)-H(10A)	109.5
C(29)-P(1)-Rh(1)	109.35(4)	C(1)-C(10)-H(10B)	109.5
C(28)-P(1)-Rh(1)	119.79(4)	H(10A)-C(10)-H(10B)	109.5
C(27)-P(1)-Rh(1)	120.82(4)	C(1)-C(10)-H(10C)	109.5
C(1)-N(1)-N(2)	106.00(9)	H(10A)-C(10)-H(10C)	109.5
C(1)-N(1)-Rh(1)	138.72(8)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	114.90(7)	C(3)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	110.83(10)	C(3)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	129.09(10)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	119.85(9)	C(3)-C(11)-H(11C)	109.5

H(11A)-C(11)-H(11C)	109.5	C(26)-C(25)-H(25)	119.8
H(11B)-C(11)-H(11C)	109.5	C(25)-C(26)-C(27)	120.41(13)
C(4)-C(12)-H(12A)	109.5	C(25)-C(26)-H(26)	119.8
C(4)-C(12)-H(12B)	109.5	C(27)-C(26)-H(26)	119.8
H(12A)-C(12)-H(12B)	109.5	C(26)-C(27)-C(22)	118.86(11)
C(4)-C(12)-H(12C)	109.5	C(26)-C(27)-P(1)	120.47(10)
H(12A)-C(12)-H(12C)	109.5	C(22)-C(27)-P(1)	120.61(9)
H(12B)-C(12)-H(12C)	109.5	P(1)-C(28)-H(28A)	109.5
C(6)-C(13)-H(13A)	109.5	P(1)-C(28)-H(28B)	109.5
C(6)-C(13)-H(13B)	109.5	H(28A)-C(28)-H(28B)	109.5
H(13A)-C(13)-H(13B)	109.5	P(1)-C(28)-H(28C)	109.5
C(6)-C(13)-H(13C)	109.5	H(28A)-C(28)-H(28C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(28B)-C(28)-H(28C)	109.5
H(13B)-C(13)-H(13C)	109.5	P(1)-C(29)-H(29A)	109.5
C(7)-C(14)-H(14A)	109.5	P(1)-C(29)-H(29B)	109.5
C(7)-C(14)-H(14B)	109.5	H(29A)-C(29)-H(29B)	109.5
H(14A)-C(14)-H(14B)	109.5	P(1)-C(29)-H(29C)	109.5
C(7)-C(14)-H(14C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(14A)-C(14)-H(14C)	109.5	H(29B)-C(29)-H(29C)	109.5
H(14B)-C(14)-H(14C)	109.5	C(31)-C(30)-H(30A)	109.5
C(9)-C(15)-H(15A)	109.5	C(31)-C(30)-H(30B)	109.5
C(9)-C(15)-H(15B)	109.5	H(30A)-C(30)-H(30B)	109.5
H(15A)-C(15)-H(15B)	109.5	C(31)-C(30)-H(30C)	109.5
C(9)-C(15)-H(15C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(30B)-C(30)-H(30C)	109.5
H(15B)-C(15)-H(15C)	109.5	C(32)-C(31)-C(30)	111.32(16)
C(17)-C(16)-C(21)	114.56(10)	C(32)-C(31)-H(31A)	109.4
C(17)-C(16)-Rh(1)	125.99(9)	C(30)-C(31)-H(31A)	109.4
C(21)-C(16)-Rh(1)	119.37(8)	C(32)-C(31)-H(31B)	109.4
F(1)-C(17)-C(18)	114.88(10)	C(30)-C(31)-H(31B)	109.4
F(1)-C(17)-C(16)	121.38(10)	H(31A)-C(31)-H(31B)	108.0
C(18)-C(17)-C(16)	123.74(11)	C(31)-C(32)-C(33)	114.51(17)
F(2)-C(18)-C(19)	119.45(11)	C(31)-C(32)-H(32A)	108.6
F(2)-C(18)-C(17)	120.48(11)	C(33)-C(32)-H(32A)	108.6
C(19)-C(18)-C(17)	120.06(11)	C(31)-C(32)-H(32B)	108.6
F(3)-C(19)-C(18)	120.33(12)	C(33)-C(32)-H(32B)	108.6
F(3)-C(19)-C(20)	121.71(12)	H(32A)-C(32)-H(32B)	107.6
C(18)-C(19)-C(20)	117.97(11)	C(34)-C(33)-C(32)	114.84(16)
F(4)-C(20)-C(21)	120.32(12)	C(34)-C(33)-H(33A)	108.6
F(4)-C(20)-C(19)	118.24(11)	C(32)-C(33)-H(33A)	108.6
C(21)-C(20)-C(19)	121.43(12)	C(34)-C(33)-H(33B)	108.6
C(20)-C(21)-C(16)	122.14(11)	C(32)-C(33)-H(33B)	108.6
C(20)-C(21)-H(21)	118.9	H(33A)-C(33)-H(33B)	107.5
C(16)-C(21)-H(21)	118.9	C(33)-C(34)-C(35)	112.34(18)
C(23)-C(22)-C(27)	120.44(12)	C(33)-C(34)-H(34A)	109.1
C(23)-C(22)-H(22)	119.8	C(35)-C(34)-H(34A)	109.1
C(27)-C(22)-H(22)	119.8	C(33)-C(34)-H(34B)	109.1
C(24)-C(23)-C(22)	120.07(13)	C(35)-C(34)-H(34B)	109.1
C(24)-C(23)-H(23)	120.0	H(34A)-C(34)-H(34B)	107.9
C(22)-C(23)-H(23)	120.0	C(34)-C(35)-H(35A)	109.5
C(25)-C(24)-C(23)	119.87(13)	C(34)-C(35)-H(35B)	109.5
C(25)-C(24)-H(24)	120.1	H(35A)-C(35)-H(35B)	109.5
C(23)-C(24)-H(24)	120.1	C(34)-C(35)-H(35C)	109.5
C(24)-C(25)-C(26)	120.31(13)	H(35A)-C(35)-H(35C)	109.5
C(24)-C(25)-H(25)	119.8	H(35B)-C(35)-H(35C)	109.5

Table S64. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **9b**. 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}
Rh1	13(1)	12(1)	11(1)	4(1)	4(1)	4(1)
P1	14(1)	14(1)	12(1)	5(1)	5(1)	5(1)
N1	15(1)	18(1)	13(1)	7(1)	4(1)	4(1)
N2	16(1)	16(1)	13(1)	5(1)	3(1)	4(1)
N3	17(1)	15(1)	14(1)	6(1)	7(1)	5(1)
N4	20(1)	16(1)	12(1)	5(1)	6(1)	3(1)
N5	16(1)	14(1)	12(1)	5(1)	4(1)	5(1)
N6	19(1)	16(1)	14(1)	7(1)	4(1)	5(1)
B1	20(1)	16(1)	14(1)	6(1)	4(1)	4(1)
C1	16(1)	18(1)	15(1)	5(1)	6(1)	2(1)
C2	15(1)	20(1)	16(1)	3(1)	4(1)	2(1)
C3	17(1)	17(1)	14(1)	3(1)	2(1)	5(1)
C4	21(1)	16(1)	19(1)	6(1)	11(1)	6(1)
C5	26(1)	19(1)	20(1)	3(1)	14(1)	5(1)
C6	24(1)	17(1)	14(1)	3(1)	9(1)	0(1)
C7	16(1)	14(1)	16(1)	6(1)	7(1)	6(1)
C8	23(1)	15(1)	20(1)	8(1)	8(1)	6(1)
C9	22(1)	18(1)	18(1)	10(1)	6(1)	7(1)
C10	20(1)	25(1)	19(1)	10(1)	7(1)	1(1)
C11	22(1)	23(1)	17(1)	5(1)	-1(1)	6(1)
C12	23(1)	28(1)	24(1)	10(1)	12(1)	13(1)
C13	29(1)	30(1)	14(1)	5(1)	8(1)	2(1)
C14	19(1)	16(1)	17(1)	5(1)	6(1)	3(1)
C15	39(1)	25(1)	22(1)	15(1)	3(1)	9(1)
C16	17(1)	14(1)	14(1)	6(1)	6(1)	5(1)
C17	16(1)	16(1)	15(1)	6(1)	6(1)	6(1)
F1	20(1)	18(1)	17(1)	5(1)	1(1)	5(1)
C18	19(1)	20(1)	18(1)	11(1)	9(1)	10(1)
F2	22(1)	29(1)	23(1)	16(1)	8(1)	14(1)
C19	26(1)	16(1)	25(1)	11(1)	14(1)	11(1)
F3	39(1)	19(1)	35(1)	16(1)	17(1)	16(1)
C20	25(1)	14(1)	20(1)	4(1)	10(1)	5(1)
F4	34(1)	13(1)	27(1)	2(1)	10(1)	4(1)
C21	19(1)	16(1)	16(1)	5(1)	6(1)	5(1)
C22	20(1)	19(1)	16(1)	4(1)	6(1)	4(1)
C23	22(1)	24(1)	19(1)	5(1)	5(1)	0(1)
C24	32(1)	20(1)	18(1)	1(1)	8(1)	-2(1)
C25	34(1)	22(1)	22(1)	-2(1)	13(1)	5(1)
C26	24(1)	21(1)	20(1)	3(1)	10(1)	6(1)
C27	20(1)	15(1)	13(1)	5(1)	7(1)	4(1)
C28	21(1)	20(1)	15(1)	8(1)	7(1)	4(1)
C29	18(1)	24(1)	19(1)	7(1)	6(1)	10(1)
C30	52(1)	46(1)	40(1)	16(1)	24(1)	18(1)
C31	38(1)	32(1)	34(1)	10(1)	14(1)	7(1)
C32	39(1)	43(1)	26(1)	7(1)	8(1)	6(1)
C33	36(1)	65(1)	36(1)	26(1)	11(1)	19(1)
C34	34(1)	43(1)	32(1)	13(1)	10(1)	8(1)

C35	45(1)	42(1)	62(1)	13(1)	24(1)	11(1)

Table S65. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **9b**.

	x	y	z	U(eq)
H1	3280(20)	8060(15)	9263(14)	22(4)
H1B	-464	7434	5791	20
H2	-3959	5255	6592	23
H5	3407	5880	5788	26
H8	1920	11200	8031	23
H10A	-820	5326	8711	34
H10B	-2506	4678	8120	34
H10C	-1974	5900	8935	34
H11A	-3184	7210	5437	35
H11B	-4359	6039	5094	35
H11C	-2991	6113	4787	35
H12A	4629	7052	8617	35
H12B	5330	6685	7813	35
H12C	4284	5771	8000	35
H13A	691	6905	4560	39
H13B	-190	5703	4441	39
H13C	1262	5880	4233	39
H14A	3859	10152	9857	27
H14B	2668	10621	10151	27
H14C	3706	11299	9768	27
H15A	-1038	9263	5832	44
H15B	339	9196	5558	44
H15C	196	10371	6085	44
H21	551	5003	7581	21
H22	4364	8995	11064	23
H23	5944	10553	12457	29
H24	5038	11761	13369	33
H25	2555	11382	12916	34
H26	966	9817	11536	27
H28A	645	7408	11235	28
H28B	1973	7033	11081	28
H28C	372	6379	10265	28
H29A	-735	8450	10319	31
H29B	-1179	7726	9164	31
H29C	-314	9015	9593	31
H30A	1936	2206	6499	67
H30B	3125	3301	6670	67
H30C	3270	2829	7553	67
H31A	3682	1274	6630	43
H31B	3461	1694	5710	43
H32A	5739	2839	7632	47
H32B	5524	3237	6703	47
H33A	7381	2339	6994	53
H33B	6139	1211	6664	53
H34A	6379	2377	5374	45
H34B	5183	1223	5050	45

H35A	7085	973	4533	76
H35B	6955	351	5287	76
H35C	8188	1505	5680	76

Table S66. Torsion angles [°] for **9b**.

C16-Rh1-P1-C29	-129.09(6)	Rh1-N5-N6-B1	-2.68(14)
N3-Rh1-P1-C29	132.8(15)	C3-N2-B1-N6	117.48(13)
N5-Rh1-P1-C29	53.26(6)	N1-N2-B1-N6	-68.65(14)
N1-Rh1-P1-C29	-36.21(6)	C3-N2-B1-N4	-122.70(13)
C16-Rh1-P1-C28	-10.23(6)	N1-N2-B1-N4	51.17(14)
N3-Rh1-P1-C28	-108.3(15)	C9-N6-B1-N2	-126.53(13)
N5-Rh1-P1-C28	172.12(6)	N5-N6-B1-N2	64.15(14)
N1-Rh1-P1-C28	82.64(6)	C9-N6-B1-N4	113.39(13)
C16-Rh1-P1-C27	111.19(6)	N5-N6-B1-N4	-55.93(14)
N3-Rh1-P1-C27	13.1(15)	C6-N4-B1-N2	117.49(13)
N5-Rh1-P1-C27	-66.45(5)	N3-N4-B1-N2	-69.79(13)
N1-Rh1-P1-C27	-155.93(5)	C6-N4-B1-N6	-122.43(13)
C16-Rh1-N1-C1	50.40(13)	N3-N4-B1-N6	50.30(13)
N3-Rh1-N1-C1	139.04(13)	N2-N1-C1-C2	-0.65(14)
N5-Rh1-N1-C1	-137.72(13)	Rh1-N1-C1-C2	171.43(10)
P1-Rh1-N1-C1	-41.17(13)	N2-N1-C1-C10	179.69(12)
C16-Rh1-N1-N2	-138.01(8)	Rh1-N1-C1-C10	-8.2(2)
N3-Rh1-N1-N2	-49.36(8)	N1-C1-C2-C3	0.12(15)
N5-Rh1-N1-N2	33.88(8)	C10-C1-C2-C3	179.77(13)
P1-Rh1-N1-N2	130.42(8)	N1-N2-C3-C2	-0.91(14)
C1-N1-N2-C3	0.97(13)	B1-N2-C3-C2	173.41(12)
Rh1-N1-N2-C3	-173.28(8)	N1-N2-C3-C11	177.65(12)
C1-N1-N2-B1	-173.95(11)	B1-N2-C3-C11	-8.0(2)
Rh1-N1-N2-B1	11.81(13)	C1-C2-C3-N2	0.47(14)
C16-Rh1-N3-C4	-43.09(12)	C1-C2-C3-C11	-177.96(13)
N5-Rh1-N3-C4	134.71(12)	N4-N3-C4-C5	-0.84(13)
P1-Rh1-N3-C4	55.0(15)	Rh1-N3-C4-C5	171.44(9)
N1-Rh1-N3-C4	-135.93(12)	N4-N3-C4-C12	177.79(11)
C16-Rh1-N3-N4	128.60(8)	Rh1-N3-C4-C12	-9.93(19)
N5-Rh1-N3-N4	-53.60(8)	N3-C4-C5-C6	0.47(14)
P1-Rh1-N3-N4	-133.3(14)	C12-C4-C5-C6	-178.06(13)
N1-Rh1-N3-N4	35.77(8)	N3-N4-C6-C5	-0.60(13)
C4-N3-N4-C6	0.90(13)	B1-N4-C6-C5	172.74(12)
Rh1-N3-N4-C6	-172.83(8)	N3-N4-C6-C13	177.31(11)
C4-N3-N4-B1	-173.20(10)	B1-N4-C6-C13	-9.3(2)
Rh1-N3-N4-B1	13.08(13)	C4-C5-C6-N4	0.09(14)
C16-Rh1-N5-C7	-106.0(3)	C4-C5-C6-C13	-177.68(13)
N3-Rh1-N5-C7	-121.46(12)	N6-N5-C7-C8	1.65(13)
P1-Rh1-N5-C7	57.43(12)	Rh1-N5-C7-C8	171.76(9)
N1-Rh1-N5-C7	152.47(12)	N6-N5-C7-C14	-175.70(11)
C16-Rh1-N5-N6	63.4(3)	Rh1-N5-C7-C14	-5.59(18)
N3-Rh1-N5-N6	47.92(8)	N5-C7-C8-C9	-1.37(14)
P1-Rh1-N5-N6	-133.18(8)	C14-C7-C8-C9	175.91(12)
N1-Rh1-N5-N6	-38.15(8)	N5-N6-C9-C8	0.49(14)
C7-N5-N6-C9	-1.33(13)	B1-N6-C9-C8	-169.78(12)
Rh1-N5-N6-C9	-173.76(8)	N5-N6-C9-C15	-179.95(13)
C7-N5-N6-B1	169.75(10)	B1-N6-C9-C15	9.8(2)

