Electronic Supplementary Information for Dalton Transactions

Supporting Information

Rh complexes derived from pincer diphosphite ligands. Rare preferred *in-plane* olefin conformation in square-planar complexes

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Representative experimental procedures

General Comments. All reactions and manipulations were performed under nitrogen or argon, either in a Braun Labmaster 100 glovebox or using standard Schlenk-type techniques. All solvents were distilled under nitrogen using the following dessicants: Sodium-benzophenone-ketyl for benzene, diethylether (Et_2O) and tetrahydrofuran (THF); sodium for petroleum ether and toluene; CaH_2 for dichloromethane (CH_2Cl_2) and NaOMe for methanol (MeOH). Chlorophosphites **1**[1] and $Rh(Cl)(PPh_3)_3$[2] were prepared according to literature procedures. NMR spectra were obtained on Bruker DPX-300, DRX-400 or DRX-500 spectrometers. $^{31}P\{^1H\}$ NMR shifts were referenced to external 85% H_3PO_4, while $^{13}C\{^1H\}$ and ^1H shifts were referenced to the residual signals of deuterated solvents. All data are reported in ppm downfield from Me_4Si. HRMS data were obtained using a Jeol JMS-SX 102A mass spectrometer. Elemental Analysis were run by the Analytical Service of the Instituto de Investigaciones Químicas. In the following section **PCP**[a] denotes the ligand resulting from deprotonation of **2a**.

***μ*-1,3-phenylene-bis[1,1'(3,3',5,5'-tetra-*tert*-butyl)biphen-2,2'-diyl]diphosphite (2a).** Over a solution of phosphorochloridite **1a** (4.74 g, 10 mmol) and NEt_3 (1.5 mL, 11 mmol) in THF (40 mL), was slowly added a resorcinol (0.55g, 5 mmol) solution in the same solvent (40 mL). After stirring for 16 h, solvent was evaporated, the residue treated with Et_2O (3 x 50 mL) and filtered through a pad of neutral alumina. Removal of the solvent yielded compound **2a** as a white foamy solid (4.29 g, 87%). ^1H RMN ($CDCl_3$, 400 MHz): δ 1.36 (s, 36H, 4 CMe_3), 1.48 (s, 36H, 4 CMe_3), 6.80 (dd, $^3J_{HH}$ = 8.4 Hz, $^4J_{HH}$ = 2.5 Hz, 2H, 2 H arom), 6.92 (m, 1H, H arom), 7.16 (t, $^3J_{HH}$ = 8.4 Hz, 1H, H arom), 7.20 (d, $^4J_{HH}$ = 2.4 Hz, 4H, 4 H arom), 7.45 (d, $^4J_{HH}$ = 2.4 Hz, 4H, 4 H arom). $^{31}P\{^1H\}$ RMN ($CDCl_3$, 202.4 MHz): δ 137.9 (s). $^{13}C\{^1H\}$ RMN ($CDCl_3$, 100.6 MHz): δ 31.3 (brs, 4 C*Me*$_3$), 31.5 (s, 4 C*Me*$_3$), 34.7 (4 *C*Me$_3$), 35.5 (4 *C*Me$_3$), 112.8 (t, J_{PC} = 8 Hz, CH arom), 115.8 (d, J_{PC} = 9 Hz, 2 CH arom), 124.4 (s, 4 CH arom), 126.6 (s, 4 CH arom), 130.0 (s, CH arom), 132.8 (d, J_{PC} = 2 Hz, 4 C_q arom), 140.3 (s, 4 C_q arom), 145.3

[1] (a) G. J. H. Buisman, P. C. J. Kamer, P. W. N. M. van Leeuwen, *Tetrahedron: Asymmetry* 1993, **4**, 1625; (b) A. Suárez, M. A. Méndez-Rojas and A. Pizzano, *Organometallics* 2002, **21** 4611.
[2] A. Osborn, F. H. Jardine, J. F. Young, G. Wilkinson, *J. Chem. Soc. (A)* 1966, 1711.

(d, J_{PC} = 6 Hz, 4 C_q arom), 146.8 (s, 4 C_q arom), 153.2 (d, J_{PC} = 7 Hz, 2 C_q arom). HRMS (FAB): *m/z* 986.5755, $[M]^+$ (exact mass calculated for $C_{62}H_{84}O_6P_2$: 986.5743)

Rh(PCP^a)(PPh$_3$) (3a). Over a suspension of $RhCl(PPh_3)_3$ (0.46 g, 0.5 mmol) in THF (5 mL) was added diphosphite **2a** (0.49 g, 0.5 mmol) dissolved in THF (10 mL). The mixture was heated over 24 h at 70ºC. An excess of NEt_3 (0.1 mL) was added and the mixture vigorously stirred for 24 h. Solvent was removed under reduced pressure and the resulting solid was purified by column chromatography on silicagel (AcOEt:Hex 1:20) yielding **3a** as an orange solid (0.58 g, 85%). ^{1}H RMN ($CDCl_3$, 400 MHz): δ 1.20 (s, 36H, 4 CMe_3), 1.38 (s, 36H, 4 CMe_3), 6.42 (d, $^3J_{HH}$ = 8 Hz, 2H, 2 H arom), 6.71 (t, $^3J_{HH}$ = 7 Hz, 6H, 6 H arom), 6.84 (t, 1H, $^3J_{HH}$ = 8 Hz, H arom), 6.97 (t, $^3J_{HH}$ = 7 Hz, 3H, 3 H arom), 7.10 (sa, 4H, 4 H arom), 7.33 (sa, 4H, 4 H arom), 7.35 (d, $^3J_{HH}$ = 7 Hz, 6H, 6 H arom). $^{31}P\{^1H\}$ RMN ($CDCl_3$, 162.1 MHz): δ 28.6 (td, J_{PRh} = 129 Hz, J_{PP} = 44 Hz, P-C), 171.5 (dd, J_{PRh} = 265 Hz, P-O). $^{13}C\{^1H\}$ RMN ($CDCl_3$, 75.5 MHz): δ 31.8 (s, 4 C*Me*$_3$), 31.9 (s, 4 C*Me*$_3$), 35.0 (4 *C*Me$_3$), 35.8 (4 *C*Me$_3$), 105.3 (t, J_{PC} = 8 Hz, 2 CH arom), 124.6 (s, 4 CH arom), 126.0 (s, CH arom), 127.6 (s, 4 CH arom), 128.0 (d, J_{PC} = 9 Hz, 6 CH arom), 129.0 (s, 3 CH arom), 131.4 (s, 4 C_q arom), 134.0 (d, J_{PC} = 13 Hz, 6 CH arom), 137.7 (d, J_{PC} = 36 Hz, 3 C_q arom), 140.1 (s, 4 C_q arom), 140.7 (ddd, J_{PC} = 58, 14 Hz, J_{RhC} = 28 Hz, C_q arom), 146.6 (s, 4 C_q arom), 147.4 (t, J_{PC} = 5 Hz, 4 OC_q arom), 159.5 (t, J_{PC} = 13 Hz, 2 OC_q arom). Anal. Calcd for: $C_{80}H_{98}O_6P_3Rh$: C 71.1, H 7.3. Found C 70.6, H 7.4.

