

Supporting Information

Part II: Crystal Structure Data

(POP)Rh pincer hydride complexes: unusual reactivity and selectivity in oxidative addition and olefin insertion reactions

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Figure A1: ORTEP diagram of $(\mu_2\text{-}^t\text{BuPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$

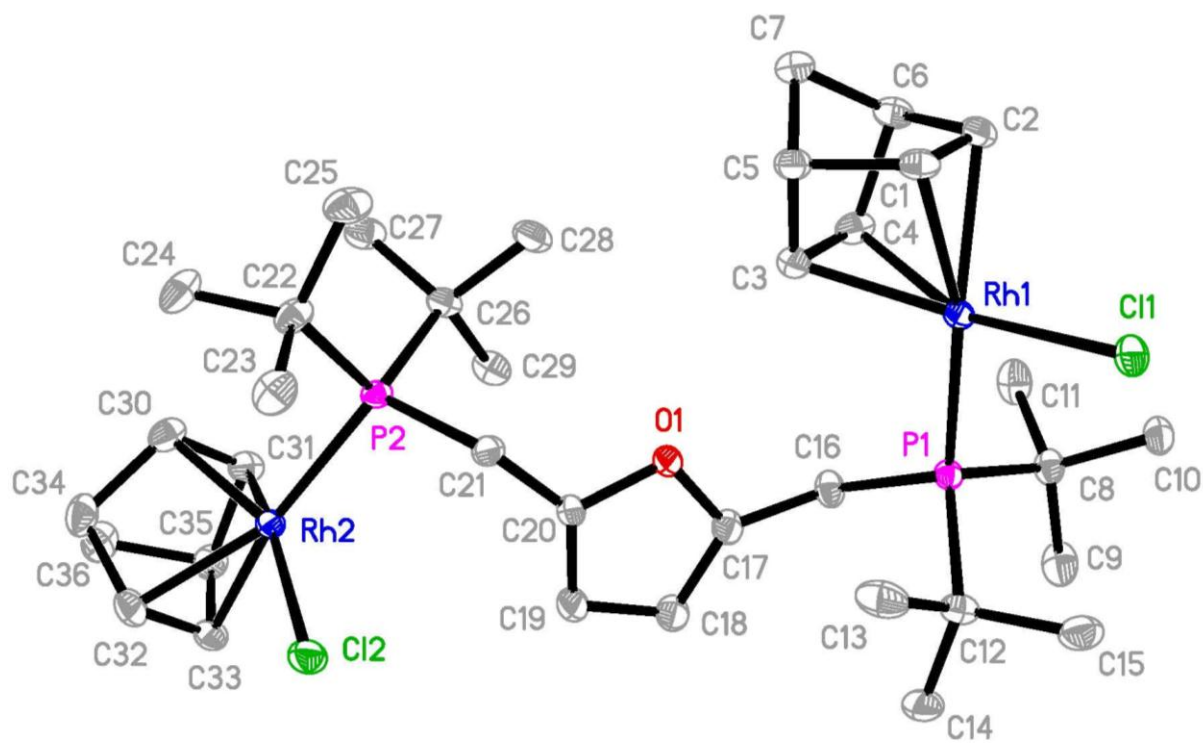


Table A2. Crystal data and structure refinement for $(\mu_2\text{-}^{\text{tBu}}\text{furPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$.

Identification code	mh301	
Empirical formula	C ₃₆ H ₅₈ Cl ₂ O ₂ P ₂ Rh ₂	
Formula weight	845.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2229(4) Å	α = 84.914(1)°.
	b = 13.3906(6) Å	β = 82.020(1)°.
	c = 15.3427(7) Å	γ = 86.259(1)°.
Volume	1866.40(14) Å ³	
Z	2	
Density (calculated)	1.504 Mg/m ³	
Absorption coefficient	1.140 mm ⁻¹	
F(000)	872	
Crystal size	0.29 x 0.23 x 0.13 mm ³	
Theta range for data collection	1.95 to 30.03°.	
Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -21 ≤ l ≤ 21	
Reflections collected	21607	
Independent reflections	10788 [R(int) = 0.0147]	
Completeness to theta = 30.03°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.746 and 0.673	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10788 / 0 / 424	
Goodness-of-fit on F ²	1.002	
Final R indices [I > 2σ(I)]	R1 = 0.0236, wR2 = 0.0552	
R indices (all data)	R1 = 0.0265, wR2 = 0.0565	
Largest diff. peak and hole	0.941 and -0.347 e.Å ⁻³	

Table A3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for $(\mu_2\text{-}^i\text{Bu}\text{furPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	7310(1)	4886(1)	6031(1)	13(1)
Rh(2)	12383(1)	9440(1)	8484(1)	15(1)
Cl(1)	7355(1)	3169(1)	5757(1)	20(1)
Cl(2)	13697(1)	7892(1)	8734(1)	24(1)
P(1)	6866(1)	4683(1)	7587(1)	13(1)
P(2)	11518(1)	8922(1)	7222(1)	14(1)
O(1)	9188(1)	6678(1)	7617(1)	17(1)
C(1)	8240(2)	5315(1)	4642(1)	18(1)
C(2)	6736(2)	5425(1)	4716(1)	19(1)
C(3)	8219(2)	6302(1)	5842(1)	20(1)
C(4)	6680(2)	6421(1)	5918(1)	20(1)
C(5)	8775(2)	6321(1)	4848(1)	19(1)
C(6)	6299(2)	6501(1)	4969(1)	20(1)
C(7)	7619(2)	7064(1)	4475(1)	22(1)
C(8)	4877(2)	4394(1)	7946(1)	18(1)
C(9)	4495(2)	4090(2)	8937(1)	28(1)
C(10)	4461(2)	3562(1)	7414(1)	21(1)
C(11)	3931(2)	5344(1)	7706(1)	26(1)
C(12)	8132(2)	3729(1)	8126(1)	20(1)
C(13)	9672(2)	3931(2)	7643(1)	29(1)
C(14)	8137(2)	3789(1)	9120(1)	26(1)
C(15)	7779(2)	2655(1)	7984(1)	28(1)
C(16)	6924(2)	5838(1)	8188(1)	19(1)
C(17)	8338(2)	6234(1)	8336(1)	19(1)

C(18)	8970(2)	6319(1)	9070(1)	23(1)
C(19)	10293(2)	6829(1)	8800(1)	22(1)
C(20)	10381(2)	7037(1)	7918(1)	17(1)
C(21)	11466(2)	7535(1)	7234(1)	16(1)
C(22)	12939(2)	9183(1)	6223(1)	20(1)
C(23)	14241(2)	8420(1)	6297(1)	26(1)
C(24)	13511(2)	10232(1)	6236(1)	27(1)
C(25)	12395(2)	9096(1)	5333(1)	26(1)
C(26)	9631(2)	9413(1)	6985(1)	18(1)
C(27)	9663(2)	10539(1)	6690(1)	24(1)
C(28)	9002(2)	8859(1)	6298(1)	24(1)
C(29)	8578(2)	9271(1)	7854(1)	23(1)
C(30)	12306(2)	11020(1)	8238(1)	23(1)
C(31)	11048(2)	10746(1)	8811(1)	21(1)
C(32)	13780(2)	10163(1)	9241(1)	24(1)
C(33)	12537(2)	9900(1)	9805(1)	22(1)
C(34)	13452(2)	11228(1)	8834(1)	27(1)
C(35)	11416(2)	10799(1)	9752(1)	23(1)
C(36)	12450(2)	11681(1)	9607(1)	29(1)

Table A4. Bond lengths [Å] and angles [°] for $(\mu_2\text{-}^t\text{BuPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$.

Rh(1)-C(4)	2.0972(16)	C(4)-C(6)	1.539(2)
Rh(1)-C(3)	2.1034(16)	C(4)-H(4)	0.92(2)
Rh(1)-C(2)	2.2044(15)	C(5)-C(7)	1.544(2)
Rh(1)-C(1)	2.2244(15)	C(5)-H(5)	1.0000
Rh(1)-P(1)	2.3590(4)	C(6)-C(7)	1.545(2)
Rh(1)-Cl(1)	2.3715(4)	C(6)-H(6)	1.0000
Rh(2)-C(30)	2.1146(16)	C(7)-H(7A)	0.9900
Rh(2)-C(31)	2.1281(16)	C(7)-H(7B)	0.9900
Rh(2)-C(32)	2.1743(16)	C(8)-C(10)	1.536(2)
Rh(2)-C(33)	2.1961(16)	C(8)-C(9)	1.536(2)
Rh(2)-Cl(2)	2.3615(4)	C(8)-C(11)	1.541(2)
Rh(2)-P(2)	2.3672(4)	C(9)-H(9A)	0.9800
P(1)-C(16)	1.8776(16)	C(9)-H(9B)	0.9800
P(1)-C(12)	1.8881(16)	C(9)-H(9C)	0.9800
P(1)-C(8)	1.8960(16)	C(10)-H(10A)	0.9800
P(2)-C(21)	1.8603(15)	C(10)-H(10B)	0.9800
P(2)-C(26)	1.8920(16)	C(10)-H(10C)	0.9800
P(2)-C(22)	1.8952(16)	C(11)-H(11A)	0.9800
O(1)-C(17)	1.3738(19)	C(11)-H(11B)	0.9800
O(1)-C(20)	1.3797(18)	C(11)-H(11C)	0.9800
C(1)-C(2)	1.376(2)	C(12)-C(14)	1.535(2)
C(1)-C(5)	1.537(2)	C(12)-C(15)	1.536(2)
C(1)-H(1)	0.95(2)	C(12)-C(13)	1.537(2)
C(2)-C(6)	1.538(2)	C(13)-H(13A)	0.9800
C(2)-H(2)	0.93(2)	C(13)-H(13B)	0.9800
C(3)-C(4)	1.408(2)	C(13)-H(13C)	0.9800
C(3)-C(5)	1.538(2)	C(14)-H(14A)	0.9800
C(3)-H(3)	0.90(2)	C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800	C(26)-C(28)	1.537(2)
C(15)-H(15A)	0.9800	C(26)-C(29)	1.542(2)
C(15)-H(15B)	0.9800	C(27)-H(27A)	0.9800
C(15)-H(15C)	0.9800	C(27)-H(27B)	0.9800
C(16)-C(17)	1.492(2)	C(27)-H(27C)	0.9800
C(16)-H(16A)	0.9900	C(28)-H(28A)	0.9800
C(16)-H(16B)	0.9900	C(28)-H(28B)	0.9800
C(17)-C(18)	1.356(2)	C(28)-H(28C)	0.9800
C(18)-C(19)	1.430(2)	C(29)-H(29A)	0.9800
C(18)-H(18)	0.9500	C(29)-H(29B)	0.9800
C(19)-C(20)	1.349(2)	C(29)-H(29C)	0.9800
C(19)-H(19)	0.9500	C(30)-C(31)	1.403(2)
C(20)-C(21)	1.489(2)	C(30)-C(34)	1.544(3)
C(21)-H(21A)	0.9900	C(30)-H(30)	0.92(2)
C(21)-H(21B)	0.9900	C(31)-C(35)	1.538(2)
C(22)-C(25)	1.535(2)	C(31)-H(31)	0.93(2)
C(22)-C(23)	1.535(2)	C(32)-C(33)	1.382(3)
C(22)-C(24)	1.535(2)	C(32)-C(34)	1.535(3)
C(23)-H(23A)	0.9800	C(32)-H(32)	0.94(2)
C(23)-H(23B)	0.9800	C(33)-C(35)	1.539(3)
C(23)-H(23C)	0.9800	C(33)-H(33)	0.95(2)
C(24)-H(24A)	0.9800	C(34)-C(36)	1.542(3)
C(24)-H(24B)	0.9800	C(34)-H(34)	1.0000
C(24)-H(24C)	0.9800	C(35)-C(36)	1.546(2)
C(25)-H(25A)	0.9800	C(35)-H(35)	1.0000
C(25)-H(25B)	0.9800	C(36)-H(36A)	0.9900
C(25)-H(25C)	0.9800	C(36)-H(36B)	0.9900
C(26)-C(27)	1.536(2)		
C(4)-Rh(1)-C(3)	39.15(7)	C(3)-Rh(1)-C(2)	78.65(6)
C(4)-Rh(1)-C(2)	66.57(6)	C(4)-Rh(1)-C(1)	78.91(6)

C(3)-Rh(1)-C(1)	65.93(6)	C(8)-P(1)-Rh(1)	109.33(5)
C(2)-Rh(1)-C(1)	36.19(6)	C(21)-P(2)-C(26)	104.42(7)
C(4)-Rh(1)-P(1)	96.08(5)	C(21)-P(2)-C(22)	100.36(7)
C(3)-Rh(1)-P(1)	100.63(4)	C(26)-P(2)-C(22)	110.83(7)
C(2)-Rh(1)-P(1)	153.76(4)	C(21)-P(2)-Rh(2)	112.92(5)
C(1)-Rh(1)-P(1)	164.06(4)	C(26)-P(2)-Rh(2)	117.94(5)
C(4)-Rh(1)-Cl(1)	157.46(5)	C(22)-P(2)-Rh(2)	108.93(5)
C(3)-Rh(1)-Cl(1)	151.58(5)	C(17)-O(1)-C(20)	107.37(12)
C(2)-Rh(1)-Cl(1)	93.83(4)	C(2)-C(1)-C(5)	106.55(14)
C(1)-Rh(1)-Cl(1)	91.80(4)	C(2)-C(1)-Rh(1)	71.11(9)
P(1)-Rh(1)-Cl(1)	97.923(14)	C(5)-C(1)-Rh(1)	94.52(9)
C(30)-Rh(2)-C(31)	38.62(7)	C(2)-C(1)-H(1)	127.6(13)
C(30)-Rh(2)-C(32)	66.97(7)	C(5)-C(1)-H(1)	125.2(13)
C(31)-Rh(2)-C(32)	79.12(7)	Rh(1)-C(1)-H(1)	108.8(12)
C(30)-Rh(2)-C(33)	79.09(6)	C(1)-C(2)-C(6)	107.03(14)
C(31)-Rh(2)-C(33)	66.12(6)	C(1)-C(2)-Rh(1)	72.70(9)
C(32)-Rh(2)-C(33)	36.86(7)	C(6)-C(2)-Rh(1)	94.30(9)
C(30)-Rh(2)-Cl(2)	150.99(5)	C(1)-C(2)-H(2)	127.3(13)
C(31)-Rh(2)-Cl(2)	157.26(5)	C(6)-C(2)-H(2)	124.8(13)
C(32)-Rh(2)-Cl(2)	90.14(5)	Rh(1)-C(2)-H(2)	108.8(13)
C(33)-Rh(2)-Cl(2)	93.32(5)	C(4)-C(3)-C(5)	106.42(13)
C(30)-Rh(2)-P(2)	102.30(5)	C(4)-C(3)-Rh(1)	70.19(9)
C(31)-Rh(2)-P(2)	104.89(5)	C(5)-C(3)-Rh(1)	99.40(10)
C(32)-Rh(2)-P(2)	157.93(5)	C(4)-C(3)-H(3)	128.2(13)
C(33)-Rh(2)-P(2)	164.02(5)	C(5)-C(3)-H(3)	121.8(13)
Cl(2)-Rh(2)-P(2)	92.618(14)	Rh(1)-C(3)-H(3)	115.3(13)
C(16)-P(1)-C(12)	104.19(7)	C(3)-C(4)-C(6)	105.89(14)
C(16)-P(1)-C(8)	99.05(7)	C(3)-C(4)-Rh(1)	70.66(9)
C(12)-P(1)-C(8)	110.97(7)	C(6)-C(4)-Rh(1)	98.61(10)
C(16)-P(1)-Rh(1)	116.66(5)	C(3)-C(4)-H(4)	126.3(13)
C(12)-P(1)-Rh(1)	115.41(5)	C(6)-C(4)-H(4)	123.6(13)

Rh(1)-C(4)-H(4)	116.3(13)	C(8)-C(10)-H(10A)	109.5
C(1)-C(5)-C(3)	100.08(12)	C(8)-C(10)-H(10B)	109.5
C(1)-C(5)-C(7)	100.80(13)	H(10A)-C(10)-H(10B)	109.5
C(3)-C(5)-C(7)	100.47(13)	C(8)-C(10)-H(10C)	109.5
C(1)-C(5)-H(5)	117.4	H(10A)-C(10)-H(10C)	109.5
C(3)-C(5)-H(5)	117.4	H(10B)-C(10)-H(10C)	109.5
C(7)-C(5)-H(5)	117.4	C(8)-C(11)-H(11A)	109.5
C(2)-C(6)-C(4)	100.34(12)	C(8)-C(11)-H(11B)	109.5
C(2)-C(6)-C(7)	100.52(13)	H(11A)-C(11)-H(11B)	109.5
C(4)-C(6)-C(7)	100.53(13)	C(8)-C(11)-H(11C)	109.5
C(2)-C(6)-H(6)	117.4	H(11A)-C(11)-H(11C)	109.5
C(4)-C(6)-H(6)	117.4	H(11B)-C(11)-H(11C)	109.5
C(7)-C(6)-H(6)	117.4	C(14)-C(12)-C(15)	107.70(14)
C(5)-C(7)-C(6)	94.25(12)	C(14)-C(12)-C(13)	108.90(14)
C(5)-C(7)-H(7A)	112.9	C(15)-C(12)-C(13)	108.50(15)
C(6)-C(7)-H(7A)	112.9	C(14)-C(12)-P(1)	115.62(12)
C(5)-C(7)-H(7B)	112.9	C(15)-C(12)-P(1)	110.98(11)
C(6)-C(7)-H(7B)	112.9	C(13)-C(12)-P(1)	104.92(11)
H(7A)-C(7)-H(7B)	110.3	C(12)-C(13)-H(13A)	109.5
C(10)-C(8)-C(9)	109.26(13)	C(12)-C(13)-H(13B)	109.5
C(10)-C(8)-C(11)	106.87(14)	H(13A)-C(13)-H(13B)	109.5
C(9)-C(8)-C(11)	108.69(14)	C(12)-C(13)-H(13C)	109.5
C(10)-C(8)-P(1)	109.64(11)	H(13A)-C(13)-H(13C)	109.5
C(9)-C(8)-P(1)	114.61(12)	H(13B)-C(13)-H(13C)	109.5
C(11)-C(8)-P(1)	107.48(11)	C(12)-C(14)-H(14A)	109.5
C(8)-C(9)-H(9A)	109.5	C(12)-C(14)-H(14B)	109.5
C(8)-C(9)-H(9B)	109.5	H(14A)-C(14)-H(14B)	109.5
H(9A)-C(9)-H(9B)	109.5	C(12)-C(14)-H(14C)	109.5
C(8)-C(9)-H(9C)	109.5	H(14A)-C(14)-H(14C)	109.5
H(9A)-C(9)-H(9C)	109.5	H(14B)-C(14)-H(14C)	109.5
H(9B)-C(9)-H(9C)	109.5	C(12)-C(15)-H(15A)	109.5

C(12)-C(15)-H(15B)	109.5	C(23)-C(22)-C(24)	107.27(15)
H(15A)-C(15)-H(15B)	109.5	C(25)-C(22)-P(2)	114.47(12)
C(12)-C(15)-H(15C)	109.5	C(23)-C(22)-P(2)	107.82(11)
H(15A)-C(15)-H(15C)	109.5	C(24)-C(22)-P(2)	109.78(11)
H(15B)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23A)	109.5
C(17)-C(16)-P(1)	121.83(11)	C(22)-C(23)-H(23B)	109.5
C(17)-C(16)-H(16A)	106.9	H(23A)-C(23)-H(23B)	109.5
P(1)-C(16)-H(16A)	106.9	C(22)-C(23)-H(23C)	109.5
C(17)-C(16)-H(16B)	106.9	H(23A)-C(23)-H(23C)	109.5
P(1)-C(16)-H(16B)	106.9	H(23B)-C(23)-H(23C)	109.5
H(16A)-C(16)-H(16B)	106.7	C(22)-C(24)-H(24A)	109.5
C(18)-C(17)-O(1)	109.05(14)	C(22)-C(24)-H(24B)	109.5
C(18)-C(17)-C(16)	133.14(15)	H(24A)-C(24)-H(24B)	109.5
O(1)-C(17)-C(16)	117.65(13)	C(22)-C(24)-H(24C)	109.5
C(17)-C(18)-C(19)	107.33(14)	H(24A)-C(24)-H(24C)	109.5
C(17)-C(18)-H(18)	126.3	H(24B)-C(24)-H(24C)	109.5
C(19)-C(18)-H(18)	126.3	C(22)-C(25)-H(25A)	109.5
C(20)-C(19)-C(18)	106.56(14)	C(22)-C(25)-H(25B)	109.5
C(20)-C(19)-H(19)	126.7	H(25A)-C(25)-H(25B)	109.5
C(18)-C(19)-H(19)	126.7	C(22)-C(25)-H(25C)	109.5
C(19)-C(20)-O(1)	109.68(14)	H(25A)-C(25)-H(25C)	109.5
C(19)-C(20)-C(21)	134.21(14)	H(25B)-C(25)-H(25C)	109.5
O(1)-C(20)-C(21)	116.11(13)	C(27)-C(26)-C(28)	109.73(13)
C(20)-C(21)-P(2)	116.77(11)	C(27)-C(26)-C(29)	108.79(13)
C(20)-C(21)-H(21A)	108.1	C(28)-C(26)-C(29)	106.78(14)
P(2)-C(21)-H(21A)	108.1	C(27)-C(26)-P(2)	109.39(11)
C(20)-C(21)-H(21B)	108.1	C(28)-C(26)-P(2)	114.61(11)
P(2)-C(21)-H(21B)	108.1	C(29)-C(26)-P(2)	107.34(11)
H(21A)-C(21)-H(21B)	107.3	C(26)-C(27)-H(27A)	109.5
C(25)-C(22)-C(23)	107.97(14)	C(26)-C(27)-H(27B)	109.5
C(25)-C(22)-C(24)	109.26(14)	H(27A)-C(27)-H(27B)	109.5

C(26)-C(27)-H(27C)	109.5	C(34)-C(32)-Rh(2)	95.13(11)
H(27A)-C(27)-H(27C)	109.5	C(33)-C(32)-H(32)	128.2(14)
H(27B)-C(27)-H(27C)	109.5	C(34)-C(32)-H(32)	124.3(14)
C(26)-C(28)-H(28A)	109.5	Rh(2)-C(32)-H(32)	108.9(13)
C(26)-C(28)-H(28B)	109.5	C(32)-C(33)-C(35)	106.64(15)
H(28A)-C(28)-H(28B)	109.5	C(32)-C(33)-Rh(2)	70.71(10)
C(26)-C(28)-H(28C)	109.5	C(35)-C(33)-Rh(2)	95.43(10)
H(28A)-C(28)-H(28C)	109.5	C(32)-C(33)-H(33)	126.3(13)
H(28B)-C(28)-H(28C)	109.5	C(35)-C(33)-H(33)	126.3(13)
C(26)-C(29)-H(29A)	109.5	Rh(2)-C(33)-H(33)	109.0(13)
C(26)-C(29)-H(29B)	109.5	C(32)-C(34)-C(36)	101.03(15)
H(29A)-C(29)-H(29B)	109.5	C(32)-C(34)-C(30)	100.48(13)
C(26)-C(29)-H(29C)	109.5	C(36)-C(34)-C(30)	100.52(15)
H(29A)-C(29)-H(29C)	109.5	C(32)-C(34)-H(34)	117.3
H(29B)-C(29)-H(29C)	109.5	C(36)-C(34)-H(34)	117.3
C(31)-C(30)-C(34)	106.01(14)	C(30)-C(34)-H(34)	117.3
C(31)-C(30)-Rh(2)	71.21(9)	C(31)-C(35)-C(33)	100.15(13)
C(34)-C(30)-Rh(2)	97.25(11)	C(31)-C(35)-C(36)	100.82(14)
C(31)-C(30)-H(30)	125.1(14)	C(33)-C(35)-C(36)	100.62(15)
C(34)-C(30)-H(30)	124.0(14)	C(31)-C(35)-H(35)	117.4
Rh(2)-C(30)-H(30)	118.1(14)	C(33)-C(35)-H(35)	117.4
C(30)-C(31)-C(35)	106.23(15)	C(36)-C(35)-H(35)	117.4
C(30)-C(31)-Rh(2)	70.17(10)	C(34)-C(36)-C(35)	94.01(13)
C(35)-C(31)-Rh(2)	98.25(11)	C(34)-C(36)-H(36A)	112.9
C(30)-C(31)-H(31)	127.2(13)	C(35)-C(36)-H(36A)	112.9
C(35)-C(31)-H(31)	122.5(13)	C(34)-C(36)-H(36B)	112.9
Rh(2)-C(31)-H(31)	117.0(13)	C(35)-C(36)-H(36B)	112.9
C(33)-C(32)-C(34)	106.53(16)	H(36A)-C(36)-H(36B)	110.3
C(33)-C(32)-Rh(2)	72.43(10)		

Table A6. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\mu_2\text{-}^t\text{Bu-furPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	14(1)	15(1)	11(1)	-2(1)	-2(1)	0(1)
Rh(2)	20(1)	14(1)	13(1)	-1(1)	-4(1)	-3(1)
Cl(1)	21(1)	18(1)	20(1)	-6(1)	-2(1)	-2(1)
Cl(2)	28(1)	18(1)	27(1)	0(1)	-12(1)	0(1)
P(1)	14(1)	14(1)	12(1)	-2(1)	-1(1)	-2(1)
P(2)	20(1)	12(1)	11(1)	-1(1)	-3(1)	-1(1)
O(1)	21(1)	18(1)	14(1)	-1(1)	-5(1)	-6(1)
C(1)	21(1)	22(1)	11(1)	-1(1)	-1(1)	2(1)
C(2)	20(1)	23(1)	14(1)	-1(1)	-5(1)	-3(1)
C(3)	26(1)	18(1)	16(1)	0(1)	-7(1)	-3(1)
C(4)	28(1)	16(1)	15(1)	-2(1)	-1(1)	4(1)
C(5)	18(1)	24(1)	16(1)	2(1)	-4(1)	-3(1)
C(6)	19(1)	23(1)	18(1)	0(1)	-5(1)	3(1)
C(7)	27(1)	22(1)	19(1)	3(1)	-6(1)	-2(1)
C(8)	17(1)	20(1)	18(1)	-4(1)	1(1)	-5(1)
C(9)	30(1)	34(1)	19(1)	-6(1)	7(1)	-13(1)
C(10)	20(1)	21(1)	21(1)	-4(1)	-2(1)	-6(1)
C(11)	15(1)	25(1)	37(1)	-8(1)	0(1)	0(1)
C(12)	22(1)	22(1)	16(1)	-1(1)	-5(1)	2(1)
C(13)	19(1)	42(1)	24(1)	1(1)	-5(1)	7(1)
C(14)	36(1)	27(1)	15(1)	1(1)	-8(1)	-2(1)
C(15)	41(1)	20(1)	24(1)	-2(1)	-12(1)	6(1)
C(16)	20(1)	19(1)	18(1)	-6(1)	0(1)	-4(1)
C(17)	22(1)	19(1)	15(1)	-4(1)	0(1)	-5(1)

C(18)	32(1)	26(1)	13(1)	-2(1)	-2(1)	-11(1)
C(19)	28(1)	25(1)	16(1)	-1(1)	-6(1)	-10(1)
C(20)	20(1)	14(1)	18(1)	-2(1)	-6(1)	-4(1)
C(21)	21(1)	14(1)	14(1)	-1(1)	-4(1)	-1(1)
C(22)	27(1)	16(1)	15(1)	-1(1)	2(1)	-1(1)
C(23)	24(1)	25(1)	26(1)	-2(1)	4(1)	0(1)
C(24)	38(1)	20(1)	21(1)	-1(1)	7(1)	-8(1)
C(25)	38(1)	26(1)	14(1)	-2(1)	0(1)	1(1)
C(26)	22(1)	18(1)	17(1)	-3(1)	-6(1)	2(1)
C(27)	33(1)	17(1)	21(1)	-3(1)	-9(1)	6(1)
C(28)	30(1)	22(1)	21(1)	-3(1)	-13(1)	1(1)
C(29)	21(1)	29(1)	21(1)	-5(1)	-4(1)	2(1)
C(30)	36(1)	15(1)	17(1)	-2(1)	-2(1)	-3(1)
C(31)	29(1)	16(1)	18(1)	-4(1)	-6(1)	1(1)
C(32)	27(1)	27(1)	22(1)	-6(1)	-9(1)	-8(1)
C(33)	31(1)	23(1)	15(1)	-2(1)	-9(1)	-6(1)
C(34)	35(1)	24(1)	25(1)	-5(1)	-2(1)	-12(1)
C(35)	32(1)	22(1)	16(1)	-5(1)	-2(1)	-5(1)
C(36)	43(1)	23(1)	23(1)	-8(1)	-4(1)	-9(1)

Table A7. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)

for $(\mu_2\text{-}^t\text{Bu}_2\text{furPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$.

	x	y	z	U(eq)
H(1)	8850(20)	4772(16)	4422(13)	22
H(2)	6100(20)	4988(16)	4552(13)	22
H(3)	8810(20)	6425(15)	6240(14)	23
H(4)	6070(20)	6659(16)	6386(14)	24
H(5)	9831	6452	4656	23
H(6)	5296	6779	4873	24
H(7A)	7674	7079	3825	27
H(7B)	7652	7751	4658	27
H(9A)	3433	4034	9080	42
H(9B)	4813	4600	9279	42
H(9C)	4997	3441	9083	42
H(10A)	5086	2955	7518	31
H(10B)	4599	3786	6783	31
H(10C)	3432	3415	7600	31
H(11A)	2897	5184	7785	39
H(11B)	4232	5584	7089	39
H(11C)	4064	5867	8091	39
H(13A)	10393	3457	7889	43
H(13B)	9907	4619	7719	43
H(13C)	9699	3847	7013	43
H(14A)	7167	3639	9436	39
H(14B)	8372	4466	9230	39
H(14C)	8875	3300	9330	39
H(15A)	7697	2608	7359	42

H(15B)	6849	2488	8343	42
H(15C)	8565	2184	8159	42
H(16A)	6390	6387	7869	23
H(16B)	6345	5712	8777	23
H(18)	8603	6082	9656	28
H(19)	10976	6991	9169	27
H(21A)	11263	7372	6647	20
H(21B)	12454	7236	7315	20
H(23A)	13963	7756	6180	39
H(23B)	14516	8391	6894	39
H(23C)	15075	8626	5865	39
H(24A)	14220	10372	5708	41
H(24B)	13990	10258	6764	41
H(24C)	12690	10735	6243	41
H(25A)	13220	9154	4858	40
H(25B)	11649	9634	5236	40
H(25C)	11969	8443	5337	40
H(27A)	8664	10813	6640	35
H(27B)	10272	10635	6116	35
H(27C)	10075	10888	7127	35
H(28A)	8947	8146	6499	36
H(28B)	9640	8932	5732	36
H(28C)	8018	9147	6224	36
H(29A)	7613	9588	7773	35
H(29B)	8969	9582	8321	35
H(29C)	8485	8552	8022	35
H(30)	12310(20)	11287(16)	7663(15)	27
H(31)	10090(20)	10776(16)	8683(14)	25
H(32)	14710(20)	9829(17)	9185(14)	29
H(33)	12450(20)	9326(16)	10219(14)	27
H(34)	14309	11618	8554	33

H(35)	10577	10831	10240	28
H(36A)	11949	12328	9429	35
H(36B)	12964	11749	10122	35

Table A8. Torsion angles [°] for $(\mu_2\text{-}^{\text{tBu}}\text{furPOP})[\text{Rh}(\text{NBD})\text{Cl}]_2$.