C7-C8-C9-N6	0.51(14)	F3-C19-C20-C21	179.58(11)
C7-C8-C9-C15	-179.01(14)	C18-C19-C20-C21	-0.47(19)
N3-Rh1-C16-C17	118.50(10)	F4-C20-C21-C16	177.58(11)
N5-Rh1-C16-C17	103.1(3)	C19-C20-C21-C16	-1.55(19)
P1-Rh1-C16-C17	-60.40(10)	C17-C16-C21-C20	3.32(17)
N1-Rh1-C16-C17	-155.60(10)	Rh1-C16-C21-C20	-179.83(9)
N3-Rh1-C16-C21	-57.96(9)	C27-C22-C23-C24	0.2(2)
N5-Rh1-C16-C21	-73.3(3)	C22-C23-C24-C25	1.1(2)
P1-Rh1-C16-C21	123.14(9)	C23-C24-C25-C26	-0.8(2)
N1-Rh1-C16-C21	27.94(9)	C24-C25-C26-C27	-0.9(2)
C21-C16-C17-F1	177.01(10)	C25-C26-C27-C22	2.2(2)
Rh1-C16-C17-F1	0.40(16)	C25-C26-C27-P1	179.41(11)
C21-C16-C17-C18	-3.37(17)	C23-C22-C27-C26	-1.86(19)
Rh1-C16-C17-C18	-179.98(9)	C23-C22-C27-P1	-179.03(10)
F1-C17-C18-F2	0.53(16)	C29-P1-C27-C26	20.53(12)
C16-C17-C18-F2	-179.11(11)	C28-P1-C27-C26	-85.22(11)
F1-C17-C18-C19	-178.77(11)	Rh1-P1-C27-C26	143.14(9)
C16-C17-C18-C19	1.59(18)	C29-P1-C27-C22	-162.34(10)
F2-C18-C19-F3	1.12(18)	C28-P1-C27-C22	91.91(11)
C17-C18-C19-F3	-179.57(11)	Rh1-P1-C27-C22	-39.73(11)
F2-C18-C19-C20	-178.84(11)	C30-C31-C32-C33	178.92(16)
C17-C18-C19-C20	0.47(18)	C31-C32-C33-C34	70.8(2)
F3-C19-C20-F4	0.43(19)	C32-C33-C34-C35	177.69(17)
C18-C19-C20-F4	-179.61(11)		

Table S67. Crystal data and structure refinement for **9c**.

Identification code	**9c**	
Empirical formula	$C_{29}H_{35}BF_4N_6PRh$	
Formula weight	688.32	
Temperature	173(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.9400(8) Å	α = 90°
	b = 18.7449(13) Å	β = 109.712(1)°
	c = 14.5298(10) Å	γ = 90°
Volume	3061.4(4) Å^3	
Z	4	
Density (calculated)	1.493 Mg/m^3	
Absorption coefficient	0.664 mm^{-1}	
F(000)	1408	
Crystal color, morphology	colorless, block	
Crystal size	0.26 x 0.22 x 0.18 mm^3	
Theta range for data collection	1.84 to 37.78°	
Index ranges	$-20 \le h \le 20$, $-32 \le k \le 32$, $-24 \le l \le 24$	
Reflections collected	74523	
Independent reflections	16316 [R(int) = 0.0421]	
Observed reflections	9949	
Completeness to theta = 37.78°	99.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8898 and 0.8462	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	16316 / 0 / 391
Goodness-of-fit on F^2	0.996
Final *R* indices [*I*>2sigma(*I*)]	R_1 = 0.0427, wR_2 = 0.1005
R indices (all data)	R_1 = 0.0826, wR_2 = 0.1209
Largest diff. peak and hole	0.953 and -0.404 e.Å^{-3}

Table S68. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **9c**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	3447(1)	3645(1)	6150(1)	35(1)
P1	4551(1)	3708(1)	7757(1)	43(1)
N1	3655(1)	2456(1)	6007(1)	39(1)
N2	3922(1)	2252(1)	5200(1)	45(1)
N3	2489(1)	3642(1)	4640(1)	35(1)
N4	2944(1)	3257(1)	4047(1)	40(1)
N5	4957(1)	3802(1)	5676(1)	45(1)
N6	5106(1)	3312(1)	5023(1)	49(1)
B1	4087(2)	2806(1)	4489(2)	46(1)
C1	3525(2)	1852(1)	6455(1)	42(1)
C2	3723(2)	1264(1)	5938(2)	49(1)
C3	3965(2)	1531(1)	5157(2)	52(1)
C4	1553(1)	4005(1)	4062(1)	39(1)
C5	1406(2)	3858(1)	3095(1)	44(1)
C6	2296(2)	3388(1)	3103(1)	42(1)
C7	5847(2)	4278(1)	5839(2)	55(1)
C8	6574(2)	4068(2)	5302(2)	70(1)
C9	6084(2)	3475(2)	4798(2)	61(1)
C10	829(2)	4487(1)	4459(2)	49(1)
C11	2563(2)	3069(1)	2258(2)	58(1)
C12	3188(2)	1822(1)	7347(2)	52(1)
C13	4275(3)	1140(2)	4370(2)	79(1)
C14	5964(2)	4927(2)	6437(2)	70(1)
C15	6491(2)	3034(2)	4102(2)	86(1)
C16	1899(2)	3567(1)	6446(1)	36(1)
C17	1541(2)	4037(1)	7040(1)	42(1)
F1	2262(1)	4581(1)	7498(1)	58(1)
C18	468(2)	4007(1)	7192(1)	44(1)
F2	232(1)	4502(1)	7783(1)	63(1)
C19	-366(2)	3504(1)	6753(2)	47(1)
C20	-60(2)	3033(1)	6152(2)	43(1)
F3	-853(1)	2528(1)	5679(1)	60(1)
C21	1022(2)	3067(1)	6008(1)	38(1)
F4	1181(1)	2574(1)	5378(1)	49(1)
C22	4608(2)	5210(1)	7990(2)	57(1)
C23	5102(2)	5840(1)	8453(2)	62(1)
C24	6129(3)	5830(1)	9228(2)	72(1)
C25	6650(3)	5194(1)	9587(2)	96(1)
C26	6145(3)	4561(1)	9145(2)	83(1)
C27	5152(2)	4558(1)	8326(1)	52(1)
C28	3928(3)	3387(1)	8668(2)	72(1)
C29	5861(2)	3156(1)	7977(2)	59(1)

Table S69. Bond lengths [Å] and angles [°] for **9c**.

Rh(1)-C(16)	2.0388(17)	C(14)-H(14B)	0.9800
Rh(1)-N(3)	2.1040(15)	C(14)-H(14C)	0.9800
Rh(1)-N(5)	2.1565(16)	C(15)-H(15A)	0.9800
Rh(1)-N(1)	2.2611(15)	C(15)-H(15B)	0.9800
Rh(1)-P(1)	2.2643(5)	C(15)-H(15C)	0.9800
Rh(1)-H(1)	1.53(2)	C(16)-C(21)	1.390(2)
P(1)-C(29)	1.812(2)	C(16)-C(17)	1.398(2)
P(1)-C(28)	1.826(3)	C(17)-F(1)	1.355(2)
P(1)-C(27)	1.828(2)	C(17)-C(18)	1.373(3)
N(1)-C(1)	1.341(2)	C(18)-F(2)	1.357(2)
N(1)-N(2)	1.368(2)	C(18)-C(19)	1.363(3)
N(2)-C(3)	1.354(3)	C(19)-C(20)	1.376(3)
N(2)-B(1)	1.524(3)	C(19)-H(19)	0.9500
N(3)-C(4)	1.335(2)	C(20)-F(3)	1.352(2)
N(3)-N(4)	1.3704(19)	C(20)-C(21)	1.378(2)
N(4)-C(6)	1.351(2)	C(21)-F(4)	1.3575(19)
N(4)-B(1)	1.548(2)	C(22)-C(23)	1.387(3)
N(5)-C(7)	1.345(3)	C(22)-C(27)	1.393(3)
N(5)-N(6)	1.374(2)	C(22)-H(22)	0.9500
N(6)-C(9)	1.349(3)	C(23)-C(24)	1.356(4)
N(6)-B(1)	1.532(3)	C(23)-H(23)	0.9500
B(1)-H(1B)	1.0000	C(24)-C(25)	1.364(4)
C(1)-C(2)	1.397(3)	C(24)-H(24)	0.9500
C(1)-C(12)	1.482(3)	C(25)-C(26)	1.388(4)
C(2)-C(3)	1.357(3)	C(25)-H(25)	0.9500
C(2)-H(2)	0.9500	C(26)-C(27)	1.368(3)
C(3)-C(13)	1.506(3)	C(26)-H(26)	0.9500
C(4)-C(5)	1.383(3)	C(28)-H(28A)	0.9800
C(4)-C(10)	1.495(3)	C(28)-H(28B)	0.9800
C(5)-C(6)	1.378(3)	C(28)-H(28C)	0.9800
C(5)-H(5)	0.9500	C(29)-H(29A)	0.9800
C(6)-C(11)	1.493(3)	C(29)-H(29B)	0.9800
C(7)-C(8)	1.404(3)	C(29)-H(29C)	0.9800
C(7)-C(14)	1.476(4)	C(16)-Rh(1)-N(3)	90.38(6)
C(8)-C(9)	1.350(4)	C(16)-Rh(1)-N(5)	172.81(6)
C(8)-H(8)	0.9500	N(3)-Rh(1)-N(5)	83.49(6)
C(9)-C(15)	1.508(4)	C(16)-Rh(1)-N(1)	94.81(6)
C(10)-H(10A)	0.9800	N(3)-Rh(1)-N(1)	86.55(5)
C(10)-H(10B)	0.9800	N(5)-Rh(1)-N(1)	88.58(6)
C(10)-H(10C)	0.9800	C(16)-Rh(1)-P(1)	92.30(5)
C(11)-H(11A)	0.9800	N(3)-Rh(1)-P(1)	176.23(4)
C(11)-H(11B)	0.9800	N(5)-Rh(1)-P(1)	93.66(5)
C(11)-H(11C)	0.9800	N(1)-Rh(1)-P(1)	95.85(4)
C(12)-H(12A)	0.9800	C(16)-Rh(1)-H(1)	87.0(7)
C(12)-H(12B)	0.9800	N(3)-Rh(1)-H(1)	90.9(7)
C(12)-H(12C)	0.9800	N(5)-Rh(1)-H(1)	89.4(7)
C(13)-H(13A)	0.9800	N(1)-Rh(1)-H(1)	176.9(7)
C(13)-H(13B)	0.9800	P(1)-Rh(1)-H(1)	86.6(7)
C(13)-H(13C)	0.9800	C(29)-P(1)-C(28)	102.85(13)
C(14)-H(14A)	0.9800	C(29)-P(1)-C(27)	103.60(11)

C(28)-P(1)-C(27)	98.78(11)	C(4)-C(10)-H(10A)	109.5
C(29)-P(1)-Rh(1)	108.66(8)	C(4)-C(10)-H(10B)	109.5
C(28)-P(1)-Rh(1)	119.54(10)	H(10A)-C(10)-H(10B)	109.5
C(27)-P(1)-Rh(1)	120.99(7)	C(4)-C(10)-H(10C)	109.5
C(1)-N(1)-N(2)	106.16(15)	H(10A)-C(10)-H(10C)	109.5
C(1)-N(1)-Rh(1)	138.93(12)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	114.75(11)	C(6)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	109.97(16)	C(6)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	129.25(16)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	120.75(15)	C(6)-C(11)-H(11C)	109.5
C(4)-N(3)-N(4)	107.34(14)	H(11A)-C(11)-H(11C)	109.5
C(4)-N(3)-Rh(1)	134.46(12)	H(11B)-C(11)-H(11C)	109.5
N(4)-N(3)-Rh(1)	117.73(10)	C(1)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.27(14)	C(1)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	130.00(15)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	120.58(14)	C(1)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.64(16)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	136.85(15)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	116.50(12)	C(3)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	109.86(19)	C(3)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	128.44(19)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	119.87(14)	C(3)-C(13)-H(13C)	109.5
N(2)-B(1)-N(6)	109.89(16)	H(13A)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	110.82(15)	H(13B)-C(13)-H(13C)	109.5
N(6)-B(1)-N(4)	108.10(16)	C(7)-C(14)-H(14A)	109.5
N(2)-B(1)-H(1B)	109.3	C(7)-C(14)-H(14B)	109.5
N(6)-B(1)-H(1B)	109.3	H(14A)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.3	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	109.66(18)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(12)	124.49(17)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(12)	125.83(18)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	106.31(18)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2)	126.8	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2)	126.8	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	107.89(17)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(13)	123.0(2)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(13)	129.1(2)	C(21)-C(16)-C(17)	111.60(15)
N(3)-C(4)-C(5)	109.30(16)	C(21)-C(16)-Rh(1)	123.27(12)
N(3)-C(4)-C(10)	122.34(16)	C(17)-C(16)-Rh(1)	124.93(13)
C(5)-C(4)-C(10)	128.36(16)	F(1)-C(17)-C(18)	115.08(15)
C(6)-C(5)-C(4)	106.61(16)	F(1)-C(17)-C(16)	120.13(16)
C(6)-C(5)-H(5)	126.7	C(18)-C(17)-C(16)	124.77(18)
C(4)-C(5)-H(5)	126.7	F(2)-C(18)-C(19)	119.60(17)
N(4)-C(6)-C(5)	107.48(16)	F(2)-C(18)-C(17)	118.57(18)
N(4)-C(6)-C(11)	123.68(18)	C(19)-C(18)-C(17)	121.83(16)
C(5)-C(6)-C(11)	128.83(18)	C(18)-C(19)-C(20)	115.57(17)
N(5)-C(7)-C(8)	108.4(2)	C(18)-C(19)-H(19)	122.2
N(5)-C(7)-C(14)	124.3(2)	C(20)-C(19)-H(19)	122.2
C(8)-C(7)-C(14)	127.2(2)	F(3)-C(20)-C(19)	118.79(16)
C(9)-C(8)-C(7)	107.2(2)	F(3)-C(20)-C(21)	119.12(16)
C(9)-C(8)-H(8)	126.4	C(19)-C(20)-C(21)	122.08(18)
C(7)-C(8)-H(8)	126.4	F(4)-C(21)-C(20)	114.98(16)
N(6)-C(9)-C(8)	107.8(2)	F(4)-C(21)-C(16)	120.87(15)
N(6)-C(9)-C(15)	122.6(3)	C(20)-C(21)-C(16)	124.14(16)
C(8)-C(9)-C(15)	129.5(2)	C(23)-C(22)-C(27)	120.3(2)