Rh(PCP^a)(CO) (4a). To a solution of compound **3a** (0.04 g, 0.03 mmol) in THF (10 mL) was added an excess of elemental selenium (0.005 g, 0.06 mmol). The mixture was introduced in a Fischer-Porter vessel and charged with 2 atm of CO. After 1h the reactor was vented and solvent removed. The solution was concentrated until started turbidity and filtered. After standing for 24 h compound **4a** was collected as yellow crystals (0.020 g, 60%). IR (nujol mull, cm^{-1}): 2017 (υ_{CO}). ^{1}H RMN ($CDCl_3$, 500 MHz): δ 1.33 (s, 36H, 4 CMe_3), 1.40 (s, 36H, 4 CMe_3), 6.64 (d, $^3J_{HH}$ = 8 Hz, 2H, 2 H arom), 7.05 (t, $^3J_{HH}$ = 8 Hz, 1H, H arom), 7.20 (d, $^4J_{HH}$ = 2 Hz, 4H, 4 H arom), 7.45 (d, $^4J_{HH}$ = 2 Hz, 4H, 4 H arom). $^{31}P\{^1H\}$ RMN ($CDCl_3$, 162.1 MHz): δ 167.3 (d, J_{PRh} = 256 Hz). $^{13}C\{^1H\}$ RMN ($CDCl_3$, 125.8 MHz): δ 31.5 (s, 4 C*Me*$_3$), 31.7 (s, 4 C*Me*$_3$), 34.7 (4 *C*Me$_3$), 35.7 (4 *C*Me$_3$), 106.1 (t, J_{PC} = 8 Hz, 2 CH arom), 125.0 (s, 4 CH arom), 126.6 (s, 4 CH arom), 129.5 (s, CH arom), 131.6 (s, 4 C_q arom), 140.2 (m, C_q arom), 140.3 (s, 4 C_q arom), 145.1 (s, 4 OC_q arom), 147.6 (s, 4 C_q arom), 160.4 (t, J_{PC} = 14 Hz, 2 OC_q

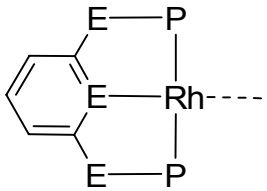
arom), 191.8 (dt, J_{RhC} = 58 Hz, J_{PC} = 16 Hz, CO). Anal. Calcd for: $C_{63}H_{83}O_7P_2Rh$: C 67.7, H 7.5. Found: C 67.9, H 7.9.

Rh(PCP^a)(η^2-C_2H_4) (5a). In a Fischer-Porter vessel compound **3a** (0.108 g, 0.08 mmol) and Se (0.010 g, 0.13 mmol) were added to THF (10 mL). The reactor was charged with 4 atm of C_2H_4 and heated at 40ºC. Reaction completion was observed after 4 d. Solvent was removed under reduce pressure and the remaining solid extracted with *n*-pentane (3x10 mL). Further filtration and concentration yielded **5a** as orange crystals (0.040 g, 45%). ^{1}H RMN (CD_2Cl_2, 400 MHz): δ 1.30 (s, 36H, 4 CMe_3), 1.39 (s, 36H, 4 CMe_3), 2.82 (brs, 4H, C_2H_4), 6.68 (d, $^3J_{HH}$ = 8 Hz, 2H, 2 H arom), 7.01 (t, $^3J_{HH}$ = 8 Hz, 1H, H arom), 7.28 (d, $^4J_{HH}$ = 2.5 Hz, 4H, 4 H arom), 7.50 (d, $^4J_{HH}$ = 2.5 Hz, 4H, 4 H arom). ^{31}P{^{1}H} RMN (CD_2Cl_2, 162.1 MHz): δ 177.3 (d, J_{PRh} = 253 Hz). ^{13}C{^{1}H} RMN ($CDCl_3$, 75.5 MHz): δ 31.5 (s, 4 C*Me*$_3$), 31.5 (s, 4 C*Me*$_3$), 34.7 (4 *C*Me$_3$), 35.6 (4 *C*Me$_3$), 58.8 (brs, C_2H_4), 105.7 (t, J_{PC} = 9 Hz, 2 CH arom), 124.8 (s, 4 CH arom), 125.2 (s, CH arom), 126.7 (s, 4 CH arom), 131.6 (s, 4 C_q arom), 139.9 (dt, J_{RhC} = 29 Hz, J_{PC} = 16 Hz, C_q arom), 140.1 (s, 4 C_q arom), 145.5 (brs, 4 OC_q arom), 147.4 (s, 4 C_q arom), 158.8 (t, J_{PC} = 16 Hz, 2 OC_q arom). Anal. Calcd for: $C_{64}H_{87}O_6P_2Rh$: C 68.8; H 7.8. Found: C 69.0, H 8.2.

QUEST3D-search Details

The QUEST3D searches commented in the text have been carried out on the Cambridge Structural Database (updated May 2006) and have the following details:

(a) Analysis of the P-M-P angles in square-planar transition metal complexes containing a pincer ligand (see chart, E is any heteroatom). The CSD search with restrictions (not disordered, no errors, $R \leq 0.075$) gave a mean value of 165º (57 fragments, 47 hits).



(b) Analysis of the C-C distance of ethylene rhodium complexes. The CSD search without any restriction, gave a mean value of 1.39 Å (139 fragments, 64 hits). A similar value (1.38 Å for 115 fragments, 52 hits) was obtained with restrictions (not disordered, no errors, $R \leq 0.075$).

Computational Details

The electronic structures and geometries of the model complexes **I-VI** were computed within the density functional theory at the B3LYP level.[3] The Rh atom was described with the Stuttgart Relativistic Small Core ECP basis set[4] and a polarization function. In all cases the atoms corresponding to the pincer ligand are described using a TZVP basis set. For the more complex models **IV-VI**, the biphenyl groups are described using a DZVP basis set. All the calculations were performed using the Gaussian03 package.[5] Figures were drawn using Molekel.[6] XYZ coordinates of all optimized complexes are available upon request.

[3] (a) A. D. *J. Chem. Phys.* 1993, **98**, 5648. (b) C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785.
[4] M. Dolg, H. Stoll, H. Preuss, R. M. Pitzer, *J. Phys. Chem*. **1993**, *97*, 5852.
[5] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.
[6] S. Portmann, H. P. Luthi, *Chimia* **2000**, *54*, 766.

Table S1. Computed energy differences of the ***ip*** and ***u*** conformers of models **I**-**VI**.

Model Complex	**Relative Energy**[a]
$RhPh(PH_3)_2(C_2H_4)$ (**I**)	+10.8
$Rh\{C_6H_3(OPH_2)_2\}(C_2H_4)$ (**II**)	-0.9
$Rh\{C_6H_3(CH_2PH_2)_2\}(C_2H_4)$ (**III**)	+1.0
$Rh\{C_6H_3(OP(OC_6H_4\text{-}OC_6H_4)_2\}(C_2H_4)$ (**IV**)	-0.1
$Rh\{C_6H_3(OP(OC_6H_3Me\text{-}OC_6H_4)_2\}(C_2H_4)$ (**V**)	-0.6
$Rh\{C_6H_3(OP(OC_6H_3tBu\text{-}OC_6H_4)_2\}(C_2H_4)$ (**VI**)	[b]

[a] A negative value for the relative energy indicates that the ***ip*** conformer is the most stable. [b] ***u*** conformation does not optimize.

Table S2. Selected bond distances and angles for model compounds **I-III**.