C(4)-Rh(1)-P(1)-C(16)	-24.20(8)	C(33)-Rh(2)-P(2)-C(22)	162.35(18)
C(3)-Rh(1)-P(1)-C(16)	15.14(8)	Cl(2)-Rh(2)-P(2)-C(22)	-85.93(5)
C(2)-Rh(1)-P(1)-C(16)	-70.72(12)	C(4)-Rh(1)-C(1)-C(2)	-65.28(10)
C(1)-Rh(1)-P(1)-C(16)	46.45(17)	C(3)-Rh(1)-C(1)-C(2)	-104.21(11)
Cl(1)-Rh(1)-P(1)-C(16)	173.51(6)	P(1)-Rh(1)-C(1)-C(2)	-138.23(14)
C(4)-Rh(1)-P(1)-C(12)	-147.02(8)	Cl(1)-Rh(1)-C(1)-C(2)	94.03(9)
C(3)-Rh(1)-P(1)-C(12)	-107.69(8)	C(4)-Rh(1)-C(1)-C(5)	40.68(10)
C(2)-Rh(1)-P(1)-C(12)	166.45(11)	C(3)-Rh(1)-C(1)-C(5)	1.75(9)
C(1)-Rh(1)-P(1)-C(12)	-76.37(17)	C(2)-Rh(1)-C(1)-C(5)	105.96(14)
Cl(1)-Rh(1)-P(1)-C(12)	50.68(6)	P(1)-Rh(1)-C(1)-C(5)	-32.3(2)
C(4)-Rh(1)-P(1)-C(8)	87.07(7)	Cl(1)-Rh(1)-C(1)-C(5)	-160.01(9)
C(3)-Rh(1)-P(1)-C(8)	126.40(7)	C(5)-C(1)-C(2)-C(6)	0.08(16)
C(2)-Rh(1)-P(1)-C(8)	40.54(11)	Rh(1)-C(1)-C(2)-C(6)	89.24(11)
C(1)-Rh(1)-P(1)-C(8)	157.72(16)	C(5)-C(1)-C(2)-Rh(1)	-89.16(10)
Cl(1)-Rh(1)-P(1)-C(8)	-75.22(6)	C(4)-Rh(1)-C(2)-C(1)	103.71(11)
C(30)-Rh(2)-P(2)-C(21)	179.61(7)	C(3)-Rh(1)-C(2)-C(1)	64.52(10)
C(31)-Rh(2)-P(2)-C(21)	-140.70(7)	P(1)-Rh(1)-C(2)-C(1)	155.57(9)
C(32)-Rh(2)-P(2)-C(21)	121.49(15)	Cl(1)-Rh(1)-C(2)-C(1)	-87.81(9)
C(33)-Rh(2)-P(2)-C(21)	-87.08(18)	C(4)-Rh(1)-C(2)-C(6)	-2.79(9)
Cl(2)-Rh(2)-P(2)-C(21)	24.65(6)	C(3)-Rh(1)-C(2)-C(6)	-41.99(10)
C(30)-Rh(2)-P(2)-C(26)	-58.37(8)	C(1)-Rh(1)-C(2)-C(6)	-106.51(14)
C(31)-Rh(2)-P(2)-C(26)	-18.67(8)	P(1)-Rh(1)-C(2)-C(6)	49.06(15)
C(32)-Rh(2)-P(2)-C(26)	-116.49(15)	Cl(1)-Rh(1)-C(2)-C(6)	165.68(9)
C(33)-Rh(2)-P(2)-C(26)	34.95(18)	C(2)-Rh(1)-C(3)-C(4)	66.69(10)
Cl(2)-Rh(2)-P(2)-C(26)	146.67(6)	C(1)-Rh(1)-C(3)-C(4)	102.41(10)
C(30)-Rh(2)-P(2)-C(22)	69.03(7)	P(1)-Rh(1)-C(3)-C(4)	-86.58(9)
C(31)-Rh(2)-P(2)-C(22)	108.73(7)	Cl(1)-Rh(1)-C(3)-C(4)	143.52(9)
C(32)-Rh(2)-P(2)-C(22)	10.91(15)	C(4)-Rh(1)-C(3)-C(5)	-104.18(13)

C(2)-Rh(1)-C(3)-C(5)	-37.49(10)	Rh(1)-C(4)-C(6)-C(7)	-106.63(11)
C(1)-Rh(1)-C(3)-C(5)	-1.76(9)	C(1)-C(5)-C(7)-C(6)	50.72(14)
P(1)-Rh(1)-C(3)-C(5)	169.24(9)	C(3)-C(5)-C(7)-C(6)	-51.78(14)
Cl(1)-Rh(1)-C(3)-C(5)	39.34(16)	C(2)-C(6)-C(7)-C(5)	-50.48(14)
C(5)-C(3)-C(4)-C(6)	0.57(17)	C(4)-C(6)-C(7)-C(5)	52.24(14)
Rh(1)-C(3)-C(4)-C(6)	-93.73(11)	C(16)-P(1)-C(8)-C(10)	170.57(11)
C(5)-C(3)-C(4)-Rh(1)	94.29(11)	C(12)-P(1)-C(8)-C(10)	-80.35(12)
C(2)-Rh(1)-C(4)-C(3)	-101.10(10)	Rh(1)-P(1)-C(8)-C(10)	48.07(12)
C(1)-Rh(1)-C(4)-C(3)	-65.32(10)	C(16)-P(1)-C(8)-C(9)	-66.15(13)
P(1)-Rh(1)-C(4)-C(3)	99.37(9)	C(12)-P(1)-C(8)-C(9)	42.93(14)
Cl(1)-Rh(1)-C(4)-C(3)	-132.43(12)	Rh(1)-P(1)-C(8)-C(9)	171.34(11)
C(3)-Rh(1)-C(4)-C(6)	103.91(14)	C(16)-P(1)-C(8)-C(11)	54.77(12)
C(2)-Rh(1)-C(4)-C(6)	2.81(9)	C(12)-P(1)-C(8)-C(11)	163.84(11)
C(1)-Rh(1)-C(4)-C(6)	38.59(10)	Rh(1)-P(1)-C(8)-C(11)	-67.74(11)
P(1)-Rh(1)-C(4)-C(6)	-156.72(9)	C(16)-P(1)-C(12)-C(14)	34.92(14)
Cl(1)-Rh(1)-C(4)-C(6)	-28.52(19)	C(8)-P(1)-C(12)-C(14)	-70.79(14)
C(2)-C(1)-C(5)-C(3)	69.41(15)	Rh(1)-P(1)-C(12)-C(14)	164.15(11)
Rh(1)-C(1)-C(5)-C(3)	-2.21(11)	C(16)-P(1)-C(12)-C(15)	157.94(12)
C(2)-C(1)-C(5)-C(7)	-33.41(16)	C(8)-P(1)-C(12)-C(15)	52.24(14)
Rh(1)-C(1)-C(5)-C(7)	-105.03(10)	Rh(1)-P(1)-C(12)-C(15)	-72.83(13)
C(4)-C(3)-C(5)-C(1)	-69.61(15)	C(16)-P(1)-C(12)-C(13)	-85.06(12)
Rh(1)-C(3)-C(5)-C(1)	2.37(12)	C(8)-P(1)-C(12)-C(13)	169.24(11)
C(4)-C(3)-C(5)-C(7)	33.47(16)	Rh(1)-P(1)-C(12)-C(13)	44.17(12)
Rh(1)-C(3)-C(5)-C(7)	105.45(11)	C(12)-P(1)-C(16)-C(17)	48.87(15)
C(1)-C(2)-C(6)-C(4)	-69.66(15)	C(8)-P(1)-C(16)-C(17)	163.33(13)
Rh(1)-C(2)-C(6)-C(4)	3.55(12)	Rh(1)-P(1)-C(16)-C(17)	-79.60(14)
C(1)-C(2)-C(6)-C(7)	33.22(16)	C(20)-O(1)-C(17)-C(18)	0.51(18)
Rh(1)-C(2)-C(6)-C(7)	106.43(10)	C(20)-O(1)-C(17)-C(16)	176.52(13)
C(3)-C(4)-C(6)-C(2)	68.47(15)	P(1)-C(16)-C(17)-C(18)	-113.7(2)
Rh(1)-C(4)-C(6)-C(2)	-3.76(13)	P(1)-C(16)-C(17)-O(1)	71.46(18)
C(3)-C(4)-C(6)-C(7)	-34.40(16)	O(1)-C(17)-C(18)-C(19)	-0.7(2)

C(16)-C(17)-C(18)-C(19)	-175.88(17)	Cl(2)-Rh(2)-C(30)-C(31)	-142.15(9)
C(17)-C(18)-C(19)-C(20)	0.7(2)	P(2)-Rh(2)-C(30)-C(31)	98.54(9)
C(18)-C(19)-C(20)-O(1)	-0.36(19)	C(31)-Rh(2)-C(30)-C(34)	104.51(14)
C(18)-C(19)-C(20)-C(21)	-179.14(17)	C(32)-Rh(2)-C(30)-C(34)	2.76(10)
C(17)-O(1)-C(20)-C(19)	-0.08(18)	C(33)-Rh(2)-C(30)-C(34)	39.30(11)
C(17)-O(1)-C(20)-C(21)	178.95(13)	Cl(2)-Rh(2)-C(30)-C(34)	-37.64(16)
C(19)-C(20)-C(21)-P(2)	-73.2(2)	P(2)-Rh(2)-C(30)-C(34)	-156.95(10)
O(1)-C(20)-C(21)-P(2)	108.05(13)	C(34)-C(30)-C(31)-C(35)	0.74(18)
C(26)-P(2)-C(21)-C(20)	-61.76(13)	Rh(2)-C(30)-C(31)-C(35)	93.09(11)
C(22)-P(2)-C(21)-C(20)	-176.61(12)	C(34)-C(30)-C(31)-Rh(2)	-92.35(12)
Rh(2)-P(2)-C(21)-C(20)	67.58(12)	C(32)-Rh(2)-C(31)-C(30)	66.56(11)
C(21)-P(2)-C(22)-C(25)	73.63(13)	C(33)-Rh(2)-C(31)-C(30)	102.86(11)
C(26)-P(2)-C(22)-C(25)	-36.28(14)	Cl(2)-Rh(2)-C(31)-C(30)	129.67(12)
Rh(2)-P(2)-C(22)-C(25)	-167.61(10)	P(2)-Rh(2)-C(31)-C(30)	-91.16(10)
C(21)-P(2)-C(22)-C(23)	-46.53(13)	C(30)-Rh(2)-C(31)-C(35)	-104.36(15)
C(26)-P(2)-C(22)-C(23)	-156.43(11)	C(32)-Rh(2)-C(31)-C(35)	-37.79(11)
Rh(2)-P(2)-C(22)-C(23)	72.24(12)	C(33)-Rh(2)-C(31)-C(35)	-1.49(10)
C(21)-P(2)-C(22)-C(24)	-163.08(12)	Cl(2)-Rh(2)-C(31)-C(35)	25.3(2)
C(26)-P(2)-C(22)-C(24)	87.01(13)	P(2)-Rh(2)-C(31)-C(35)	164.48(9)
Rh(2)-P(2)-C(22)-C(24)	-44.32(13)	C(30)-Rh(2)-C(32)-C(33)	102.97(12)
C(21)-P(2)-C(26)-C(27)	-163.56(11)	C(31)-Rh(2)-C(32)-C(33)	64.48(11)
C(22)-P(2)-C(26)-C(27)	-56.32(12)	Cl(2)-Rh(2)-C(32)-C(33)	-95.35(10)
Rh(2)-P(2)-C(26)-C(27)	70.17(11)	P(2)-Rh(2)-C(32)-C(33)	167.33(10)
C(21)-P(2)-C(26)-C(28)	-39.86(13)	C(30)-Rh(2)-C(32)-C(34)	-2.77(11)
C(22)-P(2)-C(26)-C(28)	67.39(14)	C(31)-Rh(2)-C(32)-C(34)	-41.25(11)
Rh(2)-P(2)-C(26)-C(28)	-166.13(10)	C(33)-Rh(2)-C(32)-C(34)	-105.73(16)
C(21)-P(2)-C(26)-C(29)	78.55(12)	Cl(2)-Rh(2)-C(32)-C(34)	158.92(11)
C(22)-P(2)-C(26)-C(29)	-174.21(11)	P(2)-Rh(2)-C(32)-C(34)	61.60(19)
Rh(2)-P(2)-C(26)-C(29)	-47.72(12)	C(34)-C(32)-C(33)-C(35)	0.22(17)
C(32)-Rh(2)-C(30)-C(31)	-101.75(11)	Rh(2)-C(32)-C(33)-C(35)	-90.00(11)
C(33)-Rh(2)-C(30)-C(31)	-65.21(10)	C(34)-C(32)-C(33)-Rh(2)	90.23(12)

C(30)-Rh(2)-C(33)-C(32)	-65.97(12)
C(31)-Rh(2)-C(33)-C(32)	-104.26(12)
Cl(2)-Rh(2)-C(33)-C(32)	85.79(11)
P(2)-Rh(2)-C(33)-C(32)	-162.57(14)
C(30)-Rh(2)-C(33)-C(35)	39.78(11)
C(31)-Rh(2)-C(33)-C(35)	1.48(10)
C(32)-Rh(2)-C(33)-C(35)	105.75(15)
Cl(2)-Rh(2)-C(33)-C(35)	-168.46(10)
P(2)-Rh(2)-C(33)-C(35)	-56.8(2)
C(33)-C(32)-C(34)-C(36)	33.39(17)
Rh(2)-C(32)-C(34)-C(36)	106.57(12)
C(33)-C(32)-C(34)-C(30)	-69.63(16)
Rh(2)-C(32)-C(34)-C(30)	3.55(13)
C(31)-C(30)-C(34)-C(32)	68.80(17)
Rh(2)-C(30)-C(34)-C(32)	-3.66(14)
C(31)-C(30)-C(34)-C(36)	-34.63(17)
Rh(2)-C(30)-C(34)-C(36)	-107.09(12)
C(30)-C(31)-C(35)-C(33)	-69.67(16)
Rh(2)-C(31)-C(35)-C(33)	1.98(13)
C(30)-C(31)-C(35)-C(36)	33.32(17)
Rh(2)-C(31)-C(35)-C(36)	104.97(12)
C(32)-C(33)-C(35)-C(31)	69.55(16)
Rh(2)-C(33)-C(35)-C(31)	-1.91(13)
C(32)-C(33)-C(35)-C(36)	-33.60(16)
Rh(2)-C(33)-C(35)-C(36)	-105.06(11)
C(32)-C(34)-C(36)-C(35)	-50.91(16)
C(30)-C(34)-C(36)-C(35)	52.08(16)
C(31)-C(35)-C(36)-C(34)	-51.79(16)
C(33)-C(35)-C(36)-C(34)	50.83(15)

Figure B1: ORTEP diagram of (^tBu_{xan}POP)RhCl

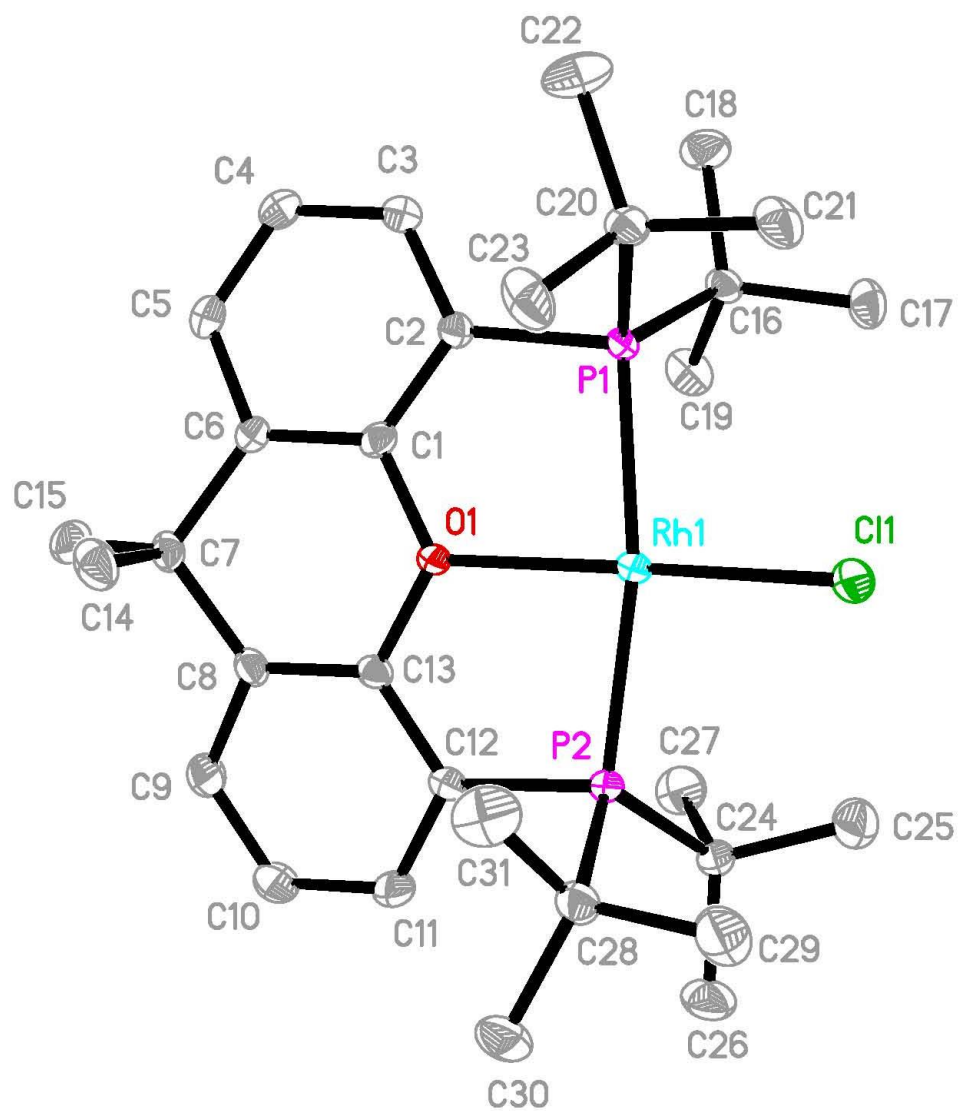


Table B2. Crystal data and structure refinement for (^tBu₃xanPOP)RhCl.

Identification code	mh307	
Empirical formula	C ₃₁ H ₄₈ Cl O P ₂ Rh	
Formula weight	636.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.2641(8) Å	α = 90°.
	b = 16.8195(13) Å	β = 107.246(1)°.
	c = 16.9432(13) Å	γ = 90°.
Volume	3065.7(4) Å ³	
Z	4	
Density (calculated)	1.380 Mg/m ³	
Absorption coefficient	0.771 mm ⁻¹	
F(000)	1336	
Crystal size	0.70 x 0.40 x 0.05 mm ³	
Theta range for data collection	1.75 to 27.10°.	
Index ranges	-14 ≤ h ≤ 14, -21 ≤ k ≤ 21, -21 ≤ l ≤ 19	
Reflections collected	21203	
Independent reflections	6706 [R(int) = 0.0260]	
Completeness to theta = 27.10°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9625 and 0.6145	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6706 / 0 / 339	
Goodness-of-fit on F ²	1.006	
Final R indices [I > 2σ(I)]	R1 = 0.0366, wR2 = 0.0891	
R indices (all data)	R1 = 0.0413, wR2 = 0.0919	
Largest diff. peak and hole	1.899 and -0.317 e.Å ⁻³	

Table B3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (**^tBu_xanPOP**)RhCl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	2941(1)	5911(1)	2808(1)	14(1)
P(1)	1755(1)	5094(1)	3335(1)	13(1)
P(2)	3709(1)	6654(1)	1959(1)	14(1)
Cl(1)	3818(1)	6649(1)	4001(1)	25(1)
O(1)	2349(2)	5147(1)	1750(1)	14(1)
C(1)	1533(2)	4512(1)	1747(2)	15(1)
C(2)	1128(2)	4429(2)	2447(2)	15(1)
C(3)	302(3)	3806(2)	2443(2)	21(1)
C(4)	-91(3)	3295(2)	1781(2)	26(1)
C(5)	356(3)	3381(2)	1111(2)	23(1)
C(6)	1190(2)	3985(1)	1080(2)	16(1)
C(7)	1794(2)	4036(2)	388(2)	17(1)
C(8)	2150(2)	4895(2)	298(2)	16(1)
C(9)	2284(3)	5191(2)	-438(2)	24(1)
C(10)	2768(3)	5940(2)	-480(2)	27(1)
C(11)	3172(3)	6399(2)	223(2)	22(1)
C(12)	3060(2)	6132(2)	976(2)	16(1)
C(13)	2505(2)	5392(1)	986(2)	14(1)
C(14)	3013(3)	3550(2)	651(2)	26(1)
C(15)	953(3)	3694(2)	-422(2)	25(1)
C(16)	346(2)	5597(2)	3494(2)	16(1)
C(17)	784(3)	6223(2)	4176(2)	22(1)
C(18)	-626(3)	5066(2)	3705(2)	27(1)
C(19)	-279(3)	6021(2)	2676(2)	24(1)
C(20)	2565(2)	4403(2)	4201(2)	18(1)
C(21)	3091(3)	4891(2)	4990(2)	23(1)

C(22)	1849(3)	3688(2)	4394(2)	33(1)
C(23)	3664(3)	4083(2)	3934(2)	27(1)
C(24)	3127(2)	7714(2)	1761(2)	18(1)
C(25)	3238(3)	8113(2)	2592(2)	28(1)
C(26)	3730(3)	8246(2)	1269(2)	31(1)
C(27)	1718(3)	7656(2)	1297(2)	29(1)
C(28)	5438(2)	6557(2)	2123(2)	20(1)
C(29)	6098(3)	7083(2)	2863(2)	35(1)
C(30)	5909(3)	6764(2)	1388(2)	30(1)
C(31)	5722(3)	5681(2)	2342(2)	33(1)

Table B4. Bond lengths [Å] and angles [°] for (^tBu_{xan}POP)RhCl.

Rh(1)-O(1)	2.1446(17)	C(14)-H(14A)	0.9800
Rh(1)-P(2)	2.2613(7)	C(14)-H(14B)	0.9800
Rh(1)-P(1)	2.2753(6)	C(14)-H(14C)	0.9800
Rh(1)-Cl(1)	2.3282(7)	C(15)-H(15A)	0.9800
P(1)-C(2)	1.839(3)	C(15)-H(15B)	0.9800
P(1)-C(20)	1.883(3)	C(15)-H(15C)	0.9800
P(1)-C(16)	1.887(3)	C(16)-C(19)	1.532(4)
P(2)-C(12)	1.833(3)	C(16)-C(17)	1.534(4)
P(2)-C(28)	1.891(3)	C(16)-C(18)	1.535(4)
P(2)-C(24)	1.895(3)	C(17)-H(17A)	0.9800
O(1)-C(1)	1.408(3)	C(17)-H(17B)	0.9800
O(1)-C(13)	1.417(3)	C(17)-H(17C)	0.9800
C(1)-C(2)	1.398(4)	C(18)-H(18A)	0.9800
C(1)-C(6)	1.398(3)	C(18)-H(18B)	0.9800
C(2)-C(3)	1.400(4)	C(18)-H(18C)	0.9800
C(3)-C(4)	1.378(4)	C(19)-H(19A)	0.9800
C(3)-H(3)	0.9500	C(19)-H(19B)	0.9800
C(4)-C(5)	1.379(4)	C(19)-H(19C)	0.9800
C(4)-H(4)	0.9500	C(20)-C(21)	1.531(4)
C(5)-C(6)	1.396(4)	C(20)-C(23)	1.536(4)
C(5)-H(5)	0.9500	C(20)-C(22)	1.536(4)
C(6)-C(7)	1.522(4)	C(21)-H(21A)	0.9800
C(7)-C(8)	1.519(3)	C(21)-H(21B)	0.9800
C(7)-C(15)	1.530(4)	C(21)-H(21C)	0.9800
C(7)-C(14)	1.546(4)	C(22)-H(22A)	0.9800
C(8)-C(9)	1.392(4)	C(22)-H(22B)	0.9800
C(8)-C(13)	1.393(3)	C(22)-H(22C)	0.9800
C(9)-C(10)	1.384(4)	C(23)-H(23A)	0.9800
C(9)-H(9)	0.9500	C(23)-H(23B)	0.9800
C(10)-C(11)	1.380(4)	C(23)-H(23C)	0.9800
C(10)-H(10)	0.9500	C(24)-C(26)	1.515(4)
C(11)-C(12)	1.394(4)	C(24)-C(25)	1.531(4)
C(11)-H(11)	0.9500	C(24)-C(27)	1.551(4)
C(12)-C(13)	1.395(3)	C(25)-H(25A)	0.9800

C(25)-H(25B)	0.9800	C(28)-C(29)	1.535(4)
C(25)-H(25C)	0.9800	C(29)-H(29A)	0.9800
C(26)-H(26A)	0.9800	C(29)-H(29B)	0.9800
C(26)-H(26B)	0.9800	C(29)-H(29C)	0.9800
C(26)-H(26C)	0.9800	C(30)-H(30A)	0.9800
C(27)-H(27A)	0.9800	C(30)-H(30B)	0.9800
C(27)-H(27B)	0.9800	C(30)-H(30C)	0.9800
C(27)-H(27C)	0.9800	C(31)-H(31A)	0.9800
C(28)-C(31)	1.530(4)	C(31)-H(31B)	0.9800
C(28)-C(30)	1.532(4)	C(31)-H(31C)	0.9800
O(1)-Rh(1)-P(2)	83.27(5)	C(1)-C(2)-P(1)	119.34(19)
O(1)-Rh(1)-P(1)	83.86(5)	C(3)-C(2)-P(1)	123.6(2)
P(2)-Rh(1)-P(1)	164.36(2)	C(4)-C(3)-C(2)	121.6(3)
O(1)-Rh(1)-Cl(1)	172.76(5)	C(4)-C(3)-H(3)	119.2
P(2)-Rh(1)-Cl(1)	96.48(2)	C(2)-C(3)-H(3)	119.2
P(1)-Rh(1)-Cl(1)	97.40(2)	C(3)-C(4)-C(5)	119.8(3)
C(2)-P(1)-C(20)	104.01(11)	C(3)-C(4)-H(4)	120.1
C(2)-P(1)-C(16)	104.71(11)	C(5)-C(4)-H(4)	120.1
C(20)-P(1)-C(16)	113.50(11)	C(4)-C(5)-C(6)	121.5(3)
C(2)-P(1)-Rh(1)	100.04(8)	C(4)-C(5)-H(5)	119.3
C(20)-P(1)-Rh(1)	118.28(8)	C(6)-C(5)-H(5)	119.3
C(16)-P(1)-Rh(1)	113.71(8)	C(5)-C(6)-C(1)	117.3(2)
C(12)-P(2)-C(28)	102.00(12)	C(5)-C(6)-C(7)	122.0(2)
C(12)-P(2)-C(24)	105.44(12)	C(1)-C(6)-C(7)	120.6(2)
C(28)-P(2)-C(24)	113.23(12)	C(8)-C(7)-C(6)	108.8(2)
C(12)-P(2)-Rh(1)	100.81(8)	C(8)-C(7)-C(15)	112.2(2)
C(28)-P(2)-Rh(1)	115.47(9)	C(6)-C(7)-C(15)	111.8(2)
C(24)-P(2)-Rh(1)	117.12(8)	C(8)-C(7)-C(14)	107.1(2)
C(1)-O(1)-C(13)	118.36(19)	C(6)-C(7)-C(14)	108.0(2)
C(1)-O(1)-Rh(1)	119.84(14)	C(15)-C(7)-C(14)	108.7(2)
C(13)-O(1)-Rh(1)	119.80(14)	C(9)-C(8)-C(13)	117.1(2)
C(2)-C(1)-C(6)	122.8(2)	C(9)-C(8)-C(7)	122.1(2)
C(2)-C(1)-O(1)	116.8(2)	C(13)-C(8)-C(7)	120.3(2)
C(6)-C(1)-O(1)	120.4(2)	C(10)-C(9)-C(8)	121.4(3)
C(1)-C(2)-C(3)	117.0(2)	C(10)-C(9)-H(9)	119.3

C(8)-C(9)-H(9)	119.3	H(17B)-C(17)-H(17C)	109.5
C(11)-C(10)-C(9)	120.0(3)	C(16)-C(18)-H(18A)	109.5
C(11)-C(10)-H(10)	120.0	C(16)-C(18)-H(18B)	109.5
C(9)-C(10)-H(10)	120.0	H(18A)-C(18)-H(18B)	109.5
C(10)-C(11)-C(12)	120.9(3)	C(16)-C(18)-H(18C)	109.5
C(10)-C(11)-H(11)	119.5	H(18A)-C(18)-H(18C)	109.5
C(12)-C(11)-H(11)	119.5	H(18B)-C(18)-H(18C)	109.5
C(11)-C(12)-C(13)	117.5(2)	C(16)-C(19)-H(19A)	109.5
C(11)-C(12)-P(2)	123.9(2)	C(16)-C(19)-H(19B)	109.5
C(13)-C(12)-P(2)	118.45(19)	H(19A)-C(19)-H(19B)	109.5
C(8)-C(13)-C(12)	122.9(2)	C(16)-C(19)-H(19C)	109.5
C(8)-C(13)-O(1)	120.5(2)	H(19A)-C(19)-H(19C)	109.5
C(12)-C(13)-O(1)	116.6(2)	H(19B)-C(19)-H(19C)	109.5
C(7)-C(14)-H(14A)	109.5	C(21)-C(20)-C(23)	108.0(2)
C(7)-C(14)-H(14B)	109.5	C(21)-C(20)-C(22)	109.0(2)
H(14A)-C(14)-H(14B)	109.5	C(23)-C(20)-C(22)	108.0(2)
C(7)-C(14)-H(14C)	109.5	C(21)-C(20)-P(1)	108.79(17)
H(14A)-C(14)-H(14C)	109.5	C(23)-C(20)-P(1)	103.49(18)
H(14B)-C(14)-H(14C)	109.5	C(22)-C(20)-P(1)	119.08(19)
C(7)-C(15)-H(15A)	109.5	C(20)-C(21)-H(21A)	109.5
C(7)-C(15)-H(15B)	109.5	C(20)-C(21)-H(21B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(7)-C(15)-H(15C)	109.5	C(20)-C(21)-H(21C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(19)-C(16)-C(17)	108.7(2)	C(20)-C(22)-H(22A)	109.5
C(19)-C(16)-C(18)	108.3(2)	C(20)-C(22)-H(22B)	109.5
C(17)-C(16)-C(18)	108.4(2)	H(22A)-C(22)-H(22B)	109.5
C(19)-C(16)-P(1)	105.10(17)	C(20)-C(22)-H(22C)	109.5
C(17)-C(16)-P(1)	108.62(17)	H(22A)-C(22)-H(22C)	109.5
C(18)-C(16)-P(1)	117.43(18)	H(22B)-C(22)-H(22C)	109.5
C(16)-C(17)-H(17A)	109.5	C(20)-C(23)-H(23A)	109.5
C(16)-C(17)-H(17B)	109.5	C(20)-C(23)-H(23B)	109.5
H(17A)-C(17)-H(17B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(16)-C(17)-H(17C)	109.5	C(20)-C(23)-H(23C)	109.5
H(17A)-C(17)-H(17C)	109.5	H(23A)-C(23)-H(23C)	109.5

H(23B)-C(23)-H(23C)	109.5	C(31)-C(28)-C(30)	108.6(2)
C(26)-C(24)-C(25)	108.7(2)	C(31)-C(28)-C(29)	110.0(3)
C(26)-C(24)-C(27)	108.4(2)	C(30)-C(28)-C(29)	109.3(2)
C(25)-C(24)-C(27)	106.6(2)	C(31)-C(28)-P(2)	104.57(18)
C(26)-C(24)-P(2)	117.8(2)	C(30)-C(28)-P(2)	116.8(2)
C(25)-C(24)-P(2)	108.66(19)	C(29)-C(28)-P(2)	107.38(19)
C(27)-C(24)-P(2)	106.18(18)	C(28)-C(29)-H(29A)	109.5
C(24)-C(25)-H(25A)	109.5	C(28)-C(29)-H(29B)	109.5
C(24)-C(25)-H(25B)	109.5	H(29A)-C(29)-H(29B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(28)-C(29)-H(29C)	109.5
C(24)-C(25)-H(25C)	109.5	H(29A)-C(29)-H(29C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(29B)-C(29)-H(29C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(28)-C(30)-H(30A)	109.5
C(24)-C(26)-H(26A)	109.5	C(28)-C(30)-H(30B)	109.5
C(24)-C(26)-H(26B)	109.5	H(30A)-C(30)-H(30B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(28)-C(30)-H(30C)	109.5
C(24)-C(26)-H(26C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(30B)-C(30)-H(30C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(28)-C(31)-H(31A)	109.5
C(24)-C(27)-H(27A)	109.5	C(28)-C(31)-H(31B)	109.5
C(24)-C(27)-H(27B)	109.5	H(31A)-C(31)-H(31B)	109.5
H(27A)-C(27)-H(27B)	109.5	C(28)-C(31)-H(31C)	109.5
C(24)-C(27)-H(27C)	109.5	H(31A)-C(31)-H(31C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(31B)-C(31)-H(31C)	109.5
H(27B)-C(27)-H(27C)	109.5		

Table B5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (**^tBu_{xan}POP**)RhCl. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Rh(1)	17(1)	14(1)	12(1)	0(1)	7(1)	-2(1)
P(1)	16(1)	11(1)	12(1)	0(1)	7(1)	0(1)
P(2)	16(1)	13(1)	14(1)	-1(1)	7(1)	-3(1)
Cl(1)	33(1)	27(1)	16(1)	-5(1)	9(1)	-12(1)
O(1)	19(1)	14(1)	11(1)	-1(1)	7(1)	-4(1)
C(1)	16(1)	11(1)	17(1)	2(1)	5(1)	1(1)
C(2)	19(1)	13(1)	16(1)	0(1)	8(1)	1(1)
C(3)	26(1)	18(1)	22(1)	-1(1)	13(1)	-3(1)
C(4)	31(2)	19(1)	30(2)	-6(1)	15(1)	-11(1)
C(5)	33(2)	16(1)	24(1)	-7(1)	12(1)	-7(1)
C(6)	20(1)	12(1)	17(1)	-1(1)	7(1)	-1(1)
C(7)	22(1)	15(1)	12(1)	-1(1)	6(1)	2(1)
C(8)	19(1)	17(1)	12(1)	-1(1)	6(1)	1(1)
C(9)	34(2)	23(1)	14(1)	-3(1)	9(1)	-4(1)
C(10)	42(2)	27(2)	14(1)	2(1)	13(1)	-6(1)
C(11)	30(1)	18(1)	20(1)	1(1)	10(1)	-6(1)
C(12)	16(1)	17(1)	15(1)	0(1)	7(1)	-1(1)
C(13)	15(1)	13(1)	14(1)	3(1)	6(1)	2(1)
C(14)	32(2)	24(1)	24(1)	4(1)	14(1)	11(1)
C(15)	37(2)	20(1)	16(1)	-3(1)	7(1)	-8(1)
C(16)	16(1)	16(1)	17(1)	0(1)	8(1)	2(1)
C(17)	26(1)	20(1)	23(1)	-4(1)	10(1)	4(1)
C(18)	26(1)	22(1)	40(2)	1(1)	22(1)	-1(1)
C(19)	22(1)	28(2)	21(1)	4(1)	6(1)	8(1)
C(20)	21(1)	14(1)	18(1)	4(1)	8(1)	5(1)
C(21)	30(1)	24(1)	15(1)	4(1)	6(1)	7(1)
C(22)	34(2)	24(2)	38(2)	15(1)	7(1)	-1(1)
C(23)	30(2)	31(2)	24(2)	4(1)	12(1)	16(1)
C(24)	25(1)	14(1)	18(1)	0(1)	10(1)	-2(1)
C(25)	35(2)	23(2)	28(2)	-1(1)	12(1)	1(1)
C(26)	42(2)	23(2)	35(2)	9(1)	24(1)	2(1)

C(27)	26(1)	26(2)	37(2)	1(1)	12(1)	4(1)
C(28)	17(1)	24(1)	21(1)	-4(1)	8(1)	-3(1)
C(29)	19(1)	54(2)	32(2)	-14(2)	9(1)	-10(1)
C(30)	25(1)	34(2)	37(2)	0(1)	20(1)	0(1)
C(31)	21(1)	33(2)	43(2)	8(1)	6(1)	7(1)

Table B6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)
for (**^tBu_xanPOP**)RhCl.

	x	y	z	U(eq)
H(3)	5	3734	2907	25
H(4)	-668	2884	1786	31
H(5)	90	3022	661	28
H(9)	2037	4871	-922	28
H(10)	2823	6138	-994	32
H(11)	3532	6905	194	26
H(14A)	3439	3596	226	38
H(14B)	2821	2990	718	38
H(14C)	3552	3756	1177	38
H(15A)	173	3994	-592	37
H(15B)	776	3135	-341	37
H(15C)	1373	3735	-851	37
H(17A)	80	6559	4191	34
H(17B)	1432	6553	4063	34
H(17C)	1120	5957	4711	34
H(18A)	-1287	5398	3798	41
H(18B)	-229	4760	4206	41
H(18C)	-983	4700	3245	41
H(19A)	-619	5626	2243	36
H(19B)	334	6351	2522	36
H(19C)	-954	6359	2741	36
H(21A)	2420	5024	5226	35
H(21B)	3461	5382	4858	35
H(21C)	3728	4581	5391	35
H(22A)	2392	3386	4857	49
H(22B)	1579	3344	3907	49
H(22C)	1121	3877	4543	49
H(23A)	4152	4529	3825	41
H(23B)	3351	3763	3432	41
H(23C)	4192	3752	4377	41

H(25A)	2832	8635	2496	42
H(25B)	4117	8180	2900	42
H(25C)	2834	7780	2912	42
H(26A)	3348	8775	1213	46
H(26B)	3611	8017	719	46
H(26C)	4622	8292	1555	46
H(27A)	1321	7293	1594	43
H(27B)	1604	7455	737	43
H(27C)	1340	8184	1267	43
H(29A)	5744	6986	3317	52
H(29B)	5986	7644	2699	52
H(29C)	6987	6956	3045	52
H(30A)	6818	6726	1556	44
H(30B)	5656	7307	1204	44
H(30C)	5555	6392	935	44
H(31A)	5260	5347	1879	50
H(31B)	5474	5549	2834	50
H(31C)	6615	5586	2455	50

Table B7. Torsion angles [°] for (^tBu_xanPOP)RhCl.