C(23)-C(22)-H(22)	119.9	C(26)-C(27)-P(1)	119.27(16)
C(27)-C(22)-H(22)	119.9	C(22)-C(27)-P(1)	122.79(17)
C(24)-C(23)-C(22)	120.6(2)	P(1)-C(28)-H(28A)	109.5
C(24)-C(23)-H(23)	119.7	P(1)-C(28)-H(28B)	109.5
C(22)-C(23)-H(23)	119.7	H(28A)-C(28)-H(28B)	109.5
C(23)-C(24)-C(25)	119.8(2)	P(1)-C(28)-H(28C)	109.5
C(23)-C(24)-H(24)	120.1	H(28A)-C(28)-H(28C)	109.5
C(25)-C(24)-H(24)	120.1	H(28B)-C(28)-H(28C)	109.5
C(24)-C(25)-C(26)	120.0(3)	P(1)-C(29)-H(29A)	109.5
C(24)-C(25)-H(25)	120.0	P(1)-C(29)-H(29B)	109.5
C(26)-C(25)-H(25)	120.0	H(29A)-C(29)-H(29B)	109.5
C(27)-C(26)-C(25)	121.3(2)	P(1)-C(29)-H(29C)	109.5
C(27)-C(26)-H(26)	119.4	H(29A)-C(29)-H(29C)	109.5
C(25)-C(26)-H(26)	119.4	H(29B)-C(29)-H(29C)	109.5
C(26)-C(27)-C(22)	117.9(2)		

Table S70. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9c**. 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}
Rh1	36(1)	37(1)	34(1)	3(1)	15(1)	5(1)
P1	56(1)	36(1)	35(1)	1(1)	12(1)	7(1)
N1	41(1)	42(1)	37(1)	2(1)	15(1)	9(1)
N2	51(1)	48(1)	39(1)	3(1)	19(1)	18(1)
N3	35(1)	38(1)	36(1)	4(1)	16(1)	7(1)
N4	39(1)	48(1)	36(1)	4(1)	18(1)	7(1)
N5	35(1)	60(1)	42(1)	7(1)	14(1)	4(1)
N6	37(1)	69(1)	44(1)	8(1)	19(1)	13(1)
B1	47(1)	58(1)	39(1)	4(1)	21(1)	16(1)
C1	42(1)	40(1)	39(1)	3(1)	9(1)	7(1)
C2	55(1)	40(1)	44(1)	1(1)	6(1)	12(1)
C3	60(1)	52(1)	43(1)	-1(1)	14(1)	22(1)
C4	35(1)	39(1)	42(1)	8(1)	13(1)	3(1)
C5	38(1)	49(1)	41(1)	10(1)	10(1)	0(1)
C6	40(1)	49(1)	36(1)	5(1)	15(1)	-4(1)
C7	37(1)	78(1)	48(1)	11(1)	10(1)	-5(1)
C8	34(1)	116(2)	62(1)	19(1)	20(1)	-1(1)
C9	35(1)	101(2)	51(1)	14(1)	20(1)	13(1)
C10	45(1)	47(1)	56(1)	9(1)	18(1)	14(1)
C11	62(1)	77(2)	40(1)	1(1)	25(1)	0(1)
C12	64(1)	45(1)	51(1)	8(1)	25(1)	2(1)
C13	115(2)	68(2)	59(1)	-5(1)	35(2)	40(2)
C14	57(1)	88(2)	61(1)	1(1)	15(1)	-25(1)
C15	52(1)	149(3)	70(2)	2(2)	36(1)	19(2)
C16	41(1)	34(1)	37(1)	4(1)	18(1)	5(1)
C17	55(1)	34(1)	45(1)	2(1)	28(1)	3(1)
F1	72(1)	47(1)	70(1)	-18(1)	41(1)	-9(1)
C18	62(1)	33(1)	51(1)	6(1)	37(1)	8(1)
F2	90(1)	47(1)	79(1)	-6(1)	62(1)	5(1)
C19	53(1)	40(1)	62(1)	11(1)	36(1)	8(1)
C20	43(1)	37(1)	54(1)	6(1)	22(1)	2(1)
F3	48(1)	53(1)	83(1)	-9(1)	27(1)	-7(1)

C21	44(1)	35(1)	40(1)	3(1)	19(1)	7(1)
F4	46(1)	49(1)	55(1)	-14(1)	20(1)	2(1)
C22	60(1)	43(1)	66(1)	0(1)	20(1)	3(1)
C23	77(2)	39(1)	73(2)	-2(1)	28(1)	5(1)
C24	114(2)	44(1)	51(1)	-11(1)	19(1)	1(1)
C25	135(3)	55(1)	55(1)	-14(1)	-23(2)	11(2)
C26	115(2)	48(1)	52(1)	-8(1)	-16(1)	17(1)
C27	72(1)	39(1)	40(1)	-2(1)	13(1)	6(1)
C28	116(2)	63(1)	42(1)	4(1)	30(1)	-4(1)
C29	64(1)	44(1)	55(1)	-5(1)	0(1)	15(1)

Table S71. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **9c**.

	x	y	z	U(eq)
H1	3311(15)	4453(10)	6191(13)	34(5)
H1B	4278	2559	3950	55
H2	3695	775	6101	59
H5	808	4044	2535	53
H8	7278	4299	5296	84
H10A	1343	4705	5068	74
H10B	202	4211	4589	74
H10C	468	4862	3981	74
H11A	1917	3183	1650	87
H11B	2633	2550	2338	87
H11C	3312	3265	2231	87
H12A	2677	2229	7354	78
H12B	3908	1839	7927	78
H12C	2758	1377	7350	78
H13A	5042	1311	4352	118
H13B	3657	1227	3736	118
H13C	4326	627	4511	118
H14A	5172	5095	6400	104
H14B	6365	5300	6191	104
H14C	6432	4819	7119	104
H15A	7255	3216	4090	129
H15B	5898	3063	3445	129
H15C	6583	2536	4320	129
H19	-1110	3481	6856	57
H22	3895	5224	7442	68
H23	4718	6281	8225	75
H24	6483	6265	9521	86
H25	7359	5186	10139	115
H26	6495	4120	9417	99
H28A	4573	3303	9288	109
H28B	3497	2940	8441	109
H28C	3381	3745	8766	109
H29A	6301	3135	8680	89
H29B	6370	3360	7638	89
H29C	5620	2673	7730	89

Table S72. Torsion angles [°] for **9c**.

C16-Rh1-P1-C29	137.57(10)	C9-N6-B1-N2	125.5(2)
N3-Rh1-P1-C29	-87.0(6)	N5-N6-B1-N2	-71.5(2)
N5-Rh1-P1-C29	-46.45(10)	C9-N6-B1-N4	-113.4(2)
N1-Rh1-P1-C29	42.49(10)	N5-N6-B1-N4	49.5(2)
C16-Rh1-P1-C28	20.10(12)	C6-N4-B1-N2	-126.27(19)
N3-Rh1-P1-C28	155.5(6)	N3-N4-B1-N2	58.8(2)
N5-Rh1-P1-C28	-163.93(12)	C6-N4-B1-N6	113.3(2)
N1-Rh1-P1-C28	-74.98(11)	N3-N4-B1-N6	-61.7(2)
C16-Rh1-P1-C27	-102.94(10)	N2-N1-C1-C2	0.7(2)
N3-Rh1-P1-C27	32.5(6)	Rh1-N1-C1-C2	175.58(14)
N5-Rh1-P1-C27	73.04(10)	N2-N1-C1-C12	-177.73(17)
N1-Rh1-P1-C27	161.99(10)	Rh1-N1-C1-C12	-2.9(3)
C16-Rh1-N1-C1	-41.78(19)	N1-C1-C2-C3	-0.7(2)
N3-Rh1-N1-C1	-131.88(19)	C12-C1-C2-C3	177.77(19)
N5-Rh1-N1-C1	144.57(19)	N1-N2-C3-C2	0.1(2)
P1-Rh1-N1-C1	51.04(19)	B1-N2-C3-C2	-177.94(19)
C16-Rh1-N1-N2	132.75(12)	N1-N2-C3-C13	-178.1(2)
N3-Rh1-N1-N2	42.66(12)	B1-N2-C3-C13	3.9(4)
N5-Rh1-N1-N2	-40.90(12)	C1-C2-C3-N2	0.3(2)
P1-Rh1-N1-N2	-134.43(11)	C1-C2-C3-C13	178.4(2)
C1-N1-N2-C3	-0.5(2)	N4-N3-C4-C5	-0.4(2)
Rh1-N1-N2-C3	-176.80(13)	Rh1-N3-C4-C5	171.17(12)
C1-N1-N2-B1	177.72(16)	N4-N3-C4-C10	180.00(16)
Rh1-N1-N2-B1	1.4(2)	Rh1-N3-C4-C10	-8.5(3)
C16-Rh1-N3-C4	49.77(17)	N3-C4-C5-C6	-0.1(2)
N5-Rh1-N3-C4	-126.47(17)	C10-C4-C5-C6	179.53(18)
N1-Rh1-N3-C4	144.56(17)	N3-N4-C6-C5	-0.7(2)
P1-Rh1-N3-C4	-85.7(6)	B1-N4-C6-C5	-176.15(19)
C16-Rh1-N3-N4	-139.35(12)	N3-N4-C6-C11	178.48(18)
N5-Rh1-N3-N4	44.41(12)	B1-N4-C6-C11	3.1(3)
N1-Rh1-N3-N4	-44.56(12)	C4-C5-C6-N4	0.5(2)
P1-Rh1-N3-N4	85.2(6)	C4-C5-C6-C11	-178.7(2)
C4-N3-N4-C6	0.69(19)	N6-N5-C7-C8	-1.7(2)
Rh1-N3-N4-C6	-172.50(11)	Rh1-N5-C7-C8	179.17(16)
C4-N3-N4-B1	176.62(16)	N6-N5-C7-C14	174.9(2)
Rh1-N3-N4-B1	3.4(2)	Rh1-N5-C7-C14	-4.2(3)
C16-Rh1-N5-C7	93.2(6)	N5-C7-C8-C9	1.8(3)
N3-Rh1-N5-C7	124.8(2)	C14-C7-C8-C9	-174.7(2)
N1-Rh1-N5-C7	-148.5(2)	N5-N6-C9-C8	0.2(2)
P1-Rh1-N5-C7	-52.8(2)	B1-N6-C9-C8	164.5(2)
C16-Rh1-N5-N6	-85.9(6)	N5-N6-C9-C15	179.7(2)
N3-Rh1-N5-N6	-54.33(13)	B1-N6-C9-C15	-16.0(4)
N1-Rh1-N5-N6	32.36(13)	C7-C8-C9-N6	-1.2(3)
P1-Rh1-N5-N6	128.13(12)	C7-C8-C9-C15	179.4(2)
C7-N5-N6-C9	0.9(2)	N3-Rh1-C16-C21	49.45(14)
Rh1-N5-N6-C9	-179.70(13)	N5-Rh1-C16-C21	80.8(6)
C7-N5-N6-B1	-164.92(17)	N1-Rh1-C16-C21	-37.12(14)
Rh1-N5-N6-B1	14.4(2)	P1-Rh1-C16-C21	-133.19(14)
C3-N2-B1-N6	-122.3(2)	N3-Rh1-C16-C17	-124.93(15)
N1-N2-B1-N6	59.8(2)	N5-Rh1-C16-C17	-93.6(6)
C3-N2-B1-N4	118.3(2)	N1-Rh1-C16-C17	148.50(15)
N1-N2-B1-N4	-59.6(2)	P1-Rh1-C16-C17	52.43(15)

C21-C16-C17-F1	-177.33(16)	Rh1-C16-C21-F4	3.0(2)
Rh1-C16-C17-F1	-2.4(2)	C17-C16-C21-C20	-0.8(2)
C21-C16-C17-C18	1.1(3)	Rh1-C16-C21-C20	-175.81(14)
Rh1-C16-C17-C18	176.03(14)	C27-C22-C23-C24	1.0(4)
F1-C17-C18-F2	-1.1(3)	C22-C23-C24-C25	-3.2(4)
C16-C17-C18-F2	-179.53(17)	C23-C24-C25-C26	1.4(5)
F1-C17-C18-C19	177.72(18)	C24-C25-C26-C27	2.7(6)
C16-C17-C18-C19	-0.8(3)	C25-C26-C27-C22	-4.8(5)
F2-C18-C19-C20	178.76(17)	C25-C26-C27-P1	178.3(3)
C17-C18-C19-C20	0.0(3)	C23-C22-C27-C26	3.0(4)
C18-C19-C20-F3	-178.91(17)	C23-C22-C27-P1	179.82(19)
C18-C19-C20-C21	0.3(3)	C29-P1-C27-C26	-33.1(3)
F3-C20-C21-F4	0.5(2)	C28-P1-C27-C26	72.5(3)
C19-C20-C21-F4	-178.73(16)	Rh1-P1-C27-C26	-155.1(2)
F3-C20-C21-C16	179.33(16)	C29-P1-C27-C22	150.1(2)
C19-C20-C21-C16	0.1(3)	C28-P1-C27-C22	-104.3(2)
C17-C16-C21-F4	178.02(15)	Rh1-P1-C27-C22	28.2(2)

Table S73. Crystal data and structure refinement for **9d**.