Selected bond distances (Å) and angles (º)	**Calculated**					
	$RhPh(PH_3)_2(C_2H_4)$ **I**		$Rh\{C_6H_3(OPH_2)_2\}(C_2H_4)$ **II**		$Rh\{C_6H_3(CH_2PH_2)_2\}(C_2H_4)$ **III**	
	ip	***u***	***ip***	***u***	***ip***	***u***
$Rh\text{-}C_{(ethylene)}$	2.335	2.239	2.250	2.255	2.260	2.249
$Rh\text{-}C_{ipso}$	2.144	2.132	2.065	2.053	2.108	2.096
Rh-P	2.326	2.308	2.260	2.273	2.283	2.288
C-C (ethylene)	1.363	1.386	1.383	1.379	1.377	1.380
P-Rh-P	174.6	176.9	155.4	157.1	158.5	162.6
Plane Rh-PCP/ plane Rh-$CC_{(ethylene)}$	0	90	0	90	14.8	76.3

Table S3. Selected bond distances and angles for model compounds **IV**-**VI** and comparison with experimental data.

	Calculated					**Experimental**	
	IV-*ip*	**IV-*u***	**V-*ip***	**V-*u***	**VI-*ip***	**5a**	**5b**
Bond distances (Å)							
Rh-$C_{(ethylene)}$	2.286	2.282	2.288	2.284	2.285	2.2184(14) 2.2353(14)	2.228(3) 2.230(3)
Rh-C_{ipso}	2.057	2.046	2.057	2.048	2.057	2.0233(12)	2.019(3)
Rh-P	2.259	2.265	2.259	2.266	2.259	2.2076(3) 2.2165(3)	2.2237(7) 2.2096(7)
C-C (ethylene)	1.374	1.372	1.374	1.372	1.373	1.377(2)	1.353(4)
Angles (º)							
P-Rh-P	155.1	156.9	155.0	157.9	155.1	155.490(13)	155.37(3)
Plane Rh-PCP/ plane Rh-$CC_{(ethylene)}$	4.1	82.7	8.8	86.9	7.9	7.4	13.0

Figure S1. Optimized structures of conformers ***ip*** (right) and ***u*** (left) of model complex $RhPh(PH_3)_2(C_2H_4)$ (**I**).

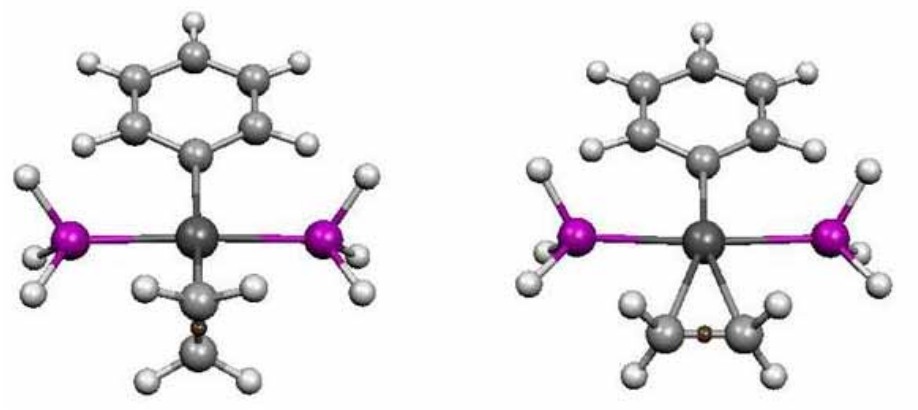


Figure S2. Optimized structures of conformers ***ip*** (right) and ***u*** (left) of model complex $Rh\{C_6H_3(OPH_2)_2\}(C_2H_4)$ (**II**).

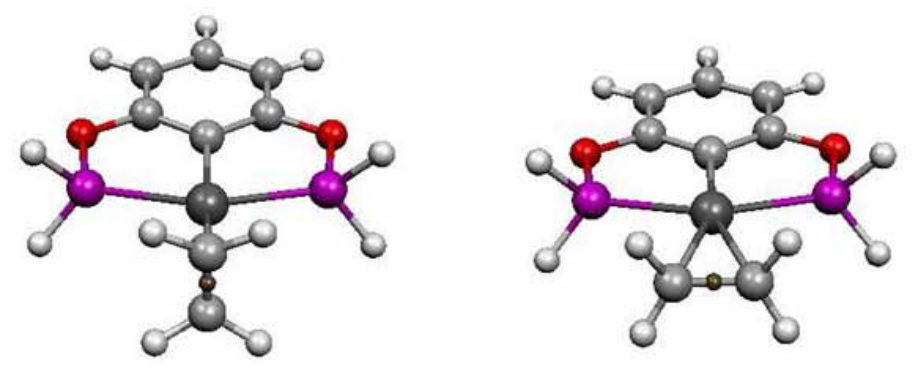


Figure S3. Optimized structures of conformers ***ip*** (right) and ***u*** (left) of model complex $Rh\{C_6H_3(CH_2PH_2)_2\}(C_2H_4)$ (**III**).

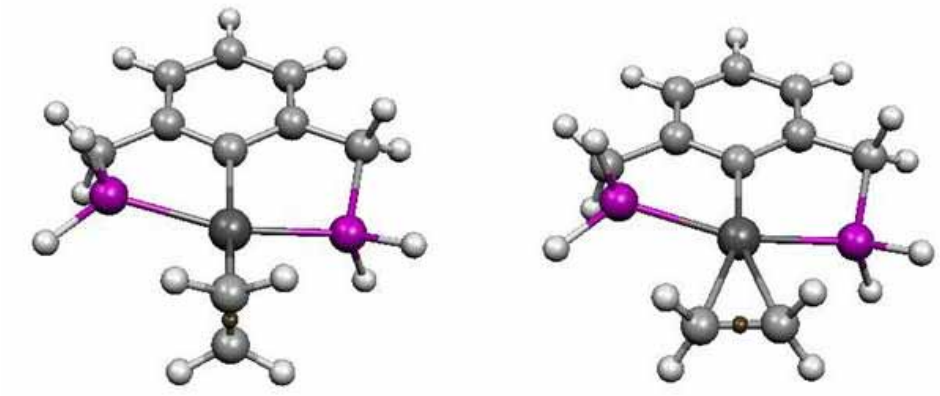


Figure S4. Optimized structures of conformers ***ip*** (top) and ***u*** (bottom) of model complex Rh{C_6H_3(OP(OC_6H_4-OC_6H_4)$_2$}(C_2H_4) (**IV**).