O(1)-Rh(1)-P(1)-C(2)	-2.54(9)	Rh(1)-P(1)-C(2)-C(1)	4.4(2)
P(2)-Rh(1)-P(1)-C(2)	32.24(13)	C(20)-P(1)-C(2)-C(3)	58.3(2)
Cl(1)-Rh(1)-P(1)-C(2)	-175.37(8)	C(16)-P(1)-C(2)-C(3)	-61.0(2)
O(1)-Rh(1)-P(1)-C(20)	109.44(11)	Rh(1)-P(1)-C(2)-C(3)	-179.0(2)
P(2)-Rh(1)-P(1)-C(20)	144.23(12)	C(1)-C(2)-C(3)-C(4)	0.3(4)
Cl(1)-Rh(1)-P(1)-C(20)	-63.38(10)	P(1)-C(2)-C(3)-C(4)	-176.4(2)
O(1)-Rh(1)-P(1)-C(16)	-113.60(10)	C(2)-C(3)-C(4)-C(5)	1.6(4)
P(2)-Rh(1)-P(1)-C(16)	-78.81(13)	C(3)-C(4)-C(5)-C(6)	-0.9(5)
Cl(1)-Rh(1)-P(1)-C(16)	73.58(9)	C(4)-C(5)-C(6)-C(1)	-1.5(4)
O(1)-Rh(1)-P(2)-C(12)	7.88(9)	C(4)-C(5)-C(6)-C(7)	173.5(3)
P(1)-Rh(1)-P(2)-C(12)	-26.95(13)	C(2)-C(1)-C(6)-C(5)	3.5(4)
Cl(1)-Rh(1)-P(2)-C(12)	-179.40(8)	O(1)-C(1)-C(6)-C(5)	-178.6(2)
O(1)-Rh(1)-P(2)-C(28)	-101.11(11)	C(2)-C(1)-C(6)-C(7)	-171.6(2)
P(1)-Rh(1)-P(2)-C(28)	-135.94(12)	O(1)-C(1)-C(6)-C(7)	6.4(4)
Cl(1)-Rh(1)-P(2)-C(28)	71.61(10)	C(5)-C(6)-C(7)-C(8)	154.7(2)
O(1)-Rh(1)-P(2)-C(24)	121.61(11)	C(1)-C(6)-C(7)-C(8)	-30.4(3)
P(1)-Rh(1)-P(2)-C(24)	86.78(13)	C(5)-C(6)-C(7)-C(15)	30.2(3)
Cl(1)-Rh(1)-P(2)-C(24)	-65.67(10)	C(1)-C(6)-C(7)-C(15)	-154.9(2)
P(2)-Rh(1)-O(1)-C(1)	-169.89(16)	C(5)-C(6)-C(7)-C(14)	-89.3(3)
P(1)-Rh(1)-O(1)-C(1)	1.20(15)	C(1)-C(6)-C(7)-C(14)	85.5(3)
Cl(1)-Rh(1)-O(1)-C(1)	101.6(4)	C(6)-C(7)-C(8)-C(9)	-155.7(2)
P(2)-Rh(1)-O(1)-C(13)	-6.23(15)	C(15)-C(7)-C(8)-C(9)	-31.5(3)
P(1)-Rh(1)-O(1)-C(13)	164.86(16)	C(14)-C(7)-C(8)-C(9)	87.7(3)
Cl(1)-Rh(1)-O(1)-C(13)	-94.7(4)	C(6)-C(7)-C(8)-C(13)	32.3(3)
C(13)-O(1)-C(1)-C(2)	-162.5(2)	C(15)-C(7)-C(8)-C(13)	156.5(2)
Rh(1)-O(1)-C(1)-C(2)	1.4(3)	C(14)-C(7)-C(8)-C(13)	-84.2(3)
C(13)-O(1)-C(1)-C(6)	19.4(3)	C(13)-C(8)-C(9)-C(10)	1.1(4)
Rh(1)-O(1)-C(1)-C(6)	-176.67(17)	C(7)-C(8)-C(9)-C(10)	-171.2(3)
C(6)-C(1)-C(2)-C(3)	-2.9(4)	C(8)-C(9)-C(10)-C(11)	2.4(5)
O(1)-C(1)-C(2)-C(3)	179.1(2)	C(9)-C(10)-C(11)-C(12)	-2.3(5)
C(6)-C(1)-C(2)-P(1)	173.91(19)	C(10)-C(11)-C(12)-C(13)	-1.1(4)
O(1)-C(1)-C(2)-P(1)	-4.1(3)	C(10)-C(11)-C(12)-P(2)	173.6(2)
C(20)-P(1)-C(2)-C(1)	-118.3(2)	C(28)-P(2)-C(12)-C(11)	-66.6(3)
C(16)-P(1)-C(2)-C(1)	122.4(2)	C(24)-P(2)-C(12)-C(11)	51.9(3)

Rh(1)-P(2)-C(12)-C(11)	174.2(2)	Rh(1)-P(2)-C(24)-C(26)	173.70(19)
C(28)-P(2)-C(12)-C(13)	108.1(2)	C(12)-P(2)-C(24)-C(25)	160.77(19)
C(24)-P(2)-C(12)-C(13)	-133.4(2)	C(28)-P(2)-C(24)-C(25)	-88.5(2)
Rh(1)-P(2)-C(12)-C(13)	-11.1(2)	Rh(1)-P(2)-C(24)-C(25)	49.7(2)
C(9)-C(8)-C(13)-C(12)	-4.7(4)	C(12)-P(2)-C(24)-C(27)	46.5(2)
C(7)-C(8)-C(13)-C(12)	167.6(2)	C(28)-P(2)-C(24)-C(27)	157.15(18)
C(9)-C(8)-C(13)-O(1)	177.4(2)	Rh(1)-P(2)-C(24)-C(27)	-64.65(19)
C(7)-C(8)-C(13)-O(1)	-10.3(3)	C(12)-P(2)-C(28)-C(31)	-71.9(2)
C(11)-C(12)-C(13)-C(8)	4.8(4)	C(24)-P(2)-C(28)-C(31)	175.35(19)
P(2)-C(12)-C(13)-C(8)	-170.27(19)	Rh(1)-P(2)-C(28)-C(31)	36.4(2)
C(11)-C(12)-C(13)-O(1)	-177.3(2)	C(12)-P(2)-C(28)-C(30)	48.2(2)
P(2)-C(12)-C(13)-O(1)	7.7(3)	C(24)-P(2)-C(28)-C(30)	-64.6(2)
C(1)-O(1)-C(13)-C(8)	-17.5(3)	Rh(1)-P(2)-C(28)-C(30)	156.45(19)
Rh(1)-O(1)-C(13)-C(8)	178.61(17)	C(12)-P(2)-C(28)-C(29)	171.3(2)
C(1)-O(1)-C(13)-C(12)	164.5(2)	C(24)-P(2)-C(28)-C(29)	58.6(2)
Rh(1)-O(1)-C(13)-C(12)	0.6(3)	Rh(1)-P(2)-C(28)-C(29)	-80.4(2)
C(2)-P(1)-C(16)-C(19)	-58.8(2)		
C(20)-P(1)-C(16)-C(19)	-171.54(17)		
Rh(1)-P(1)-C(16)-C(19)	49.41(19)		
C(2)-P(1)-C(16)-C(17)	-174.95(18)		
C(20)-P(1)-C(16)-C(17)	72.3(2)		
Rh(1)-P(1)-C(16)-C(17)	-66.76(19)		
C(2)-P(1)-C(16)-C(18)	61.6(2)		
C(20)-P(1)-C(16)-C(18)	-51.2(2)		
Rh(1)-P(1)-C(16)-C(18)	169.79(18)		
C(2)-P(1)-C(20)-C(21)	-177.97(18)		
C(16)-P(1)-C(20)-C(21)	-64.8(2)		
Rh(1)-P(1)-C(20)-C(21)	72.26(19)		
C(2)-P(1)-C(20)-C(23)	67.4(2)		
C(16)-P(1)-C(20)-C(23)	-179.39(18)		
Rh(1)-P(1)-C(20)-C(23)	-42.4(2)		
C(2)-P(1)-C(20)-C(22)	-52.3(2)		
C(16)-P(1)-C(20)-C(22)	60.9(3)		
Rh(1)-P(1)-C(20)-C(22)	-162.1(2)		
C(12)-P(2)-C(24)-C(26)	-75.2(2)		
C(28)-P(2)-C(24)-C(26)	35.5(3)		

Figure C1: ORTEP diagram of (^tBu₂furPOP)RhCl.

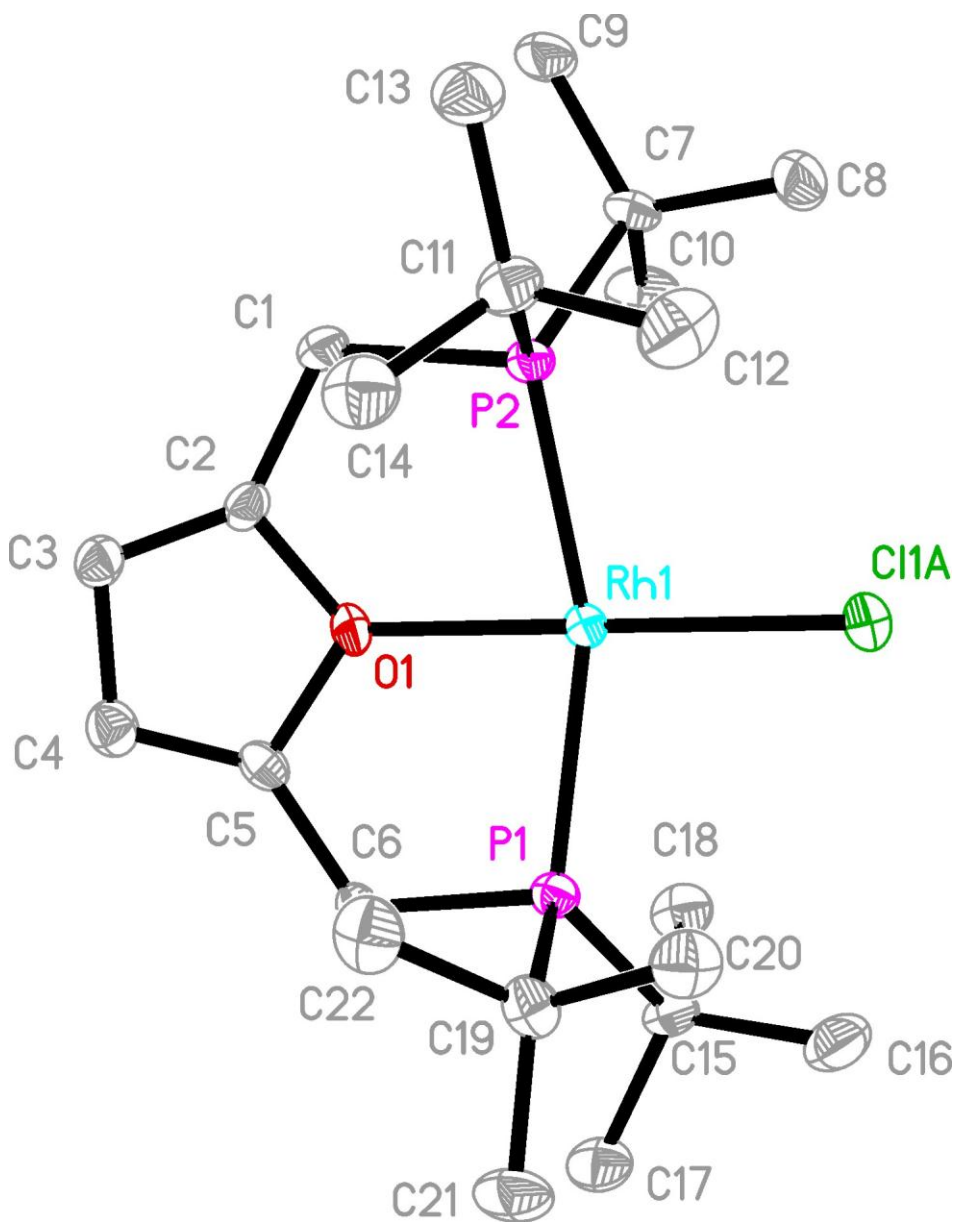


Table C2. Crystal data and structure refinement for (^tBu₂furPOP)RhCl.

Identification code	mh308a	
Empirical formula	C ₂₂ H ₄₄ Br _{0.13} Cl _{0.87} O _{P2} Rh	
Formula weight	530.65	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 15.1224(11) Å	α = 90°.
	b = 11.4949(9) Å	β = 115.2170(10)°.
	c = 15.8733(12) Å	γ = 90°.
Volume	2496.3(3) Å ³	
Z	4	
Density (calculated)	1.412 Mg/m ³	
Absorption coefficient	1.124 mm ⁻¹	
F(000)	1113	
Crystal size	0.25 x 0.20 x 0.05 mm ³	
Theta range for data collection	2.27 to 30.03°.	
Index ranges	-21 ≤ h ≤ 21, -16 ≤ k ≤ 16, -21 ≤ l ≤ 22	
Reflections collected	24848	
Independent reflections	13915 [R(int) = 0.0336]	
Completeness to theta = 30.03°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9460 and 0.7665	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	13915 / 38 / 526	
Goodness-of-fit on F ²	1.009	
Final R indices [I > 2σ(I)]	R1 = 0.0523, wR2 = 0.1186	
R indices (all data)	R1 = 0.0572, wR2 = 0.1212	
Absolute structure parameter	0.50(3)	
Largest diff. peak and hole	2.191 and -1.227 e.Å ⁻³	

Table C3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for (**^tBu₃furPOP**)RhCl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	5044(1)	133(1)	2215(1)	15(1)
Cl(1A)	6470(1)	-683(1)	3412(1)	27(1)
Br(1B)	6470(1)	-683(1)	3412(1)	27(1)
P(1)	4498(1)	-1510(1)	1323(1)	16(1)
P(2)	5025(1)	1873(1)	2912(1)	17(1)
O(1)	3855(2)	873(3)	1120(2)	19(1)
C(1)	4052(4)	2701(4)	1932(4)	20(1)
C(2)	3404(3)	1899(4)	1185(3)	17(1)
C(3)	2488(4)	1923(4)	507(4)	20(1)
C(4)	2349(4)	854(5)	-12(4)	23(1)
C(5)	3177(3)	234(4)	372(3)	18(1)
C(6)	3544(3)	-911(4)	212(3)	17(1)
C(7)	6095(4)	2901(4)	3274(4)	21(1)
C(8)	6900(4)	2465(5)	4178(4)	31(1)
C(9)	5866(4)	4182(4)	3351(4)	28(1)
C(10)	6447(4)	2786(5)	2491(4)	32(1)
C(11)	4536(4)	1793(4)	3821(4)	24(1)
C(12)	5137(5)	907(5)	4561(4)	35(1)
C(13)	4509(4)	2945(5)	4291(4)	30(1)
C(14)	3482(4)	1331(5)	3324(4)	33(1)
C(15)	5264(4)	-2389(4)	875(4)	21(1)
C(16)	6005(4)	-3120(5)	1683(4)	33(1)
C(17)	4694(4)	-3161(5)	36(4)	28(1)
C(18)	5837(4)	-1475(5)	601(4)	28(1)
C(19)	3793(4)	-2491(5)	1762(4)	23(1)

C(20)	4439(4)	-2770(5)	2797(4)	29(1)
C(21)	3428(4)	-3611(5)	1226(4)	31(1)
C(22)	2901(4)	-1782(5)	1715(4)	31(1)
Rh(2)	172(1)	2438(1)	2455(1)	16(1)
Cl(2A)	-981(1)	3177(1)	1032(1)	26(1)
Br(2B)	-981(1)	3177(1)	1032(1)	26(1)
P(3)	670(1)	4143(1)	3255(1)	21(1)
P(4)	-147(1)	512(1)	2103(1)	17(1)
O(2)	1264(3)	1769(3)	3656(3)	27(1)
C(23)	944(4)	-179(4)	3031(4)	26(1)
C(24)	1413(4)	590(5)	3861(4)	25(1)
C(25)	1984(4)	494(5)	4768(4)	34(1)
C(26)	2214(4)	1634(5)	5172(4)	33(1)
C(27)	1759(4)	2398(5)	4482(3)	27(1)
C(28)	1708(5)	3676(5)	4360(4)	35(1)
C(29)	-125(4)	-119(4)	1023(4)	23(1)
C(30)	-1100(4)	133(5)	196(3)	28(1)
C(31)	106(4)	-1416(5)	1058(4)	30(1)
C(32)	674(4)	565(5)	873(4)	33(1)
C(33)	-1189(4)	-45(4)	2324(4)	22(1)
C(34)	-2118(4)	642(4)	1711(4)	26(1)
C(35)	-1400(4)	-1362(4)	2161(4)	28(1)
C(36)	-951(4)	233(5)	3335(4)	31(1)
C(37)	-209(5)	4833(5)	3648(4)	31(1)
C(38)	-1163(4)	5115(7)	2808(5)	43(1)
C(39)	165(5)	5916(5)	4261(4)	38(1)
C(40)	-426(6)	3868(6)	4221(5)	48(2)
C(41)	1292(4)	5236(5)	2811(4)	23(1)
C(42)	520(4)	5817(5)	1950(4)	30(1)
C(43)	1926(5)	6141(6)	3515(5)	42(2)
C(44)	1958(4)	4499(5)	2495(5)	36(1)

Table C4. Bond lengths [Å] and angles [°] for (*t*Bu₃POP)RhCl.

Rh(1)-O(1)	2.077(3)	C(8)-H(8A)	0.9800
Rh(1)-P(2)	2.2915(12)	C(8)-H(8B)	0.9800
Rh(1)-P(1)	2.2924(12)	C(8)-H(8C)	0.9800
Rh(1)-Cl(1A)	2.3777(11)	C(9)-H(9A)	0.9800
Rh(1)-H(101)	1.549(15)	C(9)-H(9B)	0.9800
Rh(1)-H(102)	1.548(18)	C(9)-H(9C)	0.9800
P(1)-C(6)	1.870(5)	C(10)-H(10A)	0.9800
P(1)-C(19)	1.877(5)	C(10)-H(10B)	0.9800
P(1)-C(15)	1.890(5)	C(10)-H(10C)	0.9800
P(2)-C(1)	1.881(5)	C(11)-C(12)	1.528(8)
P(2)-C(11)	1.883(5)	C(11)-C(13)	1.529(7)
P(2)-C(7)	1.885(5)	C(11)-C(14)	1.541(8)
O(1)-C(2)	1.387(5)	C(12)-H(12A)	0.9800
O(1)-C(5)	1.401(5)	C(12)-H(12B)	0.9800
C(1)-C(2)	1.492(7)	C(12)-H(12C)	0.9800
C(1)-H(1A)	0.9900	C(13)-H(13A)	0.9800
C(1)-H(1B)	0.9900	C(13)-H(13B)	0.9800
C(2)-C(3)	1.345(7)	C(13)-H(13C)	0.9800
C(3)-C(4)	1.444(7)	C(14)-H(14A)	0.9800
C(3)-H(3)	0.9500	C(14)-H(14B)	0.9800
C(4)-C(5)	1.341(7)	C(14)-H(14C)	0.9800
C(4)-H(4)	0.9500	C(15)-C(17)	1.525(7)
C(5)-C(6)	1.492(7)	C(15)-C(18)	1.539(7)
C(6)-H(6A)	0.9900	C(15)-C(16)	1.543(8)
C(6)-H(6B)	0.9900	C(16)-H(16A)	0.9800
C(7)-C(8)	1.518(7)	C(16)-H(16B)	0.9800
C(7)-C(9)	1.530(7)	C(16)-H(16C)	0.9800
C(7)-C(10)	1.552(7)	C(17)-H(17A)	0.9800

C(17)-H(17B)	0.9800	C(23)-C(24)	1.491(8)
C(17)-H(17C)	0.9800	C(23)-H(23A)	0.9900
C(18)-H(18A)	0.9800	C(23)-H(23B)	0.9900
C(18)-H(18B)	0.9800	C(24)-C(25)	1.331(8)
C(18)-H(18C)	0.9800	C(25)-C(26)	1.435(9)
C(19)-C(21)	1.513(8)	C(25)-H(25)	0.9500
C(19)-C(20)	1.546(7)	C(26)-C(27)	1.342(8)
C(19)-C(22)	1.550(7)	C(26)-H(26)	0.9500
C(20)-H(20A)	0.9800	C(27)-C(28)	1.480(8)
C(20)-H(20B)	0.9800	C(28)-H(28A)	0.9900
C(20)-H(20C)	0.9800	C(28)-H(28B)	0.9900
C(21)-H(21A)	0.9800	C(29)-C(31)	1.527(7)
C(21)-H(21B)	0.9800	C(29)-C(30)	1.528(7)
C(21)-H(21C)	0.9800	C(29)-C(32)	1.542(7)
C(22)-H(22A)	0.9800	C(30)-H(30A)	0.9800
C(22)-H(22B)	0.9800	C(30)-H(30B)	0.9800
C(22)-H(22C)	0.9800	C(30)-H(30C)	0.9800
Rh(2)-O(2)	2.067(4)	C(31)-H(31A)	0.9800
Rh(2)-P(3)	2.2817(13)	C(31)-H(31B)	0.9800
Rh(2)-P(4)	2.2835(13)	C(31)-H(31C)	0.9800
Rh(2)-Cl(2A)	2.3470(11)	C(32)-H(32A)	0.9800
Rh(2)-H(201)	1.508(17)	C(32)-H(32B)	0.9800
Rh(2)-H(202)	1.548(17)	C(32)-H(32C)	0.9800
P(3)-C(28)	1.866(6)	C(33)-C(36)	1.521(7)
P(3)-C(37)	1.869(6)	C(33)-C(34)	1.543(7)
P(3)-C(41)	1.878(5)	C(33)-C(35)	1.547(7)
P(4)-C(23)	1.858(5)	C(34)-H(34A)	0.9800
P(4)-C(33)	1.869(5)	C(34)-H(34B)	0.9800
P(4)-C(29)	1.874(5)	C(34)-H(34C)	0.9800
O(2)-C(24)	1.390(6)	C(35)-H(35A)	0.9800
O(2)-C(27)	1.402(6)	C(35)-H(35B)	0.9800

C(35)-H(35C)	0.9800	C(40)-H(40B)	0.9800
C(36)-H(36A)	0.9800	C(40)-H(40C)	0.9800
C(36)-H(36B)	0.9800	C(41)-C(42)	1.522(8)
C(36)-H(36C)	0.9800	C(41)-C(43)	1.528(8)
C(37)-C(38)	1.526(9)	C(41)-C(44)	1.553(8)
C(37)-C(39)	1.532(8)	C(42)-H(42A)	0.9800
C(37)-C(40)	1.555(8)	C(42)-H(42B)	0.9800
C(38)-H(38A)	0.9800	C(42)-H(42C)	0.9800
C(38)-H(38B)	0.9800	C(43)-H(43A)	0.9800
C(38)-H(38C)	0.9800	C(43)-H(43B)	0.9800
C(39)-H(39A)	0.9800	C(43)-H(43C)	0.9800
C(39)-H(39B)	0.9800	C(44)-H(44A)	0.9800
C(39)-H(39C)	0.9800	C(44)-H(44B)	0.9800
C(40)-H(40A)	0.9800	C(44)-H(44C)	0.9800
O(1)-Rh(1)-P(2)	82.09(10)	C(6)-P(1)-C(15)	101.1(2)
O(1)-Rh(1)-P(1)	82.25(10)	C(19)-P(1)-C(15)	110.7(2)
P(2)-Rh(1)-P(1)	160.34(4)	C(6)-P(1)-Rh(1)	102.07(15)
O(1)-Rh(1)-Cl(1A)	176.07(10)	C(19)-P(1)-Rh(1)	112.21(18)
P(2)-Rh(1)-Cl(1A)	98.74(4)	C(15)-P(1)-Rh(1)	123.76(16)
P(1)-Rh(1)-Cl(1A)	97.69(4)	C(1)-P(2)-C(11)	103.5(2)
O(1)-Rh(1)-H(101)	99.5(9)	C(1)-P(2)-C(7)	101.7(2)
P(2)-Rh(1)-H(101)	84.3(7)	C(11)-P(2)-C(7)	111.3(2)
P(1)-Rh(1)-H(101)	86.6(8)	C(1)-P(2)-Rh(1)	102.04(15)
Cl(1A)-Rh(1)-H(101)	84.4(9)	C(11)-P(2)-Rh(1)	114.67(17)
O(1)-Rh(1)-H(102)	92.2(10)	C(7)-P(2)-Rh(1)	120.57(16)
P(2)-Rh(1)-H(102)	97.2(11)	C(2)-O(1)-C(5)	107.7(4)
P(1)-Rh(1)-H(102)	95.2(11)	C(2)-O(1)-Rh(1)	124.3(3)
Cl(1A)-Rh(1)-H(102)	83.8(10)	C(5)-O(1)-Rh(1)	123.7(3)
H(101)-Rh(1)-H(102)	168.3(13)	C(2)-C(1)-P(2)	111.2(3)
C(6)-P(1)-C(19)	103.9(2)	C(2)-C(1)-H(1A)	109.4

P(2)-C(1)-H(1A)	109.4	C(7)-C(8)-H(8C)	109.5
C(2)-C(1)-H(1B)	109.4	H(8A)-C(8)-H(8C)	109.5
P(2)-C(1)-H(1B)	109.4	H(8B)-C(8)-H(8C)	109.5
H(1A)-C(1)-H(1B)	108.0	C(7)-C(9)-H(9A)	109.5
C(3)-C(2)-O(1)	109.2(4)	C(7)-C(9)-H(9B)	109.5
C(3)-C(2)-C(1)	136.7(4)	H(9A)-C(9)-H(9B)	109.5
O(1)-C(2)-C(1)	114.1(4)	C(7)-C(9)-H(9C)	109.5
C(2)-C(3)-C(4)	106.8(4)	H(9A)-C(9)-H(9C)	109.5
C(2)-C(3)-H(3)	126.6	H(9B)-C(9)-H(9C)	109.5
C(4)-C(3)-H(3)	126.6	C(7)-C(10)-H(10A)	109.5
C(5)-C(4)-C(3)	108.2(5)	C(7)-C(10)-H(10B)	109.5
C(5)-C(4)-H(4)	125.9	H(10A)-C(10)-H(10B)	109.5
C(3)-C(4)-H(4)	125.9	C(7)-C(10)-H(10C)	109.5
C(4)-C(5)-O(1)	108.1(4)	H(10A)-C(10)-H(10C)	109.5
C(4)-C(5)-C(6)	137.3(4)	H(10B)-C(10)-H(10C)	109.5
O(1)-C(5)-C(6)	114.6(4)	C(12)-C(11)-C(13)	109.5(5)
C(5)-C(6)-P(1)	110.9(3)	C(12)-C(11)-C(14)	108.1(5)
C(5)-C(6)-H(6A)	109.5	C(13)-C(11)-C(14)	108.2(4)
P(1)-C(6)-H(6A)	109.5	C(12)-C(11)-P(2)	108.8(3)
C(5)-C(6)-H(6B)	109.5	C(13)-C(11)-P(2)	115.6(4)
P(1)-C(6)-H(6B)	109.5	C(14)-C(11)-P(2)	106.4(4)
H(6A)-C(6)-H(6B)	108.0	C(11)-C(12)-H(12A)	109.5
C(8)-C(7)-C(9)	111.1(4)	C(11)-C(12)-H(12B)	109.5
C(8)-C(7)-C(10)	108.5(5)	H(12A)-C(12)-H(12B)	109.5
C(9)-C(7)-C(10)	108.2(4)	C(11)-C(12)-H(12C)	109.5
C(8)-C(7)-P(2)	108.7(4)	H(12A)-C(12)-H(12C)	109.5
C(9)-C(7)-P(2)	115.7(4)	H(12B)-C(12)-H(12C)	109.5
C(10)-C(7)-P(2)	104.2(3)	C(11)-C(13)-H(13A)	109.5
C(7)-C(8)-H(8A)	109.5	C(11)-C(13)-H(13B)	109.5
C(7)-C(8)-H(8B)	109.5	H(13A)-C(13)-H(13B)	109.5
H(8A)-C(8)-H(8B)	109.5	C(11)-C(13)-H(13C)	109.5

H(13A)-C(13)-H(13C)	109.5	H(18B)-C(18)-H(18C)	109.5
H(13B)-C(13)-H(13C)	109.5	C(21)-C(19)-C(20)	109.6(5)
C(11)-C(14)-H(14A)	109.5	C(21)-C(19)-C(22)	108.6(4)
C(11)-C(14)-H(14B)	109.5	C(20)-C(19)-C(22)	107.7(4)
H(14A)-C(14)-H(14B)	109.5	C(21)-C(19)-P(1)	115.6(4)
C(11)-C(14)-H(14C)	109.5	C(20)-C(19)-P(1)	108.5(3)
H(14A)-C(14)-H(14C)	109.5	C(22)-C(19)-P(1)	106.6(4)
H(14B)-C(14)-H(14C)	109.5	C(19)-C(20)-H(20A)	109.5
C(17)-C(15)-C(18)	109.0(4)	C(19)-C(20)-H(20B)	109.5
C(17)-C(15)-C(16)	110.4(4)	H(20A)-C(20)-H(20B)	109.5
C(18)-C(15)-C(16)	108.0(4)	C(19)-C(20)-H(20C)	109.5
C(17)-C(15)-P(1)	115.5(3)	H(20A)-C(20)-H(20C)	109.5
C(18)-C(15)-P(1)	104.6(3)	H(20B)-C(20)-H(20C)	109.5
C(16)-C(15)-P(1)	108.9(4)	C(19)-C(21)-H(21A)	109.5
C(15)-C(16)-H(16A)	109.5	C(19)-C(21)-H(21B)	109.5
C(15)-C(16)-H(16B)	109.5	H(21A)-C(21)-H(21B)	109.5
H(16A)-C(16)-H(16B)	109.5	C(19)-C(21)-H(21C)	109.5
C(15)-C(16)-H(16C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(21B)-C(21)-H(21C)	109.5
H(16B)-C(16)-H(16C)	109.5	C(19)-C(22)-H(22A)	109.5
C(15)-C(17)-H(17A)	109.5	C(19)-C(22)-H(22B)	109.5
C(15)-C(17)-H(17B)	109.5	H(22A)-C(22)-H(22B)	109.5
H(17A)-C(17)-H(17B)	109.5	C(19)-C(22)-H(22C)	109.5
C(15)-C(17)-H(17C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(17A)-C(17)-H(17C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(17B)-C(17)-H(17C)	109.5	O(2)-Rh(2)-P(3)	82.02(11)
C(15)-C(18)-H(18A)	109.5	O(2)-Rh(2)-P(4)	82.38(11)
C(15)-C(18)-H(18B)	109.5	P(3)-Rh(2)-P(4)	162.54(5)
H(18A)-C(18)-H(18B)	109.5	O(2)-Rh(2)-Cl(2A)	175.29(12)
C(15)-C(18)-H(18C)	109.5	P(3)-Rh(2)-Cl(2A)	99.13(4)
H(18A)-C(18)-H(18C)	109.5	P(4)-Rh(2)-Cl(2A)	97.06(4)

O(2)-Rh(2)-H(201)	104.2(7)	C(25)-C(24)-C(23)	138.7(5)
P(3)-Rh(2)-H(201)	90.5(8)	O(2)-C(24)-C(23)	113.8(4)
P(4)-Rh(2)-H(201)	85.8(7)	C(24)-C(25)-C(26)	109.3(5)
Cl(2A)-Rh(2)-H(201)	80.4(7)	C(24)-C(25)-H(25)	125.4
O(2)-Rh(2)-H(202)	92.6(10)	C(26)-C(25)-H(25)	125.4
P(3)-Rh(2)-H(202)	96.7(8)	C(27)-C(26)-C(25)	106.9(5)
P(4)-Rh(2)-H(202)	91.8(9)	C(27)-C(26)-H(26)	126.6
Cl(2A)-Rh(2)-H(202)	82.7(10)	C(25)-C(26)-H(26)	126.6
H(201)-Rh(2)-H(202)	162.5(12)	C(26)-C(27)-O(2)	108.0(5)
C(28)-P(3)-C(37)	104.0(3)	C(26)-C(27)-C(28)	137.4(5)
C(28)-P(3)-C(41)	101.0(2)	O(2)-C(27)-C(28)	114.3(5)
C(37)-P(3)-C(41)	112.5(2)	C(27)-C(28)-P(3)	112.6(4)
C(28)-P(3)-Rh(2)	102.85(19)	C(27)-C(28)-H(28A)	109.1
C(37)-P(3)-Rh(2)	115.92(18)	P(3)-C(28)-H(28A)	109.1
C(41)-P(3)-Rh(2)	117.75(17)	C(27)-C(28)-H(28B)	109.1
C(23)-P(4)-C(33)	103.9(3)	P(3)-C(28)-H(28B)	109.1
C(23)-P(4)-C(29)	101.8(2)	H(28A)-C(28)-H(28B)	107.8
C(33)-P(4)-C(29)	112.6(2)	C(31)-C(29)-C(30)	109.8(4)
C(23)-P(4)-Rh(2)	101.37(17)	C(31)-C(29)-C(32)	108.7(4)
C(33)-P(4)-Rh(2)	113.12(17)	C(30)-C(29)-C(32)	107.7(5)
C(29)-P(4)-Rh(2)	121.00(16)	C(31)-C(29)-P(4)	116.0(4)
C(24)-O(2)-C(27)	108.4(4)	C(30)-C(29)-P(4)	109.0(3)
C(24)-O(2)-Rh(2)	124.4(3)	C(32)-C(29)-P(4)	105.3(3)
C(27)-O(2)-Rh(2)	124.7(3)	C(29)-C(30)-H(30A)	109.5
C(24)-C(23)-P(4)	112.0(4)	C(29)-C(30)-H(30B)	109.5
C(24)-C(23)-H(23A)	109.2	H(30A)-C(30)-H(30B)	109.5
P(4)-C(23)-H(23A)	109.2	C(29)-C(30)-H(30C)	109.5
C(24)-C(23)-H(23B)	109.2	H(30A)-C(30)-H(30C)	109.5
P(4)-C(23)-H(23B)	109.2	H(30B)-C(30)-H(30C)	109.5
H(23A)-C(23)-H(23B)	107.9	C(29)-C(31)-H(31A)	109.5
C(25)-C(24)-O(2)	107.4(5)	C(29)-C(31)-H(31B)	109.5