Identification code	**9d**	
Empirical formula	$C_{29}H_{36}BF_3N_6PRh$	
Formula weight	670.33	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.2916(14) Å	α = 90.743(2)°
	b = 11.5263(16) Å	β = 93.433(2)°
	c = 12.4406(17) Å	γ = 92.065(2)°
Volume	1472.0(3) Å^3	
Z	2	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	0.684 mm^{-1}	
F(000)	688	
Crystal color, morphology	colorless, rod	
Crystal size	0.24 x 0.18 x 0.10 mm^3	
Theta range for data collection	1.77 to 36.32°	
Index ranges	$-17 \le h \le 17$, $-19 \le k \le 19$, $-20 \le l \le 20$	
Reflections collected	34212	
Independent reflections	13969 [R(int) = 0.0365]	
Observed reflections	11895	
Completeness to theta = 36.32°	98.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9347 and 0.8530	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13969 / 0 / 382	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R_1 = 0.0332, wR_2 = 0.0785	
R indices (all data)	R_1 = 0.0424, wR_2 = 0.0830	
Largest diff. peak and hole	1.079 and -0.503 e.Å^{-3}	

Table S74. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **9d**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	2619(1)	1673(1)	1702(1)	10(1)
P1	1303(1)	2557(1)	460(1)	12(1)
N1	1080(1)	527(1)	2419(1)	13(1)
N2	1506(1)	-537(1)	2736(1)	13(1)
N3	4024(1)	931(1)	2758(1)	12(1)
N4	3936(1)	-232(1)	2946(1)	12(1)
N5	2952(1)	202(1)	686(1)	12(1)
N6	2895(1)	-868(1)	1164(1)	12(1)
B1	2805(2)	-971(1)	2393(1)	12(1)
C1	-51(1)	659(1)	2884(1)	16(1)
C2	-348(2)	-313(1)	3492(1)	20(1)
C3	662(1)	-1048(1)	3395(1)	17(1)
C4	5134(1)	1345(1)	3269(1)	13(1)
C5	5758(1)	434(1)	3793(1)	16(1)
C6	4981(1)	-553(1)	3568(1)	13(1)
C7	3282(1)	14(1)	-327(1)	13(1)
C8	3411(1)	-1177(1)	-508(1)	16(1)
C9	3169(1)	-1705(1)	449(1)	14(1)
C10	-822(2)	1726(2)	2794(1)	24(1)
C11	888(2)	-2184(1)	3923(1)	24(1)
C12	5571(1)	2593(1)	3250(1)	18(1)
C13	5200(2)	-1777(1)	3884(1)	20(1)
C14	3512(2)	956(1)	-1107(1)	18(1)
C15	3206(2)	-2961(1)	722(1)	20(1)
C16	2495(1)	2991(1)	2803(1)	13(1)
C17	2734(2)	4167(1)	2621(1)	16(1)
F1	3005(1)	4502(1)	1605(1)	23(1)
C18	2743(2)	5079(1)	3361(1)	22(1)
C19	2495(2)	4782(1)	4402(1)	23(1)
F2	2475(1)	5638(1)	5160(1)	37(1)
C20	2273(2)	3652(1)	4696(1)	20(1)
C21	2291(1)	2806(1)	3889(1)	14(1)
F3	2105(1)	1704(1)	4242(1)	18(1)
C22	1180(2)	3632(1)	-1546(1)	18(1)
C23	1632(2)	4298(1)	-2382(1)	22(1)
C24	2909(2)	4724(1)	-2328(1)	22(1)
C25	3723(2)	4494(1)	-1432(1)	20(1)
C26	3271(2)	3826(1)	-598(1)	17(1)
C27	1991(1)	3381(1)	-642(1)	14(1)
C28	198(1)	1497(1)	-240(1)	18(1)
C29	193(2)	3650(1)	899(1)	24(1)

Table S75. Bond lengths [Å] and angles [°] for **9d**.

Rh(1)-C(16)	2.0446(13)	Rh(1)-N(1)	2.2582(12)
Rh(1)-N(3)	2.1068(11)	Rh(1)-P(1)	2.2688(4)
Rh(1)-N(5)	2.1513(11)	Rh(1)-H(1)	1.469(19)

P(1)-C(28)	1.8167(15)	C(19)-F(2)	1.3569(17)
P(1)-C(29)	1.8305(16)	C(19)-C(20)	1.372(2)
P(1)-C(27)	1.8407(14)	C(20)-C(21)	1.392(2)
N(1)-C(1)	1.3427(18)	C(20)-H(20)	0.9500
N(1)-N(2)	1.3723(16)	C(21)-F(3)	1.3592(16)
N(2)-C(3)	1.3550(18)	C(22)-C(23)	1.393(2)
N(2)-B(1)	1.5262(19)	C(22)-C(27)	1.399(2)
N(3)-C(4)	1.3433(17)	C(22)-H(22)	0.9500
N(3)-N(4)	1.3643(15)	C(23)-C(24)	1.383(2)
N(4)-C(6)	1.3518(17)	C(23)-H(23)	0.9500
N(4)-B(1)	1.5403(19)	C(24)-C(25)	1.387(2)
N(5)-C(7)	1.3416(17)	C(24)-H(24)	0.9500
N(5)-N(6)	1.3762(15)	C(25)-C(26)	1.393(2)
N(6)-C(9)	1.3529(17)	C(25)-H(25)	0.9500
N(6)-B(1)	1.5428(18)	C(26)-C(27)	1.394(2)
B(1)-H(1B)	1.0000	C(26)-H(26)	0.9500
C(1)-C(2)	1.395(2)	C(28)-H(28A)	0.9800
C(1)-C(10)	1.490(2)	C(28)-H(28B)	0.9800
C(2)-C(3)	1.375(2)	C(28)-H(28C)	0.9800
C(2)-H(2)	0.9500	C(29)-H(29A)	0.9800
C(3)-C(11)	1.491(2)	C(29)-H(29B)	0.9800
C(4)-C(5)	1.3988(19)	C(29)-H(29C)	0.9800
C(4)-C(12)	1.4917(19)	C(16)-Rh(1)-N(3)	88.51(5)
C(5)-C(6)	1.383(2)	C(16)-Rh(1)-N(5)	172.37(5)
C(5)-H(5)	0.9500	N(3)-Rh(1)-N(5)	83.88(4)
C(6)-C(13)	1.4907(19)	C(16)-Rh(1)-N(1)	94.47(5)
C(7)-C(8)	1.4012(19)	N(3)-Rh(1)-N(1)	88.64(4)
C(7)-C(14)	1.4875(19)	N(5)-Rh(1)-N(1)	85.86(4)
C(8)-C(9)	1.375(2)	C(16)-Rh(1)-P(1)	92.51(4)
C(8)-H(8)	0.9500	N(3)-Rh(1)-P(1)	173.35(3)
C(9)-C(15)	1.492(2)	N(5)-Rh(1)-P(1)	94.99(3)
C(10)-H(10A)	0.9800	N(1)-Rh(1)-P(1)	97.82(3)
C(10)-H(10B)	0.9800	C(16)-Rh(1)-H(1)	86.5(8)
C(10)-H(10C)	0.9800	N(3)-Rh(1)-H(1)	89.0(7)
C(11)-H(11A)	0.9800	N(5)-Rh(1)-H(1)	92.9(8)
C(11)-H(11B)	0.9800	N(1)-Rh(1)-H(1)	177.4(7)
C(11)-H(11C)	0.9800	P(1)-Rh(1)-H(1)	84.5(7)
C(12)-H(12A)	0.9800	C(28)-P(1)-C(29)	102.42(8)
C(12)-H(12B)	0.9800	C(28)-P(1)-C(27)	103.26(7)
C(12)-H(12C)	0.9800	C(29)-P(1)-C(27)	97.77(7)
C(13)-H(13A)	0.9800	C(28)-P(1)-Rh(1)	110.36(5)
C(13)-H(13B)	0.9800	C(29)-P(1)-Rh(1)	119.58(6)
C(13)-H(13C)	0.9800	C(27)-P(1)-Rh(1)	120.80(5)
C(14)-H(14A)	0.9800	C(1)-N(1)-N(2)	105.83(11)
C(14)-H(14B)	0.9800	C(1)-N(1)-Rh(1)	137.55(10)
C(14)-H(14C)	0.9800	N(2)-N(1)-Rh(1)	114.03(8)
C(15)-H(15A)	0.9800	C(3)-N(2)-N(1)	110.47(11)
C(15)-H(15B)	0.9800	C(3)-N(2)-B(1)	128.57(12)
C(15)-H(15C)	0.9800	N(1)-N(2)-B(1)	120.87(11)
C(16)-C(17)	1.3926(19)	C(4)-N(3)-N(4)	107.14(10)
C(16)-C(21)	1.3982(19)	C(4)-N(3)-Rh(1)	133.35(9)
C(17)-F(1)	1.3671(16)	N(4)-N(3)-Rh(1)	119.25(8)
C(17)-C(18)	1.387(2)	C(6)-N(4)-N(3)	110.16(11)
C(18)-C(19)	1.381(2)	C(6)-N(4)-B(1)	130.34(11)
C(18)-H(18)	0.9500	N(3)-N(4)-B(1)	119.31(10)

C(7)-N(5)-N(6)	106.45(10)	H(12A)-C(12)-H(12C)	109.5
C(7)-N(5)-Rh(1)	137.22(9)	H(12B)-C(12)-H(12C)	109.5
N(6)-N(5)-Rh(1)	116.22(8)	C(6)-C(13)-H(13A)	109.5
C(9)-N(6)-N(5)	109.96(11)	C(6)-C(13)-H(13B)	109.5
C(9)-N(6)-B(1)	128.03(11)	H(13A)-C(13)-H(13B)	109.5
N(5)-N(6)-B(1)	120.90(10)	C(6)-C(13)-H(13C)	109.5
N(2)-B(1)-N(4)	109.89(11)	H(13A)-C(13)-H(13C)	109.5
N(2)-B(1)-N(6)	110.59(11)	H(13B)-C(13)-H(13C)	109.5
N(4)-B(1)-N(6)	107.94(11)	C(7)-C(14)-H(14A)	109.5
N(2)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14B)	109.5
N(4)-B(1)-H(1B)	109.5	H(14A)-C(14)-H(14B)	109.5
N(6)-B(1)-H(1B)	109.5	C(7)-C(14)-H(14C)	109.5
N(1)-C(1)-C(2)	110.25(13)	H(14A)-C(14)-H(14C)	109.5
N(1)-C(1)-C(10)	123.80(13)	H(14B)-C(14)-H(14C)	109.5
C(2)-C(1)-C(10)	125.88(13)	C(9)-C(15)-H(15A)	109.5
C(3)-C(2)-C(1)	106.04(13)	C(9)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2)	127.0	H(15A)-C(15)-H(15B)	109.5
C(1)-C(2)-H(2)	127.0	C(9)-C(15)-H(15C)	109.5
N(2)-C(3)-C(2)	107.39(12)	H(15A)-C(15)-H(15C)	109.5
N(2)-C(3)-C(11)	123.43(13)	H(15B)-C(15)-H(15C)	109.5
C(2)-C(3)-C(11)	129.13(13)	C(17)-C(16)-C(21)	110.51(12)
N(3)-C(4)-C(5)	109.07(12)	C(17)-C(16)-Rh(1)	125.89(10)
N(3)-C(4)-C(12)	123.00(12)	C(21)-C(16)-Rh(1)	123.26(9)
C(5)-C(4)-C(12)	127.92(13)	F(1)-C(17)-C(18)	113.91(12)
C(6)-C(5)-C(4)	106.32(12)	F(1)-C(17)-C(16)	118.40(12)
C(6)-C(5)-H(5)	126.8	C(18)-C(17)-C(16)	127.69(13)
C(4)-C(5)-H(5)	126.8	C(19)-C(18)-C(17)	116.05(14)
N(4)-C(6)-C(5)	107.31(12)	C(19)-C(18)-H(18)	122.0
N(4)-C(6)-C(13)	123.31(12)	C(17)-C(18)-H(18)	122.0
C(5)-C(6)-C(13)	129.34(13)	F(2)-C(19)-C(20)	119.08(14)
N(5)-C(7)-C(8)	109.74(12)	F(2)-C(19)-C(18)	118.72(14)
N(5)-C(7)-C(14)	123.79(12)	C(20)-C(19)-C(18)	122.20(14)
C(8)-C(7)-C(14)	126.44(12)	C(19)-C(20)-C(21)	116.94(13)
C(9)-C(8)-C(7)	106.02(12)	C(19)-C(20)-H(20)	121.5
C(9)-C(8)-H(8)	127.0	C(21)-C(20)-H(20)	121.5
C(7)-C(8)-H(8)	127.0	F(3)-C(21)-C(20)	113.85(12)
N(6)-C(9)-C(8)	107.82(12)	F(3)-C(21)-C(16)	119.57(12)
N(6)-C(9)-C(15)	123.23(12)	C(20)-C(21)-C(16)	126.57(13)
C(8)-C(9)-C(15)	128.95(13)	C(23)-C(22)-C(27)	121.38(14)
C(1)-C(10)-H(10A)	109.5	C(23)-C(22)-H(22)	119.3
C(1)-C(10)-H(10B)	109.5	C(27)-C(22)-H(22)	119.3
H(10A)-C(10)-H(10B)	109.5	C(24)-C(23)-C(22)	119.85(14)
C(1)-C(10)-H(10C)	109.5	C(24)-C(23)-H(23)	120.1
H(10A)-C(10)-H(10C)	109.5	C(22)-C(23)-H(23)	120.1
H(10B)-C(10)-H(10C)	109.5	C(23)-C(24)-C(25)	119.55(14)
C(3)-C(11)-H(11A)	109.5	C(23)-C(24)-H(24)	120.2
C(3)-C(11)-H(11B)	109.5	C(25)-C(24)-H(24)	120.2
H(11A)-C(11)-H(11B)	109.5	C(24)-C(25)-C(26)	120.58(15)
C(3)-C(11)-H(11C)	109.5	C(24)-C(25)-H(25)	119.7
H(11A)-C(11)-H(11C)	109.5	C(26)-C(25)-H(25)	119.7
H(11B)-C(11)-H(11C)	109.5	C(25)-C(26)-C(27)	120.71(14)
C(4)-C(12)-H(12A)	109.5	C(25)-C(26)-H(26)	119.6
C(4)-C(12)-H(12B)	109.5	C(27)-C(26)-H(26)	119.6
H(12A)-C(12)-H(12B)	109.5	C(26)-C(27)-C(22)	117.92(13)
C(4)-C(12)-H(12C)	109.5	C(26)-C(27)-P(1)	123.08(10)

C(22)-C(27)-P(1)	118.91(11)	P(1)-C(29)-H(29A)	109.5
P(1)-C(28)-H(28A)	109.5	P(1)-C(29)-H(29B)	109.5
P(1)-C(28)-H(28B)	109.5	H(29A)-C(29)-H(29B)	109.5
H(28A)-C(28)-H(28B)	109.5	P(1)-C(29)-H(29C)	109.5
P(1)-C(28)-H(28C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(28A)-C(28)-H(28C)	109.5	H(29B)-C(29)-H(29C)	109.5
H(28B)-C(28)-H(28C)	109.5		

Table S76. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9d**. 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}
Rh1	11(1)	9(1)	10(1)	1(1)	1(1)	1(1)
P1	13(1)	11(1)	12(1)	2(1)	1(1)	2(1)
N1	12(1)	13(1)	14(1)	1(1)	1(1)	1(1)
N2	12(1)	14(1)	13(1)	2(1)	2(1)	0(1)
N3	12(1)	11(1)	12(1)	1(1)	0(1)	1(1)
N4	13(1)	11(1)	12(1)	1(1)	0(1)	1(1)
N5	13(1)	11(1)	11(1)	1(1)	2(1)	1(1)
N6	14(1)	10(1)	12(1)	0(1)	1(1)	1(1)
B1	14(1)	12(1)	12(1)	0(1)	1(1)	0(1)
C1	14(1)	18(1)	18(1)	2(1)	3(1)	2(1)
C2	15(1)	24(1)	22(1)	5(1)	7(1)	0(1)
C3	16(1)	18(1)	17(1)	4(1)	4(1)	-2(1)
C4	12(1)	15(1)	14(1)	-1(1)	2(1)	0(1)
C5	14(1)	19(1)	14(1)	0(1)	-2(1)	2(1)
C6	15(1)	15(1)	11(1)	0(1)	0(1)	3(1)
C7	13(1)	14(1)	11(1)	-1(1)	1(1)	2(1)
C8	16(1)	16(1)	14(1)	-3(1)	2(1)	3(1)
C9	14(1)	12(1)	16(1)	-2(1)	1(1)	2(1)
C10	18(1)	26(1)	30(1)	6(1)	8(1)	8(1)
C11	24(1)	21(1)	27(1)	10(1)	7(1)	0(1)
C12	15(1)	15(1)	22(1)	-1(1)	0(1)	-2(1)
C13	23(1)	16(1)	19(1)	2(1)	-3(1)	6(1)
C14	21(1)	19(1)	13(1)	2(1)	5(1)	2(1)
C15	25(1)	12(1)	23(1)	-2(1)	2(1)	2(1)
C16	14(1)	12(1)	12(1)	0(1)	1(1)	2(1)
C17	22(1)	13(1)	14(1)	1(1)	1(1)	0(1)
F1	39(1)	14(1)	17(1)	2(1)	6(1)	-3(1)
C18	34(1)	12(1)	19(1)	-2(1)	-1(1)	1(1)
C19	37(1)	16(1)	16(1)	-6(1)	-3(1)	6(1)
F2	73(1)	19(1)	19(1)	-8(1)	-3(1)	8(1)
C20	28(1)	19(1)	13(1)	-1(1)	0(1)	4(1)
C21	16(1)	13(1)	14(1)	0(1)	0(1)	2(1)
F3	26(1)	15(1)	14(1)	2(1)	2(1)	-1(1)
C22	19(1)	21(1)	16(1)	4(1)	1(1)	1(1)
C23	30(1)	22(1)	14(1)	5(1)	0(1)	2(1)
C24	33(1)	18(1)	16(1)	4(1)	5(1)	-1(1)
C25	24(1)	17(1)	20(1)	2(1)	5(1)	-4(1)
C26	20(1)	15(1)	16(1)	2(1)	2(1)	-2(1)
C27	17(1)	13(1)	12(1)	1(1)	1(1)	1(1)
C28	15(1)	18(1)	22(1)	2(1)	-3(1)	-2(1)