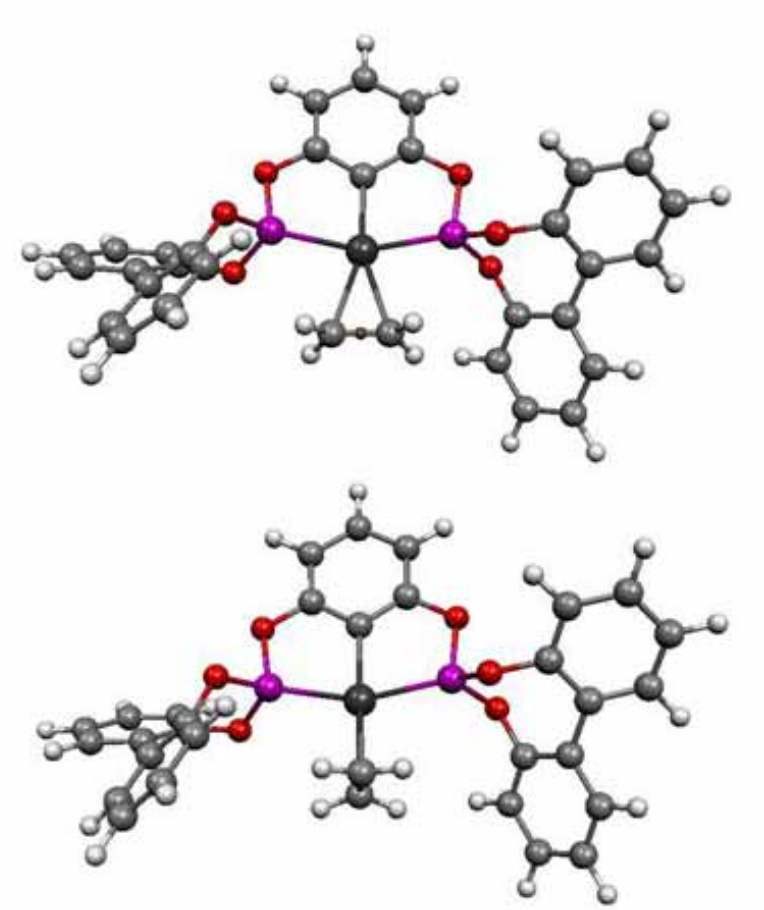


Figure S5. Optimized structures of the conformers ***ip*** (top) and ***u*** (bottom) of model complex Rh{C_6H_3(OP(OC_6H_3Me-OC_6H_4)$_2$}(C_2H_4) (**V**).

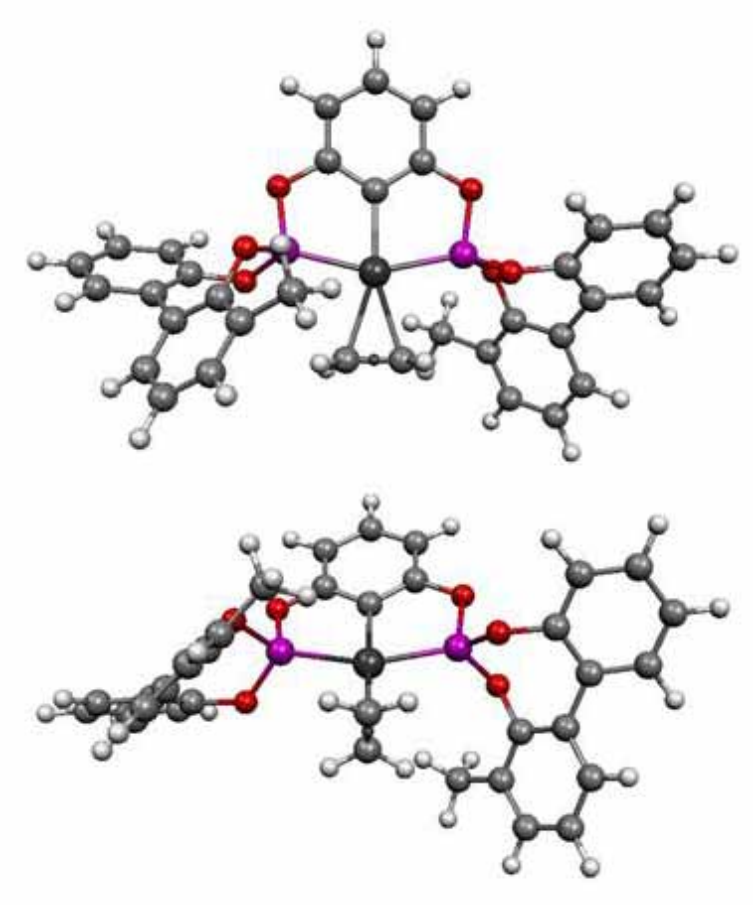
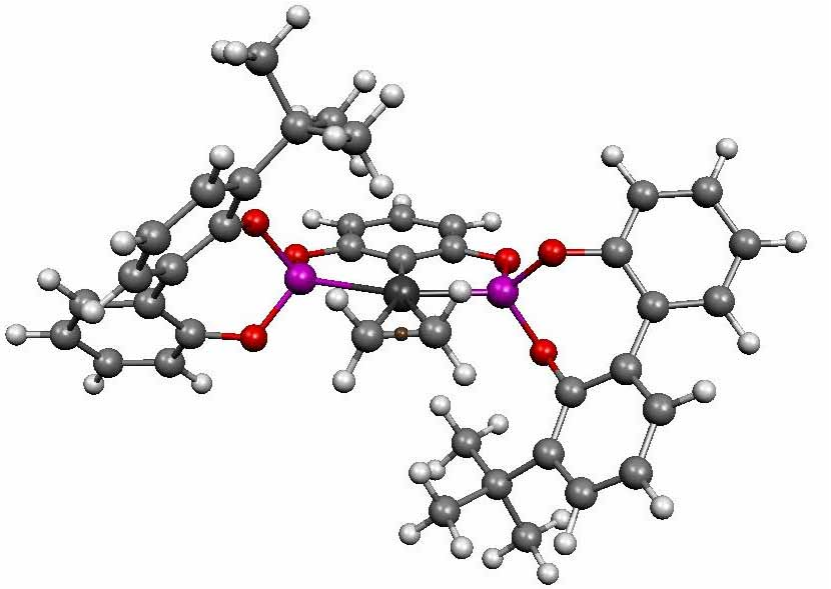


Figure S6. Optimized structures of the conformer ***ip*** of model complex Rh{C_6H_3(OP(OC_6H_3-*t*-Bu-OC_6H_4)$_2$}(C_2H_4) (**VI**)