H(31A)-C(31)-H(31B)	109.5	C(33)-C(36)-H(36C)	109.5
C(29)-C(31)-H(31C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(36B)-C(36)-H(36C)	109.5
H(31B)-C(31)-H(31C)	109.5	C(38)-C(37)-C(39)	109.8(5)
C(29)-C(32)-H(32A)	109.5	C(38)-C(37)-C(40)	107.8(5)
C(29)-C(32)-H(32B)	109.5	C(39)-C(37)-C(40)	108.8(5)
H(32A)-C(32)-H(32B)	109.5	C(38)-C(37)-P(3)	109.9(4)
C(29)-C(32)-H(32C)	109.5	C(39)-C(37)-P(3)	115.7(4)
H(32A)-C(32)-H(32C)	109.5	C(40)-C(37)-P(3)	104.5(4)
H(32B)-C(32)-H(32C)	109.5	C(37)-C(38)-H(38A)	109.5
C(36)-C(33)-C(34)	107.5(4)	C(37)-C(38)-H(38B)	109.5
C(36)-C(33)-C(35)	108.8(4)	H(38A)-C(38)-H(38B)	109.5
C(34)-C(33)-C(35)	109.2(4)	C(37)-C(38)-H(38C)	109.5
C(36)-C(33)-P(4)	106.7(3)	H(38A)-C(38)-H(38C)	109.5
C(34)-C(33)-P(4)	108.7(3)	H(38B)-C(38)-H(38C)	109.5
C(35)-C(33)-P(4)	115.7(4)	C(37)-C(39)-H(39A)	109.5
C(33)-C(34)-H(34A)	109.5	C(37)-C(39)-H(39B)	109.5
C(33)-C(34)-H(34B)	109.5	H(39A)-C(39)-H(39B)	109.5
H(34A)-C(34)-H(34B)	109.5	C(37)-C(39)-H(39C)	109.5
C(33)-C(34)-H(34C)	109.5	H(39A)-C(39)-H(39C)	109.5
H(34A)-C(34)-H(34C)	109.5	H(39B)-C(39)-H(39C)	109.5
H(34B)-C(34)-H(34C)	109.5	C(37)-C(40)-H(40A)	109.5
C(33)-C(35)-H(35A)	109.5	C(37)-C(40)-H(40B)	109.5
C(33)-C(35)-H(35B)	109.5	H(40A)-C(40)-H(40B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(37)-C(40)-H(40C)	109.5
C(33)-C(35)-H(35C)	109.5	H(40A)-C(40)-H(40C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(40B)-C(40)-H(40C)	109.5
H(35B)-C(35)-H(35C)	109.5	C(42)-C(41)-C(43)	111.1(5)
C(33)-C(36)-H(36A)	109.5	C(42)-C(41)-C(44)	107.7(5)
C(33)-C(36)-H(36B)	109.5	C(43)-C(41)-C(44)	108.4(5)
H(36A)-C(36)-H(36B)	109.5	C(42)-C(41)-P(3)	108.3(3)

C(43)-C(41)-P(3)	116.1(4)	H(43A)-C(43)-H(43B)	109.5
C(44)-C(41)-P(3)	104.7(4)	C(41)-C(43)-H(43C)	109.5
C(41)-C(42)-H(42A)	109.5	H(43A)-C(43)-H(43C)	109.5
C(41)-C(42)-H(42B)	109.5	H(43B)-C(43)-H(43C)	109.5
H(42A)-C(42)-H(42B)	109.5	C(41)-C(44)-H(44A)	109.5
C(41)-C(42)-H(42C)	109.5	C(41)-C(44)-H(44B)	109.5
H(42A)-C(42)-H(42C)	109.5	H(44A)-C(44)-H(44B)	109.5
H(42B)-C(42)-H(42C)	109.5	C(41)-C(44)-H(44C)	109.5
C(41)-C(43)-H(43A)	109.5	H(44A)-C(44)-H(44C)	109.5
C(41)-C(43)-H(43B)	109.5	H(44B)-C(44)-H(44C)	109.5

Table C5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (**^tBu₂furPOP**)RhCl. The anisotropic

displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Rh(1)	14(1)	14(1)	14(1)	0(1)	5(1)	0(1)
Cl(1A)	19(1)	26(1)	27(1)	-3(1)	1(1)	3(1)
Br(1B)	19(1)	26(1)	27(1)	-3(1)	1(1)	3(1)
P(1)	16(1)	16(1)	18(1)	-2(1)	8(1)	-2(1)
P(2)	19(1)	13(1)	17(1)	-1(1)	5(1)	0(1)
O(1)	11(1)	21(2)	20(2)	0(1)	3(1)	0(1)
C(1)	23(2)	13(2)	21(2)	0(2)	7(2)	3(2)
C(2)	19(2)	13(2)	20(2)	3(2)	8(2)	3(2)
C(3)	19(2)	16(2)	24(2)	4(2)	7(2)	1(2)
C(4)	21(2)	24(2)	20(2)	2(2)	6(2)	0(2)
C(5)	18(2)	22(2)	12(2)	-2(2)	5(2)	-3(2)
C(6)	15(2)	21(2)	13(2)	0(2)	5(2)	-1(2)
C(7)	21(2)	16(2)	23(3)	-6(2)	6(2)	-7(2)
C(8)	24(2)	22(2)	34(3)	0(2)	0(2)	-3(2)
C(9)	30(3)	17(2)	29(3)	-3(2)	6(2)	-6(2)
C(10)	38(3)	30(3)	37(3)	-7(2)	24(3)	-12(2)
C(11)	26(3)	24(2)	26(3)	-2(2)	16(2)	1(2)
C(12)	52(4)	33(3)	25(3)	9(2)	21(3)	9(3)
C(13)	31(3)	33(3)	29(3)	-7(2)	16(3)	0(2)
C(14)	33(3)	35(3)	37(3)	-3(2)	22(3)	-2(2)
C(15)	23(2)	15(2)	28(3)	-2(2)	14(2)	-1(2)
C(16)	34(3)	22(2)	45(4)	-2(2)	19(3)	4(2)
C(17)	33(3)	26(3)	28(3)	-7(2)	18(2)	0(2)
C(18)	28(3)	27(2)	34(3)	-2(2)	19(2)	-1(2)
C(19)	20(2)	27(2)	22(2)	2(2)	10(2)	-3(2)

C(20)	36(3)	27(3)	25(3)	3(2)	15(2)	-1(2)
C(21)	33(3)	22(2)	43(4)	-5(2)	21(3)	-12(2)
C(22)	26(3)	36(3)	36(3)	4(2)	19(2)	-2(2)
Rh(2)	17(1)	15(1)	14(1)	2(1)	4(1)	-1(1)
Cl(2A)	25(1)	18(1)	24(1)	3(1)	-1(1)	2(1)
Br(2B)	25(1)	18(1)	24(1)	3(1)	-1(1)	2(1)
P(3)	25(1)	18(1)	18(1)	2(1)	6(1)	-3(1)
P(4)	15(1)	15(1)	20(1)	3(1)	7(1)	2(1)
O(2)	28(2)	21(2)	25(2)	8(2)	3(2)	-1(2)
C(23)	25(3)	20(2)	27(3)	7(2)	6(2)	5(2)
C(24)	25(3)	22(2)	30(3)	8(2)	13(2)	3(2)
C(25)	26(3)	33(3)	33(3)	13(2)	3(2)	1(2)
C(26)	31(3)	39(3)	20(3)	10(2)	4(2)	2(2)
C(27)	24(2)	30(2)	19(2)	-1(2)	2(2)	-7(2)
C(28)	39(3)	32(3)	22(3)	1(2)	3(3)	-9(2)
C(29)	21(2)	22(2)	27(3)	-3(2)	13(2)	2(2)
C(30)	35(3)	28(2)	23(2)	-4(2)	12(2)	1(2)
C(31)	28(3)	23(2)	40(3)	-8(2)	15(3)	2(2)
C(32)	37(3)	35(3)	38(3)	-4(2)	25(3)	-1(2)
C(33)	21(2)	26(3)	21(2)	-2(2)	10(2)	-7(2)
C(34)	18(2)	22(2)	37(3)	3(2)	12(2)	2(2)
C(35)	30(3)	22(2)	36(3)	5(2)	17(2)	-2(2)
C(36)	34(3)	38(3)	27(3)	-3(2)	17(2)	-13(3)
C(37)	43(3)	28(3)	32(3)	-9(2)	26(3)	-7(2)
C(38)	28(3)	53(4)	52(4)	-8(4)	22(3)	5(3)
C(39)	60(4)	29(3)	29(3)	-3(2)	24(3)	-7(3)
C(40)	74(5)	32(3)	62(5)	-11(3)	53(4)	-18(3)
C(41)	23(2)	21(2)	25(2)	-2(2)	9(2)	-5(2)
C(42)	36(3)	27(3)	30(3)	6(2)	16(3)	-3(2)
C(43)	46(4)	37(3)	39(4)	-2(3)	14(3)	-19(3)
C(44)	29(3)	32(3)	48(4)	6(3)	16(3)	-3(2)

Table C6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)

for (**^tBu₄furPOP**)RhCl.

	x	y	z	U(eq)
H(101)	4523(17)	-338(15)	2800(17)	22
H(102)	5754(17)	500(20)	1792(18)	22
H(1A)	3654	3151	2177	24
H(1B)	4365	3258	1667	24
H(3)	2021	2526	392	24
H(4)	1770	628	-535	27
H(6A)	3825	-815	-245	20
H(6B)	2993	-1466	-51	20
H(8A)	7511	2872	4295	46
H(8B)	6990	1627	4131	46
H(8C)	6720	2615	4692	46
H(9A)	5776	4301	3921	42
H(9B)	5266	4400	2809	42
H(9C)	6409	4665	3372	42
H(10A)	7016	3290	2633	48
H(10B)	5919	3019	1896	48
H(10C)	6629	1977	2452	48
H(12A)	5807	1194	4898	53
H(12B)	5146	165	4260	53
H(12C)	4843	792	4998	53
H(13A)	4131	2847	4658	45
H(13B)	4201	3543	3815	45
H(13C)	5177	3184	4702	45
H(14A)	3483	590	3018	49
H(14B)	3078	1896	2856	49

H(14C)	3214	1210	3781	49
H(16A)	5660	-3741	1844	49
H(16B)	6342	-2619	2227	49
H(16C)	6485	-3463	1492	49
H(17A)	4156	-2714	-430	41
H(17B)	4430	-3832	235	41
H(17C)	5131	-3432	-235	41
H(18A)	6318	-1867	436	42
H(18B)	6176	-949	1126	42
H(18C)	5384	-1029	65	42
H(20A)	4094	-3313	3028	43
H(20B)	4580	-2050	3163	43
H(20C)	5053	-3123	2858	43
H(21A)	3017	-4025	1467	47
H(21B)	3986	-4101	1298	47
H(21C)	3043	-3434	565	47
H(22A)	2431	-1689	1063	46
H(22B)	3119	-1014	1995	46
H(22C)	2589	-2195	2056	46
H(201)	-725(15)	2426(16)	2644(13)	25
H(202)	852(17)	2490(20)	1953(16)	25
H(23A)	748	-918	3223	31
H(23B)	1425	-365	2780	31
H(25)	2205	-217	5096	41
H(26)	2612	1813	5807	39
H(28A)	2329	3956	4363	41
H(28B)	1637	4040	4893	41
H(30A)	-1054	-65	-384	43
H(30B)	-1258	961	192	43
H(30C)	-1616	-334	250	43
H(31A)	-413	-1862	1125	46
H(31B)	732	-1574	1590	46

H(31C)	148	-1645	481	46
H(32A)	1305	448	1409	50
H(32B)	510	1395	809	50
H(32C)	714	286	307	50
H(34A)	-2638	468	1905	38
H(34B)	-2331	418	1058	38
H(34C)	-1976	1478	1780	38
H(35A)	-793	-1800	2492	42
H(35B)	-1661	-1530	1493	42
H(35C)	-1879	-1592	2394	42
H(36A)	-750	1049	3463	47
H(36B)	-419	-271	3744	47
H(36C)	-1532	100	3448	47
H(38A)	-1653	5364	3020	64
H(38B)	-1397	4421	2416	64
H(38C)	-1050	5741	2446	64
H(39A)	217	6563	3883	57
H(39B)	809	5753	4765	57
H(39C)	-292	6123	4526	57
H(40A)	-913	4152	4426	72
H(40B)	177	3669	4765	72
H(40C)	-679	3176	3831	72
H(42A)	130	6350	2137	45
H(42B)	92	5221	1533	45
H(42C)	839	6252	1627	45
H(43A)	2300	6580	3248	63
H(43B)	2376	5747	4084	63
H(43C)	1507	6674	3663	63
H(44A)	2372	5018	2328	54
H(44B)	1551	4028	1954	54
H(44C)	2370	3987	3005	54

Table C7. Torsion angles [°] for (^tBu₂furPOP)RhCl

O(1)-Rh(1)-P(1)-C(6)	9.20(17)	Rh(1)-O(1)-C(2)-C(3)	-157.7(3)
P(2)-Rh(1)-P(1)-C(6)	46.7(2)	C(5)-O(1)-C(2)-C(1)	-177.7(4)
Cl(1A)-Rh(1)-P(1)-C(6)	-166.83(14)	Rh(1)-O(1)-C(2)-C(1)	25.2(5)
O(1)-Rh(1)-P(1)-C(19)	-101.4(2)	P(2)-C(1)-C(2)-C(3)	156.1(5)
P(2)-Rh(1)-P(1)-C(19)	-64.0(2)	P(2)-C(1)-C(2)-O(1)	-28.0(5)
Cl(1A)-Rh(1)-P(1)-C(19)	82.55(18)	O(1)-C(2)-C(3)-C(4)	0.3(5)
O(1)-Rh(1)-P(1)-C(15)	121.5(2)	C(1)-C(2)-C(3)-C(4)	176.3(5)
P(2)-Rh(1)-P(1)-C(15)	158.9(2)	C(2)-C(3)-C(4)-C(5)	0.2(5)
Cl(1A)-Rh(1)-P(1)-C(15)	-54.6(2)	C(3)-C(4)-C(5)-O(1)	-0.6(5)
O(1)-Rh(1)-P(2)-C(1)	-5.97(19)	C(3)-C(4)-C(5)-C(6)	179.5(5)
P(1)-Rh(1)-P(2)-C(1)	-43.4(2)	C(2)-O(1)-C(5)-C(4)	0.7(5)
Cl(1A)-Rh(1)-P(2)-C(1)	170.15(17)	Rh(1)-O(1)-C(5)-C(4)	158.0(3)
O(1)-Rh(1)-P(2)-C(11)	105.2(2)	C(2)-O(1)-C(5)-C(6)	-179.3(4)
P(1)-Rh(1)-P(2)-C(11)	67.7(2)	Rh(1)-O(1)-C(5)-C(6)	-22.0(5)
Cl(1A)-Rh(1)-P(2)-C(11)	-78.7(2)	C(4)-C(5)-C(6)-P(1)	-151.6(5)
O(1)-Rh(1)-P(2)-C(7)	-117.5(2)	O(1)-C(5)-C(6)-P(1)	28.4(5)
P(1)-Rh(1)-P(2)-C(7)	-154.9(2)	C(19)-P(1)-C(6)-C(5)	94.4(3)
Cl(1A)-Rh(1)-P(2)-C(7)	58.7(2)	C(15)-P(1)-C(6)-C(5)	-150.8(3)
P(2)-Rh(1)-O(1)-C(2)	-9.4(3)	Rh(1)-P(1)-C(6)-C(5)	-22.4(3)
P(1)-Rh(1)-O(1)-C(2)	158.7(3)	C(1)-P(2)-C(7)-C(8)	169.9(4)
Cl(1A)-Rh(1)-O(1)-C(2)	-111.9(14)	C(11)-P(2)-C(7)-C(8)	60.3(4)
P(2)-Rh(1)-O(1)-C(5)	-162.9(3)	Rh(1)-P(2)-C(7)-C(8)	-78.4(4)
P(1)-Rh(1)-O(1)-C(5)	5.2(3)	C(1)-P(2)-C(7)-C(9)	44.2(4)
Cl(1A)-Rh(1)-O(1)-C(5)	94.5(15)	C(11)-P(2)-C(7)-C(9)	-65.5(5)
C(11)-P(2)-C(1)-C(2)	-99.9(4)	Rh(1)-P(2)-C(7)-C(9)	155.8(3)
C(7)-P(2)-C(1)-C(2)	144.6(3)	C(1)-P(2)-C(7)-C(10)	-74.5(4)
Rh(1)-P(2)-C(1)-C(2)	19.5(4)	C(11)-P(2)-C(7)-C(10)	175.9(4)
C(5)-O(1)-C(2)-C(3)	-0.6(5)	Rh(1)-P(2)-C(7)-C(10)	37.2(4)

C(1)-P(2)-C(11)-C(12)	167.1(4)	P(4)-Rh(2)-P(3)-C(37)	-83.7(3)
C(7)-P(2)-C(11)-C(12)	-84.4(4)	Cl(2A)-Rh(2)-P(3)-C(37)	74.1(2)
Rh(1)-P(2)-C(11)-C(12)	56.8(4)	O(2)-Rh(2)-P(3)-C(41)	112.0(2)
C(1)-P(2)-C(11)-C(13)	-69.3(4)	P(4)-Rh(2)-P(3)-C(41)	138.9(2)
C(7)-P(2)-C(11)-C(13)	39.2(5)	Cl(2A)-Rh(2)-P(3)-C(41)	-63.33(19)
Rh(1)-P(2)-C(11)-C(13)	-179.6(3)	O(2)-Rh(2)-P(4)-C(23)	-10.6(2)
C(1)-P(2)-C(11)-C(14)	50.9(4)	P(3)-Rh(2)-P(4)-C(23)	-37.4(2)
C(7)-P(2)-C(11)-C(14)	159.4(4)	Cl(2A)-Rh(2)-P(4)-C(23)	164.66(19)
Rh(1)-P(2)-C(11)-C(14)	-59.4(4)	O(2)-Rh(2)-P(4)-C(33)	100.0(2)
C(6)-P(1)-C(15)-C(17)	-46.1(4)	P(3)-Rh(2)-P(4)-C(33)	73.2(2)
C(19)-P(1)-C(15)-C(17)	63.5(4)	Cl(2A)-Rh(2)-P(4)-C(33)	-84.75(18)
Rh(1)-P(1)-C(15)-C(17)	-158.9(3)	O(2)-Rh(2)-P(4)-C(29)	-121.9(2)
C(6)-P(1)-C(15)-C(18)	73.8(4)	P(3)-Rh(2)-P(4)-C(29)	-148.7(2)
C(19)-P(1)-C(15)-C(18)	-176.7(3)	Cl(2A)-Rh(2)-P(4)-C(29)	53.33(19)
Rh(1)-P(1)-C(15)-C(18)	-39.0(4)	P(3)-Rh(2)-O(2)-C(24)	169.6(4)
C(6)-P(1)-C(15)-C(16)	-171.0(3)	P(4)-Rh(2)-O(2)-C(24)	-2.6(4)
C(19)-P(1)-C(15)-C(16)	-61.4(4)	Cl(2A)-Rh(2)-O(2)-C(24)	-86.0(14)
Rh(1)-P(1)-C(15)-C(16)	76.2(4)	P(3)-Rh(2)-O(2)-C(27)	9.6(4)
C(6)-P(1)-C(19)-C(21)	72.0(4)	P(4)-Rh(2)-O(2)-C(27)	-162.5(4)
C(15)-P(1)-C(19)-C(21)	-35.7(5)	Cl(2A)-Rh(2)-O(2)-C(27)	114.1(13)
Rh(1)-P(1)-C(19)-C(21)	-178.5(4)	C(33)-P(4)-C(23)-C(24)	-94.4(4)
C(6)-P(1)-C(19)-C(20)	-164.5(3)	C(29)-P(4)-C(23)-C(24)	148.5(4)
C(15)-P(1)-C(19)-C(20)	87.8(4)	Rh(2)-P(4)-C(23)-C(24)	23.2(4)
Rh(1)-P(1)-C(19)-C(20)	-55.0(4)	C(27)-O(2)-C(24)-C(25)	-0.8(6)
C(6)-P(1)-C(19)-C(22)	-48.8(4)	Rh(2)-O(2)-C(24)-C(25)	-163.5(4)
C(15)-P(1)-C(19)-C(22)	-156.5(4)	C(27)-O(2)-C(24)-C(23)	-178.3(4)
Rh(1)-P(1)-C(19)-C(22)	60.7(4)	Rh(2)-O(2)-C(24)-C(23)	18.9(6)
O(2)-Rh(2)-P(3)-C(28)	2.2(2)	P(4)-C(23)-C(24)-C(25)	156.3(6)
P(4)-Rh(2)-P(3)-C(28)	29.0(3)	P(4)-C(23)-C(24)-O(2)	-27.3(6)
Cl(2A)-Rh(2)-P(3)-C(28)	-173.2(2)	O(2)-C(24)-C(25)-C(26)	0.3(6)
O(2)-Rh(2)-P(3)-C(37)	-110.5(2)	C(23)-C(24)-C(25)-C(26)	176.8(6)

C(24)-C(25)-C(26)-C(27)	0.4(7)	C(41)-P(3)-C(37)-C(38)	79.2(5)
C(25)-C(26)-C(27)-O(2)	-0.9(6)	Rh(2)-P(3)-C(37)-C(38)	-60.4(5)
C(25)-C(26)-C(27)-C(28)	-175.2(7)	C(28)-P(3)-C(37)-C(39)	62.6(5)
C(24)-O(2)-C(27)-C(26)	1.0(6)	C(41)-P(3)-C(37)-C(39)	-45.8(5)
Rh(2)-O(2)-C(27)-C(26)	163.7(4)	Rh(2)-P(3)-C(37)-C(39)	174.6(4)
C(24)-O(2)-C(27)-C(28)	176.9(5)	C(28)-P(3)-C(37)-C(40)	-57.0(5)
Rh(2)-O(2)-C(27)-C(28)	-20.5(6)	C(41)-P(3)-C(37)-C(40)	-165.3(4)
C(26)-C(27)-C(28)-P(3)	-165.7(6)	Rh(2)-P(3)-C(37)-C(40)	55.1(5)
O(2)-C(27)-C(28)-P(3)	20.1(6)	C(28)-P(3)-C(41)-C(42)	-173.9(4)
C(37)-P(3)-C(28)-C(27)	108.9(5)	C(37)-P(3)-C(41)-C(42)	-63.6(4)
C(41)-P(3)-C(28)-C(27)	-134.4(4)	Rh(2)-P(3)-C(41)-C(42)	75.2(4)
Rh(2)-P(3)-C(28)-C(27)	-12.4(5)	C(28)-P(3)-C(41)-C(43)	-48.1(5)
C(23)-P(4)-C(29)-C(31)	42.6(4)	C(37)-P(3)-C(41)-C(43)	62.2(5)
C(33)-P(4)-C(29)-C(31)	-68.0(4)	Rh(2)-P(3)-C(41)-C(43)	-159.0(4)
Rh(2)-P(4)-C(29)-C(31)	153.7(3)	C(28)-P(3)-C(41)-C(44)	71.4(4)
C(23)-P(4)-C(29)-C(30)	167.1(4)	C(37)-P(3)-C(41)-C(44)	-178.4(4)
C(33)-P(4)-C(29)-C(30)	56.5(4)	Rh(2)-P(3)-C(41)-C(44)	-39.6(4)
Rh(2)-P(4)-C(29)-C(30)	-81.8(4)		
C(23)-P(4)-C(29)-C(32)	-77.6(4)		
C(33)-P(4)-C(29)-C(32)	171.8(4)		
Rh(2)-P(4)-C(29)-C(32)	33.5(4)		
C(23)-P(4)-C(33)-C(36)	54.0(4)		
C(29)-P(4)-C(33)-C(36)	163.3(4)		
Rh(2)-P(4)-C(33)-C(36)	-55.0(4)		
C(23)-P(4)-C(33)-C(34)	169.7(4)		
C(29)-P(4)-C(33)-C(34)	-81.0(4)		
Rh(2)-P(4)-C(33)-C(34)	60.6(4)		
C(23)-P(4)-C(33)-C(35)	-67.2(4)		
C(29)-P(4)-C(33)-C(35)	42.1(5)		
Rh(2)-P(4)-C(33)-C(35)	-176.2(3)		
C(28)-P(3)-C(37)-C(38)	-172.4(4)		

Figure D1: ORTEP diagram of *cis*-(^tBu_{xan}POP)Rh(H)₂Cl

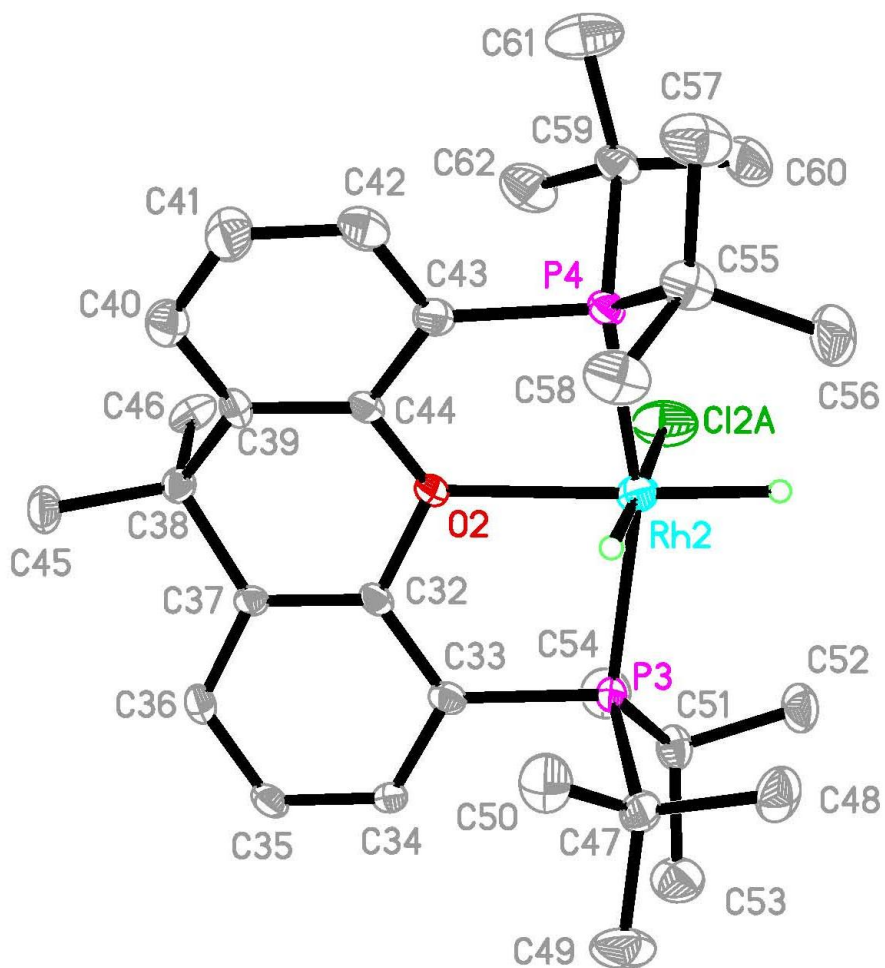


Table D2. Crystal data and structure refinement for *cis*-(^tBu₃xanPOP)Rh(H)₂Cl.

Identification code	mh310_xtl2	
Empirical formula	C31.05 H50.05 Cl1.05 O P2 Rh	
Formula weight	641.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 32.468(2) Å	α = 90°.
	b = 11.6622(9) Å	β = 97.443(1)°.
	c = 16.7338(12) Å	γ = 90°.
Volume	6282.7(8) Å ³	
Z	8	
Density (calculated)	1.356 Mg/m ³	
Absorption coefficient	0.756 mm ⁻¹	
F(000)	2697	
Crystal size	0.49 x 0.06 x 0.05 mm ³	
Theta range for data collection	1.86 to 29.57°.	
Index ranges	-45<=h<=45, -16<=k<=16, -23<=l<=23	
Reflections collected	68829	
Independent reflections	17599 [R(int) = 0.0661]	
Completeness to theta = 29.57°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9632 and 0.7082	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17599 / 1060 / 702	
Goodness-of-fit on F ²	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0820, wR2 = 0.1836	
R indices (all data)	R1 = 0.1046, wR2 = 0.1955	
Largest diff. peak and hole	3.994 and -1.958 e.Å ⁻³	

Table D3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *cis*-(^tBu₂xanPOP)Rh(H)₂Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	1017(1)	5250(1)	4509(1)	11(1)
P(1)	600(1)	6722(1)	3982(1)	11(1)
P(2)	1481(1)	3760(1)	4654(1)	13(1)
Cl(1)	1539(1)	6615(1)	5200(1)	18(1)
O(1)	1363(1)	5691(3)	3465(2)	11(1)
C(1)	1760(2)	5196(4)	3493(3)	14(1)
C(2)	1866(2)	4297(4)	4031(3)	16(1)
C(3)	2257(2)	3798(5)	4032(3)	20(1)
C(4)	2528(2)	4166(5)	3516(3)	25(1)
C(5)	2411(2)	5041(5)	2969(3)	20(1)
C(6)	2025(1)	5566(4)	2940(3)	13(1)
C(7)	1863(2)	6436(4)	2302(3)	14(1)
C(8)	1559(2)	7239(4)	2635(3)	13(1)
C(9)	1486(2)	8358(4)	2360(3)	18(1)
C(10)	1171(2)	9021(5)	2606(3)	20(1)
C(11)	909(2)	8556(4)	3108(3)	16(1)
C(12)	968(1)	7435(4)	3402(3)	12(1)
C(13)	1307(1)	6815(4)	3176(3)	10(1)
C(14)	2213(2)	7094(5)	1967(3)	17(1)
C(15)	1620(2)	5747(4)	1601(3)	19(1)
C(16)	1296(2)	2413(4)	4088(4)	21(1)
C(17)	941(2)	1889(5)	4502(5)	35(2)
C(18)	1628(2)	1508(5)	3996(5)	36(2)
C(19)	1114(2)	2779(5)	3228(4)	26(1)
C(20)	1755(2)	3408(4)	5698(3)	18(1)
C(21)	1426(2)	3542(6)	6267(4)	30(1)
C(22)	1949(2)	2214(5)	5819(4)	27(1)
C(23)	2099(2)	4287(5)	5946(3)	23(1)

C(24)	180(2)	6313(4)	3136(3)	14(1)
C(25)	-162(2)	5653(5)	3492(4)	27(1)
C(26)	-8(2)	7305(5)	2610(3)	22(1)
C(27)	381(2)	5512(5)	2568(4)	26(1)
C(28)	390(2)	7777(4)	4693(3)	17(1)
C(29)	253(2)	7042(5)	5374(3)	26(1)
C(30)	18(2)	8509(5)	4347(3)	23(1)
C(31)	741(2)	8570(5)	5051(4)	27(1)
Rh(2)	3918(1)	4757(1)	1551(1)	20(1)
P(3)	3947(1)	6561(1)	2112(1)	15(1)
P(4)	3890(1)	3429(1)	525(1)	16(1)
Cl(2A)	3496(1)	3810(2)	2518(1)	39(1)
Cl(2B)	3496(1)	3810(2)	2518(1)	39(1)
C(63B)	4090(20)	3040(60)	2830(40)	30
Cl(3B)	4414(8)	4145(19)	2161(11)	71(7)
O(2)	3369(1)	5493(3)	744(2)	16(1)
C(32)	3264(2)	6635(4)	893(3)	14(1)
C(33)	3483(2)	7216(4)	1536(3)	16(1)
C(34)	3350(2)	8320(4)	1693(3)	17(1)
C(35)	3016(2)	8822(4)	1226(3)	19(1)
C(36)	2809(2)	8230(4)	576(3)	17(1)
C(37)	2924(2)	7124(4)	404(3)	14(1)
C(38)	2679(2)	6399(4)	-257(3)	15(1)
C(39)	2981(2)	5579(4)	-590(3)	15(1)
C(40)	2931(2)	5183(5)	-1383(3)	24(1)
C(41)	3180(2)	4317(6)	-1621(3)	28(1)
C(42)	3467(2)	3787(5)	-1064(4)	25(1)
C(43)	3535(2)	4158(4)	-263(3)	18(1)
C(44)	3299(2)	5088(4)	-52(3)	14(1)
C(45)	2440(2)	7133(5)	-903(3)	23(1)
C(46)	2364(2)	5652(5)	128(3)	23(1)
C(47)	4389(2)	7476(5)	1825(3)	22(1)

C(48)	4795(2)	6839(6)	2097(4)	29(1)
C(49)	4427(2)	8684(6)	2163(5)	39(2)
C(50)	4329(2)	7586(6)	908(4)	32(1)
C(51)	3881(2)	6740(5)	3219(3)	23(1)
C(52)	4174(2)	5880(5)	3686(3)	27(1)
C(53)	3989(2)	7932(6)	3626(4)	35(1)
C(54)	3432(2)	6485(6)	3311(4)	33(1)
C(55)	4384(2)	3187(5)	77(4)	25(1)
C(56)	4740(2)	3070(6)	781(4)	35(2)
C(57)	4404(2)	2136(6)	-463(5)	37(2)
C(58)	4477(2)	4262(6)	-407(4)	31(1)
C(59)	3604(2)	2042(5)	655(3)	20(1)
C(60)	3832(2)	1444(5)	1403(4)	35(2)
C(61)	3544(3)	1206(6)	-49(5)	44(2)
C(62)	3166(2)	2395(6)	809(4)	34(1)

Table D4. Bond lengths [Å] and angles [°] for *cis*-(^tBu_{xanPOP})Rh(H)₂Cl.