C29	29(1)	23(1)	22(1)	7(1)	8(1)	13(1)

Table S77. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **9d**.

	x	y	z	U(eq)
H1	3664(18)	2381(17)	1252(15)	17(5)
H1B	2889	-1801	2602	15
H2	-1097	-441	3891	24
H5	6556	483	4218	19
H8	3622	-1546	-1159	19
H10A	-253	2409	2979	36
H10B	-1526	1681	3291	36
H10C	-1194	1792	2055	36
H11A	1734	-2147	4329	35
H11B	881	-2799	3372	35
H11C	197	-2350	4414	35
H12A	5397	2895	2525	26
H12B	6507	2666	3447	26
H12C	5095	3036	3766	26
H13A	4412	-2108	4184	29
H13B	5929	-1794	4427	29
H13C	5403	-2233	3249	29
H14A	3892	1646	-720	27
H14B	2683	1149	-1479	27
H14C	4112	695	-1635	27
H15A	2368	-3217	989	30
H15B	3902	-3075	1279	30
H15C	3372	-3415	76	30
H18	2909	5861	3163	26
H20	2115	3456	5417	24
H22	302	3343	-1590	22
H23	1066	4460	-2988	26
H24	3226	5171	-2899	27
H25	4596	4796	-1388	24
H26	3842	3671	8	20
H28A	-397	1895	-743	27
H28B	-304	1075	284	27
H28C	701	948	-640	27
H29A	-397	3858	289	36
H29B	697	4344	1165	36
H29C	-316	3335	1476	36

Table S78. Torsion angles [°] for **9d**.

C16-Rh1-P1-C28	-140.06(7)	N3-Rh1-P1-C29	-120.5(3)
N3-Rh1-P1-C28	121.2(3)	N5-Rh1-P1-C29	159.61(7)
N5-Rh1-P1-C28	41.30(6)	N1-Rh1-P1-C29	73.12(8)
N1-Rh1-P1-C28	-45.20(6)	C16-Rh1-P1-C27	99.54(6)
C16-Rh1-P1-C29	-21.75(8)	N3-Rh1-P1-C27	0.8(3)

N5-Rh1-P1-C27	-79.11(6)	C10-C1-C2-C3	-176.18(15)
N1-Rh1-P1-C27	-165.60(6)	N1-N2-C3-C2	1.23(16)
C16-Rh1-N1-C1	36.81(15)	B1-N2-C3-C2	178.03(13)
N3-Rh1-N1-C1	125.21(14)	N1-N2-C3-C11	-176.57(14)
N5-Rh1-N1-C1	-150.83(14)	B1-N2-C3-C11	0.2(2)
P1-Rh1-N1-C1	-56.35(14)	C1-C2-C3-N2	-1.25(17)
C16-Rh1-N1-N2	-121.61(9)	C1-C2-C3-C11	176.38(16)
N3-Rh1-N1-N2	-33.22(9)	N4-N3-C4-C5	-0.27(15)
N5-Rh1-N1-N2	50.75(9)	Rh1-N3-C4-C5	-174.18(10)
P1-Rh1-N1-N2	145.23(8)	N4-N3-C4-C12	179.98(12)
C1-N1-N2-C3	-0.69(15)	Rh1-N3-C4-C12	6.1(2)
Rh1-N1-N2-C3	164.36(9)	N3-C4-C5-C6	0.54(16)
C1-N1-N2-B1	-177.77(12)	C12-C4-C5-C6	-179.72(14)
Rh1-N1-N2-B1	-12.73(15)	N3-N4-C6-C5	0.45(15)
C16-Rh1-N3-C4	-51.94(13)	B1-N4-C6-C5	175.32(13)
N5-Rh1-N3-C4	127.58(13)	N3-N4-C6-C13	-177.67(13)
N1-Rh1-N3-C4	-146.44(13)	B1-N4-C6-C13	-2.8(2)
P1-Rh1-N3-C4	47.0(4)	C4-C5-C6-N4	-0.60(15)
C16-Rh1-N3-N4	134.73(10)	C4-C5-C6-C13	177.37(14)
N5-Rh1-N3-N4	-45.76(9)	N6-N5-C7-C8	1.23(15)
N1-Rh1-N3-N4	40.22(9)	Rh1-N5-C7-C8	177.08(10)
P1-Rh1-N3-N4	-126.3(2)	N6-N5-C7-C14	-176.88(12)
C4-N3-N4-C6	-0.12(14)	Rh1-N5-C7-C14	-1.0(2)
Rh1-N3-N4-C6	174.82(9)	N5-C7-C8-C9	-1.16(16)
C4-N3-N4-B1	-175.63(11)	C14-C7-C8-C9	176.90(13)
Rh1-N3-N4-B1	-0.70(15)	N5-N6-C9-C8	0.14(15)
C16-Rh1-N5-C7	-121.8(3)	B1-N6-C9-C8	-167.73(13)
N3-Rh1-N5-C7	-125.45(14)	N5-N6-C9-C15	179.16(13)
N1-Rh1-N5-C7	145.48(14)	B1-N6-C9-C15	11.3(2)
P1-Rh1-N5-C7	47.97(13)	C7-C8-C9-N6	0.60(16)
C16-Rh1-N5-N6	53.8(4)	C7-C8-C9-C15	-178.35(14)
N3-Rh1-N5-N6	50.11(9)	N3-Rh1-C16-C17	121.30(13)
N1-Rh1-N5-N6	-38.96(9)	N5-Rh1-C16-C17	117.6(3)
P1-Rh1-N5-N6	-136.47(9)	N1-Rh1-C16-C17	-150.18(12)
C7-N5-N6-C9	-0.86(14)	P1-Rh1-C16-C17	-52.13(12)
Rh1-N5-N6-C9	-177.71(9)	N3-Rh1-C16-C21	-51.41(12)
C7-N5-N6-B1	168.02(12)	N5-Rh1-C16-C21	-55.1(4)
Rh1-N5-N6-B1	-8.84(15)	N1-Rh1-C16-C21	37.11(12)
C3-N2-B1-N4	-108.25(15)	P1-Rh1-C16-C21	135.16(11)
N1-N2-B1-N4	68.26(15)	C21-C16-C17-F1	177.57(13)
C3-N2-B1-N6	132.67(14)	Rh1-C16-C17-F1	4.1(2)
N1-N2-B1-N6	-50.82(16)	C21-C16-C17-C18	-2.0(2)
C6-N4-B1-N2	124.76(14)	Rh1-C16-C17-C18	-175.51(13)
N3-N4-B1-N2	-60.77(15)	F1-C17-C18-C19	-179.02(14)
C6-N4-B1-N6	-114.56(14)	C16-C17-C18-C19	0.6(3)
N3-N4-B1-N6	59.91(15)	C17-C18-C19-F2	-179.22(15)
C9-N6-B1-N2	-126.76(14)	C17-C18-C19-C20	1.0(3)
N5-N6-B1-N2	66.55(15)	F2-C19-C20-C21	179.37(15)
C9-N6-B1-N4	113.00(14)	C18-C19-C20-C21	-0.9(3)
N5-N6-B1-N4	-53.69(15)	C19-C20-C21-F3	178.05(14)
N2-N1-C1-C2	-0.13(16)	C19-C20-C21-C16	-0.9(2)
Rh1-N1-C1-C2	-159.69(11)	C17-C16-C21-F3	-176.73(12)
N2-N1-C1-C10	176.99(14)	Rh1-C16-C21-F3	-3.03(18)
Rh1-N1-C1-C10	17.4(2)	C17-C16-C21-C20	2.2(2)
N1-C1-C2-C3	0.86(18)	Rh1-C16-C21-C20	175.87(12)

C27-C22-C23-C24	0.1(2)	C23-C22-C27-P1	177.00(12)
C22-C23-C24-C25	-0.8(2)	C28-P1-C27-C26	-145.25(12)
C23-C24-C25-C26	1.0(2)	C29-P1-C27-C26	109.97(13)
C24-C25-C26-C27	-0.4(2)	Rh1-P1-C27-C26	-21.42(14)
C25-C26-C27-C22	-0.3(2)	C28-P1-C27-C22	38.41(13)
C25-C26-C27-P1	-176.65(11)	C29-P1-C27-C22	-66.37(13)
C23-C22-C27-C26	0.5(2)	Rh1-P1-C27-C22	162.23(10)

Table S79. Crystal data and structure refinement for **9e**.

Identification code	**9e**	
Empirical formula	$C_{29}H_{37}BF_2N_6PRh$	
Formula weight	652.34	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.2523(9) Å	α = 92.716(2)°
	b = 11.6983(10) Å	β = 95.959(2)°
	c = 12.3627(11) Å	γ = 92.041(2)°
Volume	1471.8(2) Å^3	
Z	2	
Density (calculated)	1.472 Mg/m^3	
Absorption coefficient	0.677 mm^{-1}	
F(000)	672	
Crystal color, morphology	colorless, needle	
Crystal size	0.18 x 0.10 x 0.06 mm^3	
Theta range for data collection	1.66 to 31.50°	
Index ranges	$-15 \le h \le 15$, $-17 \le k \le 17$, $-18 \le l \le 18$	
Reflections collected	26065	
Independent reflections	9759 [R(int) = 0.0961]	
Observed reflections	6497	
Completeness to theta = 31.50°	99.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9605 and 0.8878	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9759 / 0 / 373	
Goodness-of-fit on F^2	0.968	
Final R indices [I>2sigma(I)]	R_1 = 0.0568, wR_2 = 0.1055	
R indices (all data)	R_1 = 0.1019, wR_2 = 0.1230	
Largest diff. peak and hole	1.058 and -0.796 e.Å^{-3}	

Table S80. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **9e**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	2689(1)	6700(1)	6725(1)	13(1)
P1	1325(1)	7545(1)	5484(1)	16(1)
N1	1193(3)	5584(2)	7452(2)	16(1)
N2	1651(3)	4543(2)	7765(2)	16(1)

N3	2996(3)	5200(2)	5700(2)	16(1)
N4	2967(3)	4164(2)	6181(2)	15(1)
N5	4149(3)	6019(2)	7820(2)	15(1)
N6	4103(3)	4871(2)	7988(2)	14(1)
B1	2946(4)	4111(3)	7422(3)	17(1)
C1	46(3)	5693(3)	7873(3)	20(1)
C2	-227(4)	4738(3)	8452(3)	23(1)
C3	801(4)	4034(3)	8376(3)	20(1)
C4	3270(3)	4971(3)	4677(3)	17(1)
C5	3411(3)	3802(3)	4502(3)	19(1)
C6	3224(3)	3311(3)	5462(3)	18(1)
C7	5273(3)	6455(3)	8356(3)	16(1)
C8	5949(3)	5575(3)	8860(3)	18(1)
C9	5187(3)	4591(3)	8609(3)	15(1)
C10	-770(4)	6707(4)	7743(3)	29(1)
C11	1044(4)	2904(3)	8877(3)	28(1)
C12	3445(4)	5875(3)	3892(3)	21(1)
C13	3277(4)	2089(3)	5753(3)	24(1)
C14	5682(4)	7689(3)	8375(3)	23(1)
C15	5473(4)	3391(3)	8888(3)	23(1)
C16	2573(3)	8003(3)	7848(3)	17(1)
C17	2902(4)	9141(3)	7738(3)	22(1)
F1	3233(2)	9517(2)	6778(2)	31(1)
C18	2918(4)	9971(3)	8578(3)	28(1)
F2	3284(3)	11063(2)	8378(2)	43(1)
C19	2616(5)	9714(4)	9586(4)	34(1)
C20	2284(4)	8583(4)	9739(3)	29(1)
C21	2265(4)	7750(3)	8895(3)	21(1)
C22	3253(4)	8779(3)	4460(3)	22(1)
C23	3681(4)	9434(3)	3648(3)	26(1)
C24	2828(4)	9660(3)	2759(3)	28(1)
C25	1549(4)	9234(4)	2670(3)	27(1)
C26	1122(4)	8575(3)	3480(3)	25(1)
C27	1977(4)	8334(3)	4387(3)	18(1)
C28	283(4)	8661(3)	5947(3)	25(1)
C29	164(4)	6500(3)	4753(3)	22(1)

Table S81. Bond lengths [Å] and angles [°] for **9e**.