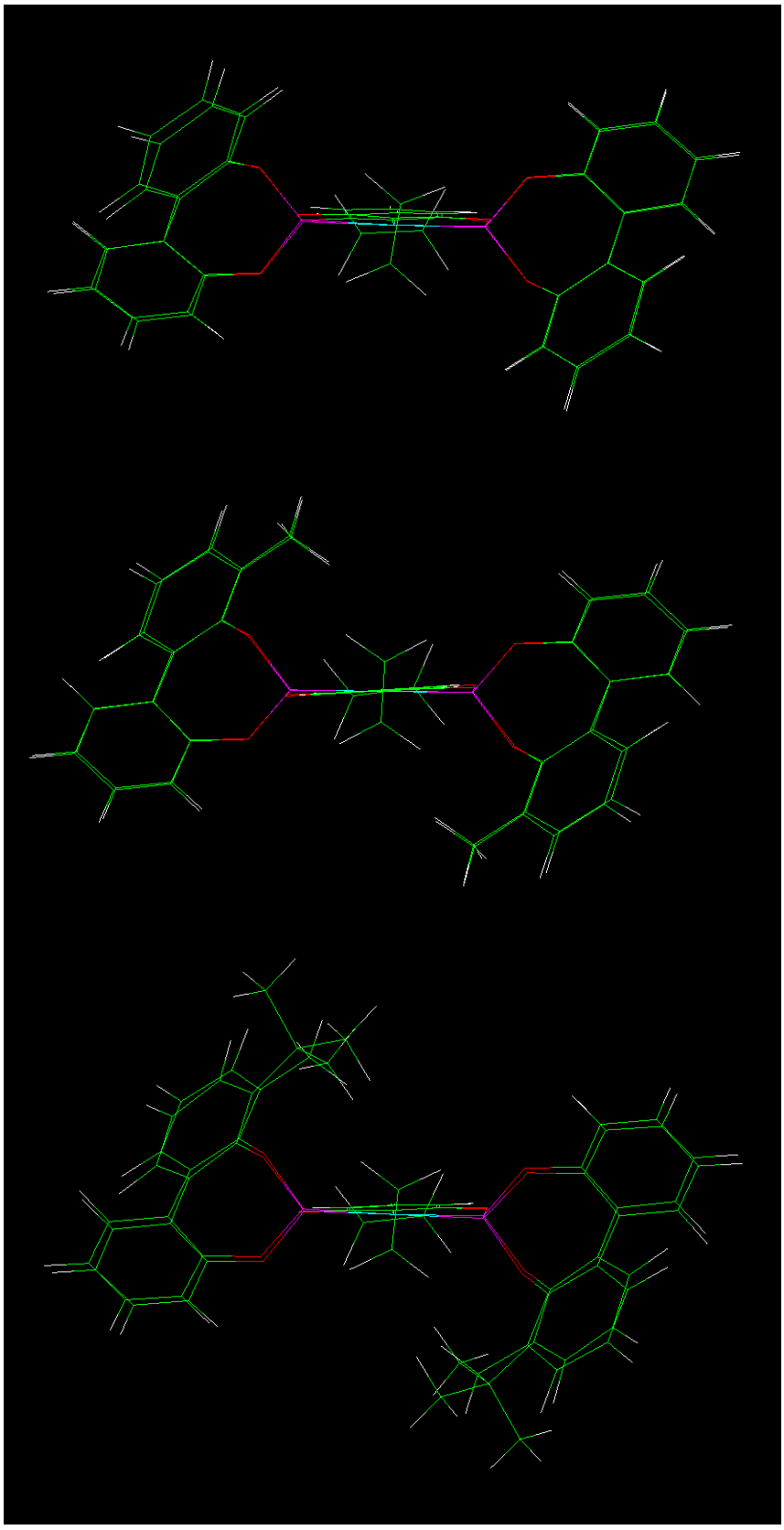


Figure S7. Superposition of ethylene conformers: **IV**-***ip*** and **IV**-***u*** (top), **V**-***ip*** and **V**-***u*** (middle), **VI**-***ip*** and **V**-***u*** (bottom).

Figure S8. ORTEP view (30% ellipsoids) of one single enantiomer of the racemate present in the crystallographic unit cell of **5a**. H atoms (except for ethylene) and solvent have been omitted for clarity.

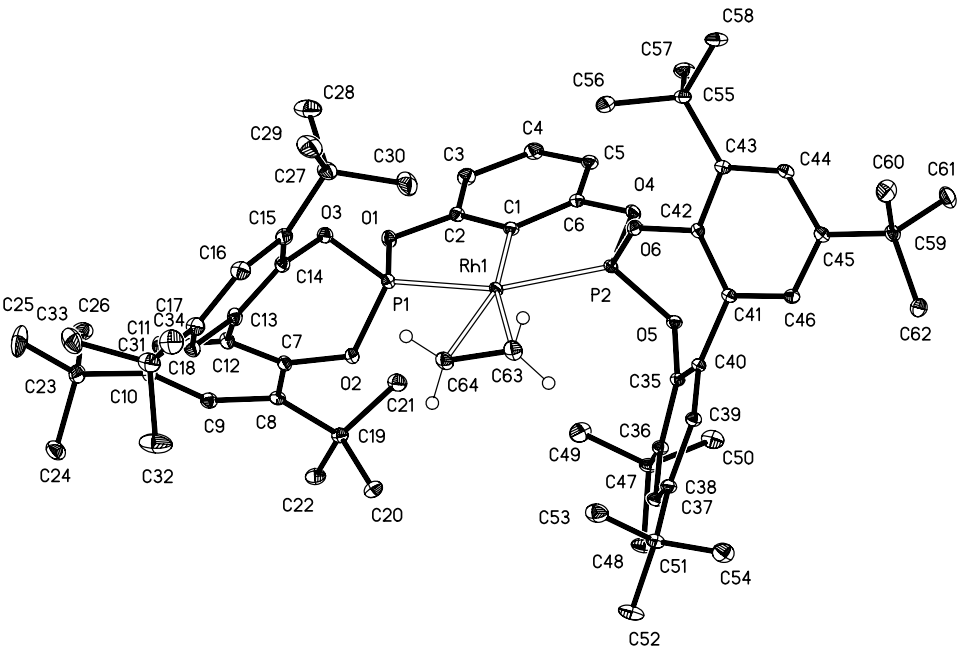


Table S4. Crystal data and structure refinement for **5a**.

Empirical formula	$C_{69}\ H_{99}\ O_6\ P_2\ Rh$	
	$[C_{64}\ H_{87}\ O_6\ P_2\ Rh,\ C_5\ H_{12}]$	
Formula weight	1189.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.2239(5) Å	α= 90°.
	b = 19.2234(6) Å	β= 97.7050(10)°.
	c = 20.3456(6) Å	γ = 90°.
Volume	6675.6(3) $Å^3$	
Z	4	
Density (calculated)	1.183 Mg/m^3	
Absorption coefficient	0.351 mm^{-1}	
F(000)	2544	
Crystal size	0.30 x 0.26 x 0.24 mm^3	
Theta range for data collection	2.35 to 30.52°.	
Index ranges	-20<=h<=24, -27<=k<=26, -29<=l<=29	
Reflections collected	153626	
Independent reflections	20381 [R(int) = 0.0346]	
Completeness to theta = 30.52°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9205 and 0.9020	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20381 / 35 / 719	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0797	
R indices (all data)	R1 = 0.0392, wR2 = 0.0850	
Largest diff. peak and hole	0.883 and -0.796 $e.Å^{-3}$	

Table S5. Bond lengths [Å] and angles [°] for **5a**

Rh(1)-C(1)	2.0233(12)	C(12)-C(13)	1.4853(18)
Rh(1)-P(1)	2.2076(3)	C(13)-C(18)	1.3972(19)
Rh(1)-P(2)	2.2165(3)	C(13)-C(14)	1.3981(18)
Rh(1)-C(64)	2.2184(14)	C(14)-C(15)	1.4022(18)
Rh(1)-C(63)	2.2353(14)	C(15)-C(16)	1.4009(19)
P(1)-O(2)	1.6053(9)	C(15)-C(27)	1.5455(19)
P(1)-O(1)	1.6187(10)	C(16)-C(17)	1.395(2)
P(1)-O(3)	1.6194(10)	C(16)-H(16)	0.9500
P(2)-O(6)	1.5974(10)	C(17)-C(18)	1.3888(19)
P(2)-O(4)	1.6220(10)	C(17)-C(31)	1.530(2)
P(2)-O(5)	1.6234(10)	C(18)-H(18)	0.9500
O(1)-C(2)	1.4030(15)	C(19)-C(22)	1.5390(19)
O(2)-C(7)	1.4039(15)	C(19)-C(21)	1.5396(19)
O(3)-C(14)	1.4015(16)	C(19)-C(20)	1.5446(19)
O(4)-C(6)	1.4051(15)	C(20)-H(20A)	0.9800
O(5)-C(35)	1.4036(15)	C(20)-H(20B)	0.9800
O(6)-C(42)	1.3941(15)	C(20)-H(20C)	0.9800
C(1)-C(2)	1.3947(18)	C(21)-H(21A)	0.9800
C(1)-C(6)	1.3947(17)	C(21)-H(21B)	0.9799
C(2)-C(3)	1.3896(18)	C(21)-H(21C)	0.9800
C(3)-C(4)	1.395(2)	C(22)-H(22A)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22B)	0.9800
C(4)-C(5)	1.389(2)	C(22)-H(22C)	0.9800
C(4)-H(4)	0.9500	C(23)-C(25)	1.533(2)
C(5)-C(6)	1.3870(18)	C(23)-C(26)	1.536(2)
C(5)-H(5)	0.9500	C(23)-C(24)	1.536(2)
C(7)-C(12)	1.3915(18)	C(24)-H(24A)	0.9800
C(7)-C(8)	1.4030(17)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.3984(18)	C(24)-H(24C)	0.9800
C(8)-C(19)	1.5389(18)	C(25)-H(25A)	0.9800
C(9)-C(10)	1.4036(19)	C(25)-H(25B)	0.9800
C(9)-H(9)	0.9500	C(25)-H(25C)	0.9800
C(10)-C(11)	1.3900(19)	C(26)-H(26A)	0.9800
C(10)-C(23)	1.5343(19)	C(26)-H(26B)	0.9800
C(11)-C(12)	1.4016(18)	C(26)-H(26C)	0.9800
C(11)-H(11)	0.9500	C(27)-C(30)	1.528(2)