Rh(1)-O(1)	2.254(3)	C(9)-H(9)	0.9500
Rh(1)-P(2)	2.2919(13)	C(10)-C(11)	1.382(7)
Rh(1)-P(1)	2.2924(12)	C(10)-H(10)	0.9500
Rh(1)-Cl(1)	2.4958(13)	C(11)-C(12)	1.401(7)
Rh(1)-H(1)	1.595(10)	C(11)-H(11)	0.9500
Rh(1)-H(2)	1.597(10)	C(12)-C(13)	1.409(6)
P(1)-C(12)	1.834(5)	C(14)-H(14A)	0.9800
P(1)-C(24)	1.894(5)	C(14)-H(14B)	0.9800
P(1)-C(28)	1.896(5)	C(14)-H(14C)	0.9800
P(2)-C(2)	1.839(5)	C(15)-H(15A)	0.9800
P(2)-C(16)	1.893(5)	C(15)-H(15B)	0.9800
P(2)-C(20)	1.899(5)	C(15)-H(15C)	0.9800
O(1)-C(13)	1.400(5)	C(16)-C(18)	1.531(8)
O(1)-C(1)	1.408(5)	C(16)-C(19)	1.543(8)
C(1)-C(2)	1.395(7)	C(16)-C(17)	1.545(9)
C(1)-C(6)	1.411(7)	C(17)-H(17A)	0.9800
C(2)-C(3)	1.396(7)	C(17)-H(17B)	0.9800
C(3)-C(4)	1.378(8)	C(17)-H(17C)	0.9800
C(3)-H(3)	0.9500	C(18)-H(18A)	0.9800
C(4)-C(5)	1.389(8)	C(18)-H(18B)	0.9800
C(4)-H(4)	0.9500	C(18)-H(18C)	0.9800
C(5)-C(6)	1.392(7)	C(19)-H(19A)	0.9800
C(5)-H(5)	0.9500	C(19)-H(19B)	0.9800
C(6)-C(7)	1.516(7)	C(19)-H(19C)	0.9800
C(7)-C(8)	1.518(7)	C(20)-C(21)	1.527(8)
C(7)-C(14)	1.535(7)	C(20)-C(22)	1.531(7)
C(7)-C(15)	1.551(7)	C(20)-C(23)	1.533(8)
C(8)-C(13)	1.388(6)	C(21)-H(21A)	0.9800
C(8)-C(9)	1.394(7)	C(21)-H(21B)	0.9800
C(9)-C(10)	1.386(8)	C(21)-H(21C)	0.9800

C(22)-H(22A)	0.9800	Rh(2)-P(3)	2.3005(14)
C(22)-H(22B)	0.9800	Rh(2)-P(4)	2.3054(14)
C(22)-H(22C)	0.9800	Rh(2)-Cl(2A)	2.5081(17)
C(23)-H(23A)	0.9800	Rh(2)-H(4A)	1.582(10)
C(23)-H(23B)	0.9800	Rh(2)-H(3A)	1.597(10)
C(23)-H(23C)	0.9800	P(3)-C(33)	1.845(5)
C(24)-C(26)	1.532(7)	P(3)-C(47)	1.899(5)
C(24)-C(25)	1.534(7)	P(3)-C(51)	1.905(6)
C(24)-C(27)	1.538(7)	P(4)-C(43)	1.841(6)
C(25)-H(25A)	0.9800	P(4)-C(55)	1.879(6)
C(25)-H(25B)	0.9800	P(4)-C(59)	1.892(5)
C(25)-H(25C)	0.9800	C(63B)-Cl(3B)	2.09(7)
C(26)-H(26A)	0.9800	C(63B)-H(63A)	0.9900
C(26)-H(26B)	0.9800	C(63B)-H(63B)	0.9900
C(26)-H(26C)	0.9800	Cl(3B)-H(3A)	0.64(8)
C(27)-H(27A)	0.9800	O(2)-C(44)	1.403(6)
C(27)-H(27B)	0.9800	O(2)-C(32)	1.405(6)
C(27)-H(27C)	0.9800	C(32)-C(33)	1.387(7)
C(28)-C(31)	1.527(8)	C(32)-C(37)	1.407(7)
C(28)-C(30)	1.530(7)	C(33)-C(34)	1.395(7)
C(28)-C(29)	1.539(7)	C(34)-C(35)	1.381(7)
C(29)-H(29A)	0.9800	C(34)-H(34)	0.9500
C(29)-H(29B)	0.9800	C(35)-C(36)	1.387(7)
C(29)-H(29C)	0.9800	C(35)-H(35)	0.9500
C(30)-H(30A)	0.9800	C(36)-C(37)	1.383(7)
C(30)-H(30B)	0.9800	C(36)-H(36)	0.9500
C(30)-H(30C)	0.9800	C(37)-C(38)	1.530(7)
C(31)-H(31A)	0.9800	C(38)-C(45)	1.511(7)
C(31)-H(31B)	0.9800	C(38)-C(39)	1.525(7)
C(31)-H(31C)	0.9800	C(38)-C(46)	1.546(7)
Rh(2)-Cl(3B)	1.928(19)	C(39)-C(40)	1.394(7)
Rh(2)-O(2)	2.263(4)	C(39)-C(44)	1.401(7)

C(40)-C(41)	1.385(8)	C(53)-H(53A)	0.9800
C(40)-H(40)	0.9500	C(53)-H(53B)	0.9800
C(41)-C(42)	1.376(8)	C(53)-H(53C)	0.9800
C(41)-H(41)	0.9500	C(54)-H(54A)	0.9800
C(42)-C(43)	1.399(8)	C(54)-H(54B)	0.9800
C(42)-H(42)	0.9500	C(54)-H(54C)	0.9800
C(43)-C(44)	1.400(7)	C(55)-C(57)	1.529(9)
C(45)-H(45A)	0.9800	C(55)-C(58)	1.543(8)
C(45)-H(45B)	0.9800	C(55)-C(56)	1.546(9)
C(45)-H(45C)	0.9800	C(56)-H(56A)	0.9800
C(46)-H(46A)	0.9800	C(56)-H(56B)	0.9800
C(46)-H(46B)	0.9800	C(56)-H(56C)	0.9800
C(46)-H(46C)	0.9800	C(57)-H(57A)	0.9800
C(47)-C(49)	1.517(9)	C(57)-H(57B)	0.9800
C(47)-C(50)	1.528(8)	C(57)-H(57C)	0.9800
C(47)-C(48)	1.530(8)	C(58)-H(58A)	0.9800
C(48)-H(48A)	0.9800	C(58)-H(58B)	0.9800
C(48)-H(48B)	0.9800	C(58)-H(58C)	0.9800
C(48)-H(48C)	0.9800	C(59)-C(61)	1.522(9)
C(49)-H(49A)	0.9800	C(59)-C(62)	1.532(8)
C(49)-H(49B)	0.9800	C(59)-C(60)	1.537(8)
C(49)-H(49C)	0.9800	C(60)-H(60A)	0.9800
C(50)-H(50A)	0.9800	C(60)-H(60B)	0.9800
C(50)-H(50B)	0.9800	C(60)-H(60C)	0.9800
C(50)-H(50C)	0.9800	C(61)-H(61A)	0.9800
C(51)-C(54)	1.513(8)	C(61)-H(61B)	0.9800
C(51)-C(52)	1.525(8)	C(61)-H(61C)	0.9800
C(51)-C(53)	1.567(9)	C(62)-H(62A)	0.9800
C(52)-H(52A)	0.9800	C(62)-H(62B)	0.9800
C(52)-H(52B)	0.9800	C(62)-H(62C)	0.9800
C(52)-H(52C)	0.9800		

O(1)-Rh(1)-P(2)	82.48(9)	O(1)-C(1)-C(6)	119.0(4)
O(1)-Rh(1)-P(1)	81.95(9)	C(1)-C(2)-C(3)	117.6(5)
P(2)-Rh(1)-P(1)	163.06(5)	C(1)-C(2)-P(2)	119.4(4)
O(1)-Rh(1)-Cl(1)	80.66(9)	C(3)-C(2)-P(2)	122.8(4)
P(2)-Rh(1)-Cl(1)	92.15(4)	C(4)-C(3)-C(2)	121.5(5)
P(1)-Rh(1)-Cl(1)	91.89(4)	C(4)-C(3)-H(3)	119.3
O(1)-Rh(1)-H(1)	174(2)	C(2)-C(3)-H(3)	119.3
P(2)-Rh(1)-H(1)	98(2)	C(3)-C(4)-C(5)	120.0(5)
P(1)-Rh(1)-H(1)	99(2)	C(3)-C(4)-H(4)	120.0
Cl(1)-Rh(1)-H(1)	93(2)	C(5)-C(4)-H(4)	120.0
O(1)-Rh(1)-H(2)	107(2)	C(4)-C(5)-C(6)	120.9(5)
P(2)-Rh(1)-H(2)	91(2)	C(4)-C(5)-H(5)	119.6
P(1)-Rh(1)-H(2)	87(2)	C(6)-C(5)-H(5)	119.6
Cl(1)-Rh(1)-H(2)	172(2)	C(5)-C(6)-C(1)	117.8(4)
H(1)-Rh(1)-H(2)	80(3)	C(5)-C(6)-C(7)	123.2(4)
C(12)-P(1)-C(24)	100.0(2)	C(1)-C(6)-C(7)	118.8(4)
C(12)-P(1)-C(28)	110.4(2)	C(6)-C(7)-C(8)	109.7(4)
C(24)-P(1)-C(28)	110.6(2)	C(6)-C(7)-C(14)	112.8(4)
C(12)-P(1)-Rh(1)	98.57(16)	C(8)-C(7)-C(14)	111.8(4)
C(24)-P(1)-Rh(1)	115.54(16)	C(6)-C(7)-C(15)	106.3(4)
C(28)-P(1)-Rh(1)	119.09(17)	C(8)-C(7)-C(15)	107.9(4)
C(2)-P(2)-C(16)	101.2(2)	C(14)-C(7)-C(15)	108.1(4)
C(2)-P(2)-C(20)	108.9(2)	C(13)-C(8)-C(9)	117.4(4)
C(16)-P(2)-C(20)	111.2(2)	C(13)-C(8)-C(7)	119.1(4)
C(2)-P(2)-Rh(1)	99.64(16)	C(9)-C(8)-C(7)	123.2(4)
C(16)-P(2)-Rh(1)	114.48(17)	C(10)-C(9)-C(8)	121.6(5)
C(20)-P(2)-Rh(1)	118.97(17)	C(10)-C(9)-H(9)	119.2
C(13)-O(1)-C(1)	118.3(4)	C(8)-C(9)-H(9)	119.2
C(13)-O(1)-Rh(1)	115.2(3)	C(11)-C(10)-C(9)	119.9(5)
C(1)-O(1)-Rh(1)	115.2(3)	C(11)-C(10)-H(10)	120.0
C(2)-C(1)-O(1)	118.7(4)	C(9)-C(10)-H(10)	120.0
C(2)-C(1)-C(6)	122.1(4)	C(10)-C(11)-C(12)	120.8(5)

C(10)-C(11)-H(11)	119.6	C(16)-C(18)-H(18A)	109.5
C(12)-C(11)-H(11)	119.6	C(16)-C(18)-H(18B)	109.5
C(11)-C(12)-C(13)	117.4(4)	H(18A)-C(18)-H(18B)	109.5
C(11)-C(12)-P(1)	122.7(4)	C(16)-C(18)-H(18C)	109.5
C(13)-C(12)-P(1)	119.7(3)	H(18A)-C(18)-H(18C)	109.5
C(8)-C(13)-O(1)	119.8(4)	H(18B)-C(18)-H(18C)	109.5
C(8)-C(13)-C(12)	122.7(4)	C(16)-C(19)-H(19A)	109.5
O(1)-C(13)-C(12)	117.3(4)	C(16)-C(19)-H(19B)	109.5
C(7)-C(14)-H(14A)	109.5	H(19A)-C(19)-H(19B)	109.5
C(7)-C(14)-H(14B)	109.5	C(16)-C(19)-H(19C)	109.5
H(14A)-C(14)-H(14B)	109.5	H(19A)-C(19)-H(19C)	109.5
C(7)-C(14)-H(14C)	109.5	H(19B)-C(19)-H(19C)	109.5
H(14A)-C(14)-H(14C)	109.5	C(21)-C(20)-C(22)	108.6(5)
H(14B)-C(14)-H(14C)	109.5	C(21)-C(20)-C(23)	107.9(5)
C(7)-C(15)-H(15A)	109.5	C(22)-C(20)-C(23)	107.4(4)
C(7)-C(15)-H(15B)	109.5	C(21)-C(20)-P(2)	105.6(4)
H(15A)-C(15)-H(15B)	109.5	C(22)-C(20)-P(2)	117.0(4)
C(7)-C(15)-H(15C)	109.5	C(23)-C(20)-P(2)	110.0(3)
H(15A)-C(15)-H(15C)	109.5	C(20)-C(21)-H(21A)	109.5
H(15B)-C(15)-H(15C)	109.5	C(20)-C(21)-H(21B)	109.5
C(18)-C(16)-C(19)	106.6(5)	H(21A)-C(21)-H(21B)	109.5
C(18)-C(16)-C(17)	110.4(5)	C(20)-C(21)-H(21C)	109.5
C(19)-C(16)-C(17)	108.1(5)	H(21A)-C(21)-H(21C)	109.5
C(18)-C(16)-P(2)	116.1(4)	H(21B)-C(21)-H(21C)	109.5
C(19)-C(16)-P(2)	107.2(4)	C(20)-C(22)-H(22A)	109.5
C(17)-C(16)-P(2)	108.1(4)	C(20)-C(22)-H(22B)	109.5
C(16)-C(17)-H(17A)	109.5	H(22A)-C(22)-H(22B)	109.5
C(16)-C(17)-H(17B)	109.5	C(20)-C(22)-H(22C)	109.5
H(17A)-C(17)-H(17B)	109.5	H(22A)-C(22)-H(22C)	109.5
C(16)-C(17)-H(17C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(17A)-C(17)-H(17C)	109.5	C(20)-C(23)-H(23A)	109.5
H(17B)-C(17)-H(17C)	109.5	C(20)-C(23)-H(23B)	109.5

H(23A)-C(23)-H(23B)	109.5	C(30)-C(28)-P(1)	117.0(4)
C(20)-C(23)-H(23C)	109.5	C(29)-C(28)-P(1)	105.4(4)
H(23A)-C(23)-H(23C)	109.5	C(28)-C(29)-H(29A)	109.5
H(23B)-C(23)-H(23C)	109.5	C(28)-C(29)-H(29B)	109.5
C(26)-C(24)-C(25)	110.2(4)	H(29A)-C(29)-H(29B)	109.5
C(26)-C(24)-C(27)	105.9(4)	C(28)-C(29)-H(29C)	109.5
C(25)-C(24)-C(27)	108.8(5)	H(29A)-C(29)-H(29C)	109.5
C(26)-C(24)-P(1)	115.7(3)	H(29B)-C(29)-H(29C)	109.5
C(25)-C(24)-P(1)	108.8(4)	C(28)-C(30)-H(30A)	109.5
C(27)-C(24)-P(1)	107.1(3)	C(28)-C(30)-H(30B)	109.5
C(24)-C(25)-H(25A)	109.5	H(30A)-C(30)-H(30B)	109.5
C(24)-C(25)-H(25B)	109.5	C(28)-C(30)-H(30C)	109.5
H(25A)-C(25)-H(25B)	109.5	H(30A)-C(30)-H(30C)	109.5
C(24)-C(25)-H(25C)	109.5	H(30B)-C(30)-H(30C)	109.5
H(25A)-C(25)-H(25C)	109.5	C(28)-C(31)-H(31A)	109.5
H(25B)-C(25)-H(25C)	109.5	C(28)-C(31)-H(31B)	109.5
C(24)-C(26)-H(26A)	109.5	H(31A)-C(31)-H(31B)	109.5
C(24)-C(26)-H(26B)	109.5	C(28)-C(31)-H(31C)	109.5
H(26A)-C(26)-H(26B)	109.5	H(31A)-C(31)-H(31C)	109.5
C(24)-C(26)-H(26C)	109.5	H(31B)-C(31)-H(31C)	109.5
H(26A)-C(26)-H(26C)	109.5	Cl(3B)-Rh(2)-O(2)	175.0(7)
H(26B)-C(26)-H(26C)	109.5	Cl(3B)-Rh(2)-P(3)	97.8(7)
C(24)-C(27)-H(27A)	109.5	O(2)-Rh(2)-P(3)	83.33(9)
C(24)-C(27)-H(27B)	109.5	Cl(3B)-Rh(2)-P(4)	95.5(7)
H(27A)-C(27)-H(27B)	109.5	O(2)-Rh(2)-P(4)	81.83(9)
C(24)-C(27)-H(27C)	109.5	P(3)-Rh(2)-P(4)	156.00(5)
H(27A)-C(27)-H(27C)	109.5	Cl(3B)-Rh(2)-Cl(2A)	89.1(7)
H(27B)-C(27)-H(27C)	109.5	O(2)-Rh(2)-Cl(2A)	95.62(11)
C(31)-C(28)-C(30)	108.8(4)	P(3)-Rh(2)-Cl(2A)	97.85(5)
C(31)-C(28)-C(29)	108.6(5)	P(4)-Rh(2)-Cl(2A)	102.27(5)
C(30)-C(28)-C(29)	107.5(4)	Cl(3B)-Rh(2)-H(4A)	93.5(7)
C(31)-C(28)-P(1)	109.2(4)	O(2)-Rh(2)-H(4A)	81.9(4)

P(3)-Rh(2)-H(4A)	79.8(2)	O(2)-C(32)-C(37)	118.1(4)
P(4)-Rh(2)-H(4A)	79.5(2)	C(32)-C(33)-C(34)	117.1(5)
Cl(2A)-Rh(2)-H(4A)	176.7(3)	C(32)-C(33)-P(3)	120.3(4)
Cl(3B)-Rh(2)-H(3A)	18(3)	C(34)-C(33)-P(3)	122.5(4)
O(2)-Rh(2)-H(3A)	167(3)	C(35)-C(34)-C(33)	121.7(5)
P(3)-Rh(2)-H(3A)	96(3)	C(35)-C(34)-H(34)	119.1
P(4)-Rh(2)-H(3A)	103(3)	C(33)-C(34)-H(34)	119.1
Cl(2A)-Rh(2)-H(3A)	72(3)	C(34)-C(35)-C(36)	119.8(5)
H(4A)-Rh(2)-H(3A)	111(3)	C(34)-C(35)-H(35)	120.1
C(33)-P(3)-C(47)	103.2(2)	C(36)-C(35)-H(35)	120.1
C(33)-P(3)-C(51)	106.0(2)	C(37)-C(36)-C(35)	120.7(5)
C(47)-P(3)-C(51)	111.6(3)	C(37)-C(36)-H(36)	119.6
C(33)-P(3)-Rh(2)	100.27(16)	C(35)-C(36)-H(36)	119.6
C(47)-P(3)-Rh(2)	113.78(19)	C(36)-C(37)-C(32)	118.0(5)
C(51)-P(3)-Rh(2)	119.56(19)	C(36)-C(37)-C(38)	122.4(4)
C(43)-P(4)-C(55)	105.7(3)	C(32)-C(37)-C(38)	119.4(4)
C(43)-P(4)-C(59)	101.9(2)	C(45)-C(38)-C(39)	112.9(4)
C(55)-P(4)-C(59)	112.1(3)	C(45)-C(38)-C(37)	112.0(4)
C(43)-P(4)-Rh(2)	100.59(17)	C(39)-C(38)-C(37)	108.2(4)
C(55)-P(4)-Rh(2)	116.37(19)	C(45)-C(38)-C(46)	108.1(4)
C(59)-P(4)-Rh(2)	117.46(18)	C(39)-C(38)-C(46)	106.8(4)
Cl(3B)-C(63B)-H(63A)	112.4	C(37)-C(38)-C(46)	108.6(4)
Cl(3B)-C(63B)-H(63B)	112.4	C(40)-C(39)-C(44)	117.5(5)
H(63A)-C(63B)-H(63B)	110.0	C(40)-C(39)-C(38)	123.6(5)
Rh(2)-Cl(3B)-C(63B)	94(2)	C(44)-C(39)-C(38)	118.5(4)
Rh(2)-Cl(3B)-H(3A)	50(3)	C(41)-C(40)-C(39)	121.0(5)
C(63B)-Cl(3B)-H(3A)	49(6)	C(41)-C(40)-H(40)	119.5
C(44)-O(2)-C(32)	118.3(4)	C(39)-C(40)-H(40)	119.5
C(44)-O(2)-Rh(2)	117.2(3)	C(42)-C(41)-C(40)	120.2(5)
C(32)-O(2)-Rh(2)	116.4(3)	C(42)-C(41)-H(41)	119.9
C(33)-C(32)-O(2)	119.3(4)	C(40)-C(41)-H(41)	119.9
C(33)-C(32)-C(37)	122.5(5)	C(41)-C(42)-C(43)	121.3(5)

C(41)-C(42)-H(42)	119.4	C(47)-C(49)-H(49A)	109.5
C(43)-C(42)-H(42)	119.4	C(47)-C(49)-H(49B)	109.5
C(42)-C(43)-C(44)	117.2(5)	H(49A)-C(49)-H(49B)	109.5
C(42)-C(43)-P(4)	123.3(4)	C(47)-C(49)-H(49C)	109.5
C(44)-C(43)-P(4)	119.3(4)	H(49A)-C(49)-H(49C)	109.5
C(43)-C(44)-C(39)	122.5(5)	H(49B)-C(49)-H(49C)	109.5
C(43)-C(44)-O(2)	118.3(4)	C(47)-C(50)-H(50A)	109.5
C(39)-C(44)-O(2)	119.1(4)	C(47)-C(50)-H(50B)	109.5
C(38)-C(45)-H(45A)	109.5	H(50A)-C(50)-H(50B)	109.5
C(38)-C(45)-H(45B)	109.5	C(47)-C(50)-H(50C)	109.5
H(45A)-C(45)-H(45B)	109.5	H(50A)-C(50)-H(50C)	109.5
C(38)-C(45)-H(45C)	109.5	H(50B)-C(50)-H(50C)	109.5
H(45A)-C(45)-H(45C)	109.5	C(54)-C(51)-C(52)	111.3(5)
H(45B)-C(45)-H(45C)	109.5	C(54)-C(51)-C(53)	107.2(5)
C(38)-C(46)-H(46A)	109.5	C(52)-C(51)-C(53)	105.7(5)
C(38)-C(46)-H(46B)	109.5	C(54)-C(51)-P(3)	107.9(4)
H(46A)-C(46)-H(46B)	109.5	C(52)-C(51)-P(3)	106.6(4)
C(38)-C(46)-H(46C)	109.5	C(53)-C(51)-P(3)	118.2(4)
H(46A)-C(46)-H(46C)	109.5	C(51)-C(52)-H(52A)	109.5
H(46B)-C(46)-H(46C)	109.5	C(51)-C(52)-H(52B)	109.5
C(49)-C(47)-C(50)	106.8(5)	H(52A)-C(52)-H(52B)	109.5
C(49)-C(47)-C(48)	108.4(5)	C(51)-C(52)-H(52C)	109.5
C(50)-C(47)-C(48)	109.5(5)	H(52A)-C(52)-H(52C)	109.5
C(49)-C(47)-P(3)	117.1(4)	H(52B)-C(52)-H(52C)	109.5
C(50)-C(47)-P(3)	107.4(4)	C(51)-C(53)-H(53A)	109.5
C(48)-C(47)-P(3)	107.6(4)	C(51)-C(53)-H(53B)	109.5
C(47)-C(48)-H(48A)	109.5	H(53A)-C(53)-H(53B)	109.5
C(47)-C(48)-H(48B)	109.5	C(51)-C(53)-H(53C)	109.5
H(48A)-C(48)-H(48B)	109.5	H(53A)-C(53)-H(53C)	109.5
C(47)-C(48)-H(48C)	109.5	H(53B)-C(53)-H(53C)	109.5
H(48A)-C(48)-H(48C)	109.5	C(51)-C(54)-H(54A)	109.5
H(48B)-C(48)-H(48C)	109.5	C(51)-C(54)-H(54B)	109.5

H(54A)-C(54)-H(54B)	109.5	H(58A)-C(58)-H(58C)	109.5
C(51)-C(54)-H(54C)	109.5	H(58B)-C(58)-H(58C)	109.5
H(54A)-C(54)-H(54C)	109.5	C(61)-C(59)-C(62)	106.0(5)
H(54B)-C(54)-H(54C)	109.5	C(61)-C(59)-C(60)	109.8(5)
C(57)-C(55)-C(58)	108.4(5)	C(62)-C(59)-C(60)	110.1(5)
C(57)-C(55)-C(56)	107.2(5)	C(61)-C(59)-P(4)	118.2(4)
C(58)-C(55)-C(56)	107.1(5)	C(62)-C(59)-P(4)	105.6(4)
C(57)-C(55)-P(4)	117.3(4)	C(60)-C(59)-P(4)	106.9(4)
C(58)-C(55)-P(4)	108.8(4)	C(59)-C(60)-H(60A)	109.5
C(56)-C(55)-P(4)	107.6(4)	C(59)-C(60)-H(60B)	109.5
C(55)-C(56)-H(56A)	109.5	H(60A)-C(60)-H(60B)	109.5
C(55)-C(56)-H(56B)	109.5	C(59)-C(60)-H(60C)	109.5
H(56A)-C(56)-H(56B)	109.5	H(60A)-C(60)-H(60C)	109.5
C(55)-C(56)-H(56C)	109.5	H(60B)-C(60)-H(60C)	109.5
H(56A)-C(56)-H(56C)	109.5	C(59)-C(61)-H(61A)	109.5
H(56B)-C(56)-H(56C)	109.5	C(59)-C(61)-H(61B)	109.5
C(55)-C(57)-H(57A)	109.5	H(61A)-C(61)-H(61B)	109.5
C(55)-C(57)-H(57B)	109.5	C(59)-C(61)-H(61C)	109.5
H(57A)-C(57)-H(57B)	109.5	H(61A)-C(61)-H(61C)	109.5
C(55)-C(57)-H(57C)	109.5	H(61B)-C(61)-H(61C)	109.5
H(57A)-C(57)-H(57C)	109.5	C(59)-C(62)-H(62A)	109.5
H(57B)-C(57)-H(57C)	109.5	C(59)-C(62)-H(62B)	109.5
C(55)-C(58)-H(58A)	109.5	H(62A)-C(62)-H(62B)	109.5
C(55)-C(58)-H(58B)	109.5	C(59)-C(62)-H(62C)	109.5
H(58A)-C(58)-H(58B)	109.5	H(62A)-C(62)-H(62C)	109.5
C(55)-C(58)-H(58C)	109.5	H(62B)-C(62)-H(62C)	109.5

Table D5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *cis*-(^tBu₂xanPOP)Rh(H)₂Cl. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Rh(1)	13(1)	7(1)	14(1)	2(1)	3(1)	0(1)
P(1)	12(1)	8(1)	13(1)	0(1)	2(1)	0(1)
P(2)	14(1)	8(1)	16(1)	2(1)	2(1)	1(1)
Cl(1)	22(1)	14(1)	18(1)	-2(1)	-3(1)	1(1)
O(1)	8(1)	10(2)	16(2)	3(1)	3(1)	2(1)
C(1)	12(2)	13(2)	16(2)	-4(2)	0(2)	1(2)
C(2)	14(2)	15(2)	18(2)	0(2)	2(2)	2(2)
C(3)	15(2)	22(2)	21(2)	2(2)	0(2)	6(2)
C(4)	17(2)	33(3)	25(3)	4(2)	5(2)	9(2)
C(5)	15(2)	25(3)	19(2)	3(2)	3(2)	1(2)
C(6)	8(2)	14(2)	16(2)	0(2)	1(2)	0(2)
C(7)	19(2)	11(2)	13(2)	-2(2)	5(2)	0(2)
C(8)	13(2)	14(2)	13(2)	0(2)	0(2)	0(2)
C(9)	22(2)	14(2)	18(2)	4(2)	4(2)	-4(2)
C(10)	25(3)	13(2)	22(2)	6(2)	1(2)	2(2)
C(11)	16(2)	11(2)	22(2)	2(2)	3(2)	1(2)
C(12)	12(2)	11(2)	12(2)	0(2)	0(2)	-3(2)
C(13)	8(2)	8(2)	14(2)	0(2)	0(2)	-2(2)
C(14)	14(2)	23(2)	15(2)	2(2)	3(2)	-4(2)
C(15)	23(3)	15(2)	17(2)	-2(2)	1(2)	-2(2)
C(16)	20(2)	8(2)	32(3)	-4(2)	-4(2)	2(2)
C(17)	36(3)	15(3)	54(4)	2(3)	3(3)	-10(2)
C(18)	34(3)	18(3)	53(4)	-17(3)	-11(3)	12(2)
C(19)	26(3)	22(3)	27(3)	-12(2)	-6(2)	1(2)
C(20)	21(2)	14(2)	19(2)	6(2)	3(2)	3(2)
C(21)	29(3)	38(3)	22(3)	10(2)	7(2)	6(3)
C(22)	34(3)	17(2)	29(3)	9(2)	-4(2)	5(2)
C(23)	29(3)	18(2)	21(3)	0(2)	-4(2)	3(2)
C(24)	14(2)	11(2)	17(2)	-2(2)	-2(2)	-4(2)
C(25)	14(2)	27(3)	39(3)	8(3)	-4(2)	-8(2)
C(26)	25(3)	21(3)	16(2)	0(2)	-7(2)	3(2)

C(27)	30(3)	18(3)	27(3)	-9(2)	-6(2)	5(2)
C(28)	22(2)	13(2)	18(2)	-1(2)	6(2)	5(2)
C(29)	35(3)	27(3)	19(3)	6(2)	13(2)	11(2)
C(30)	26(3)	19(3)	23(3)	0(2)	5(2)	9(2)
C(31)	25(3)	20(3)	34(3)	-14(2)	-4(2)	7(2)
Rh(2)	18(1)	18(1)	24(1)	-3(1)	1(1)	-1(1)
P(3)	13(1)	14(1)	16(1)	1(1)	-2(1)	0(1)
P(4)	13(1)	12(1)	24(1)	-1(1)	2(1)	1(1)
Cl(2A)	53(1)	31(1)	35(1)	-2(1)	17(1)	-12(1)
Cl(2B)	53(1)	31(1)	35(1)	-2(1)	17(1)	-12(1)
Cl(3B)	47(9)	67(13)	96(14)	-46(11)	-2(8)	11(9)
O(2)	20(2)	11(2)	17(2)	-2(1)	-2(1)	3(1)
C(32)	12(2)	10(2)	21(2)	3(2)	3(2)	0(2)
C(33)	19(2)	12(2)	16(2)	1(2)	3(2)	-2(2)
C(34)	16(2)	13(2)	22(2)	-2(2)	-2(2)	-1(2)
C(35)	18(2)	11(2)	29(3)	1(2)	1(2)	3(2)
C(36)	16(2)	16(2)	18(2)	4(2)	1(2)	3(2)
C(37)	12(2)	11(2)	18(2)	1(2)	1(2)	-3(2)
C(38)	14(2)	16(2)	15(2)	0(2)	1(2)	1(2)
C(39)	14(2)	15(2)	17(2)	4(2)	2(2)	2(2)
C(40)	28(3)	24(3)	20(2)	1(2)	1(2)	2(2)
C(41)	35(3)	33(3)	17(2)	-3(2)	3(2)	8(3)
C(42)	27(3)	22(3)	27(3)	-7(2)	7(2)	8(2)
C(43)	19(2)	16(2)	21(2)	-1(2)	3(2)	-1(2)
C(44)	16(2)	10(2)	17(2)	1(2)	2(2)	0(2)
C(45)	21(3)	25(3)	21(3)	2(2)	-3(2)	7(2)
C(46)	20(3)	28(3)	21(3)	-7(2)	3(2)	-8(2)
C(47)	14(2)	21(3)	28(3)	3(2)	1(2)	-4(2)
C(48)	17(3)	36(3)	34(3)	5(3)	2(2)	-2(2)
C(49)	27(3)	24(3)	68(5)	-6(3)	12(3)	-10(2)
C(50)	25(3)	37(3)	33(3)	12(3)	8(2)	-6(3)
C(51)	25(3)	25(3)	18(2)	4(2)	0(2)	3(2)
C(52)	30(3)	30(3)	20(3)	4(2)	-3(2)	6(2)
C(53)	49(4)	29(3)	26(3)	-6(3)	2(3)	0(3)
C(54)	33(3)	36(3)	31(3)	5(3)	10(3)	-3(3)
C(55)	17(2)	24(3)	36(3)	-2(2)	13(2)	-2(2)

C(56)	17(3)	34(3)	51(4)	3(3)	0(3)	6(2)
C(57)	28(3)	30(3)	55(4)	-11(3)	17(3)	-2(3)
C(58)	24(3)	27(3)	44(4)	-2(3)	17(3)	-5(2)
C(59)	22(2)	14(2)	27(3)	2(2)	7(2)	-3(2)
C(60)	36(3)	20(3)	47(4)	9(3)	0(3)	-1(2)
C(61)	54(4)	33(4)	46(4)	-11(3)	16(3)	-22(3)
C(62)	36(3)	24(3)	46(4)	5(3)	13(3)	-4(3)

Table D6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$)
for *cis*-(^tBu_{xan}POP)Rh(H)₂Cl.

	x	y	z	U(eq)
H(1)	807(17)	5020(50)	5300(20)	17
H(2)	649(13)	4410(40)	4160(30)	17
H(3)	2338	3190	4397	23
H(4)	2794	3822	3534	30
H(5)	2598	5284	2611	24
H(9)	1656	8674	1994	22
H(10)	1136	9793	2431	24
H(11)	686	9003	3256	19
H(14A)	2364	7559	2397	26
H(14B)	2093	7595	1527	26
H(14C)	2404	6549	1765	26
H(15A)	1801	5153	1421	28
H(15B)	1529	6266	1152	28
H(15C)	1378	5386	1787	28
H(17A)	811	1261	4171	53
H(17B)	733	2480	4563	53
H(17C)	1053	1595	5034	53
H(18A)	1507	892	3643	55
H(18B)	1732	1190	4527	55
H(18C)	1858	1863	3761	55
H(19A)	1336	3096	2949	39
H(19B)	900	3363	3257	39
H(19C)	992	2111	2931	39
H(21A)	1554	3411	6823	44
H(21B)	1204	2983	6124	44
H(21C)	1311	4319	6218	44
H(22A)	2070	2122	6383	41
H(22B)	2167	2126	5470	41
H(22C)	1735	1630	5681	41
H(23A)	1985	5063	5878	35
H(23B)	2321	4193	5606	35

H(23C)	2212	4166	6512	35
H(25A)	-301	6166	3837	41
H(25B)	-39	5007	3813	41
H(25C)	-365	5364	3054	41
H(26A)	-201	6999	2161	33
H(26B)	214	7732	2398	33
H(26C)	-159	7818	2935	33
H(27A)	511	4861	2875	38
H(27B)	593	5934	2321	38
H(27C)	168	5230	2145	38
H(29A)	491	6604	5636	39
H(29B)	34	6512	5150	39
H(29C)	147	7541	5772	39
H(30A)	-67	8996	4773	34
H(30B)	-212	8008	4135	34
H(30C)	97	8992	3912	34
H(31A)	810	9103	4636	41
H(31B)	986	8111	5247	41
H(31C)	651	9003	5499	41
H(4A)	4167(3)	5416(7)	939(5)	30
H(3A)	4230(20)	4180(70)	2250(40)	25
H(63A)	4181	3084	3416	36
H(63B)	4093	2236	2645	36
H(34)	3492	8738	2132	20
H(35)	2928	9571	1351	23
H(36)	2586	8588	244	20
H(40)	2723	5513	-1765	29
H(41)	3153	4088	-2170	34
H(42)	3622	3158	-1227	30
H(45A)	2244	7620	-660	34
H(45B)	2287	6638	-1312	34
H(45C)	2634	7615	-1155	34
H(46A)	2160	6147	340	34
H(46B)	2512	5197	568	34
H(46C)	2221	5137	-281	34
H(48A)	5030	7286	1951	43

H(48B)	4789	6088	1833	43
H(48C)	4827	6733	2683	43
H(49A)	4491	8650	2751	59
H(49B)	4165	9093	2017	59
H(49C)	4651	9089	1939	59
H(50A)	4071	8004	734	47
H(50B)	4313	6820	665	47
H(50C)	4564	8005	736	47
H(52A)	4144	5927	4261	41
H(52B)	4461	6057	3608	41
H(52C)	4103	5104	3489	41
H(53A)	3848	8541	3292	52
H(53B)	4290	8055	3678	52
H(53C)	3897	7945	4161	52
H(54A)	3352	5749	3054	49
H(54B)	3254	7094	3052	49
H(54C)	3400	6447	3884	49
H(56A)	4682	2427	1126	52
H(56B)	4763	3779	1098	52
H(56C)	5002	2929	565	52
H(57A)	4162	2131	-879	55
H(57B)	4403	1438	-136	55
H(57C)	4658	2164	-719	55
H(58A)	4769	4255	-498	46
H(58B)	4422	4951	-104	46
H(58C)	4299	4261	-927	46
H(60A)	3666	793	1549	53
H(60B)	3872	1988	1852	53
H(60C)	4102	1169	1284	53
H(61A)	3336	632	45	65
H(61B)	3808	823	-99	65
H(61C)	3451	1625	-547	65
H(62A)	3013	2698	311	52
H(62B)	3186	2988	1227	52
H(62C)	3020	1727	988	52

Table D7. Torsion angles [°] for *cis*-(^tBu_{xan}POP)Rh(H)₂Cl.