Rh(1)-C(16)	2.028(4)	N(3)-N(4)	1.376(4)
Rh(1)-N(5)	2.115(3)	N(4)-C(6)	1.355(4)
Rh(1)-N(3)	2.167(3)	N(4)-B(1)	1.541(5)
Rh(1)-P(1)	2.2545(10)	N(5)-C(7)	1.340(4)
Rh(1)-N(1)	2.263(3)	N(5)-N(6)	1.369(4)
Rh(1)-H(1)	1.45(4)	N(6)-C(9)	1.343(4)
P(1)-C(29)	1.815(4)	N(6)-B(1)	1.542(5)
P(1)-C(28)	1.825(4)	B(1)-H(1B)	1.0000
P(1)-C(27)	1.844(4)	C(1)-C(2)	1.391(5)
N(1)-C(1)	1.342(4)	C(1)-C(10)	1.481(5)
N(1)-N(2)	1.378(4)	C(2)-C(3)	1.369(5)
N(2)-C(3)	1.351(4)	C(2)-H(2)	0.9500
N(2)-B(1)	1.531(5)	C(3)-C(11)	1.504(5)
N(3)-C(4)	1.341(4)	C(4)-C(5)	1.389(5)

C(4)-C(12)	1.487(5)	C(16)-Rh(1)-N(5)	87.87(13)
C(5)-C(6)	1.371(5)	C(16)-Rh(1)-N(3)	171.88(12)
C(5)-H(5)	0.9500	N(5)-Rh(1)-N(3)	84.06(11)
C(6)-C(13)	1.491(5)	C(16)-Rh(1)-P(1)	91.89(10)
C(7)-C(8)	1.396(5)	N(5)-Rh(1)-P(1)	173.30(8)
C(7)-C(14)	1.487(5)	N(3)-Rh(1)-P(1)	96.24(8)
C(8)-C(9)	1.372(5)	C(16)-Rh(1)-N(1)	92.88(12)
C(8)-H(8)	0.9500	N(5)-Rh(1)-N(1)	87.82(11)
C(9)-C(15)	1.494(5)	N(3)-Rh(1)-N(1)	85.88(11)
C(10)-H(10A)	0.9800	P(1)-Rh(1)-N(1)	98.88(8)
C(10)-H(10B)	0.9800	C(16)-Rh(1)-H(1)	88.0(15)
C(10)-H(10C)	0.9800	N(5)-Rh(1)-H(1)	84.2(15)
C(11)-H(11A)	0.9800	N(3)-Rh(1)-H(1)	92.1(15)
C(11)-H(11B)	0.9800	P(1)-Rh(1)-H(1)	89.1(15)
C(11)-H(11C)	0.9800	N(1)-Rh(1)-H(1)	172.0(15)
C(12)-H(12A)	0.9800	C(29)-P(1)-C(28)	103.52(18)
C(12)-H(12B)	0.9800	C(29)-P(1)-C(27)	103.38(17)
C(12)-H(12C)	0.9800	C(28)-P(1)-C(27)	97.05(17)
C(13)-H(13A)	0.9800	C(29)-P(1)-Rh(1)	110.86(12)
C(13)-H(13B)	0.9800	C(28)-P(1)-Rh(1)	118.90(13)
C(13)-H(13C)	0.9800	C(27)-P(1)-Rh(1)	120.65(12)
C(14)-H(14A)	0.9800	C(1)-N(1)-N(2)	106.0(3)
C(14)-H(14B)	0.9800	C(1)-N(1)-Rh(1)	138.5(3)
C(14)-H(14C)	0.9800	N(2)-N(1)-Rh(1)	114.0(2)
C(15)-H(15A)	0.9800	C(3)-N(2)-N(1)	109.8(3)
C(15)-H(15B)	0.9800	C(3)-N(2)-B(1)	129.0(3)
C(15)-H(15C)	0.9800	N(1)-N(2)-B(1)	121.2(3)
C(16)-C(17)	1.378(5)	C(4)-N(3)-N(4)	106.0(3)
C(16)-C(21)	1.407(5)	C(4)-N(3)-Rh(1)	137.4(2)
C(17)-F(1)	1.356(4)	N(4)-N(3)-Rh(1)	116.5(2)
C(17)-C(18)	1.386(5)	C(6)-N(4)-N(3)	110.2(3)
C(18)-F(2)	1.359(5)	C(6)-N(4)-B(1)	127.8(3)
C(18)-C(19)	1.360(6)	N(3)-N(4)-B(1)	120.7(3)
C(19)-C(20)	1.382(6)	C(7)-N(5)-N(6)	106.8(3)
C(19)-H(19)	0.9500	C(7)-N(5)-Rh(1)	133.5(2)
C(20)-C(21)	1.391(5)	N(6)-N(5)-Rh(1)	119.3(2)
C(20)-H(20)	0.9500	C(9)-N(6)-N(5)	110.1(3)
C(21)-H(21)	0.9500	C(9)-N(6)-B(1)	130.6(3)
C(22)-C(27)	1.383(5)	N(5)-N(6)-B(1)	119.3(3)
C(22)-C(23)	1.389(5)	N(2)-B(1)-N(4)	110.4(3)
C(22)-H(22A)	0.9500	N(2)-B(1)-N(6)	109.8(3)
C(23)-C(24)	1.373(6)	N(4)-B(1)-N(6)	108.3(3)
C(23)-H(23)	0.9500	N(2)-B(1)-H(1B)	109.4
C(24)-C(25)	1.378(6)	N(4)-B(1)-H(1B)	109.4
C(24)-H(24)	0.9500	N(6)-B(1)-H(1B)	109.4
C(25)-C(26)	1.389(5)	N(1)-C(1)-C(2)	110.0(3)
C(25)-H(25)	0.9500	N(1)-C(1)-C(10)	123.7(3)
C(26)-C(27)	1.396(5)	C(2)-C(1)-C(10)	126.3(3)
C(26)-H(26)	0.9500	C(3)-C(2)-C(1)	106.3(3)
C(28)-H(28A)	0.9800	C(3)-C(2)-H(2)	126.9
C(28)-H(28B)	0.9800	C(1)-C(2)-H(2)	126.9
C(28)-H(28C)	0.9800	N(2)-C(3)-C(2)	107.9(3)
C(29)-H(29A)	0.9800	N(2)-C(3)-C(11)	122.9(3)
C(29)-H(29B)	0.9800	C(2)-C(3)-C(11)	129.2(3)
C(29)-H(29C)	0.9800	N(3)-C(4)-C(5)	110.0(3)

N(3)-C(4)-C(12)	123.0(3)	H(15A)-C(15)-H(15C)	109.5
C(5)-C(4)-C(12)	126.9(3)	H(15B)-C(15)-H(15C)	109.5
C(6)-C(5)-C(4)	106.6(3)	C(17)-C(16)-C(21)	114.1(3)
C(6)-C(5)-H(5)	126.7	C(17)-C(16)-Rh(1)	126.5(3)
C(4)-C(5)-H(5)	126.7	C(21)-C(16)-Rh(1)	119.1(3)
N(4)-C(6)-C(5)	107.2(3)	F(1)-C(17)-C(16)	121.0(3)
N(4)-C(6)-C(13)	122.6(3)	F(1)-C(17)-C(18)	115.6(3)
C(5)-C(6)-C(13)	130.2(3)	C(16)-C(17)-C(18)	123.3(4)
N(5)-C(7)-C(8)	109.1(3)	F(2)-C(18)-C(19)	120.1(4)
N(5)-C(7)-C(14)	123.2(3)	F(2)-C(18)-C(17)	118.0(4)
C(8)-C(7)-C(14)	127.7(3)	C(19)-C(18)-C(17)	121.9(4)
C(9)-C(8)-C(7)	106.4(3)	C(18)-C(19)-C(20)	117.0(4)
C(9)-C(8)-H(8)	126.8	C(18)-C(19)-H(19)	121.5
C(7)-C(8)-H(8)	126.8	C(20)-C(19)-H(19)	121.5
N(6)-C(9)-C(8)	107.7(3)	C(19)-C(20)-C(21)	121.1(4)
N(6)-C(9)-C(15)	123.3(3)	C(19)-C(20)-H(20)	119.5
C(8)-C(9)-C(15)	128.9(3)	C(21)-C(20)-H(20)	119.5
C(1)-C(10)-H(10A)	109.5	C(20)-C(21)-C(16)	122.6(4)
C(1)-C(10)-H(10B)	109.5	C(20)-C(21)-H(21)	118.7
H(10A)-C(10)-H(10B)	109.5	C(16)-C(21)-H(21)	118.7
C(1)-C(10)-H(10C)	109.5	C(27)-C(22)-C(23)	121.1(4)
H(10A)-C(10)-H(10C)	109.5	C(27)-C(22)-H(22A)	119.4
H(10B)-C(10)-H(10C)	109.5	C(23)-C(22)-H(22A)	119.4
C(3)-C(11)-H(11A)	109.5	C(24)-C(23)-C(22)	120.0(4)
C(3)-C(11)-H(11B)	109.5	C(24)-C(23)-H(23)	120.0
H(11A)-C(11)-H(11B)	109.5	C(22)-C(23)-H(23)	120.0
C(3)-C(11)-H(11C)	109.5	C(23)-C(24)-C(25)	120.1(4)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(24)-H(24)	119.9
H(11B)-C(11)-H(11C)	109.5	C(25)-C(24)-H(24)	119.9
C(4)-C(12)-H(12A)	109.5	C(24)-C(25)-C(26)	119.9(4)
C(4)-C(12)-H(12B)	109.5	C(24)-C(25)-H(25)	120.0
H(12A)-C(12)-H(12B)	109.5	C(26)-C(25)-H(25)	120.0
C(4)-C(12)-H(12C)	109.5	C(25)-C(26)-C(27)	120.7(4)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(26)-H(26)	119.6
H(12B)-C(12)-H(12C)	109.5	C(27)-C(26)-H(26)	119.6
C(6)-C(13)-H(13A)	109.5	C(22)-C(27)-C(26)	118.1(3)
C(6)-C(13)-H(13B)	109.5	C(22)-C(27)-P(1)	122.9(3)
H(13A)-C(13)-H(13B)	109.5	C(26)-C(27)-P(1)	118.7(3)
C(6)-C(13)-H(13C)	109.5	P(1)-C(28)-H(28A)	109.5
H(13A)-C(13)-H(13C)	109.5	P(1)-C(28)-H(28B)	109.5
H(13B)-C(13)-H(13C)	109.5	H(28A)-C(28)-H(28B)	109.5
C(7)-C(14)-H(14A)	109.5	P(1)-C(28)-H(28C)	109.5
C(7)-C(14)-H(14B)	109.5	H(28A)-C(28)-H(28C)	109.5
H(14A)-C(14)-H(14B)	109.5	H(28B)-C(28)-H(28C)	109.5
C(7)-C(14)-H(14C)	109.5	P(1)-C(29)-H(29A)	109.5
H(14A)-C(14)-H(14C)	109.5	P(1)-C(29)-H(29B)	109.5
H(14B)-C(14)-H(14C)	109.5	H(29A)-C(29)-H(29B)	109.5
C(9)-C(15)-H(15A)	109.5	P(1)-C(29)-H(29C)	109.5
C(9)-C(15)-H(15B)	109.5	H(29A)-C(29)-H(29C)	109.5
H(15A)-C(15)-H(15B)	109.5	H(29B)-C(29)-H(29C)	109.5
C(9)-C(15)-H(15C)	109.5		

Table S82. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9e**. 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}
Rh1	14(1)	13(1)	13(1)	1(1)	2(1)	1(1)
P1	16(1)	15(1)	16(1)	3(1)	2(1)	1(1)
N1	18(2)	17(2)	14(1)	1(1)	2(1)	0(1)
N2	14(1)	16(2)	17(1)	4(1)	1(1)	-3(1)
N3	20(2)	16(2)	13(1)	2(1)	1(1)	2(1)
N4	15(1)	15(1)	14(1)	1(1)	0(1)	0(1)
N5	16(1)	14(1)	16(1)	3(1)	3(1)	2(1)
N6	14(1)	14(1)	16(1)	2(1)	4(1)	1(1)
B1	19(2)	15(2)	17(2)	4(2)	1(2)	2(2)
C1	16(2)	27(2)	17(2)	-1(2)	3(1)	1(2)
C2	17(2)	31(2)	22(2)	4(2)	9(1)	0(2)
C3	18(2)	22(2)	20(2)	1(1)	6(1)	-7(1)
C4	14(2)	22(2)	14(2)	0(1)	0(1)	0(1)
C5	17(2)	23(2)	17(2)	-5(1)	3(1)	3(1)
C6	16(2)	18(2)	20(2)	-3(1)	0(1)	2(1)
C7	19(2)	18(2)	14(2)	-1(1)	5(1)	0(1)
C8	17(2)	23(2)	15(2)	-1(1)	0(1)	3(1)
C9	15(2)	19(2)	12(2)	0(1)	2(1)	2(1)
C10	22(2)	36(2)	29(2)	6(2)	9(2)	7(2)
C11	27(2)	26(2)	30(2)	9(2)	4(2)	-5(2)
C12	22(2)	25(2)	16(2)	1(2)	3(1)	3(2)
C13	27(2)	20(2)	25(2)	-3(2)	0(2)	5(2)
C14	20(2)	22(2)	26(2)	-1(2)	2(2)	-1(2)
C15	29(2)	20(2)	21(2)	3(2)	0(2)	3(2)
C16	16(2)	14(2)	22(2)	2(1)	2(1)	2(1)
C17	28(2)	20(2)	19(2)	1(2)	3(2)	4(2)
F1	44(2)	22(1)	26(1)	4(1)	8(1)	-4(1)
C18	37(2)	15(2)	32(2)	-2(2)	-1(2)	2(2)
F2	74(2)	16(1)	39(2)	-3(1)	6(1)	-4(1)
C19	49(3)	24(2)	27(2)	-7(2)	1(2)	8(2)
C20	38(2)	29(2)	20(2)	-2(2)	3(2)	5(2)
C21	24(2)	19(2)	20(2)	0(1)	4(2)	2(2)
C22	27(2)	19(2)	20(2)	4(1)	2(2)	-1(2)
C23	29(2)	20(2)	29(2)	5(2)	9(2)	-3(2)
C24	43(3)	20(2)	23(2)	6(2)	8(2)	-1(2)
C25	35(2)	30(2)	17(2)	7(2)	-3(2)	1(2)
C26	27(2)	26(2)	23(2)	5(2)	-1(2)	-2(2)
C27	25(2)	16(2)	15(2)	5(1)	3(1)	1(1)
C28	27(2)	26(2)	24(2)	7(2)	4(2)	8(2)
C29	20(2)	21(2)	26(2)	5(2)	0(2)	-1(2)

Table S83. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2\ x\ 10^3$) for **9e**.

	x	y	z	U(eq)
H1	3790(40)	7330(30)	6350(30)	24(11)
H1B	3050	3303	7635	20
H2	-977	4601	8826	27

H5	3600	3418	3846	23
H8	6774	5644	9290	22
H10A	-245	7399	8012	43
H10B	-1526	6625	8161	43
H10C	-1077	6769	6972	43
H11A	1866	2964	9361	41
H11B	1106	2310	8301	41
H11C	317	2701	9297	41
H12A	3807	6580	4289	31
H12B	2594	6022	3496	31
H12C	4049	5619	3375	31
H13A	2475	1867	6072	36
H13B	4041	1996	6282	36
H13C	3348	1603	5096	36
H14A	5465	7981	7651	34
H14B	6631	7780	8579	34
H14C	5220	8119	8907	34
H15A	4682	3013	9110	35
H15B	6179	3402	9488	35
H15C	5746	2971	8250	35
H19	2633	10287	10160	40
H20	2066	8370	10432	35
H21	2034	6981	9032	25
H22A	3847	8635	5076	26
H23	4564	9726	3706	31
H24	3120	10110	2205	34
H25	960	9391	2055	33
H26	238	8286	3417	30
H28A	-427	8780	5374	38
H28B	808	9376	6113	38
H28C	-92	8427	6604	38
H29A	-479	6895	4278	33
H29B	-290	6072	5275	33
H29C	635	5969	4311	33

Table S84. Torsion angles [°] for **9e**.