C(27)-C(29)	1.533(2)	C(43)-C(55)	1.5391(18)
C(27)-C(28)	1.549(2)	C(44)-C(45)	1.4000(18)
C(28)-H(28A)	0.9800	C(44)-H(44)	0.9500
C(28)-H(28B)	0.9800	C(45)-C(46)	1.3896(17)
C(28)-H(28C)	0.9800	C(45)-C(59)	1.5330(18)
C(29)-H(29A)	0.9800	C(46)-H(46)	0.9499
C(29)-H(29B)	0.9800	C(47)-C(49)	1.535(2)
C(29)-H(29C)	0.9800	C(47)-C(48)	1.5372(18)
C(30)-H(30A)	0.9800	C(47)-C(50)	1.541(2)
C(30)-H(30B)	0.9800	C(48)-H(48A)	0.9800
C(30)-H(30C)	0.9800	C(48)-H(48B)	0.9800
C(31)-C(34)	1.534(2)	C(48)-H(48C)	0.9800
C(31)-C(33)	1.537(2)	C(49)-H(49A)	0.9800
C(31)-C(32)	1.539(2)	C(49)-H(49B)	0.9800
C(32)-H(32A)	0.9800	C(49)-H(49C)	0.9800
C(32)-H(32B)	0.9800	C(50)-H(50A)	0.9801
C(32)-H(32C)	0.9800	C(50)-H(50B)	0.9800
C(33)-H(33A)	0.9800	C(50)-H(50C)	0.9800
C(33)-H(33B)	0.9800	C(51)-C(52)	1.5315(18)
C(33)-H(33C)	0.9800	C(51)-C(54)	1.535(2)
C(34)-H(34A)	0.9800	C(51)-C(53)	1.539(2)
C(34)-H(34B)	0.9800	C(52)-H(52A)	0.9800
C(34)-H(34C)	0.9800	C(52)-H(52B)	0.9800
C(35)-C(40)	1.3951(17)	C(52)-H(52C)	0.9800
C(35)-C(36)	1.4037(17)	C(53)-H(53A)	0.9800
C(36)-C(37)	1.4012(18)	C(53)-H(53B)	0.9800
C(36)-C(47)	1.5412(18)	C(53)-H(53C)	0.9800
C(37)-C(38)	1.3968(18)	C(54)-H(54A)	0.9800
C(37)-H(37)	0.9500	C(54)-H(54B)	0.9800
C(38)-C(39)	1.3988(17)	C(54)-H(54C)	0.9800
C(38)-C(51)	1.5333(18)	C(55)-C(57)	1.538(2)
C(39)-C(40)	1.3962(17)	C(55)-C(58)	1.5404(19)
C(39)-H(39)	0.9500	C(55)-C(56)	1.544(2)
C(40)-C(41)	1.4935(17)	C(56)-H(56A)	0.9800
C(41)-C(42)	1.3932(17)	C(56)-H(56B)	0.9800
C(41)-C(46)	1.4023(17)	C(56)-H(56C)	0.9800
C(42)-C(43)	1.4078(17)	C(57)-H(57A)	0.9800
C(43)-C(44)	1.3935(18)	C(57)-H(57B)	0.9800

C(57)-H(57C)	0.9800	C(1)-Rh(1)-P(1)	77.68(4)
C(58)-H(58A)	0.9800	C(1)-Rh(1)-P(2)	77.87(4)
C(58)-H(58B)	0.9800	P(1)-Rh(1)-P(2)	155.490(13)
C(58)-H(58C)	0.9800	C(1)-Rh(1)-C(64)	160.39(5)
C(59)-C(62)	1.5319(19)	P(1)-Rh(1)-C(64)	83.21(4)
C(59)-C(61)	1.535(2)	P(2)-Rh(1)-C(64)	121.30(4)
C(59)-C(60)	1.540(2)	C(1)-Rh(1)-C(63)	163.41(5)
C(60)-H(60A)	0.9800	P(1)-Rh(1)-C(63)	118.91(4)
C(60)-H(60B)	0.9800	P(2)-Rh(1)-C(63)	85.54(4)
C(60)-H(60C)	0.9800	C(64)-Rh(1)-C(63)	36.01(5)
C(61)-H(61A)	0.9800	O(2)-P(1)-O(1)	105.75(5)
C(61)-H(61B)	0.9800	O(2)-P(1)-O(3)	103.74(5)
C(61)-H(61C)	0.9800	O(1)-P(1)-O(3)	95.53(5)
C(62)-H(62A)	0.9800	O(2)-P(1)-Rh(1)	114.13(4)
C(62)-H(62B)	0.9800	O(1)-P(1)-Rh(1)	110.47(4)
C(62)-H(62C)	0.9800	O(3)-P(1)-Rh(1)	124.51(4)
C(63)-C(64)	1.377(2)	O(6)-P(2)-O(4)	105.11(5)
C(63)-H(63A)	0.926(14)	O(6)-P(2)-O(5)	103.56(5)
C(63)-H(63B)	0.947(15)	O(4)-P(2)-O(5)	95.35(5)
C(64)-H(64A)	0.953(14)	O(6)-P(2)-Rh(1)	113.70(4)
C(64)-H(64B)	0.964(14)	O(4)-P(2)-Rh(1)	110.00(4)
C(65)-C(66)	1.550(11)	O(5)-P(2)-Rh(1)	126.12(4)
C(65)-H(65A)	0.9800	C(2)-O(1)-P(1)	111.77(8)
C(65)-H(65B)	0.9800	C(7)-O(2)-P(1)	123.72(8)
C(65)-H(65C)	0.9800	C(14)-O(3)-P(1)	120.55(8)
C(66)-C(67)	1.506(10)	C(6)-O(4)-P(2)	111.77(8)
C(66)-H(66A)	0.9900	C(35)-O(5)-P(2)	115.25(8)
C(66)-H(66B)	0.9900	C(42)-O(6)-P(2)	131.16(8)
C(67)-C(68)	1.505(11)	C(2)-C(1)-C(6)	115.07(11)
C(67)-H(67A)	0.9900	C(2)-C(1)-Rh(1)	122.46(9)
C(67)-H(67B)	0.9900	C(6)-C(1)-Rh(1)	122.43(9)
C(68)-C(69)	1.423(12)	C(3)-C(2)-C(1)	124.05(12)
C(68)-H(68A)	0.9900	C(3)-C(2)-O(1)	118.61(12)
C(68)-H(68B)	0.9900	C(1)-C(2)-O(1)	117.34(11)
C(69)-H(69A)	0.9800	C(2)-C(3)-C(4)	117.72(13)
C(69)-H(69B)	0.9800	C(2)-C(3)-H(3)	121.1
C(69)-H(69C)	0.9800	C(4)-C(3)-H(3)	121.2
		C(5)-C(4)-C(3)	121.08(12)