O(1)-Rh(1)-P(1)-C(12)	-20.61(17)	O(1)-C(1)-C(2)-P(2)	2.1(6)
P(2)-Rh(1)-P(1)-C(12)	-44.0(2)	C(6)-C(1)-C(2)-P(2)	-173.3(4)
Cl(1)-Rh(1)-P(1)-C(12)	59.68(15)	C(16)-P(2)-C(2)-C(1)	101.4(4)
O(1)-Rh(1)-P(1)-C(24)	84.9(2)	C(20)-P(2)-C(2)-C(1)	-141.3(4)
P(2)-Rh(1)-P(1)-C(24)	61.5(2)	Rh(1)-P(2)-C(2)-C(1)	-16.1(4)
Cl(1)-Rh(1)-P(1)-C(24)	165.18(18)	C(16)-P(2)-C(2)-C(3)	-74.5(5)
O(1)-Rh(1)-P(1)-C(28)	-139.8(2)	C(20)-P(2)-C(2)-C(3)	42.8(5)
P(2)-Rh(1)-P(1)-C(28)	-163.2(2)	Rh(1)-P(2)-C(2)-C(3)	168.0(4)
Cl(1)-Rh(1)-P(1)-C(28)	-59.5(2)	C(1)-C(2)-C(3)-C(4)	-0.7(8)
O(1)-Rh(1)-P(2)-C(2)	16.22(19)	P(2)-C(2)-C(3)-C(4)	175.3(4)
P(1)-Rh(1)-P(2)-C(2)	39.6(2)	C(2)-C(3)-C(4)-C(5)	-1.1(9)
Cl(1)-Rh(1)-P(2)-C(2)	-64.07(17)	C(3)-C(4)-C(5)-C(6)	0.8(9)
O(1)-Rh(1)-P(2)-C(16)	-90.9(2)	C(4)-C(5)-C(6)-C(1)	1.2(8)
P(1)-Rh(1)-P(2)-C(16)	-67.5(3)	C(4)-C(5)-C(6)-C(7)	-173.5(5)
Cl(1)-Rh(1)-P(2)-C(16)	-171.1(2)	C(2)-C(1)-C(6)-C(5)	-3.1(7)
O(1)-Rh(1)-P(2)-C(20)	134.2(2)	O(1)-C(1)-C(6)-C(5)	-178.5(4)
P(1)-Rh(1)-P(2)-C(20)	157.6(2)	C(2)-C(1)-C(6)-C(7)	171.8(4)
Cl(1)-Rh(1)-P(2)-C(20)	53.90(19)	O(1)-C(1)-C(6)-C(7)	-3.6(7)
P(2)-Rh(1)-O(1)-C(13)	-162.6(3)	C(5)-C(6)-C(7)-C(8)	-152.8(5)
P(1)-Rh(1)-O(1)-C(13)	24.1(3)	C(1)-C(6)-C(7)-C(8)	32.6(6)
Cl(1)-Rh(1)-O(1)-C(13)	-69.2(3)	C(5)-C(6)-C(7)-C(14)	-27.4(7)
P(2)-Rh(1)-O(1)-C(1)	-19.5(3)	C(1)-C(6)-C(7)-C(14)	158.0(4)
P(1)-Rh(1)-O(1)-C(1)	167.2(3)	C(5)-C(6)-C(7)-C(15)	90.8(6)
Cl(1)-Rh(1)-O(1)-C(1)	73.9(3)	C(1)-C(6)-C(7)-C(15)	-83.8(5)
C(13)-O(1)-C(1)-C(2)	156.5(4)	C(6)-C(7)-C(8)-C(13)	-34.2(6)
Rh(1)-O(1)-C(1)-C(2)	14.6(5)	C(14)-C(7)-C(8)-C(13)	-160.0(4)
C(13)-O(1)-C(1)-C(6)	-27.9(6)	C(15)-C(7)-C(8)-C(13)	81.3(5)
Rh(1)-O(1)-C(1)-C(6)	-169.8(3)	C(6)-C(7)-C(8)-C(9)	153.2(5)
O(1)-C(1)-C(2)-C(3)	178.2(4)	C(14)-C(7)-C(8)-C(9)	27.4(7)
C(6)-C(1)-C(2)-C(3)	2.8(7)	C(15)-C(7)-C(8)-C(9)	-91.3(6)

C(13)-C(8)-C(9)-C(10)	-0.7(7)	Rh(1)-P(2)-C(16)-C(17)	-69.7(4)
C(7)-C(8)-C(9)-C(10)	172.1(5)	C(2)-P(2)-C(20)-C(21)	153.2(4)
C(8)-C(9)-C(10)-C(11)	-3.0(8)	C(16)-P(2)-C(20)-C(21)	-96.2(4)
C(9)-C(10)-C(11)-C(12)	2.8(8)	Rh(1)-P(2)-C(20)-C(21)	40.1(4)
C(10)-C(11)-C(12)-C(13)	0.9(7)	C(2)-P(2)-C(20)-C(22)	-85.9(5)
C(10)-C(11)-C(12)-P(1)	-173.4(4)	C(16)-P(2)-C(20)-C(22)	24.8(5)
C(24)-P(1)-C(12)-C(11)	77.9(4)	Rh(1)-P(2)-C(20)-C(22)	161.1(4)
C(28)-P(1)-C(12)-C(11)	-38.6(5)	C(2)-P(2)-C(20)-C(23)	37.0(4)
Rh(1)-P(1)-C(12)-C(11)	-164.1(4)	C(16)-P(2)-C(20)-C(23)	147.6(4)
C(24)-P(1)-C(12)-C(13)	-96.3(4)	Rh(1)-P(2)-C(20)-C(23)	-76.1(4)
C(28)-P(1)-C(12)-C(13)	147.2(4)	C(12)-P(1)-C(24)-C(26)	-57.1(4)
Rh(1)-P(1)-C(12)-C(13)	21.7(4)	C(28)-P(1)-C(24)-C(26)	59.3(4)
C(9)-C(8)-C(13)-O(1)	179.2(4)	Rh(1)-P(1)-C(24)-C(26)	-161.7(3)
C(7)-C(8)-C(13)-O(1)	6.2(7)	C(12)-P(1)-C(24)-C(25)	178.2(4)
C(9)-C(8)-C(13)-C(12)	4.7(7)	C(28)-P(1)-C(24)-C(25)	-65.4(4)
C(7)-C(8)-C(13)-C(12)	-168.4(4)	Rh(1)-P(1)-C(24)-C(25)	73.6(4)
C(1)-O(1)-C(13)-C(8)	26.7(6)	C(12)-P(1)-C(24)-C(27)	60.7(4)
Rh(1)-O(1)-C(13)-C(8)	168.6(3)	C(28)-P(1)-C(24)-C(27)	177.1(4)
C(1)-O(1)-C(13)-C(12)	-158.4(4)	Rh(1)-P(1)-C(24)-C(27)	-43.9(4)
Rh(1)-O(1)-C(13)-C(12)	-16.5(5)	C(12)-P(1)-C(28)-C(31)	-39.2(4)
C(11)-C(12)-C(13)-C(8)	-4.8(7)	C(24)-P(1)-C(28)-C(31)	-148.9(4)
P(1)-C(12)-C(13)-C(8)	169.7(4)	Rh(1)-P(1)-C(28)-C(31)	73.7(4)
C(11)-C(12)-C(13)-O(1)	-179.5(4)	C(12)-P(1)-C(28)-C(30)	84.9(4)
P(1)-C(12)-C(13)-O(1)	-5.0(6)	C(24)-P(1)-C(28)-C(30)	-24.9(5)
C(2)-P(2)-C(16)-C(18)	59.5(5)	Rh(1)-P(1)-C(28)-C(30)	-162.2(3)
C(20)-P(2)-C(16)-C(18)	-56.0(5)	C(12)-P(1)-C(28)-C(29)	-155.7(4)
Rh(1)-P(2)-C(16)-C(18)	165.6(4)	C(24)-P(1)-C(28)-C(29)	94.5(4)
C(2)-P(2)-C(16)-C(19)	-59.5(4)	Rh(1)-P(1)-C(28)-C(29)	-42.8(4)
C(20)-P(2)-C(16)-C(19)	-175.0(4)	Cl(3B)-Rh(2)-P(3)-C(33)	178.8(7)
Rh(1)-P(2)-C(16)-C(19)	46.6(4)	O(2)-Rh(2)-P(3)-C(33)	3.72(19)
C(2)-P(2)-C(16)-C(17)	-175.8(4)	P(4)-Rh(2)-P(3)-C(33)	55.8(2)
C(20)-P(2)-C(16)-C(17)	68.7(4)	Cl(2A)-Rh(2)-P(3)-C(33)	-91.07(17)

Cl(3B)-Rh(2)-P(3)-C(47)	69.3(7)	C(44)-O(2)-C(32)-C(33)	-150.9(5)
O(2)-Rh(2)-P(3)-C(47)	-105.8(2)	Rh(2)-O(2)-C(32)-C(33)	-3.2(6)
P(4)-Rh(2)-P(3)-C(47)	-53.7(2)	C(44)-O(2)-C(32)-C(37)	32.3(6)
Cl(2A)-Rh(2)-P(3)-C(47)	159.46(19)	Rh(2)-O(2)-C(32)-C(37)	-180.0(3)
Cl(3B)-Rh(2)-P(3)-C(51)	-66.1(8)	O(2)-C(32)-C(33)-C(34)	-175.7(4)
O(2)-Rh(2)-P(3)-C(51)	118.8(2)	C(37)-C(32)-C(33)-C(34)	0.9(7)
P(4)-Rh(2)-P(3)-C(51)	170.9(2)	O(2)-C(32)-C(33)-P(3)	7.4(6)
Cl(2A)-Rh(2)-P(3)-C(51)	24.1(2)	C(37)-C(32)-C(33)-P(3)	-176.0(4)
Cl(3B)-Rh(2)-P(4)-C(43)	-162.6(8)	C(47)-P(3)-C(33)-C(32)	110.4(4)
O(2)-Rh(2)-P(4)-C(43)	13.1(2)	C(51)-P(3)-C(33)-C(32)	-132.2(4)
P(3)-Rh(2)-P(4)-C(43)	-39.2(2)	Rh(2)-P(3)-C(33)-C(32)	-7.2(4)
Cl(2A)-Rh(2)-P(4)-C(43)	107.17(18)	C(47)-P(3)-C(33)-C(34)	-66.3(5)
Cl(3B)-Rh(2)-P(4)-C(55)	-49.0(8)	C(51)-P(3)-C(33)-C(34)	51.1(5)
O(2)-Rh(2)-P(4)-C(55)	126.8(2)	Rh(2)-P(3)-C(33)-C(34)	176.1(4)
P(3)-Rh(2)-P(4)-C(55)	74.4(3)	C(32)-C(33)-C(34)-C(35)	-0.6(8)
Cl(2A)-Rh(2)-P(4)-C(55)	-139.2(2)	P(3)-C(33)-C(34)-C(35)	176.3(4)
Cl(3B)-Rh(2)-P(4)-C(59)	87.9(8)	C(33)-C(34)-C(35)-C(36)	-1.0(8)
O(2)-Rh(2)-P(4)-C(59)	-96.4(2)	C(34)-C(35)-C(36)-C(37)	2.3(8)
P(3)-Rh(2)-P(4)-C(59)	-148.7(2)	C(35)-C(36)-C(37)-C(32)	-1.9(7)
Cl(2A)-Rh(2)-P(4)-C(59)	-2.4(2)	C(35)-C(36)-C(37)-C(38)	174.1(5)
O(2)-Rh(2)-Cl(3B)-C(63B)	-148(8)	C(33)-C(32)-C(37)-C(36)	0.4(7)
P(3)-Rh(2)-Cl(3B)-C(63B)	110(2)	O(2)-C(32)-C(37)-C(36)	177.0(4)
P(4)-Rh(2)-Cl(3B)-C(63B)	-90(2)	C(33)-C(32)-C(37)-C(38)	-175.8(5)
Cl(2A)-Rh(2)-Cl(3B)-C(63B)	12(2)	O(2)-C(32)-C(37)-C(38)	0.8(7)
Cl(3B)-Rh(2)-O(2)-C(44)	44(9)	C(36)-C(37)-C(38)-C(45)	25.2(7)
P(3)-Rh(2)-O(2)-C(44)	146.9(3)	C(32)-C(37)-C(38)-C(45)	-158.7(5)
P(4)-Rh(2)-O(2)-C(44)	-14.2(3)	C(36)-C(37)-C(38)-C(39)	150.3(5)
Cl(2A)-Rh(2)-O(2)-C(44)	-115.8(3)	C(32)-C(37)-C(38)-C(39)	-33.7(6)
Cl(3B)-Rh(2)-O(2)-C(32)	-104(9)	C(36)-C(37)-C(38)-C(46)	-94.1(6)
P(3)-Rh(2)-O(2)-C(32)	-1.2(3)	C(32)-C(37)-C(38)-C(46)	81.9(6)
P(4)-Rh(2)-O(2)-C(32)	-162.3(3)	C(45)-C(38)-C(39)-C(40)	-25.3(7)
Cl(2A)-Rh(2)-O(2)-C(32)	96.1(3)	C(37)-C(38)-C(39)-C(40)	-149.8(5)

C(46)-C(38)-C(39)-C(40)	93.4(6)	C(51)-P(3)-C(47)-C(50)	-161.8(4)
C(45)-C(38)-C(39)-C(44)	162.5(5)	Rh(2)-P(3)-C(47)-C(50)	59.3(4)
C(37)-C(38)-C(39)-C(44)	38.0(6)	C(33)-P(3)-C(47)-C(48)	-166.1(4)
C(46)-C(38)-C(39)-C(44)	-78.8(6)	C(51)-P(3)-C(47)-C(48)	80.5(4)
C(44)-C(39)-C(40)-C(41)	1.6(8)	Rh(2)-P(3)-C(47)-C(48)	-58.4(4)
C(38)-C(39)-C(40)-C(41)	-170.6(5)	C(33)-P(3)-C(51)-C(54)	41.8(5)
C(39)-C(40)-C(41)-C(42)	3.6(10)	C(47)-P(3)-C(51)-C(54)	153.4(4)
C(40)-C(41)-C(42)-C(43)	-4.5(10)	Rh(2)-P(3)-C(51)-C(54)	-70.3(4)
C(41)-C(42)-C(43)-C(44)	0.1(9)	C(33)-P(3)-C(51)-C(52)	161.4(4)
C(41)-C(42)-C(43)-P(4)	175.9(5)	C(47)-P(3)-C(51)-C(52)	-87.0(4)
C(55)-P(4)-C(43)-C(42)	47.8(5)	Rh(2)-P(3)-C(51)-C(52)	49.3(4)
C(59)-P(4)-C(43)-C(42)	-69.5(5)	C(33)-P(3)-C(51)-C(53)	-79.9(5)
Rh(2)-P(4)-C(43)-C(42)	169.2(5)	C(47)-P(3)-C(51)-C(53)	31.7(5)
C(55)-P(4)-C(43)-C(44)	-136.5(4)	Rh(2)-P(3)-C(51)-C(53)	168.0(4)
C(59)-P(4)-C(43)-C(44)	106.3(4)	C(43)-P(4)-C(55)-C(57)	-82.8(5)
Rh(2)-P(4)-C(43)-C(44)	-15.0(4)	C(59)-P(4)-C(55)-C(57)	27.4(6)
C(42)-C(43)-C(44)-C(39)	5.4(8)	Rh(2)-P(4)-C(55)-C(57)	166.5(4)
P(4)-C(43)-C(44)-C(39)	-170.6(4)	C(43)-P(4)-C(55)-C(58)	40.6(5)
C(42)-C(43)-C(44)-O(2)	-178.6(5)	C(59)-P(4)-C(55)-C(58)	150.8(4)
P(4)-C(43)-C(44)-O(2)	5.4(6)	Rh(2)-P(4)-C(55)-C(58)	-70.1(5)
C(40)-C(39)-C(44)-C(43)	-6.3(8)	C(43)-P(4)-C(55)-C(56)	156.3(4)
C(38)-C(39)-C(44)-C(43)	166.4(5)	C(59)-P(4)-C(55)-C(56)	-93.4(4)
C(40)-C(39)-C(44)-O(2)	177.8(5)	Rh(2)-P(4)-C(55)-C(56)	45.7(5)
C(38)-C(39)-C(44)-O(2)	-9.5(7)	C(43)-P(4)-C(59)-C(61)	65.3(6)
C(32)-O(2)-C(44)-C(43)	155.9(4)	C(55)-P(4)-C(59)-C(61)	-47.3(6)
Rh(2)-O(2)-C(44)-C(43)	8.5(6)	Rh(2)-P(4)-C(59)-C(61)	174.0(5)
C(32)-O(2)-C(44)-C(39)	-28.0(6)	C(43)-P(4)-C(59)-C(62)	-53.1(5)
Rh(2)-O(2)-C(44)-C(39)	-175.4(3)	C(55)-P(4)-C(59)-C(62)	-165.7(4)
C(33)-P(3)-C(47)-C(49)	71.7(5)	Rh(2)-P(4)-C(59)-C(62)	55.7(4)
C(51)-P(3)-C(47)-C(49)	-41.7(5)	C(43)-P(4)-C(59)-C(60)	-170.4(4)
Rh(2)-P(3)-C(47)-C(49)	179.3(4)	C(55)-P(4)-C(59)-C(60)	77.0(5)
C(33)-P(3)-C(47)-C(50)	-48.4(4)	Rh(2)-P(4)-C(59)-C(60)	-61.6(4)

Figure E1: ORTEP diagram of [*trans*-(^tBu_{xan}POP)Rh(H)₂(OH₂)]SbF₆

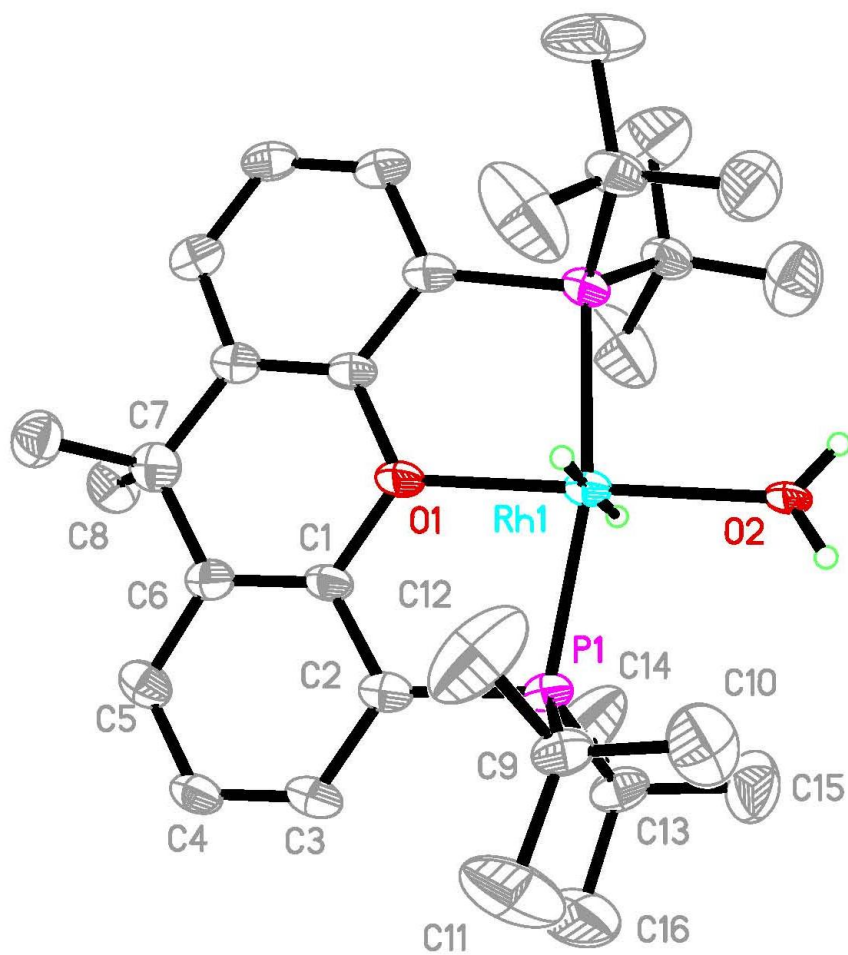


Table E2. Crystal data and structure refinement for [*trans*-(^tBu₃xanPOP)Rh(H)₂(OH₂)]SbF₆.

Identification code	mh311_c2	
Empirical formula	C ₃₇ H ₅₈ F ₆ O ₂ P ₂ Rh Sb	
Formula weight	935.43	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 19.017(3) Å	α = 90°.
	b = 11.5983(17) Å	β = 126.613(2)°.
	c = 11.3433(16) Å	γ = 90°.
Volume	2008.3(5) Å ³	
Z	2	
Density (calculated)	1.547 Mg/m ³	
Absorption coefficient	1.222 mm ⁻¹	
F(000)	952	
Crystal size	0.24 x 0.13 x 0.03 mm ³	
Theta range for data collection	2.21 to 30.02°.	
Index ranges	-26 ≤ h ≤ 26, -16 ≤ k ≤ 16, -15 ≤ l ≤ 15	
Reflections collected	11611	
Independent reflections	5622 [R(int) = 0.0384]	
Completeness to theta = 30.02°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7462 and 0.6352	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5622 / 350 / 238	
Goodness-of-fit on F ²	1.015	
Final R indices [I > 2σ(I)]	R1 = 0.0562, wR2 = 0.1293	
R indices (all data)	R1 = 0.0693, wR2 = 0.1379	
Absolute structure parameter	0.04(4)	
Largest diff. peak and hole	1.527 and -0.479 e.Å ⁻³	

Table E3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\textit{trans}\text{-}(\textit{tBu}\text{-xanPOP})\text{Rh}(\text{H})_2(\text{OH}_2)]\text{SbF}_6$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	0	-4(1)	0	24(1)
P(1)	-1501(1)	195(1)	-1501(2)	26(1)
O(1)	0	1847(5)	0	27(1)
O(2)	0	-1920(5)	0	32(1)
C(1)	-800(3)	2450(5)	-800(5)	25(1)
C(2)	-1576(3)	1767(6)	-1576(6)	28(1)
C(3)	-2375(3)	2366(6)	-2377(6)	30(1)
C(4)	-2414(4)	3541(8)	-2417(8)	30(1)
C(5)	-1640(4)	4190(6)	-1638(6)	30(1)
C(6)	-830(4)	3654(5)	-823(6)	27(1)
C(7)	0	4359(9)	0	36(2)
C(8)	3(5)	5189(7)	-1095(8)	38(2)
C(9)	-2045(4)	-298(5)	-642(6)	31(1)
C(10)	-1937(6)	-1569(7)	-401(11)	59(2)
C(11)	-3009(5)	5(10)	-1473(11)	76(3)
C(12)	-1526(7)	315(10)	859(9)	80(3)
C(13)	-2045(4)	-298(6)	-3447(6)	33(1)
C(14)	-1521(7)	303(10)	-3892(10)	80(3)
C(15)	-1939(6)	-1572(7)	-3479(9)	61(2)
C(16)	-3001(5)	7(10)	-4542(8)	77(3)
Sb(1)	0	2290(1)	5000	46(1)
F(1)	-1202(3)	2271(9)	3809(8)	122(3)
F(2)	4(6)	1252(12)	3816(12)	203(5)
F(3)	-9(9)	3339(13)	3795(17)	271(8)
C(21)	1(5)	-1650(8)	-4402(10)	59(2)
C(22)	1(4)	-2671(12)	-3767(8)	53(2)
C(23)	2(5)	-3707(8)	-4399(9)	52(2)

Table E4. Bond lengths [\AA] and angles [$^\circ$] for $[\textit{trans}\text{-}(\textit{tBu}\text{xanPOP})\text{Rh}(\text{H})_2(\text{OH}_2)]\text{SbF}_6$.

Rh(1)-O(1)	2.147(6)	C(10)-H(10C)	0.9600
Rh(1)-O(2)	2.223(6)	C(11)-H(11A)	0.9600
Rh(1)-P(1)#1	2.3032(14)	C(11)-H(11B)	0.9600
Rh(1)-P(1)	2.3032(14)	C(11)-H(11C)	0.9600
Rh(1)-H(1)	1.556(19)	C(12)-H(12A)	0.9600
P(1)-C(2)	1.827(6)	C(12)-H(12B)	0.9600
P(1)-C(9)	1.883(6)	C(12)-H(12C)	0.9600
P(1)-C(13)	1.883(5)	C(13)-C(15)	1.494(10)
O(1)-C(1)#1	1.407(6)	C(13)-C(16)	1.510(9)
O(1)-C(1)	1.407(6)	C(13)-C(14)	1.528(10)
O(2)-H(2)	0.838(10)	C(14)-H(14A)	0.9600
C(1)-C(6)	1.397(8)	C(14)-H(14B)	0.9600
C(1)-C(2)	1.424(7)	C(14)-H(14C)	0.9600
C(2)-C(3)	1.403(7)	C(15)-H(15A)	0.9600
C(3)-C(4)	1.364(11)	C(15)-H(15B)	0.9600
C(3)-H(3)	0.9300	C(15)-H(15C)	0.9600
C(4)-C(5)	1.401(10)	C(16)-H(16A)	0.9600
C(4)-H(4)	0.9300	C(16)-H(16B)	0.9600
C(5)-C(6)	1.385(8)	C(16)-H(16C)	0.9600
C(5)-H(5)	0.9300	Sb(1)-F(2)	1.806(7)
C(6)-C(7)	1.508(8)	Sb(1)-F(2)#2	1.806(7)
C(7)-C(6)#1	1.508(8)	Sb(1)-F(3)#2	1.823(9)
C(7)-C(8)#1	1.574(9)	Sb(1)-F(3)	1.823(9)
C(7)-C(8)	1.574(9)	Sb(1)-F(1)	1.835(5)
C(8)-H(8A)	0.9600	Sb(1)-F(1)#2	1.835(5)
C(8)-H(8B)	0.9600	C(21)-C(21)#3	1.355(19)
C(8)-H(8C)	0.9600	C(21)-C(22)	1.386(15)
C(9)-C(10)	1.491(10)	C(21)-H(21)	0.9300
C(9)-C(11)	1.521(9)	C(22)-C(23)	1.400(14)
C(9)-C(12)	1.541(10)	C(22)-H(22)	0.9300
C(10)-H(10A)	0.9600	C(23)-C(23)#3	1.359(17)
C(10)-H(10B)	0.9600	C(23)-H(23)	0.9300

O(1)-Rh(1)-O(2)	180.0	C(6)-C(5)-H(5)	119.6
O(1)-Rh(1)-P(1)#1	84.25(4)	C(4)-C(5)-H(5)	119.6
O(2)-Rh(1)-P(1)#1	95.75(4)	C(5)-C(6)-C(1)	118.6(5)
O(1)-Rh(1)-P(1)	84.25(4)	C(5)-C(6)-C(7)	120.5(6)
O(2)-Rh(1)-P(1)	95.75(4)	C(1)-C(6)-C(7)	121.0(5)
P(1)#1-Rh(1)-P(1)	168.51(9)	C(6)#1-C(7)-C(6)	114.3(8)
O(1)-Rh(1)-H(1)	91.4(3)	C(6)#1-C(7)-C(8)#1	109.8(4)
O(2)-Rh(1)-H(1)	88.6(3)	C(6)-C(7)-C(8)#1	109.0(4)
P(1)#1-Rh(1)-H(1)	90.5(4)	C(6)#1-C(7)-C(8)	109.0(4)
P(1)-Rh(1)-H(1)	89.8(4)	C(6)-C(7)-C(8)	109.8(4)
C(2)-P(1)-C(9)	106.0(3)	C(8)#1-C(7)-C(8)	104.6(8)
C(2)-P(1)-C(13)	106.0(3)	C(7)-C(8)-H(8A)	109.5
C(9)-P(1)-C(13)	115.3(3)	C(7)-C(8)-H(8B)	109.5
C(2)-P(1)-Rh(1)	99.30(18)	H(8A)-C(8)-H(8B)	109.5
C(9)-P(1)-Rh(1)	114.08(19)	C(7)-C(8)-H(8C)	109.5
C(13)-P(1)-Rh(1)	114.08(19)	H(8A)-C(8)-H(8C)	109.5
C(1)#1-O(1)-C(1)	120.5(6)	H(8B)-C(8)-H(8C)	109.5
C(1)#1-O(1)-Rh(1)	119.8(3)	C(10)-C(9)-C(11)	109.0(7)
C(1)-O(1)-Rh(1)	119.8(3)	C(10)-C(9)-C(12)	109.0(7)
Rh(1)-O(2)-H(2)	125.1(12)	C(11)-C(9)-C(12)	108.6(7)
C(6)-C(1)-O(1)	121.6(5)	C(10)-C(9)-P(1)	109.7(5)
C(6)-C(1)-C(2)	121.9(5)	C(11)-C(9)-P(1)	116.1(4)
O(1)-C(1)-C(2)	116.5(5)	C(12)-C(9)-P(1)	104.2(4)
C(3)-C(2)-C(1)	116.6(6)	C(9)-C(10)-H(10A)	109.5
C(3)-C(2)-P(1)	123.2(5)	C(9)-C(10)-H(10B)	109.5
C(1)-C(2)-P(1)	120.2(4)	H(10A)-C(10)-H(10B)	109.5
C(4)-C(3)-C(2)	122.2(6)	C(9)-C(10)-H(10C)	109.5
C(4)-C(3)-H(3)	118.9	H(10A)-C(10)-H(10C)	109.5
C(2)-C(3)-H(3)	118.9	H(10B)-C(10)-H(10C)	109.5
C(3)-C(4)-C(5)	120.0(6)	C(9)-C(11)-H(11A)	109.5
C(3)-C(4)-H(4)	120.0	C(9)-C(11)-H(11B)	109.5
C(5)-C(4)-H(4)	120.0	H(11A)-C(11)-H(11B)	109.5
C(6)-C(5)-C(4)	120.8(6)	C(9)-C(11)-H(11C)	109.5

H(11A)-C(11)-H(11C)	109.5	H(16A)-C(16)-H(16B)	109.5
H(11B)-C(11)-H(11C)	109.5	C(13)-C(16)-H(16C)	109.5
C(9)-C(12)-H(12A)	109.5	H(16A)-C(16)-H(16C)	109.5
C(9)-C(12)-H(12B)	109.5	H(16B)-C(16)-H(16C)	109.5
H(12A)-C(12)-H(12B)	109.5	F(2)-Sb(1)-F(2)#2	96.5(10)
C(9)-C(12)-H(12C)	109.5	F(2)-Sb(1)-F(3)#2	179.4(6)
H(12A)-C(12)-H(12C)	109.5	F(2)#2-Sb(1)-F(3)#2	83.6(6)
H(12B)-C(12)-H(12C)	109.5	F(2)-Sb(1)-F(3)	83.6(6)
C(15)-C(13)-C(16)	109.0(7)	F(2)#2-Sb(1)-F(3)	179.4(6)
C(15)-C(13)-C(14)	108.7(7)	F(3)#2-Sb(1)-F(3)	96.3(12)
C(16)-C(13)-C(14)	108.9(8)	F(2)-Sb(1)-F(1)	90.0(4)
C(15)-C(13)-P(1)	109.9(5)	F(2)#2-Sb(1)-F(1)	89.1(4)
C(16)-C(13)-P(1)	116.3(5)	F(3)#2-Sb(1)-F(1)	90.6(6)
C(14)-C(13)-P(1)	103.8(4)	F(3)-Sb(1)-F(1)	90.3(5)
C(13)-C(14)-H(14A)	109.5	F(2)-Sb(1)-F(1)#2	89.1(4)
C(13)-C(14)-H(14B)	109.5	F(2)#2-Sb(1)-F(1)#2	90.0(4)
H(14A)-C(14)-H(14B)	109.5	F(3)#2-Sb(1)-F(1)#2	90.3(5)
C(13)-C(14)-H(14C)	109.5	F(3)-Sb(1)-F(1)#2	90.6(6)
H(14A)-C(14)-H(14C)	109.5	F(1)-Sb(1)-F(1)#2	178.7(7)
H(14B)-C(14)-H(14C)	109.5	C(21)#3-C(21)-C(22)	121.3(5)
C(13)-C(15)-H(15A)	109.5	C(21)#3-C(21)-H(21)	119.3
C(13)-C(15)-H(15B)	109.5	C(22)-C(21)-H(21)	119.3
H(15A)-C(15)-H(15B)	109.5	C(21)-C(22)-C(23)	117.8(7)
C(13)-C(15)-H(15C)	109.5	C(21)-C(22)-H(22)	121.1
H(15A)-C(15)-H(15C)	109.5	C(23)-C(22)-H(22)	121.1
H(15B)-C(15)-H(15C)	109.5	C(23)#3-C(23)-C(22)	120.9(5)
C(13)-C(16)-H(16A)	109.5	C(23)#3-C(23)-H(23)	119.6
C(13)-C(16)-H(16B)	109.5	C(22)-C(23)-H(23)	119.6