C16-Rh1-P1-C29	-138.35(17)	C16-Rh1-N1-N2	-122.2(2)
N5-Rh1-P1-C29	133.8(7)	N5-Rh1-N1-N2	-34.4(2)
N3-Rh1-P1-C29	41.64(16)	N3-Rh1-N1-N2	49.8(2)
N1-Rh1-P1-C29	-45.14(16)	P1-Rh1-N1-N2	145.4(2)
C16-Rh1-P1-C28	-18.60(19)	C1-N1-N2-C3	-0.6(4)
N5-Rh1-P1-C28	-106.4(7)	Rh1-N1-N2-C3	168.1(2)
N3-Rh1-P1-C28	161.39(17)	C1-N1-N2-B1	179.3(3)
N1-Rh1-P1-C28	74.61(17)	Rh1-N1-N2-B1	-12.0(4)
C16-Rh1-P1-C27	100.74(17)	C16-Rh1-N3-C4	-133.7(9)
N5-Rh1-P1-C27	12.9(8)	N5-Rh1-N3-C4	-126.9(4)
N3-Rh1-P1-C27	-79.26(16)	P1-Rh1-N3-C4	46.4(4)
N1-Rh1-P1-C27	-166.04(15)	N1-Rh1-N3-C4	144.9(4)
C16-Rh1-N1-C1	41.3(4)	C16-Rh1-N3-N4	43.2(10)
N5-Rh1-N1-C1	129.0(4)	N5-Rh1-N3-N4	50.0(2)
N3-Rh1-N1-C1	-146.8(4)	P1-Rh1-N3-N4	-136.8(2)
P1-Rh1-N1-C1	-51.1(4)	N1-Rh1-N3-N4	-38.3(2)

C4-N3-N4-C6	0.2(4)	C4-C5-C6-N4	0.6(4)
Rh1-N3-N4-C6	-177.6(2)	C4-C5-C6-C13	-179.1(4)
C4-N3-N4-B1	168.0(3)	N6-N5-C7-C8	0.5(4)
Rh1-N3-N4-B1	-9.8(4)	Rh1-N5-C7-C8	-171.9(2)
C16-Rh1-N5-C7	-52.8(3)	N6-N5-C7-C14	-179.8(3)
N3-Rh1-N5-C7	128.2(3)	Rh1-N5-C7-C14	7.8(5)
P1-Rh1-N5-C7	35.3(10)	N5-C7-C8-C9	-0.2(4)
N1-Rh1-N5-C7	-145.7(3)	C14-C7-C8-C9	-179.9(3)
C16-Rh1-N5-N6	135.5(2)	N5-N6-C9-C8	0.5(4)
N3-Rh1-N5-N6	-43.5(2)	B1-N6-C9-C8	176.3(3)
P1-Rh1-N5-N6	-136.4(6)	N5-N6-C9-C15	-176.4(3)
N1-Rh1-N5-N6	42.6(2)	B1-N6-C9-C15	-0.6(6)
C7-N5-N6-C9	-0.6(4)	C7-C8-C9-N6	-0.2(4)
Rh1-N5-N6-C9	173.1(2)	C7-C8-C9-C15	176.5(3)
C7-N5-N6-B1	-177.0(3)	N5-Rh1-C16-C17	114.8(3)
Rh1-N5-N6-B1	-3.3(4)	N3-Rh1-C16-C17	121.5(9)
C3-N2-B1-N4	128.3(4)	P1-Rh1-C16-C17	-58.5(3)
N1-N2-B1-N4	-51.6(4)	N1-Rh1-C16-C17	-157.5(3)
C3-N2-B1-N6	-112.3(4)	N5-Rh1-C16-C21	-57.9(3)
N1-N2-B1-N6	67.8(4)	N3-Rh1-C16-C21	-51.2(11)
C6-N4-B1-N2	-127.3(4)	P1-Rh1-C16-C21	128.8(3)
N3-N4-B1-N2	67.2(4)	N1-Rh1-C16-C21	29.8(3)
C6-N4-B1-N6	112.5(4)	C21-C16-C17-F1	179.5(3)
N3-N4-B1-N6	-53.1(4)	Rh1-C16-C17-F1	6.5(5)
C9-N6-B1-N2	125.5(4)	C21-C16-C17-C18	-0.6(6)
N5-N6-B1-N2	-59.1(4)	Rh1-C16-C17-C18	-173.6(3)
C9-N6-B1-N4	-113.9(4)	F1-C17-C18-F2	-1.3(6)
N5-N6-B1-N4	61.6(4)	C16-C17-C18-F2	178.7(4)
N2-N1-C1-C2	0.3(4)	F1-C17-C18-C19	-179.6(4)
Rh1-N1-C1-C2	-164.1(3)	C16-C17-C18-C19	0.5(7)
N2-N1-C1-C10	179.0(3)	F2-C18-C19-C20	-178.4(4)
Rh1-N1-C1-C10	14.7(6)	C17-C18-C19-C20	-0.3(7)
N1-C1-C2-C3	0.2(4)	C18-C19-C20-C21	0.1(7)
C10-C1-C2-C3	-178.5(4)	C19-C20-C21-C16	-0.2(6)
N1-N2-C3-C2	0.8(4)	C17-C16-C21-C20	0.4(5)
B1-N2-C3-C2	-179.2(3)	Rh1-C16-C21-C20	174.0(3)
N1-N2-C3-C11	-177.7(3)	C27-C22-C23-C24	0.7(6)
B1-N2-C3-C11	2.4(6)	C22-C23-C24-C25	-0.2(6)
C1-C2-C3-N2	-0.6(4)	C23-C24-C25-C26	0.0(6)
C1-C2-C3-C11	177.8(4)	C24-C25-C26-C27	-0.3(6)
N4-N3-C4-C5	0.2(4)	C23-C22-C27-C26	-1.0(6)
Rh1-N3-C4-C5	177.3(3)	C23-C22-C27-P1	-175.6(3)
N4-N3-C4-C12	-177.4(3)	C25-C26-C27-C22	0.7(6)
Rh1-N3-C4-C12	-0.3(5)	C25-C26-C27-P1	175.6(3)
N3-C4-C5-C6	-0.5(4)	C29-P1-C27-C22	-146.9(3)
C12-C4-C5-C6	177.0(3)	C28-P1-C27-C22	107.3(3)
N3-N4-C6-C5	-0.5(4)	Rh1-P1-C27-C22	-22.4(4)
B1-N4-C6-C5	-167.2(3)	C29-P1-C27-C26	38.4(3)
N3-N4-C6-C13	179.2(3)	C28-P1-C27-C26	-67.3(3)
B1-N4-C6-C13	12.4(5)	Rh1-P1-C27-C26	162.9(3)

Table S85. Crystal data and structure refinement for **9g**.

Identification code	**9g**	
Empirical formula	$C_{29}H_{37}BF_2N_6PRh$	
Formula weight	652.34	
Temperature	100.0(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.1914(10) Å	α = 99.310(2)°
	b = 10.5164(11) Å	β = 99.180(2)°
	c = 15.794(2) Å	γ = 115.370(2)°
Volume	1458.8(3) Å^3	
Z	2	
Density (calculated)	1.485 Mg/m^3	
Absorption coefficient	0.683 mm^{-1}	
F(000)	672	
Crystal color, morphology	colorless, plate	
Crystal size	0.26 x 0.18 x 0.08 mm^3	
Theta range for data collection	2.22 to 36.32°	
Index ranges	$-16 \le h \le 16$, $-17 \le k \le 17$, $-26 \le l \le 26$	
Reflections collected	39002	
Independent reflections	13918 [R(int) = 0.0391]	
Observed reflections	11379	
Completeness to theta = 36.32°	98.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9474 and 0.8424	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13918 / 0 / 373	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R_1 = 0.0401, wR_2 = 0.0960	
R indices (all data)	R_1 = 0.0532, wR_2 = 0.1029	
Largest diff. peak and hole	2.512 and -0.395 e.Å^{-3}	

Table S86. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **9g**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Rh1	8914(1)	6987(1)	7821(1)	16(1)
P1	6402(1)	6019(1)	7241(1)	21(1)
N1	9763(2)	7694(2)	6660(1)	18(1)
N2	10820(2)	9131(1)	6855(1)	17(1)
N3	11206(2)	7864(1)	8488(1)	16(1)
N4	12208(2)	9072(1)	8296(1)	17(1)
N5	9289(2)	9172(2)	8361(1)	19(1)
N6	10604(2)	10296(2)	8321(1)	18(1)
B1	11646(2)	9986(2)	7822(1)	18(1)
C1	9473(2)	7170(2)	5779(1)	21(1)
C2	10325(2)	8272(2)	5410(1)	22(1)
C3	11172(2)	9498(2)	6107(1)	20(1)
C4	11998(2)	7406(2)	9005(1)	18(1)
C5	13527(2)	8318(2)	9130(1)	21(1)
C6	13626(2)	9358(2)	8672(1)	19(1)
C7	8764(2)	9760(2)	8954(1)	22(1)
C8	9722(2)	11239(2)	9290(1)	25(1)
C9	10891(2)	11553(2)	8887(1)	21(1)
C10	8413(2)	5625(2)	5300(1)	28(1)

C11	12306(2)	10977(2)	6108(1)	25(1)
C12	11276(2)	6117(2)	9366(1)	22(1)
C13	14967(2)	10601(2)	8563(1)	26(1)
C14	7367(2)	8881(2)	9206(1)	27(1)
C15	12262(2)	12959(2)	9021(1)	28(1)
C16	8917(2)	5041(2)	7475(1)	20(1)
C17	8048(2)	3749(2)	7677(1)	26(1)
F1	6917(1)	3663(1)	8068(1)	38(1)
C18	8228(2)	2509(2)	7533(1)	30(1)
C19	9380(2)	2512(2)	7172(1)	27(1)
C20	10279(2)	3779(2)	6975(1)	21(1)
F2	11460(1)	3836(1)	6646(1)	26(1)
C21	10078(2)	5004(2)	7110(1)	19(1)
C22	4348(2)	7095(2)	6793(1)	29(1)
C23	3833(2)	7924(2)	6385(2)	31(1)
C24	4742(2)	8909(2)	5979(1)	28(1)
C25	6164(2)	9082(2)	6002(1)	30(1)
C26	6685(2)	8251(2)	6413(1)	28(1)
C27	5771(2)	7230(2)	6802(1)	21(1)
C28	5190(2)	5343(2)	7976(2)	32(1)
C29	5485(2)	4429(2)	6287(2)	31(1)

Table S87. Bond lengths [Å] and angles [°] for **9g**.

Rh(1)-C(16)	2.0329(16)	C(6)-C(13)	1.490(2)
Rh(1)-N(3)	2.1146(13)	C(7)-C(8)	1.386(3)
Rh(1)-N(5)	2.1595(14)	C(7)-C(14)	1.487(2)
Rh(1)-N(1)	2.2482(13)	C(8)-C(9)	1.379(2)
Rh(1)-P(1)	2.2681(5)	C(8)-H(8)	0.9500
Rh(1)-H(1)	1.49(2)	C(9)-C(15)	1.489(3)
P(1)-C(29)	1.826(2)	C(10)-H(10A)	0.9800
P(1)-C(28)	1.8320(19)	C(10)-H(10B)	0.9800
P(1)-C(27)	1.8337(17)	C(10)-H(10C)	0.9800
N(1)-C(1)	1.345(2)	C(11)-H(11A)	0.9800
N(1)-N(2)	1.3730(19)	C(11)-H(11B)	0.9800
N(2)-C(3)	1.3563(19)	C(11)-H(11C)	0.9800
N(2)-B(1)	1.532(2)	C(12)-H(12A)	0.9800
N(3)-C(4)	1.342(2)	C(12)-H(12B)	0.9800
N(3)-N(4)	1.3646(18)	C(12)-H(12C)	0.9800
N(4)-C(6)	1.353(2)	C(13)-H(13A)	0.9800
N(4)-B(1)	1.542(2)	C(13)-H(13B)	0.9800
N(5)-C(7)	1.342(2)	C(13)-H(13C)	0.9800
N(5)-N(6)	1.3754(19)	C(14)-H(14A)	0.9800
N(6)-C(9)	1.355(2)	C(14)-H(14B)	0.9800
N(6)-B(1)	1.528(2)	C(14)-H(14C)	0.9800
B(1)-H(1B)	1.0000	C(15)-H(15A)	0.9800
C(1)-C(2)	1.398(2)	C(15)-H(15B)	0.9800
C(1)-C(10)	1.489(3)	C(15)-H(15C)	0.9800
C(2)-C(3)	1.379(2)	C(16)-C(17)	1.390(2)
C(2)-H(2)	0.9500	C(16)-C(21)	1.408(2)
C(3)-C(11)	1.488(2)	C(17)-F(1)	1.369(2)
C(4)-C(5)	1.396(2)	C(17)-C(18)	1.382(3)
C(4)-C(12)	1.494(2)	C(18)-C(19)	1.383(3)
C(5)-C(6)	1.384(2)	C(18)-H(18)	0.9500
C(5)-H(5)	0.9500	C(19)-C(20)	1.375(2)