C(5)-C(4)-H(4)	119.5	C(18)-C(17)-C(16)	117.52(13)
C(3)-C(4)-H(4)	119.4	C(18)-C(17)-C(31)	120.34(13)
C(6)-C(5)-C(4)	118.28(12)	C(16)-C(17)-C(31)	122.11(13)
C(6)-C(5)-H(5)	120.9	C(17)-C(18)-C(13)	121.51(13)
C(4)-C(5)-H(5)	120.9	C(17)-C(18)-H(18)	119.3
C(5)-C(6)-C(1)	123.77(12)	C(13)-C(18)-H(18)	119.2
C(5)-C(6)-O(4)	118.76(11)	C(8)-C(19)-C(22)	111.26(11)
C(1)-C(6)-O(4)	117.46(11)	C(8)-C(19)-C(21)	111.81(10)
C(12)-C(7)-C(8)	123.16(12)	C(22)-C(19)-C(21)	107.84(11)
C(12)-C(7)-O(2)	117.28(11)	C(8)-C(19)-C(20)	109.61(11)
C(8)-C(7)-O(2)	119.32(11)	C(22)-C(19)-C(20)	107.22(11)
C(9)-C(8)-C(7)	115.46(12)	C(21)-C(19)-C(20)	108.96(11)
C(9)-C(8)-C(19)	122.03(11)	C(19)-C(20)-H(20A)	109.5
C(7)-C(8)-C(19)	122.38(11)	C(19)-C(20)-H(20B)	109.4
C(8)-C(9)-C(10)	123.55(12)	H(20A)-C(20)-H(20B)	109.5
C(8)-C(9)-H(9)	118.2	C(19)-C(20)-H(20C)	109.5
C(10)-C(9)-H(9)	118.2	H(20A)-C(20)-H(20C)	109.5
C(11)-C(10)-C(9)	117.86(12)	H(20B)-C(20)-H(20C)	109.5
C(11)-C(10)-C(23)	122.28(12)	C(19)-C(21)-H(21A)	109.4
C(9)-C(10)-C(23)	119.86(12)	C(19)-C(21)-H(21B)	109.5
C(10)-C(11)-C(12)	121.13(13)	H(21A)-C(21)-H(21B)	109.5
C(10)-C(11)-H(11)	119.4	C(19)-C(21)-H(21C)	109.5
C(12)-C(11)-H(11)	119.4	H(21A)-C(21)-H(21C)	109.5
C(7)-C(12)-C(11)	118.26(12)	H(21B)-C(21)-H(21C)	109.5
C(7)-C(12)-C(13)	122.13(12)	C(19)-C(22)-H(22A)	109.5
C(11)-C(12)-C(13)	119.47(12)	C(19)-C(22)-H(22B)	109.5
C(18)-C(13)-C(14)	118.50(12)	H(22A)-C(22)-H(22B)	109.5
C(18)-C(13)-C(12)	118.61(12)	C(19)-C(22)-H(22C)	109.4
C(14)-C(13)-C(12)	122.89(12)	H(22A)-C(22)-H(22C)	109.5
C(13)-C(14)-O(3)	116.81(11)	H(22B)-C(22)-H(22C)	109.5
C(13)-C(14)-C(15)	122.45(12)	C(25)-C(23)-C(10)	112.08(12)
O(3)-C(14)-C(15)	120.55(12)	C(25)-C(23)-C(26)	108.44(14)
C(16)-C(15)-C(14)	115.72(12)	C(10)-C(23)-C(26)	108.67(12)
C(16)-C(15)-C(27)	120.44(12)	C(25)-C(23)-C(24)	108.29(14)
C(14)-C(15)-C(27)	123.75(12)	C(10)-C(23)-C(24)	109.95(12)
C(17)-C(16)-C(15)	123.93(13)	C(26)-C(23)-C(24)	109.36(12)
C(17)-C(16)-H(16)	118.0	C(23)-C(24)-H(24A)	109.5
C(15)-C(16)-H(16)	118.0	C(23)-C(24)-H(24B)	109.5

H(24A)-C(24)-H(24B)	109.5	H(30A)-C(30)-H(30C)	109.5
C(23)-C(24)-H(24C)	109.4	H(30B)-C(30)-H(30C)	109.5
H(24A)-C(24)-H(24C)	109.5	C(17)-C(31)-C(34)	111.75(13)
H(24B)-C(24)-H(24C)	109.5	C(17)-C(31)-C(33)	109.17(13)
C(23)-C(25)-H(25A)	109.4	C(34)-C(31)-C(33)	108.92(13)
C(23)-C(25)-H(25B)	109.5	C(17)-C(31)-C(32)	110.36(12)
H(25A)-C(25)-H(25B)	109.5	C(34)-C(31)-C(32)	107.28(15)
C(23)-C(25)-H(25C)	109.5	C(33)-C(31)-C(32)	109.32(15)
H(25A)-C(25)-H(25C)	109.5	C(31)-C(32)-H(32A)	109.5
H(25B)-C(25)-H(25C)	109.5	C(31)-C(32)-H(32B)	109.5
C(23)-C(26)-H(26A)	109.4	H(32A)-C(32)-H(32B)	109.5
C(23)-C(26)-H(26B)	109.5	C(31)-C(32)-H(32C)	109.5
H(26A)-C(26)-H(26B)	109.5	H(32A)-C(32)-H(32C)	109.5
C(23)-C(26)-H(26C)	109.5	H(32B)-C(32)-H(32C)	109.5
H(26A)-C(26)-H(26C)	109.5	C(31)-C(33)-H(33A)	109.4
H(26B)-C(26)-H(26C)	109.5	C(31)-C(33)-H(33B)	109.5
C(30)-C(27)-C(29)	107.52(14)	H(33A)-C(33)-H(33B)	109.5
C(30)-C(27)-C(15)	112.29(12)	C(31)-C(33)-H(33C)	109.5
C(29)-C(27)-C(15)	111.69(13)	H(33A)-C(33)-H(33C)	109.5
C(30)-C(27)-C(28)	109.35(14)	H(33B)-C(33)-H(33C)	109.5
C(29)-C(27)-C(28)	106.66(13)	C(31)-C(34)-H(34A)	109.6
C(15)-C(27)-C(28)	109.15(13)	C(31)-C(34)-H(34B)	109.4
C(27)-C(28)-H(28A)	109.4	H(34A)-C(34)-H(34B)	109.5
C(27)-C(28)-H(28B)	109.5	C(31)-C(34)-H(34C)	109.4
H(28A)-C(28)-H(28B)	109.5	H(34A)-C(34)-H(34C)	109.5
C(27)-C(28)-H(28C)	109.4	H(34B)-C(34)-H(34C)	109.5
H(28A)-C(28)-H(28C)	109.5	C(40)-C(35)-O(5)	117.16(11)
H(28B)-C(28)-H(28C)	109.5	C(40)-C(35)-C(36)	122.74(11)
C(27)-C(29)-H(29A)	109.4	O(5)-C(35)-C(36)	120.10(11)
C(27)-C(29)-H(29B)	109.5	C(37)-C(36)-C(35)	115.90(11)
H(29A)-C(29)-H(29B)	109.5	C(37)-C(36)-C(47)	121.68(11)
C(27)-C(29)-H(29C)	109.5	C(35)-C(36)-C(47)	122.41(11)
H(29A)-C(29)-H(29C)	109.5	C(38)-C(37)-C(36)	123.40(11)
H(29B)-C(29)-H(29C)	109.5	C(38)-C(37)-H(37)	118.3
C(27)-C(30)-H(30A)	109.4	C(36)-C(37)-H(37)	118.3
C(27)-C(30)-H(30B)	109.6	C(37)-C(38)-C(39)	117.47(12)
H(30A)-C(30)-H(30B)	109.5	C(37)-C(38)-C(51)	122.99(11)
C(27)-C(30)-H(30C)	109.5	C(39)-C(38)-C(51)	119.52(11)