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z #2 -x,y,-z+1 #3 -x,y,-z-1

Table E5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{trans}-(\text{t}^{\text{Bu}}\text{xanPOP})\text{Rh}(\text{H})_2(\text{OH}_2)]\text{SbF}_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Rh(1)	15(1)	29(1)	24(1)	0	9(1)	0
P(1)	18(1)	30(1)	25(1)	-2(1)	10(1)	-4(1)
O(1)	14(2)	31(3)	31(3)	0	11(2)	0
O(2)	9(2)	27(3)	43(4)	0	7(3)	0
C(1)	15(2)	32(3)	24(2)	0(2)	10(2)	2(2)
C(2)	19(2)	38(3)	23(2)	1(2)	11(2)	1(2)
C(3)	20(2)	43(3)	25(2)	4(2)	12(2)	6(2)
C(4)	19(3)	41(3)	26(3)	0(2)	12(2)	6(2)
C(5)	28(3)	40(3)	26(3)	4(2)	18(2)	8(2)
C(6)	22(2)	33(3)	23(2)	-1(2)	12(2)	-1(2)
C(7)	32(4)	35(5)	37(5)	0	18(4)	0
C(8)	41(3)	37(4)	40(3)	6(3)	26(3)	3(3)
C(9)	24(2)	40(3)	29(3)	-1(2)	15(2)	-7(2)
C(10)	66(5)	52(4)	82(6)	14(4)	57(5)	3(4)
C(11)	45(4)	111(7)	96(6)	46(6)	55(4)	21(5)
C(12)	113(7)	94(7)	49(4)	-27(4)	57(5)	-54(6)
C(13)	29(3)	46(3)	21(2)	-7(2)	13(2)	-8(2)
C(14)	113(7)	97(7)	67(5)	-46(5)	73(5)	-59(6)
C(15)	76(6)	41(4)	38(4)	-9(3)	20(4)	4(4)
C(16)	47(4)	109(7)	32(3)	-27(5)	1(3)	18(5)
Sb(1)	31(1)	30(1)	62(1)	0	18(1)	0
F(1)	50(3)	172(8)	113(5)	14(6)	32(3)	31(5)
F(2)	79(6)	307(11)	178(9)	-134(8)	53(6)	-2(7)
F(3)	210(12)	296(13)	275(13)	149(10)	127(10)	-23(9)
C(21)	35(4)	63(5)	60(5)	-29(4)	18(4)	-1(3)
C(22)	28(3)	87(6)	37(3)	-8(4)	16(3)	-3(4)
C(23)	21(3)	70(5)	49(4)	7(3)	11(3)	-6(3)

Table E6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $[\textit{trans}\text{-}(\textit{tBu}\text{-xanPOP})\text{Rh}(\text{H})_2(\text{OH}_2)]\text{SbF}_6$.

	x	y	z	U(eq)
H(1)	-7(7)	-36(7)	1365(18)	36
H(2)	434(13)	-2336(17)	280(70)	47
H(3)	-2894	1947	-2899	37
H(4)	-2955	3911	-2960	36
H(5)	-1671	4991	-1669	36
H(8A)	2	4740	-1807	57
H(8B)	518	5664	-559	57
H(8C)	-509	5669	-1587	57
H(10A)	-2027	-1780	318	88
H(10B)	-1356	-1786	-57	88
H(10C)	-2358	-1959	-1308	88
H(11A)	-3337	-344	-2429	114
H(11B)	-3079	827	-1574	114
H(11C)	-3220	-277	-940	114
H(12A)	-1924	583	1056	120
H(12B)	-1215	958	843	120
H(12C)	-1117	-216	1613	120
H(14A)	-1107	-229	-3812	120
H(14B)	-1213	950	-3256	120
H(14C)	-1912	567	-4888	120
H(15A)	-2321	-1961	-3318	91
H(15B)	-1343	-1782	-2721	91
H(15C)	-2087	-1790	-4418	91
H(16A)	-3210	-274	-5496	115
H(16B)	-3070	829	-4579	115
H(16C)	-3332	-342	-4248	115
H(21)	2	-951	-3999	71
H(22)	0	-2668	-2948	63
H(23)	5	-4404	-3992	63

Table E7. Torsion angles [°] for *[trans-(^tBu_{xan}POP)Rh(H)₂(OH₂)]SbF₆*.

O(1)-Rh(1)-P(1)-C(2)	0.02(17)	C(4)-C(5)-C(6)-C(7)	179.4(5)
O(2)-Rh(1)-P(1)-C(2)	-179.98(17)	O(1)-C(1)-C(6)-C(5)	179.7(4)
P(1)#1-Rh(1)-P(1)-C(2)	0.02(17)	C(2)-C(1)-C(6)-C(5)	-0.6(8)
O(1)-Rh(1)-P(1)-C(9)	-112.3(2)	O(1)-C(1)-C(6)-C(7)	0.7(7)
O(2)-Rh(1)-P(1)-C(9)	67.7(2)	C(2)-C(1)-C(6)-C(7)	-179.6(4)
P(1)#1-Rh(1)-P(1)-C(9)	-112.3(2)	C(5)-C(6)-C(7)-C(6)#1	-179.4(6)
O(1)-Rh(1)-P(1)-C(13)	112.3(2)	C(1)-C(6)-C(7)-C(6)#1	-0.4(3)
O(2)-Rh(1)-P(1)-C(13)	-67.7(2)	C(5)-C(6)-C(7)-C(8)#1	57.4(7)
P(1)#1-Rh(1)-P(1)-C(13)	112.3(2)	C(1)-C(6)-C(7)-C(8)#1	-123.6(6)
O(2)-Rh(1)-O(1)-C(1)#1	0(76)	C(5)-C(6)-C(7)-C(8)	-56.6(7)
P(1)#1-Rh(1)-O(1)-C(1)#1	0.0(2)	C(1)-C(6)-C(7)-C(8)	122.4(6)
P(1)-Rh(1)-O(1)-C(1)#1	-180.0(2)	C(2)-P(1)-C(9)-C(10)	-174.4(5)
O(2)-Rh(1)-O(1)-C(1)	0(100)	C(13)-P(1)-C(9)-C(10)	68.6(6)
P(1)#1-Rh(1)-O(1)-C(1)	-180.0(2)	Rh(1)-P(1)-C(9)-C(10)	-66.2(5)
P(1)-Rh(1)-O(1)-C(1)	0.0(2)	C(2)-P(1)-C(9)-C(11)	61.4(7)
C(1)#1-O(1)-C(1)-C(6)	-0.4(4)	C(13)-P(1)-C(9)-C(11)	-55.5(7)
Rh(1)-O(1)-C(1)-C(6)	179.6(4)	Rh(1)-P(1)-C(9)-C(11)	169.7(6)
C(1)#1-O(1)-C(1)-C(2)	180.0(5)	C(2)-P(1)-C(9)-C(12)	-57.9(6)
Rh(1)-O(1)-C(1)-C(2)	0.0(5)	C(13)-P(1)-C(9)-C(12)	-174.8(6)
C(6)-C(1)-C(2)-C(3)	0.5(8)	Rh(1)-P(1)-C(9)-C(12)	50.4(6)
O(1)-C(1)-C(2)-C(3)	-179.9(4)	C(2)-P(1)-C(13)-C(15)	174.5(5)
C(6)-C(1)-C(2)-P(1)	-179.6(4)	C(9)-P(1)-C(13)-C(15)	-68.6(6)
O(1)-C(1)-C(2)-P(1)	0.1(6)	Rh(1)-P(1)-C(13)-C(15)	66.3(6)
C(9)-P(1)-C(2)-C(3)	-61.6(5)	C(2)-P(1)-C(13)-C(16)	-61.2(7)
C(13)-P(1)-C(2)-C(3)	61.4(5)	C(9)-P(1)-C(13)-C(16)	55.8(7)
Rh(1)-P(1)-C(2)-C(3)	179.9(4)	Rh(1)-P(1)-C(13)-C(16)	-169.4(6)
C(9)-P(1)-C(2)-C(1)	118.4(4)	C(2)-P(1)-C(13)-C(14)	58.4(6)
C(13)-P(1)-C(2)-C(1)	-118.5(4)	C(9)-P(1)-C(13)-C(14)	175.4(6)
Rh(1)-P(1)-C(2)-C(1)	-0.1(4)	Rh(1)-P(1)-C(13)-C(14)	-49.8(6)
C(1)-C(2)-C(3)-C(4)	-0.1(9)	C(21)#3-C(21)-C(22)-C(23)	0.2(14)
P(1)-C(2)-C(3)-C(4)	180.0(5)	C(21)-C(22)-C(23)-C(23)#3	-0.3(12)
C(2)-C(3)-C(4)-C(5)	-0.1(10)		
C(3)-C(4)-C(5)-C(6)	0.0(9)		
C(4)-C(5)-C(6)-C(1)	0.4(8)		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z #2 -x,y,-z+1 #3 -x,y,-z-1

Figure F1: ORTEP diagram of $[(^t\text{Bu}_2\text{xanPOP})\text{Rh}(\text{H})_2]\text{SbF}_6$

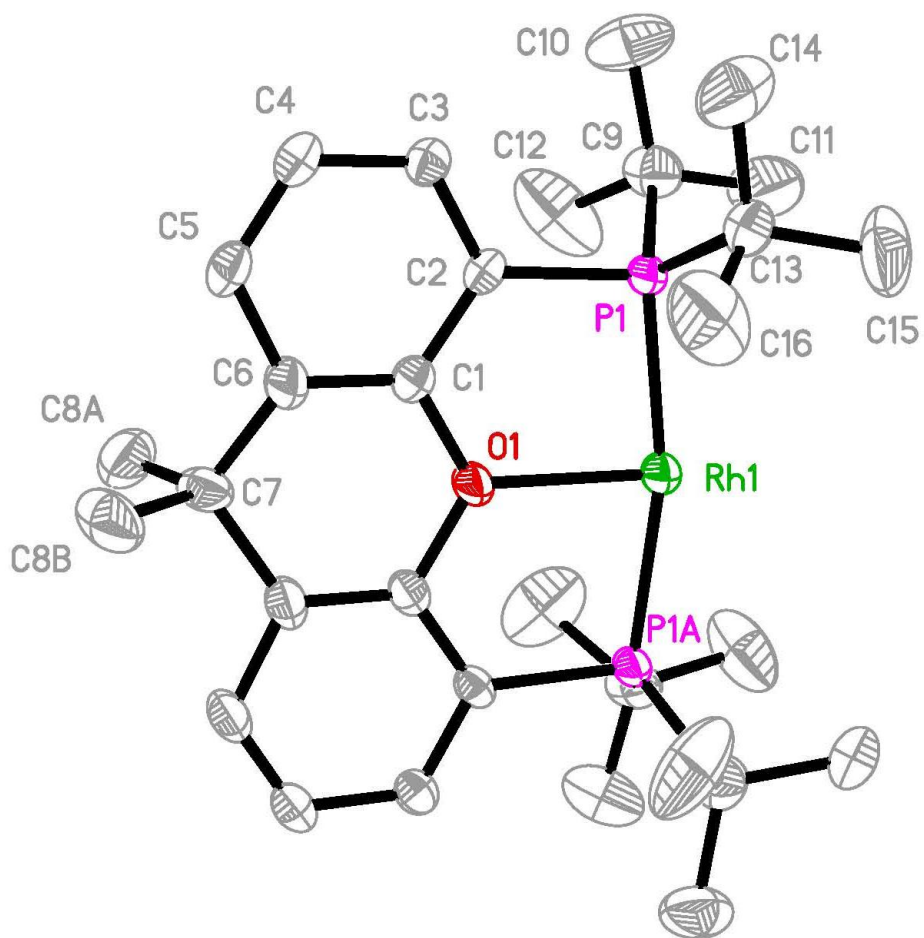


Table F2. Crystal data and structure refinement for [(^tBu₃xanPOP)Rh(H)₂]SbF₆.

Identification code	mh315-c2	
Empirical formula	C ₃₂ H ₅₂ Cl ₂ F ₆ O ₂ P ₂ Rh Sb	
Formula weight	924.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 19.814(2) Å	α = 90°.
	b = 10.6736(11) Å	β = 124.295(2)°.
	c = 11.1660(12) Å	γ = 90°.
Volume	1950.9(4) Å ³	
Z	2	
Density (calculated)	1.573 Mg/m ³	
Absorption coefficient	1.387 mm ⁻¹	
F(000)	932	
Crystal size	0.57 x 0.09 x 0.03 mm ³	
Theta range for data collection	2.21 to 31.00°.	
Index ranges	-28 ≤ h ≤ 28, -15 ≤ k ≤ 15, -16 ≤ l ≤ 15	
Reflections collected	11953	
Independent reflections	5989 [R(int) = 0.0308]	
Completeness to theta = 31.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9596 and 0.5053	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5989 / 381 / 253	
Goodness-of-fit on F ²	1.006	
Final R indices [I > 2σ(I)]	R1 = 0.0644, wR2 = 0.1513	
R indices (all data)	R1 = 0.0703, wR2 = 0.1555	
Absolute structure parameter	-0.04(4)	
Largest diff. peak and hole	1.863 and -1.107 e.Å ⁻³	

Table F3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(^t\text{Bu}\text{xanPOP})\text{Rh}(\text{H})_2]\text{SbF}_6$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Rh(1)	5000	0	5000	25(1)
P(1)	6389(1)	237(1)	6389(2)	26(1)
O(1)	5000	2037(5)	5000	34(1)
C(1)	5744(3)	2692(5)	5747(6)	30(1)
C(2)	6453(3)	1966(5)	6455(6)	22(1)
C(3)	7192(3)	2578(5)	7192(5)	25(1)
C(4)	7231(4)	3895(6)	7228(7)	30(1)
C(5)	6530(4)	4582(6)	6516(8)	35(1)
C(6)	5755(4)	3994(6)	5739(9)	39(2)
C(7)	5000	4771(11)	4706(10)	36(3)
C(8A)	5000	5372(18)	3490(17)	55(4)
C(8B)	5000	5870(15)	5538(19)	58(4)
C(9)	6898(5)	-285(6)	5481(9)	41(2)
C(10)	7786(5)	-19(12)	6232(10)	62(2)
C(11)	6740(6)	-1647(9)	5126(15)	72(3)
C(12)	6485(8)	437(13)	4060(11)	85(3)
C(13)	6895(5)	-292(6)	8307(9)	41(2)
C(14)	7787(6)	-28(12)	9340(9)	63(2)
C(15)	6745(7)	-1654(9)	8368(11)	78(3)
C(16)	6491(8)	468(13)	8921(12)	82(3)
Sb(1)	5000	-2338(1)	0	40(1)
F(1A)	5003(6)	-2278(14)	1617(9)	93(3)
F(2A)	5825(7)	-3473(10)	822(15)	98(4)
F(3A)	5817(6)	-1053(8)	819(11)	70(2)
F(1B)	4202(10)	-2620(20)	355(19)	66(4)
F(2B)	5803(10)	-2590(20)	1968(18)	65(4)
F(3B)	5000	-910(18)	0	90(4)
Cl(1)	4984(9)	3272(13)	1991(17)	186(5)
Cl(2)	5618(12)	2330(20)	510(20)	227(6)
C(17)	5060(40)	3570(50)	560(50)	206(12)

Table F4. Bond lengths [\AA] and angles [$^\circ$] for $[(\text{tBu}\text{xanPOP})\text{Rh}(\text{H})_2]\text{SbF}_6$.

Rh(1)-O(1)	2.175(6)	C(9)-C(11)	1.492(11)
Rh(1)-P(1)#1	2.2871(15)	C(9)-C(12)	1.523(13)
Rh(1)-P(1)	2.2872(15)	C(10)-H(10A)	0.9800
Rh(1)-H(1)	1.54469(11)	C(10)-H(10B)	0.9800
P(1)-C(2)	1.849(5)	C(10)-H(10C)	0.9800
P(1)-C(13)	1.869(8)	C(11)-H(11A)	0.9800
P(1)-C(9)	1.873(8)	C(11)-H(11B)	0.9800
O(1)-C(1)#1	1.405(6)	C(11)-H(11C)	0.9800
O(1)-C(1)	1.405(6)	C(12)-H(12A)	0.9800
C(1)-C(6)	1.390(8)	C(12)-H(12B)	0.9800
C(1)-C(2)	1.395(8)	C(12)-H(12C)	0.9800
C(2)-C(3)	1.375(7)	C(13)-C(14)	1.496(12)
C(3)-C(4)	1.407(8)	C(13)-C(15)	1.493(11)
C(3)-H(3)	0.9500	C(13)-C(16)	1.544(13)
C(4)-C(5)	1.361(10)	C(14)-H(14A)	0.9800
C(4)-H(4)	0.9500	C(14)-H(14B)	0.9800
C(5)-C(6)	1.415(9)	C(14)-H(14C)	0.9800
C(5)-H(5)	0.9500	C(15)-H(15A)	0.9800
C(6)-C(7)	1.520(10)	C(15)-H(15B)	0.9800
C(6)-C(7)#1	1.527(10)	C(15)-H(15C)	0.9800
C(7)-C(8B)	1.496(15)	C(16)-H(16A)	0.9800
C(7)-C(8A)	1.502(15)	C(16)-H(16B)	0.9800
C(7)-C(6)#1	1.527(10)	C(16)-H(16C)	0.9800
C(8A)-H(8A1)	0.9800	Sb(1)-F(3B)	1.525(19)
C(8A)-H(8A2)	0.9800	Sb(1)-F(2A)#2	1.814(9)
C(8A)-H(8A3)	0.9800	Sb(1)-F(2A)	1.814(9)
C(8B)-H(8B1)	0.9800	Sb(1)-F(1A)#2	1.804(8)
C(8B)-H(8B2)	0.9800	Sb(1)-F(1A)	1.804(8)
C(8B)-H(8B3)	0.9800	Sb(1)-F(1B)	1.858(15)
C(9)-C(10)	1.489(11)	Sb(1)-F(1B)#2	1.859(15)

Sb(1)-F(2B)#2	1.868(16)	Cl(1)-C(17)	1.72(2)
Sb(1)-F(2B)	1.868(16)	Cl(2)-C(17)	1.75(2)
Sb(1)-F(3A)#2	1.916(8)	C(17)-H(17A)	0.9900
Sb(1)-F(3A)	1.916(8)	C(17)-H(17B)	0.9900
O(1)-Rh(1)-P(1)#1	83.66(3)	C(4)-C(5)-C(6)	121.2(6)
O(1)-Rh(1)-P(1)	83.66(3)	C(4)-C(5)-H(5)	119.4
P(1)#1-Rh(1)-P(1)	167.32(7)	C(6)-C(5)-H(5)	119.4
O(1)-Rh(1)-H(1)	133.708(4)	C(1)-C(6)-C(5)	117.0(6)
P(1)#1-Rh(1)-H(1)	94.38(4)	C(1)-C(6)-C(7)	122.6(7)
P(1)-Rh(1)-H(1)	94.37(4)	C(5)-C(6)-C(7)	119.2(7)
C(2)-P(1)-C(13)	106.0(3)	C(1)-C(6)-C(7)#1	122.0(7)
C(2)-P(1)-C(9)	105.8(3)	C(5)-C(6)-C(7)#1	118.9(7)
C(13)-P(1)-C(9)	115.2(3)	C(7)-C(6)-C(7)#1	24.9(8)
C(2)-P(1)-Rh(1)	99.60(18)	C(8B)-C(7)-C(8A)	103.1(15)
C(13)-P(1)-Rh(1)	114.1(2)	C(8B)-C(7)-C(6)	107.5(7)
C(9)-P(1)-Rh(1)	114.2(2)	C(8A)-C(7)-C(6)	114.7(6)
C(1)#1-O(1)-C(1)	120.3(6)	C(8B)-C(7)-C(6)#1	106.6(7)
C(1)#1-O(1)-Rh(1)	119.8(3)	C(8A)-C(7)-C(6)#1	115.9(6)
C(1)-O(1)-Rh(1)	119.8(3)	C(6)-C(7)-C(6)#1	108.3(9)
C(6)-C(1)-C(2)	123.0(5)	C(7)-C(8A)-H(8A1)	109.5
C(6)-C(1)-O(1)	120.5(5)	C(7)-C(8A)-H(8A2)	109.5
C(2)-C(1)-O(1)	116.4(5)	H(8A1)-C(8A)-H(8A2)	109.5
C(3)-C(2)-C(1)	117.9(5)	C(7)-C(8A)-H(8A3)	109.5
C(3)-C(2)-P(1)	121.6(4)	H(8A1)-C(8A)-H(8A3)	109.5
C(1)-C(2)-P(1)	120.5(4)	H(8A2)-C(8A)-H(8A3)	109.5
C(2)-C(3)-C(4)	120.9(6)	C(7)-C(8B)-H(8B1)	109.5
C(2)-C(3)-H(3)	119.5	C(7)-C(8B)-H(8B2)	109.5
C(4)-C(3)-H(3)	119.5	H(8B1)-C(8B)-H(8B2)	109.5
C(5)-C(4)-C(3)	120.0(6)	C(7)-C(8B)-H(8B3)	109.5
C(5)-C(4)-H(4)	120.0	H(8B1)-C(8B)-H(8B3)	109.5
C(3)-C(4)-H(4)	120.0	H(8B2)-C(8B)-H(8B3)	109.5

C(10)-C(9)-C(11)	109.9(8)	H(14A)-C(14)-H(14B)	109.5
C(10)-C(9)-C(12)	105.1(9)	C(13)-C(14)-H(14C)	109.5
C(11)-C(9)-C(12)	107.9(9)	H(14A)-C(14)-H(14C)	109.5
C(10)-C(9)-P(1)	117.7(5)	H(14B)-C(14)-H(14C)	109.5
C(11)-C(9)-P(1)	109.7(6)	C(13)-C(15)-H(15A)	109.5
C(12)-C(9)-P(1)	106.1(5)	C(13)-C(15)-H(15B)	109.5
C(9)-C(10)-H(10A)	109.5	H(15A)-C(15)-H(15B)	109.5
C(9)-C(10)-H(10B)	109.5	C(13)-C(15)-H(15C)	109.5
H(10A)-C(10)-H(10B)	109.5	H(15A)-C(15)-H(15C)	109.5
C(9)-C(10)-H(10C)	109.5	H(15B)-C(15)-H(15C)	109.5
H(10A)-C(10)-H(10C)	109.5	C(13)-C(16)-H(16A)	109.5
H(10B)-C(10)-H(10C)	109.5	C(13)-C(16)-H(16B)	109.5
C(9)-C(11)-H(11A)	109.5	H(16A)-C(16)-H(16B)	109.5
C(9)-C(11)-H(11B)	109.5	C(13)-C(16)-H(16C)	109.5
H(11A)-C(11)-H(11B)	109.5	H(16A)-C(16)-H(16C)	109.5
C(9)-C(11)-H(11C)	109.5	H(16B)-C(16)-H(16C)	109.5
H(11A)-C(11)-H(11C)	109.5	F(3B)-Sb(1)-F(2A)#2	131.9(4)
H(11B)-C(11)-H(11C)	109.5	F(3B)-Sb(1)-F(2A)	131.9(4)
C(9)-C(12)-H(12A)	109.5	F(2A)#2-Sb(1)-F(2A)	96.2(8)
C(9)-C(12)-H(12B)	109.5	F(3B)-Sb(1)-F(1A)#2	87.9(5)
H(12A)-C(12)-H(12B)	109.5	F(2A)#2-Sb(1)-F(1A)#2	91.4(6)
C(9)-C(12)-H(12C)	109.5	F(2A)-Sb(1)-F(1A)#2	91.4(6)
H(12A)-C(12)-H(12C)	109.5	F(3B)-Sb(1)-F(1A)	87.9(5)
H(12B)-C(12)-H(12C)	109.5	F(2A)#2-Sb(1)-F(1A)	91.4(6)
C(14)-C(13)-C(15)	109.1(8)	F(2A)-Sb(1)-F(1A)	91.4(6)
C(14)-C(13)-C(16)	104.0(9)	F(1A)#2-Sb(1)-F(1A)	175.9(9)
C(15)-C(13)-C(16)	109.0(9)	F(3B)-Sb(1)-F(1B)	99.4(8)
C(14)-C(13)-P(1)	117.7(5)	F(2A)#2-Sb(1)-F(1B)	50.7(8)
C(15)-C(13)-P(1)	110.7(6)	F(2A)-Sb(1)-F(1B)	114.6(8)
C(16)-C(13)-P(1)	105.8(5)	F(1A)#2-Sb(1)-F(1B)	134.1(6)
C(13)-C(14)-H(14A)	109.5	F(1A)-Sb(1)-F(1B)	46.8(6)
C(13)-C(14)-H(14B)	109.5	F(3B)-Sb(1)-F(1B)#2	99.4(8)

F(2A)#2-Sb(1)-F(1B)#2	114.6(8)	F(1A)#2-Sb(1)-F(3A)#2	88.4(5)
F(2A)-Sb(1)-F(1B)#2	50.7(8)	F(1A)-Sb(1)-F(3A)#2	88.7(5)
F(1A)#2-Sb(1)-F(1B)#2	46.8(6)	F(1B)-Sb(1)-F(3A)#2	68.1(8)
F(1A)-Sb(1)-F(1B)#2	134.1(6)	F(1B)#2-Sb(1)-F(3A)#2	127.3(8)
F(1B)-Sb(1)-F(1B)#2	161.3(15)	F(2B)#2-Sb(1)-F(3A)#2	67.0(7)
F(3B)-Sb(1)-F(2B)#2	98.2(7)	F(2B)-Sb(1)-F(3A)#2	126.4(7)
F(2A)#2-Sb(1)-F(2B)#2	51.9(8)	F(3B)-Sb(1)-F(3A)	44.3(3)
F(2A)-Sb(1)-F(2B)#2	115.3(8)	F(2A)#2-Sb(1)-F(3A)	176.2(5)
F(1A)#2-Sb(1)-F(2B)#2	46.2(6)	F(2A)-Sb(1)-F(3A)	87.6(5)
F(1A)-Sb(1)-F(2B)#2	134.6(6)	F(1A)#2-Sb(1)-F(3A)	88.7(5)
F(1B)-Sb(1)-F(2B)#2	88.0(8)	F(1A)-Sb(1)-F(3A)	88.4(5)
F(1B)#2-Sb(1)-F(2B)#2	89.4(8)	F(1B)-Sb(1)-F(3A)	127.3(8)
F(3B)-Sb(1)-F(2B)	98.2(7)	F(1B)#2-Sb(1)-F(3A)	68.1(8)
F(2A)#2-Sb(1)-F(2B)	115.3(8)	F(2B)#2-Sb(1)-F(3A)	126.4(7)
F(2A)-Sb(1)-F(2B)	51.9(8)	F(2B)-Sb(1)-F(3A)	67.0(7)
F(1A)#2-Sb(1)-F(2B)	134.6(6)	F(3A)#2-Sb(1)-F(3A)	88.6(6)
F(1A)-Sb(1)-F(2B)	46.2(6)	Cl(1)-C(17)-Cl(2)	106.3(15)
F(1B)-Sb(1)-F(2B)	89.4(8)	Cl(1)-C(17)-H(17A)	110.5
F(1B)#2-Sb(1)-F(2B)	88.0(8)	Cl(2)-C(17)-H(17A)	110.5
F(2B)#2-Sb(1)-F(2B)	163.6(14)	Cl(1)-C(17)-H(17B)	110.5
F(3B)-Sb(1)-F(3A)#2	44.3(3)	Cl(2)-C(17)-H(17B)	110.5
F(2A)#2-Sb(1)-F(3A)#2	87.6(5)	H(17A)-C(17)-H(17B)	108.7
F(2A)-Sb(1)-F(3A)#2	176.2(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1 #2 -x+1,y,-z

Table F5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[(^t\text{Bu})\text{xanPOP}]\text{Rh}(\text{H})_2]\text{SbF}_6$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	22(1)	19(1)	31(1)	0	13(1)	0
P(1)	19(1)	17(1)	34(1)	0(1)	11(1)	0(1)
O(1)	19(2)	18(2)	49(3)	0	9(2)	0
C(1)	24(2)	21(2)	37(3)	-2(2)	13(2)	-4(2)
C(2)	25(2)	22(2)	22(2)	-2(2)	14(2)	-6(2)
C(3)	27(2)	25(2)	24(2)	0(2)	14(2)	-2(2)
C(4)	33(3)	27(2)	31(3)	-4(2)	19(2)	-9(2)
C(5)	34(3)	23(2)	42(3)	-3(2)	18(2)	-9(2)
C(6)	29(3)	21(2)	53(3)	-2(2)	14(2)	-2(2)
C(7)	26(4)	34(5)	46(5)	-10(3)	19(4)	2(4)
C(8A)	42(6)	50(7)	61(6)	16(5)	23(5)	-6(5)
C(8B)	40(6)	42(6)	70(7)	-25(5)	16(6)	3(5)
C(9)	36(3)	41(4)	43(3)	-10(2)	21(3)	0(2)
C(10)	46(4)	91(5)	63(4)	-31(4)	39(3)	-19(4)
C(11)	62(5)	50(4)	118(7)	-33(4)	59(5)	-4(3)
C(12)	108(6)	102(6)	48(4)	6(4)	46(4)	54(5)
C(13)	39(3)	38(3)	51(3)	13(2)	28(3)	1(2)
C(14)	52(4)	89(5)	37(3)	14(4)	18(3)	-19(4)
C(15)	72(5)	45(4)	59(5)	24(3)	0(4)	-11(4)
C(16)	107(6)	97(6)	73(5)	42(4)	71(5)	37(5)
Sb(1)	13(1)	70(1)	28(1)	0	7(1)	0
F(1A)	81(5)	163(7)	53(4)	15(5)	48(4)	-1(5)
F(2A)	55(5)	61(4)	135(8)	7(5)	28(5)	22(4)
F(3A)	41(4)	62(4)	86(5)	-7(4)	23(4)	-13(3)
F(1B)	54(6)	99(8)	64(7)	2(7)	45(5)	7(6)
F(2B)	54(6)	83(7)	53(5)	0(6)	27(5)	-4(6)
F(3B)	85(7)	86(6)	89(7)	0	43(5)	0
Cl(1)	184(9)	155(8)	190(8)	49(6)	88(7)	-19(7)
Cl(2)	236(10)	163(9)	255(11)	-15(8)	123(8)	-30(8)
C(17)	202(16)	213(17)	205(14)	2(9)	117(12)	-12(9)

Table F6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for mh315-C2.

	x	y	z	U(eq)
H(1)	5000	-1000	6000	38
H(3)	7684	2105	7685	30
H(4)	7746	4305	7748	36
H(5)	6561	5470	6542	42
H(8A1)	4495	5853	2879	82
H(8A2)	5033	4721	2906	82
H(8A3)	5471	5933	3891	82
H(8B1)	4511	6379	4907	87
H(8B2)	5489	6378	5885	87
H(8B3)	5000	5572	6368	87
H(10A)	7885	877	6452	93
H(10B)	7963	-259	5603	93
H(10C)	8095	-501	7136	93
H(11A)	6154	-1815	4625	108
H(11B)	7044	-2138	6023	108
H(11C)	6919	-1882	4498	108
H(12A)	6583	1336	4264	128
H(12B)	5896	274	3487	128
H(12C)	6710	165	3514	128
H(14A)	7890	865	9303	95
H(14B)	8097	-525	9068	95
H(14C)	7960	-251	10326	95
H(15A)	6161	-1832	7694	118
H(15B)	6920	-1876	9355	118
H(15C)	7055	-2147	8094	118
H(16A)	6586	1364	8883	122
H(16B)	6729	220	9928	122
H(16C)	5903	302	8340	122
H(17A)	5349	4377	711	247
H(17B)	4513	3621	-355	247

Table F7. Torsion angles [°] for [(^tBu_{xanPOP})Rh(H)₂]SbF₆.