C(19)-H(19)	0.9500	C(7)-N(5)-Rh(1)	134.28(12)
C(20)-F(2)	1.368(2)	N(6)-N(5)-Rh(1)	116.85(9)
C(20)-C(21)	1.378(2)	C(9)-N(6)-N(5)	110.20(13)
C(21)-H(21)	0.9500	C(9)-N(6)-B(1)	128.34(15)
C(22)-C(23)	1.385(3)	N(5)-N(6)-B(1)	120.46(13)
C(22)-C(27)	1.392(2)	N(6)-B(1)-N(2)	111.30(13)
C(22)-H(22)	0.9500	N(6)-B(1)-N(4)	107.57(12)
C(23)-C(24)	1.387(3)	N(2)-B(1)-N(4)	109.12(13)
C(23)-H(23)	0.9500	N(6)-B(1)-H(1B)	109.6
C(24)-C(25)	1.375(3)	N(2)-B(1)-H(1B)	109.6
C(24)-H(24)	0.9500	N(4)-B(1)-H(1B)	109.6
C(25)-C(26)	1.392(3)	N(1)-C(1)-C(2)	109.95(15)
C(25)-H(25)	0.9500	N(1)-C(1)-C(10)	123.30(15)
C(26)-C(27)	1.392(2)	C(2)-C(1)-C(10)	126.74(15)
C(26)-H(26)	0.9500	C(3)-C(2)-C(1)	106.15(14)
C(28)-H(28A)	0.9800	C(3)-C(2)-H(2)	126.9
C(28)-H(28B)	0.9800	C(1)-C(2)-H(2)	126.9
C(28)-H(28C)	0.9800	N(2)-C(3)-C(2)	107.32(14)
C(29)-H(29A)	0.9800	N(2)-C(3)-C(11)	122.94(15)
C(29)-H(29B)	0.9800	C(2)-C(3)-C(11)	129.73(15)
C(29)-H(29C)	0.9800	N(3)-C(4)-C(5)	108.92(14)
C(16)-Rh(1)-N(3)	86.98(6)	N(3)-C(4)-C(12)	122.84(15)
C(16)-Rh(1)-N(5)	169.58(6)	C(5)-C(4)-C(12)	128.25(15)
N(3)-Rh(1)-N(5)	82.97(5)	C(6)-C(5)-C(4)	106.44(14)
C(16)-Rh(1)-N(1)	92.85(6)	C(6)-C(5)-H(5)	126.8
N(3)-Rh(1)-N(1)	85.50(5)	C(4)-C(5)-H(5)	126.8
N(5)-Rh(1)-N(1)	89.14(5)	N(4)-C(6)-C(5)	107.34(14)
C(16)-Rh(1)-P(1)	93.52(5)	N(4)-C(6)-C(13)	122.21(14)
N(3)-Rh(1)-P(1)	174.10(4)	C(5)-C(6)-C(13)	130.45(15)
N(5)-Rh(1)-P(1)	96.19(4)	N(5)-C(7)-C(8)	110.25(15)
N(1)-Rh(1)-P(1)	100.34(4)	N(5)-C(7)-C(14)	122.60(16)
C(16)-Rh(1)-H(1)	86.3(9)	C(8)-C(7)-C(14)	127.12(15)
N(3)-Rh(1)-H(1)	88.7(9)	C(9)-C(8)-C(7)	106.34(14)
N(5)-Rh(1)-H(1)	90.7(9)	C(9)-C(8)-H(8)	126.8
N(1)-Rh(1)-H(1)	174.2(9)	C(7)-C(8)-H(8)	126.8
P(1)-Rh(1)-H(1)	85.5(9)	N(6)-C(9)-C(8)	107.17(15)
C(29)-P(1)-C(28)	99.65(10)	N(6)-C(9)-C(15)	123.28(15)
C(29)-P(1)-C(27)	99.82(9)	C(8)-C(9)-C(15)	129.53(16)
C(28)-P(1)-C(27)	103.28(8)	C(1)-C(10)-H(10A)	109.5
C(29)-P(1)-Rh(1)	118.64(7)	C(1)-C(10)-H(10B)	109.5
C(28)-P(1)-Rh(1)	116.98(7)	H(10A)-C(10)-H(10B)	109.5
C(27)-P(1)-Rh(1)	115.61(6)	C(1)-C(10)-H(10C)	109.5
C(1)-N(1)-N(2)	106.13(13)	H(10A)-C(10)-H(10C)	109.5
C(1)-N(1)-Rh(1)	139.28(12)	H(10B)-C(10)-H(10C)	109.5
N(2)-N(1)-Rh(1)	114.32(9)	C(3)-C(11)-H(11A)	109.5
C(3)-N(2)-N(1)	110.45(13)	C(3)-C(11)-H(11B)	109.5
C(3)-N(2)-B(1)	128.19(14)	H(11A)-C(11)-H(11B)	109.5
N(1)-N(2)-B(1)	120.08(12)	C(3)-C(11)-H(11C)	109.5
C(4)-N(3)-N(4)	107.49(13)	H(11A)-C(11)-H(11C)	109.5
C(4)-N(3)-Rh(1)	134.42(11)	H(11B)-C(11)-H(11C)	109.5
N(4)-N(3)-Rh(1)	117.47(9)	C(4)-C(12)-H(12A)	109.5
C(6)-N(4)-N(3)	109.80(12)	C(4)-C(12)-H(12B)	109.5
C(6)-N(4)-B(1)	129.73(14)	H(12A)-C(12)-H(12B)	109.5
N(3)-N(4)-B(1)	119.96(13)	C(4)-C(12)-H(12C)	109.5
C(7)-N(5)-N(6)	106.01(14)	H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
C(6)-C(13)-H(13A)	109.5
C(6)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(6)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(7)-C(14)-H(14A)	109.5
C(7)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(7)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(9)-C(15)-H(15A)	109.5
C(9)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(9)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	113.23(15)
C(17)-C(16)-Rh(1)	127.97(13)
C(21)-C(16)-Rh(1)	118.00(11)
F(1)-C(17)-C(18)	115.20(15)
F(1)-C(17)-C(16)	118.97(15)
C(18)-C(17)-C(16)	125.82(17)
C(17)-C(18)-C(19)	119.34(17)
C(17)-C(18)-H(18)	120.3
C(19)-C(18)-H(18)	120.3
C(20)-C(19)-C(18)	116.55(16)
C(20)-C(19)-H(19)	121.7
C(18)-C(19)-H(19)	121.7
F(2)-C(20)-C(19)	118.02(15)
F(2)-C(20)-C(21)	118.27(15)
C(19)-C(20)-C(21)	123.69(16)
C(20)-C(21)-C(16)	121.35(15)
C(20)-C(21)-H(21)	119.3
C(16)-C(21)-H(21)	119.3
C(23)-C(22)-C(27)	121.05(18)
C(23)-C(22)-H(22)	119.5
C(27)-C(22)-H(22)	119.5
C(22)-C(23)-C(24)	119.85(17)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(25)-C(24)-C(23)	119.84(17)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.35(18)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	120.50(17)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(26)-C(27)-C(22)	118.38(16)
C(26)-C(27)-P(1)	119.81(13)
C(22)-C(27)-P(1)	121.66(13)
P(1)-C(28)-H(28A)	109.5
P(1)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
P(1)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
P(1)-C(29)-H(29A)	109.5
P(1)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
P(1)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5

Table S88. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9g**. 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}
Rh1	14(1)	18(1)	20(1)	8(1)	6(1)	9(1)
P1	15(1)	21(1)	29(1)	11(1)	6(1)	8(1)
N1	17(1)	19(1)	19(1)	6(1)	4(1)	9(1)
N2	18(1)	18(1)	18(1)	7(1)	6(1)	10(1)
N3	16(1)	15(1)	19(1)	6(1)	4(1)	9(1)
N4	16(1)	17(1)	19(1)	6(1)	6(1)	8(1)
N5	19(1)	23(1)	20(1)	9(1)	8(1)	13(1)
N6	21(1)	19(1)	21(1)	7(1)	7(1)	12(1)
B1	19(1)	18(1)	19(1)	6(1)	6(1)	10(1)
C1	19(1)	25(1)	19(1)	5(1)	3(1)	11(1)
C2	25(1)	25(1)	18(1)	7(1)	6(1)	12(1)
C3	22(1)	24(1)	19(1)	10(1)	8(1)	14(1)
C4	21(1)	20(1)	17(1)	5(1)	5(1)	12(1)
C5	20(1)	25(1)	21(1)	8(1)	4(1)	13(1)
C6	17(1)	20(1)	19(1)	5(1)	5(1)	9(1)
C7	24(1)	30(1)	20(1)	10(1)	8(1)	20(1)
C8	32(1)	30(1)	23(1)	7(1)	10(1)	23(1)
C9	28(1)	22(1)	20(1)	6(1)	6(1)	17(1)
C10	27(1)	27(1)	21(1)	3(1)	1(1)	7(1)
C11	31(1)	23(1)	26(1)	12(1)	12(1)	13(1)
C12	26(1)	22(1)	23(1)	10(1)	7(1)	13(1)
C13	17(1)	29(1)	28(1)	10(1)	5(1)	7(1)
C14	25(1)	39(1)	26(1)	12(1)	11(1)	20(1)
C15	37(1)	21(1)	29(1)	6(1)	9(1)	16(1)
C16	18(1)	19(1)	24(1)	10(1)	6(1)	9(1)
C17	22(1)	24(1)	35(1)	14(1)	12(1)	11(1)
F1	34(1)	33(1)	66(1)	29(1)	31(1)	19(1)
C18	30(1)	22(1)	42(1)	16(1)	12(1)	11(1)
C19	30(1)	20(1)	33(1)	9(1)	7(1)	14(1)
C20	22(1)	20(1)	20(1)	4(1)	4(1)	11(1)
F2	27(1)	24(1)	30(1)	5(1)	9(1)	15(1)
C21	19(1)	18(1)	20(1)	5(1)	4(1)	9(1)
C22	16(1)	28(1)	42(1)	15(1)	5(1)	10(1)
C23	22(1)	33(1)	44(1)	12(1)	5(1)	17(1)
C24	32(1)	31(1)	28(1)	10(1)	5(1)	22(1)
C25	34(1)	36(1)	35(1)	20(1)	15(1)	23(1)
C26	25(1)	34(1)	35(1)	19(1)	12(1)	19(1)
C27	18(1)	22(1)	23(1)	6(1)	3(1)	9(1)
C28	21(1)	38(1)	45(1)	25(1)	13(1)	14(1)
C29	21(1)	21(1)	44(1)	6(1)	2(1)	6(1)

Table S89. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **9g**.

	x	y	z	U(eq)
H1	8510(30)	6570(30)	8634(15)	27(6)
H1B	12521	10926	7840	21
H2	10322	8192	4802	26
H5	14340	8240	9463	25

H8	9599	11904	9712	30
H10A	8150	5044	5731	43
H10B	8891	5244	4910	43
H10C	7500	5570	4944	43
H11A	12100	11710	6443	38
H11B	12252	11061	5496	38
H11C	13312	11135	6387	38
H12A	10266	5956	9395	34
H12B	11882	6297	9962	34
H12C	11209	5253	8976	34
H13A	14919	11509	8760	39
H13B	14984	10447	7937	39
H13C	15882	10663	8922	39
H14A	7400	8023	9353	40
H14B	6494	8569	8708	40
H14C	7288	9473	9723	40
H15A	13158	12831	9187	42
H15B	12282	13700	9495	42
H15C	12248	13272	8469	42
H18	7569	1662	7680	36
H19	9541	1681	7065	32
H21	10735	5841	6953	23
H22	3722	6424	7071	35
H23	2858	7819	6383	38
H24	4382	9462	5685	33
H25	6795	9773	5736	36
H26	7671	8382	6428	33
H28A	4157	4693	7621	48
H28B	5212	6168	8382	48
H28C	5550	4808	8321	48
H29A	4393	4045	6166	46
H29B	5753	3677	6416	46
H29C	5817	4711	5766	46

Table S90. Torsion angles [°] for **9g**.

C16-Rh1-P1-C29	-30.37(9)	C1-N1-N2-C3	0.52(17)
N3-Rh1-P1-C29	-125.1(4)	Rh1-N1-N2-C3	-174.65(10)
N5-Rh1-P1-C29	153.43(9)	C1-N1-N2-B1	-167.59(13)
N1-Rh1-P1-C29	63.18(9)	Rh1-N1-N2-B1	17.24(16)
C16-Rh1-P1-C28	89.12(9)	C16-Rh1-N3-C4	-41.83(15)
N3-Rh1-P1-C28	-5.6(4)	N5-Rh1-N3-C4	135.38(15)
N5-Rh1-P1-C28	-87.08(9)	N1-Rh1-N3-C4	-134.93(15)
N1-Rh1-P1-C28	-177.33(9)	P1-Rh1-N3-C4	53.2(4)
C16-Rh1-P1-C27	-148.89(8)	C16-Rh1-N3-N4	127.75(11)
N3-Rh1-P1-C27	116.4(3)	N5-Rh1-N3-N4	-55.03(10)
N5-Rh1-P1-C27	34.92(7)	N1-Rh1-N3-N4	34.65(10)
N1-Rh1-P1-C27	-55.34(7)	P1-Rh1-N3-N4	-137.2(3)
C16-Rh1-N1-C1	47.77(17)	C4-N3-N4-C6	1.36(16)
N3-Rh1-N1-C1	134.51(17)	Rh1-N3-N4-C6	-170.86(10)
N5-Rh1-N1-C1	-142.47(17)	C4-N3-N4-B1	-171.24(13)
P1-Rh1-N1-C1	-46.34(17)	Rh1-N3-N4-B1	16.54(17)
C16-Rh1-N1-N2	-139.36(11)	C16-Rh1-N5-C7	-99.3(3)
N3-Rh1-N1-N2	-52.61(10)	N3-Rh1-N5-C7	-114.83(16)
N5-Rh1-N1-N2	30.40(10)	N1-Rh1-N5-C7	159.60(16)
P1-Rh1-N1-N2	126.54(10)	P1-Rh1-N5-C7	59.29(16)

C16-Rh1-N5-N6	58.5(3)	N5-Rh1-C16-C17	104.5(3)
N3-Rh1-N5-N6	42.93(11)	N1-Rh1-C16-C17	-154.65(16)
N1-Rh1-N5-N6	-42.65(11)	P1-Rh1-C16-C17	-54.10(16)
P1-Rh1-N5-N6	-142.95(10)	N3-Rh1-C16-C21	-48.93(13)
C7-N5-N6-C9	0.65(17)	N5-Rh1-C16-C21	-64.4(3)
Rh1-N5-N6-C9	-162.97(10)	N1-Rh1-C16-C21	36.41(13)
C7-N5-N6-B1	170.14(14)	P1-Rh1-C16-C21	136.96(12)
Rh1-N5-N6-B1	6.52(18)	C21-C16-C17-F1	177.52(16)
C9-N6-B1-N2	-136.30(16)	Rh1-C16-C17-F1	8.1(3)
N5-N6-B1-N2	56.31(18)	C21-C16-C17-C18	-1.3(3)
C9-N6-B1-N4	104.22(18)	Rh1-C16-C17-C18	-170.64(16)
N5-N6-B1-N4	-63.18(18)	F1-C17-C18-C19	-177.55(18)
C3-N2-B1-N6	123.07(16)	C16-C17-C18-C19	1.3(3)
N1-N2-B1-N6	-71.15(17)	C17-C18-C19-C20	-0.2(3)
C3-N2-B1-N4	-118.38(16)	C18-C19-C20-F2	177.71(16)
N1-N2-B1-N4	47.40(18)	C18-C19-C20-C21	-0.6(3)
C6-N4-B1-N6	-121.28(16)	F2-C20-C21-C16	-177.74(14)
N3-N4-B1-N6	49.66(18)	C19-C20-C21-C16	0.6(3)
C6-N4-B1-N2	117.86(17)	C17-C16-C21-C20	0.3(2)
N3-N4-B1-N2	-71.20(16)	Rh1-C16-C21-C20	170.84(12)
N2-N1-C1-C2	-0.82(18)	C27-C22-C23-C24	-0.1(3)
Rh1-N1-C1-C2	172.42(13)	C22-C23-C24-C25	-1.6(3)
N2-N1-C1-C10	178.04(16)	C23-C24-C25-C26	1.5(3)
Rh1-N1-C1-C10	-8.7(3)	C24-C25-C26-C27	0.3(3)
N1-C1-C2-C3	0.82(19)	C25-C26-C27-C22	-1.9(3)
C10-C1-C2-C3	-177.99(17)	C25-C26-C27-P1	173.84(16)
N1-N2-C3-C2	-0.02(18)	C23-C22-C27-C26	1.8(3)
B1-N2-C3-C2	166.87(15)	C23-C22-C27-P1	-173.83(16)
N1-N2-C3-C11	-178.90(15)	C29-P1-C27-C26	-95.23(16)
B1-N2-C3-C11	-12.0(2)	C28-P1-C27-C26	162.31(16)
C1-C2-C3-N2	-0.47(18)	Rh1-P1-C27-C26	33.26(17)
C1-C2-C3-C11	178.31(17)	C29-P1-C27-C22	80.35(17)
N4-N3-C4-C5	-1.16(17)	C28-P1-C27-C22	-22.11(18)
Rh1-N3-C4-C5	169.16(11)	Rh1-P1-C27-C22	-151.16(14)
N4-N3-C4-C12	178.71(14)		
Rh1-N3-C4-C12	-11.0(2)		
N3-C4-C5-C6	0.55(18)		
C12-C4-C5-C6	-179.31(15)		
N3-N4-C6-C5	-1.01(17)		
B1-N4-C6-C5	170.65(15)		
N3-N4-C6-C13	178.83(14)		
B1-N4-C6-C13	-9.5(2)		
C4-C5-C6-N4	0.28(18)		
C4-C5-C6-C13	-179.54(16)		
N6-N5-C7-C8	0.10(18)		
Rh1-N5-C7-C8	159.52(13)		
N6-N5-C7-C14	-178.27(15)		
Rh1-N5-C7-C14	-18.8(2)		
N5-C7-C8-C9	-0.78(19)		
C14-C7-C8-C9	177.49(16)		
N5-N6-C9-C8	-1.14(18)		
B1-N6-C9-C8	-169.57(15)		
N5-N6-C9-C15	177.83(15)		
B1-N6-C9-C15	9.4(3)		
C7-C8-C9-N6	1.15(19)		
C7-C8-C9-C15	-177.73(17)		
N3-Rh1-C16-C17	120.01(16)		