O(1)-Rh(1)-P(1)-C(2)	0.08(17)	C(4)-C(5)-C(6)-C(1)	0.5(11)
P(1)#1-Rh(1)-P(1)-C(2)	0.09(17)	C(4)-C(5)-C(6)-C(7)	-167.1(7)
O(1)-Rh(1)-P(1)-C(13)	112.5(3)	C(4)-C(5)-C(6)-C(7)#1	164.4(7)
P(1)#1-Rh(1)-P(1)-C(13)	112.5(3)	C(1)-C(6)-C(7)-C(8B)	139.6(11)
O(1)-Rh(1)-P(1)-C(9)	-112.2(3)	C(5)-C(6)-C(7)-C(8B)	-53.5(13)
P(1)#1-Rh(1)-P(1)-C(9)	-112.2(3)	C(7)#1-C(6)-C(7)-C(8B)	43.0(10)
P(1)#1-Rh(1)-O(1)-C(1)#1	-0.2(3)	C(1)-C(6)-C(7)-C(8A)	-106.4(12)
P(1)-Rh(1)-O(1)-C(1)#1	179.8(3)	C(5)-C(6)-C(7)-C(8A)	60.5(13)
P(1)#1-Rh(1)-O(1)-C(1)	179.8(3)	C(7)#1-C(6)-C(7)-C(8A)	157.0(10)
P(1)-Rh(1)-O(1)-C(1)	-0.2(3)	C(1)-C(6)-C(7)-C(6)#1	24.8(9)
C(1)#1-O(1)-C(1)-C(6)	-1.0(5)	C(5)-C(6)-C(7)-C(6)#1	-168.3(9)
Rh(1)-O(1)-C(1)-C(6)	179.0(5)	C(7)#1-C(6)-C(7)-C(6)#1	-71.8(6)
C(1)#1-O(1)-C(1)-C(2)	-179.8(6)	C(2)-P(1)-C(9)-C(10)	64.1(8)
Rh(1)-O(1)-C(1)-C(2)	0.2(6)	C(13)-P(1)-C(9)-C(10)	-52.6(8)
C(6)-C(1)-C(2)-C(3)	1.0(10)	Rh(1)-P(1)-C(9)-C(10)	172.6(7)
O(1)-C(1)-C(2)-C(3)	179.7(4)	C(2)-P(1)-C(9)-C(11)	-169.4(7)
C(6)-C(1)-C(2)-P(1)	-178.9(6)	C(13)-P(1)-C(9)-C(11)	73.9(8)
O(1)-C(1)-C(2)-P(1)	-0.1(7)	Rh(1)-P(1)-C(9)-C(11)	-60.9(7)
C(13)-P(1)-C(2)-C(3)	61.6(5)	C(2)-P(1)-C(9)-C(12)	-53.2(8)
C(9)-P(1)-C(2)-C(3)	-61.2(5)	C(13)-P(1)-C(9)-C(12)	-169.8(7)
Rh(1)-P(1)-C(2)-C(3)	-179.9(4)	Rh(1)-P(1)-C(9)-C(12)	55.3(7)
C(13)-P(1)-C(2)-C(1)	-118.6(5)	C(2)-P(1)-C(13)-C(14)	-64.1(8)
C(9)-P(1)-C(2)-C(1)	118.6(5)	C(9)-P(1)-C(13)-C(14)	52.5(8)
Rh(1)-P(1)-C(2)-C(1)	0.0(5)	Rh(1)-P(1)-C(13)-C(14)	-172.6(7)
C(1)-C(2)-C(3)-C(4)	-0.1(8)	C(2)-P(1)-C(13)-C(15)	169.4(7)
P(1)-C(2)-C(3)-C(4)	179.7(4)	C(9)-P(1)-C(13)-C(15)	-74.0(8)
C(2)-C(3)-C(4)-C(5)	-0.5(9)	Rh(1)-P(1)-C(13)-C(15)	60.9(8)
C(3)-C(4)-C(5)-C(6)	0.3(10)	C(2)-P(1)-C(13)-C(16)	51.5(7)
C(2)-C(1)-C(6)-C(5)	-1.2(11)	C(9)-P(1)-C(13)-C(16)	168.1(7)
O(1)-C(1)-C(6)-C(5)	-179.9(6)	Rh(1)-P(1)-C(13)-C(16)	-57.0(7)
C(2)-C(1)-C(6)-C(7)	166.0(7)		
O(1)-C(1)-C(6)-C(7)	-12.8(11)		
C(2)-C(1)-C(6)-C(7)#1	-164.5(7)		
O(1)-C(1)-C(6)-C(7)#1	16.7(11)		

Symmetry transformations used to generate equivalent atoms: #1 $-x+1,y,-z+1$ #2 $-x+1,y,-z$

Figure G1: ORTEP diagram of (^tBu_{xan}POP)Rh(H)

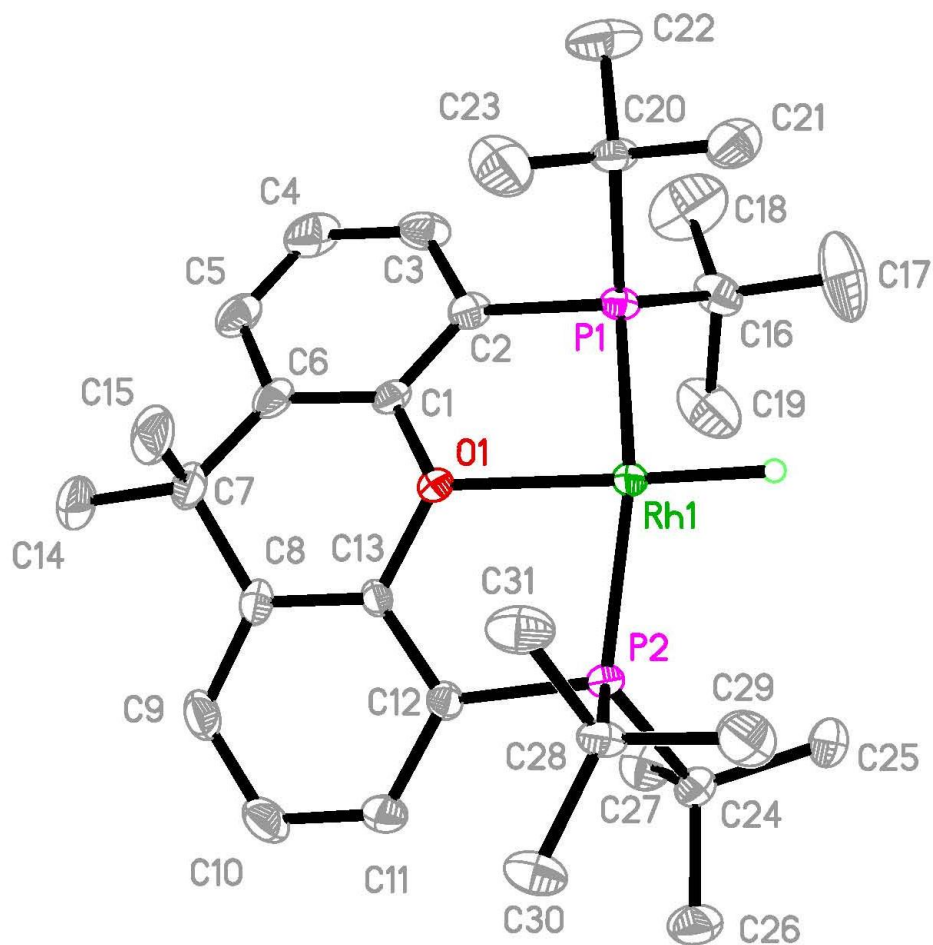


Table G2. Crystal data and structure refinement for (^tBu₃xanPOP)Rh(H).

Identification code	mh316	
Empirical formula	C ₃₁ H ₄₉ O P ₂ Rh	
Formula weight	602.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 15.2555(12) Å	α = 90°.
	b = 19.6805(15) Å	β = 90°.
	c = 20.5255(16) Å	γ = 90°.
Volume	6162.5(8) Å ³	
Z	8	
Density (calculated)	1.299 Mg/m ³	
Absorption coefficient	0.679 mm ⁻¹	
F(000)	2544	
Crystal size	0.38 x 0.18 x 0.04 mm ³	
Theta range for data collection	1.96 to 30.03°.	
Index ranges	0 ≤ h ≤ 21, 0 ≤ k ≤ 27, 0 ≤ l ≤ 28	
Reflections collected	9007	
Independent reflections	9007 [R(int) = 0.0000]	
Completeness to theta = 30.03°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9734 and 0.7825	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9007 / 1 / 334	
Goodness-of-fit on F ²	1.001	
Final R indices [I > 2σ(I)]	R1 = 0.0577, wR2 = 0.1215	
R indices (all data)	R1 = 0.0786, wR2 = 0.1306	
Largest diff. peak and hole	1.157 and -0.802 e.Å ⁻³	

Table G3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (**^tBu_xanPOP**)Rh(**H**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Rh(1)	7894(1)	1346(1)	6023(1)	16(1)
P(1)	8926(1)	1151(1)	6766(1)	17(1)
P(2)	7181(1)	1751(1)	5155(1)	16(1)
O(1)	8236(2)	2411(1)	6187(1)	16(1)
C(1)	8963(2)	2556(2)	6578(2)	17(1)
C(2)	9414(2)	2006(2)	6854(2)	20(1)
C(3)	10141(2)	2166(2)	7241(2)	28(1)
C(4)	10394(3)	2834(2)	7345(2)	34(1)
C(5)	9912(3)	3358(2)	7082(2)	29(1)
C(6)	9179(2)	3235(2)	6701(2)	21(1)
C(7)	8556(3)	3784(2)	6465(2)	24(1)
C(8)	8194(2)	3570(2)	5809(2)	20(1)
C(9)	7963(3)	4028(2)	5318(2)	28(1)
C(10)	7546(3)	3807(2)	4759(2)	30(1)
C(11)	7314(2)	3134(2)	4696(2)	24(1)
C(12)	7521(2)	2649(2)	5175(2)	18(1)
C(13)	7993(2)	2889(2)	5710(2)	16(1)
C(14)	8966(3)	4492(2)	6447(2)	35(1)
C(15)	7770(3)	3801(2)	6950(2)	34(1)
C(16)	9843(2)	570(2)	6494(2)	26(1)
C(17)	9494(3)	-149(2)	6479(3)	58(2)
C(18)	10699(4)	592(4)	6880(3)	67(2)
C(19)	10054(4)	783(3)	5805(2)	53(1)
C(20)	8560(2)	977(2)	7632(2)	23(1)
C(21)	7972(3)	351(2)	7622(2)	36(1)
C(22)	9267(3)	866(3)	8147(2)	45(1)
C(23)	7997(4)	1587(2)	7819(2)	47(1)
C(24)	7543(3)	1428(2)	4330(2)	23(1)

C(25)	7576(3)	644(2)	4378(2)	32(1)
C(26)	6977(3)	1619(2)	3746(2)	34(1)
C(27)	8484(3)	1681(2)	4226(2)	33(1)
C(28)	5951(2)	1815(2)	5222(2)	21(1)
C(29)	5568(3)	1100(2)	5154(2)	35(1)
C(30)	5468(3)	2308(2)	4771(2)	30(1)
C(31)	5795(3)	2064(2)	5925(2)	32(1)

Table G4. Bond lengths [Å] and angles [°] for (^tBu_{xan}POP)Rh(H).

Rh(1)-O(1)	2.186(2)	C(11)-H(11)	0.9500
Rh(1)-P(1)	2.2261(9)	C(12)-C(13)	1.397(4)
Rh(1)-P(2)	2.2342(8)	C(14)-H(14A)	0.9800
Rh(1)-H(1)	1.607(10)	C(14)-H(14B)	0.9800
P(1)-C(2)	1.849(3)	C(14)-H(14C)	0.9800
P(1)-C(16)	1.890(4)	C(15)-H(15A)	0.9800
P(1)-C(20)	1.894(3)	C(15)-H(15B)	0.9800
P(2)-C(12)	1.841(3)	C(15)-H(15C)	0.9800
P(2)-C(28)	1.886(4)	C(16)-C(19)	1.510(6)
P(2)-C(24)	1.892(3)	C(16)-C(17)	1.512(6)
O(1)-C(1)	1.399(4)	C(16)-C(18)	1.528(6)
O(1)-C(13)	1.406(4)	C(17)-H(17A)	0.9800
C(1)-C(6)	1.400(4)	C(17)-H(17B)	0.9800
C(1)-C(2)	1.401(5)	C(17)-H(17C)	0.9800
C(2)-C(3)	1.401(5)	C(18)-H(18A)	0.9800
C(3)-C(4)	1.386(5)	C(18)-H(18B)	0.9800
C(3)-H(3)	0.9500	C(18)-H(18C)	0.9800
C(4)-C(5)	1.377(6)	C(19)-H(19A)	0.9800
C(4)-H(4)	0.9500	C(19)-H(19B)	0.9800
C(5)-C(6)	1.386(5)	C(19)-H(19C)	0.9800
C(5)-H(5)	0.9500	C(20)-C(21)	1.524(5)
C(6)-C(7)	1.518(5)	C(20)-C(23)	1.525(6)
C(7)-C(8)	1.515(5)	C(20)-C(22)	1.527(5)
C(7)-C(14)	1.528(5)	C(21)-H(21A)	0.9800
C(7)-C(15)	1.558(5)	C(21)-H(21B)	0.9800
C(8)-C(13)	1.389(4)	C(21)-H(21C)	0.9800
C(8)-C(9)	1.397(5)	C(22)-H(22A)	0.9800
C(9)-C(10)	1.383(6)	C(22)-H(22B)	0.9800
C(9)-H(9)	0.9500	C(22)-H(22C)	0.9800
C(10)-C(11)	1.378(5)	C(23)-H(23A)	0.9800
C(10)-H(10)	0.9500	C(23)-H(23B)	0.9800
C(11)-C(12)	1.407(4)	C(23)-H(23C)	0.9800

C(24)-C(26)	1.524(5)	C(28)-C(30)	1.530(5)
C(24)-C(27)	1.533(6)	C(28)-C(29)	1.531(5)
C(24)-C(25)	1.546(5)	C(28)-C(31)	1.543(5)
C(25)-H(25A)	0.9800	C(29)-H(29A)	0.9800
C(25)-H(25B)	0.9800	C(29)-H(29B)	0.9800
C(25)-H(25C)	0.9800	C(29)-H(29C)	0.9800
C(26)-H(26A)	0.9800	C(30)-H(30A)	0.9800
C(26)-H(26B)	0.9800	C(30)-H(30B)	0.9800
C(26)-H(26C)	0.9800	C(30)-H(30C)	0.9800
C(27)-H(27A)	0.9800	C(31)-H(31A)	0.9800
C(27)-H(27B)	0.9800	C(31)-H(31B)	0.9800
C(27)-H(27C)	0.9800	C(31)-H(31C)	0.9800
O(1)-Rh(1)-P(1)	83.75(6)	O(1)-C(1)-C(6)	118.9(3)
O(1)-Rh(1)-P(2)	84.04(6)	O(1)-C(1)-C(2)	117.7(3)
P(1)-Rh(1)-P(2)	162.20(3)	C(6)-C(1)-C(2)	123.3(3)
O(1)-Rh(1)-H(1)	175.2(15)	C(3)-C(2)-C(1)	116.4(3)
P(1)-Rh(1)-H(1)	96.8(15)	C(3)-C(2)-P(1)	125.3(3)
P(2)-Rh(1)-H(1)	96.4(15)	C(1)-C(2)-P(1)	117.8(2)
C(2)-P(1)-C(16)	106.36(17)	C(4)-C(3)-C(2)	121.4(4)
C(2)-P(1)-C(20)	101.14(15)	C(4)-C(3)-H(3)	119.3
C(16)-P(1)-C(20)	112.70(16)	C(2)-C(3)-H(3)	119.3
C(2)-P(1)-Rh(1)	101.20(11)	C(5)-C(4)-C(3)	120.0(4)
C(16)-P(1)-Rh(1)	115.15(13)	C(5)-C(4)-H(4)	120.0
C(20)-P(1)-Rh(1)	117.70(12)	C(3)-C(4)-H(4)	120.0
C(12)-P(2)-C(28)	102.38(15)	C(4)-C(5)-C(6)	121.5(3)
C(12)-P(2)-C(24)	105.06(15)	C(4)-C(5)-H(5)	119.3
C(28)-P(2)-C(24)	112.18(16)	C(6)-C(5)-H(5)	119.3
C(12)-P(2)-Rh(1)	100.86(11)	C(5)-C(6)-C(1)	117.2(3)
C(28)-P(2)-Rh(1)	116.75(11)	C(5)-C(6)-C(7)	124.1(3)
C(24)-P(2)-Rh(1)	116.89(12)	C(1)-C(6)-C(7)	118.4(3)
C(1)-O(1)-C(13)	118.2(2)	C(8)-C(7)-C(6)	108.2(3)
C(1)-O(1)-Rh(1)	118.19(18)	C(8)-C(7)-C(14)	112.4(3)
C(13)-O(1)-Rh(1)	118.13(18)	C(6)-C(7)-C(14)	113.6(3)

C(8)-C(7)-C(15)	107.0(3)	C(19)-C(16)-C(18)	107.2(4)
C(6)-C(7)-C(15)	107.1(3)	C(17)-C(16)-C(18)	109.8(4)
C(14)-C(7)-C(15)	108.1(3)	C(19)-C(16)-P(1)	105.5(3)
C(13)-C(8)-C(9)	117.5(3)	C(17)-C(16)-P(1)	108.2(3)
C(13)-C(8)-C(7)	118.6(3)	C(18)-C(16)-P(1)	117.5(3)
C(9)-C(8)-C(7)	123.6(3)	C(16)-C(17)-H(17A)	109.5
C(10)-C(9)-C(8)	120.8(3)	C(16)-C(17)-H(17B)	109.5
C(10)-C(9)-H(9)	119.6	H(17A)-C(17)-H(17B)	109.5
C(8)-C(9)-H(9)	119.6	C(16)-C(17)-H(17C)	109.5
C(11)-C(10)-C(9)	119.9(3)	H(17A)-C(17)-H(17C)	109.5
C(11)-C(10)-H(10)	120.1	H(17B)-C(17)-H(17C)	109.5
C(9)-C(10)-H(10)	120.1	C(16)-C(18)-H(18A)	109.5
C(10)-C(11)-C(12)	121.9(3)	C(16)-C(18)-H(18B)	109.5
C(10)-C(11)-H(11)	119.0	H(18A)-C(18)-H(18B)	109.5
C(12)-C(11)-H(11)	119.0	C(16)-C(18)-H(18C)	109.5
C(13)-C(12)-C(11)	115.9(3)	H(18A)-C(18)-H(18C)	109.5
C(13)-C(12)-P(2)	119.1(2)	H(18B)-C(18)-H(18C)	109.5
C(11)-C(12)-P(2)	125.0(3)	C(16)-C(19)-H(19A)	109.5
C(8)-C(13)-C(12)	123.7(3)	C(16)-C(19)-H(19B)	109.5
C(8)-C(13)-O(1)	119.0(3)	H(19A)-C(19)-H(19B)	109.5
C(12)-C(13)-O(1)	117.2(3)	C(16)-C(19)-H(19C)	109.5
C(7)-C(14)-H(14A)	109.5	H(19A)-C(19)-H(19C)	109.5
C(7)-C(14)-H(14B)	109.5	H(19B)-C(19)-H(19C)	109.5
H(14A)-C(14)-H(14B)	109.5	C(21)-C(20)-C(23)	108.0(4)
C(7)-C(14)-H(14C)	109.5	C(21)-C(20)-C(22)	108.0(3)
H(14A)-C(14)-H(14C)	109.5	C(23)-C(20)-C(22)	109.7(4)
H(14B)-C(14)-H(14C)	109.5	C(21)-C(20)-P(1)	107.9(2)
C(7)-C(15)-H(15A)	109.5	C(23)-C(20)-P(1)	105.0(3)
C(7)-C(15)-H(15B)	109.5	C(22)-C(20)-P(1)	117.8(3)
H(15A)-C(15)-H(15B)	109.5	C(20)-C(21)-H(21A)	109.5
C(7)-C(15)-H(15C)	109.5	C(20)-C(21)-H(21B)	109.5
H(15A)-C(15)-H(15C)	109.5	H(21A)-C(21)-H(21B)	109.5
H(15B)-C(15)-H(15C)	109.5	C(20)-C(21)-H(21C)	109.5
C(19)-C(16)-C(17)	108.3(4)	H(21A)-C(21)-H(21C)	109.5

H(21B)-C(21)-H(21C)	109.5	C(24)-C(27)-H(27A)	109.5
C(20)-C(22)-H(22A)	109.5	C(24)-C(27)-H(27B)	109.5
C(20)-C(22)-H(22B)	109.5	H(27A)-C(27)-H(27B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(24)-C(27)-H(27C)	109.5
C(20)-C(22)-H(22C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(27B)-C(27)-H(27C)	109.5
H(22B)-C(22)-H(22C)	109.5	C(30)-C(28)-C(29)	110.1(3)
C(20)-C(23)-H(23A)	109.5	C(30)-C(28)-C(31)	106.9(3)
C(20)-C(23)-H(23B)	109.5	C(29)-C(28)-C(31)	108.5(3)
H(23A)-C(23)-H(23B)	109.5	C(30)-C(28)-P(2)	118.5(2)
C(20)-C(23)-H(23C)	109.5	C(29)-C(28)-P(2)	108.2(3)
H(23A)-C(23)-H(23C)	109.5	C(31)-C(28)-P(2)	104.0(2)
H(23B)-C(23)-H(23C)	109.5	C(28)-C(29)-H(29A)	109.5
C(26)-C(24)-C(27)	110.0(3)	C(28)-C(29)-H(29B)	109.5
C(26)-C(24)-C(25)	108.3(3)	H(29A)-C(29)-H(29B)	109.5
C(27)-C(24)-C(25)	107.6(3)	C(28)-C(29)-H(29C)	109.5
C(26)-C(24)-P(2)	117.1(3)	H(29A)-C(29)-H(29C)	109.5
C(27)-C(24)-P(2)	106.7(2)	H(29B)-C(29)-H(29C)	109.5
C(25)-C(24)-P(2)	106.7(3)	C(28)-C(30)-H(30A)	109.5
C(24)-C(25)-H(25A)	109.5	C(28)-C(30)-H(30B)	109.5
C(24)-C(25)-H(25B)	109.5	H(30A)-C(30)-H(30B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(28)-C(30)-H(30C)	109.5
C(24)-C(25)-H(25C)	109.5	H(30A)-C(30)-H(30C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(30B)-C(30)-H(30C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(28)-C(31)-H(31A)	109.5
C(24)-C(26)-H(26A)	109.5	C(28)-C(31)-H(31B)	109.5
C(24)-C(26)-H(26B)	109.5	H(31A)-C(31)-H(31B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(28)-C(31)-H(31C)	109.5
C(24)-C(26)-H(26C)	109.5	H(31A)-C(31)-H(31C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(31B)-C(31)-H(31C)	109.5
H(26B)-C(26)-H(26C)	109.5		

Table G5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (^tBu xanPOP)Rh(H). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	19(1)	14(1)	15(1)	1(1)	-4(1)	0(1)
P(1)	16(1)	20(1)	15(1)	3(1)	-2(1)	0(1)
P(2)	19(1)	16(1)	13(1)	0(1)	-3(1)	0(1)
O(1)	19(1)	16(1)	14(1)	-1(1)	-3(1)	-1(1)
C(1)	20(2)	21(2)	12(1)	-2(1)	1(1)	-5(1)
C(2)	20(2)	24(2)	17(2)	1(1)	-1(1)	-6(1)
C(3)	24(2)	36(2)	25(2)	8(2)	-7(2)	-7(2)
C(4)	29(2)	45(2)	28(2)	1(2)	-8(2)	-19(2)
C(5)	33(2)	31(2)	21(2)	-4(1)	0(2)	-15(2)
C(6)	25(2)	24(2)	14(1)	-4(1)	5(1)	-7(1)
C(7)	33(2)	18(2)	22(2)	-5(1)	5(1)	-4(1)
C(8)	24(2)	16(1)	21(2)	-4(1)	5(1)	-3(1)
C(9)	39(2)	14(1)	30(2)	2(1)	4(2)	0(1)
C(10)	40(2)	22(2)	26(2)	9(1)	2(2)	3(2)
C(11)	32(2)	24(2)	17(2)	5(1)	-2(1)	-2(1)
C(12)	23(2)	15(1)	15(1)	1(1)	3(1)	-1(1)
C(13)	22(2)	12(1)	14(1)	0(1)	4(1)	1(1)
C(14)	49(3)	21(2)	35(2)	-6(2)	-3(2)	-7(2)
C(15)	41(2)	28(2)	33(2)	-10(2)	9(2)	8(2)
C(16)	21(2)	28(2)	28(2)	6(1)	4(1)	7(1)
C(17)	44(3)	26(2)	106(5)	-4(3)	28(3)	6(2)
C(18)	42(3)	97(5)	64(4)	-19(3)	-13(3)	36(3)
C(19)	67(3)	47(3)	45(3)	13(2)	31(3)	24(3)
C(20)	26(2)	29(2)	14(1)	3(1)	-2(1)	-6(1)
C(21)	46(3)	40(2)	22(2)	1(2)	6(2)	-22(2)
C(22)	36(2)	75(3)	23(2)	10(2)	-9(2)	-14(2)
C(23)	61(3)	42(2)	37(2)	7(2)	23(2)	13(2)
C(24)	30(2)	22(2)	18(2)	-3(1)	-2(1)	2(1)

C(25)	47(2)	21(2)	29(2)	-7(1)	-5(2)	5(2)
C(26)	46(3)	38(2)	18(2)	-1(2)	-5(2)	8(2)
C(27)	32(2)	39(2)	28(2)	-2(2)	8(2)	4(2)
C(28)	21(2)	25(2)	18(2)	5(1)	-4(1)	0(1)
C(29)	27(2)	34(2)	44(2)	8(2)	-10(2)	-8(2)
C(30)	24(2)	37(2)	27(2)	9(2)	-3(2)	6(2)
C(31)	26(2)	47(2)	22(2)	6(2)	4(1)	5(2)

Table G6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for (**^tBu_xanPOP**)Rh(**H**).

	x	y	z	U(eq)
H(1)	7580(30)	572(9)	5950(20)	29(11)
H(3)	10468	1810	7436	34
H(4)	10900	2930	7598	41
H(5)	10086	3813	7163	34
H(9)	8095	4496	5370	33
H(10)	7420	4120	4419	35
H(11)	7004	2993	4317	29
H(14A)	9449	4497	6133	53
H(14B)	9190	4608	6881	53
H(14C)	8522	4825	6317	53
H(15A)	7334	4130	6798	51
H(15B)	7980	3934	7383	51
H(15C)	7503	3349	6974	51
H(17A)	8931	-157	6248	87
H(17B)	9411	-313	6925	87
H(17C)	9913	-443	6252	87
H(18A)	11080	219	6740	101
H(18B)	10571	545	7346	101
H(18C)	10994	1027	6802	101
H(19A)	10485	469	5619	79
H(19B)	10295	1244	5807	79
H(19C)	9518	774	5542	79
H(21A)	8327	-53	7528	54
H(21B)	7523	404	7284	54
H(21C)	7689	298	8048	54
H(22A)	9669	1254	8149	67
H(22B)	9595	450	8047	67

H(22C)	8993	821	8577	67
H(23A)	7723	1505	8243	70
H(23B)	7541	1655	7489	70
H(23C)	8366	1994	7844	70
H(25A)	6979	466	4420	48
H(25B)	7921	512	4760	48
H(25C)	7848	458	3984	48
H(26A)	6946	2115	3709	51
H(26B)	6385	1435	3806	51
H(26C)	7234	1429	3349	51
H(27A)	8744	1445	3853	49
H(27B)	8832	1588	4618	49
H(27C)	8476	2171	4143	49
H(29A)	4942	1110	5262	52
H(29B)	5872	791	5452	52
H(29C)	5643	941	4705	52
H(30A)	5591	2190	4316	44
H(30B)	5667	2773	4857	44
H(30C)	4836	2277	4850	44
H(31A)	5164	2079	6013	47
H(31B)	6044	2520	5978	47
H(31C)	6078	1752	6232	47

Table G7. Torsion angles [°] for (^tBu_{xan}POP)Rh(H).

O(1)-Rh(1)-P(1)-C(2)	-9.15(13)	C(1)-C(2)-C(3)-C(4)	0.2(5)
P(2)-Rh(1)-P(1)-C(2)	37.75(16)	P(1)-C(2)-C(3)-C(4)	-171.5(3)
O(1)-Rh(1)-P(1)-C(16)	-123.37(14)	C(2)-C(3)-C(4)-C(5)	2.0(6)
P(2)-Rh(1)-P(1)-C(16)	-76.47(17)	C(3)-C(4)-C(5)-C(6)	-1.1(6)
O(1)-Rh(1)-P(1)-C(20)	99.89(14)	C(4)-C(5)-C(6)-C(1)	-1.9(5)
P(2)-Rh(1)-P(1)-C(20)	146.80(15)	C(4)-C(5)-C(6)-C(7)	172.1(4)
O(1)-Rh(1)-P(2)-C(12)	6.31(13)	O(1)-C(1)-C(6)-C(5)	-179.0(3)
P(1)-Rh(1)-P(2)-C(12)	-40.56(16)	C(2)-C(1)-C(6)-C(5)	4.3(5)
O(1)-Rh(1)-P(2)-C(28)	-103.63(14)	O(1)-C(1)-C(6)-C(7)	6.6(4)
P(1)-Rh(1)-P(2)-C(28)	-150.51(15)	C(2)-C(1)-C(6)-C(7)	-170.1(3)
O(1)-Rh(1)-P(2)-C(24)	119.51(15)	C(5)-C(6)-C(7)-C(8)	148.2(3)
P(1)-Rh(1)-P(2)-C(24)	72.64(17)	C(1)-C(6)-C(7)-C(8)	-37.8(4)
P(1)-Rh(1)-O(1)-C(1)	7.7(2)	C(5)-C(6)-C(7)-C(14)	22.6(5)
P(2)-Rh(1)-O(1)-C(1)	-159.3(2)	C(1)-C(6)-C(7)-C(14)	-163.4(3)
P(1)-Rh(1)-O(1)-C(13)	161.2(2)	C(5)-C(6)-C(7)-C(15)	-96.7(4)
P(2)-Rh(1)-O(1)-C(13)	-5.9(2)	C(1)-C(6)-C(7)-C(15)	77.3(4)
C(13)-O(1)-C(1)-C(6)	28.1(4)	C(6)-C(7)-C(8)-C(13)	38.6(4)
Rh(1)-O(1)-C(1)-C(6)	-178.4(2)	C(14)-C(7)-C(8)-C(13)	164.9(3)
C(13)-O(1)-C(1)-C(2)	-154.9(3)	C(15)-C(7)-C(8)-C(13)	-76.5(4)
Rh(1)-O(1)-C(1)-C(2)	-1.5(4)	C(6)-C(7)-C(8)-C(9)	-148.3(3)
O(1)-C(1)-C(2)-C(3)	179.7(3)	C(14)-C(7)-C(8)-C(9)	-22.0(5)
C(6)-C(1)-C(2)-C(3)	-3.5(5)	C(15)-C(7)-C(8)-C(9)	96.6(4)
O(1)-C(1)-C(2)-P(1)	-7.9(4)	C(13)-C(8)-C(9)-C(10)	0.4(6)
C(6)-C(1)-C(2)-P(1)	168.9(3)	C(7)-C(8)-C(9)-C(10)	-172.8(4)
C(16)-P(1)-C(2)-C(3)	-55.4(4)	C(8)-C(9)-C(10)-C(11)	3.3(6)
C(20)-P(1)-C(2)-C(3)	62.5(3)	C(9)-C(10)-C(11)-C(12)	-2.8(6)
Rh(1)-P(1)-C(2)-C(3)	-176.0(3)	C(10)-C(11)-C(12)-C(13)	-1.4(5)
C(16)-P(1)-C(2)-C(1)	133.0(3)	C(10)-C(11)-C(12)-P(2)	176.2(3)
C(20)-P(1)-C(2)-C(1)	-109.1(3)	C(28)-P(2)-C(12)-C(13)	112.7(3)
Rh(1)-P(1)-C(2)-C(1)	12.4(3)	C(24)-P(2)-C(12)-C(13)	-130.0(3)

Rh(1)-P(2)-C(12)-C(13)	-8.1(3)	C(16)-P(1)-C(20)-C(22)	44.2(4)
C(28)-P(2)-C(12)-C(11)	-64.8(3)	Rh(1)-P(1)-C(20)-C(22)	-178.1(3)
C(24)-P(2)-C(12)-C(11)	52.6(3)	C(12)-P(2)-C(24)-C(26)	-78.1(3)
Rh(1)-P(2)-C(12)-C(11)	174.5(3)	C(28)-P(2)-C(24)-C(26)	32.4(3)
C(9)-C(8)-C(13)-C(12)	-4.9(5)	Rh(1)-P(2)-C(24)-C(26)	171.1(2)
C(7)-C(8)-C(13)-C(12)	168.6(3)	C(12)-P(2)-C(24)-C(27)	45.7(3)
C(9)-C(8)-C(13)-O(1)	178.3(3)	C(28)-P(2)-C(24)-C(27)	156.1(2)
C(7)-C(8)-C(13)-O(1)	-8.2(5)	Rh(1)-P(2)-C(24)-C(27)	-65.1(3)
C(11)-C(12)-C(13)-C(8)	5.3(5)	C(12)-P(2)-C(24)-C(25)	160.5(3)
P(2)-C(12)-C(13)-C(8)	-172.4(3)	C(28)-P(2)-C(24)-C(25)	-89.1(3)
C(11)-C(12)-C(13)-O(1)	-177.9(3)	Rh(1)-P(2)-C(24)-C(25)	49.7(3)
P(2)-C(12)-C(13)-O(1)	4.5(4)	C(12)-P(2)-C(28)-C(30)	49.1(3)
C(1)-O(1)-C(13)-C(8)	-27.4(4)	C(24)-P(2)-C(28)-C(30)	-63.0(3)
Rh(1)-O(1)-C(13)-C(8)	179.1(2)	Rh(1)-P(2)-C(28)-C(30)	158.2(2)
C(1)-O(1)-C(13)-C(12)	155.6(3)	C(12)-P(2)-C(28)-C(29)	175.3(2)
Rh(1)-O(1)-C(13)-C(12)	2.1(4)	C(24)-P(2)-C(28)-C(29)	63.2(3)
C(2)-P(1)-C(16)-C(19)	-69.6(3)	Rh(1)-P(2)-C(28)-C(29)	-75.6(3)
C(20)-P(1)-C(16)-C(19)	-179.5(3)	C(12)-P(2)-C(28)-C(31)	-69.4(3)
Rh(1)-P(1)-C(16)-C(19)	41.6(3)	C(24)-P(2)-C(28)-C(31)	178.5(2)
C(2)-P(1)-C(16)-C(17)	174.7(3)	Rh(1)-P(2)-C(28)-C(31)	39.7(3)
C(20)-P(1)-C(16)-C(17)	64.7(4)		
Rh(1)-P(1)-C(16)-C(17)	-74.1(4)		
C(2)-P(1)-C(16)-C(18)	49.8(4)		
C(20)-P(1)-C(16)-C(18)	-60.2(4)		
Rh(1)-P(1)-C(16)-C(18)	160.9(4)		
C(2)-P(1)-C(20)-C(21)	168.5(3)		
C(16)-P(1)-C(20)-C(21)	-78.4(3)		
Rh(1)-P(1)-C(20)-C(21)	59.4(3)		
C(2)-P(1)-C(20)-C(23)	53.4(3)		
C(16)-P(1)-C(20)-C(23)	166.6(3)		
Rh(1)-P(1)-C(20)-C(23)	-55.7(3)		
C(2)-P(1)-C(20)-C(22)	-69.0(3)		