C(40)-C(39)-C(38)	121.61(12)	H(49A)-C(49)-H(49B)	109.5
C(40)-C(39)-H(39)	119.2	C(47)-C(49)-H(49C)	109.5
C(38)-C(39)-H(39)	119.2	H(49A)-C(49)-H(49C)	109.5
C(35)-C(40)-C(39)	118.01(11)	H(49B)-C(49)-H(49C)	109.5
C(35)-C(40)-C(41)	122.73(11)	C(47)-C(50)-H(50A)	109.4
C(39)-C(40)-C(41)	119.21(11)	C(47)-C(50)-H(50B)	109.5
C(42)-C(41)-C(46)	118.14(11)	H(50A)-C(50)-H(50B)	109.5
C(42)-C(41)-C(40)	124.14(11)	C(47)-C(50)-H(50C)	109.5
C(46)-C(41)-C(40)	117.66(11)	H(50A)-C(50)-H(50C)	109.5
C(41)-C(42)-O(6)	119.78(11)	H(50B)-C(50)-H(50C)	109.5
C(41)-C(42)-C(43)	122.49(11)	C(52)-C(51)-C(38)	112.64(11)
O(6)-C(42)-C(43)	117.35(11)	C(52)-C(51)-C(54)	108.58(12)
C(44)-C(43)-C(42)	116.18(11)	C(38)-C(51)-C(54)	110.02(11)
C(44)-C(43)-C(55)	121.06(11)	C(52)-C(51)-C(53)	107.94(12)
C(42)-C(43)-C(55)	122.74(11)	C(38)-C(51)-C(53)	108.41(11)
C(43)-C(44)-C(45)	123.57(12)	C(54)-C(51)-C(53)	109.19(12)
C(43)-C(44)-H(44)	118.2	C(51)-C(52)-H(52A)	109.4
C(45)-C(44)-H(44)	118.2	C(51)-C(52)-H(52B)	109.5
C(46)-C(45)-C(44)	117.54(12)	H(52A)-C(52)-H(52B)	109.5
C(46)-C(45)-C(59)	123.00(11)	C(51)-C(52)-H(52C)	109.5
C(44)-C(45)-C(59)	119.46(11)	H(52A)-C(52)-H(52C)	109.5
C(45)-C(46)-C(41)	121.74(12)	H(52B)-C(52)-H(52C)	109.5
C(45)-C(46)-H(46)	119.1	C(51)-C(53)-H(53A)	109.5
C(41)-C(46)-H(46)	119.2	C(51)-C(53)-H(53B)	109.5
C(49)-C(47)-C(48)	107.24(12)	H(53A)-C(53)-H(53B)	109.5
C(49)-C(47)-C(50)	110.28(12)	C(51)-C(53)-H(53C)	109.5
C(48)-C(47)-C(50)	106.95(12)	H(53A)-C(53)-H(53C)	109.5
C(49)-C(47)-C(36)	111.35(11)	H(53B)-C(53)-H(53C)	109.5
C(48)-C(47)-C(36)	111.02(11)	C(51)-C(54)-H(54A)	109.5
C(50)-C(47)-C(36)	109.88(11)	C(51)-C(54)-H(54B)	109.5
C(47)-C(48)-H(48A)	109.5	H(54A)-C(54)-H(54B)	109.5
C(47)-C(48)-H(48B)	109.6	C(51)-C(54)-H(54C)	109.4
H(48A)-C(48)-H(48B)	109.5	H(54A)-C(54)-H(54C)	109.5
C(47)-C(48)-H(48C)	109.4	H(54B)-C(54)-H(54C)	109.5
H(48A)-C(48)-H(48C)	109.5	C(57)-C(55)-C(43)	110.20(11)
H(48B)-C(48)-H(48C)	109.5	C(57)-C(55)-C(58)	108.35(11)
C(47)-C(49)-H(49A)	109.4	C(43)-C(55)-C(58)	110.74(11)
C(47)-C(49)-H(49B)	109.5	C(57)-C(55)-C(56)	110.40(12)

C(43)-C(55)-C(56)	110.97(11)	C(59)-C(62)-H(62A)	109.5
C(58)-C(55)-C(56)	106.06(12)	C(59)-C(62)-H(62B)	109.5
C(55)-C(56)-H(56A)	109.6	H(62A)-C(62)-H(62B)	109.5
C(55)-C(56)-H(56B)	109.4	C(59)-C(62)-H(62C)	109.5
H(56A)-C(56)-H(56B)	109.5	H(62A)-C(62)-H(62C)	109.5
C(55)-C(56)-H(56C)	109.4	H(62B)-C(62)-H(62C)	109.5
H(56A)-C(56)-H(56C)	109.5	C(64)-C(63)-Rh(1)	71.32(8)
H(56B)-C(56)-H(56C)	109.5	C(64)-C(63)-H(63A)	122.3(12)
C(55)-C(57)-H(57A)	109.4	Rh(1)-C(63)-H(63A)	107.9(12)
C(55)-C(57)-H(57B)	109.4	C(64)-C(63)-H(63B)	120.4(12)
H(57A)-C(57)-H(57B)	109.5	Rh(1)-C(63)-H(63B)	108.0(12)
C(55)-C(57)-H(57C)	109.6	H(63A)-C(63)-H(63B)	114.4(17)
H(57A)-C(57)-H(57C)	109.5	C(63)-C(64)-Rh(1)	72.66(8)
H(57B)-C(57)-H(57C)	109.5	C(63)-C(64)-H(64A)	120.1(12)
C(55)-C(58)-H(58A)	109.5	Rh(1)-C(64)-H(64A)	107.5(12)
C(55)-C(58)-H(58B)	109.5	C(63)-C(64)-H(64B)	120.3(12)
H(58A)-C(58)-H(58B)	109.5	Rh(1)-C(64)-H(64B)	109.2(11)
C(55)-C(58)-H(58C)	109.4	H(64A)-C(64)-H(64B)	115.7(16)
H(58A)-C(58)-H(58C)	109.5	C(66)-C(65)-H(65A)	109.5
H(58B)-C(58)-H(58C)	109.5	C(66)-C(65)-H(65B)	109.4
C(62)-C(59)-C(45)	111.88(11)	H(65A)-C(65)-H(65B)	109.5
C(62)-C(59)-C(61)	108.41(12)	C(66)-C(65)-H(65C)	109.5
C(45)-C(59)-C(61)	108.28(11)	H(65A)-C(65)-H(65C)	109.5
C(62)-C(59)-C(60)	108.34(12)	H(65B)-C(65)-H(65C)	109.5
C(45)-C(59)-C(60)	111.03(11)	C(67)-C(66)-C(65)	112.8(5)
C(61)-C(59)-C(60)	108.82(12)	C(67)-C(66)-H(66A)	109.0
C(59)-C(60)-H(60A)	109.5	C(65)-C(66)-H(66A)	109.0
C(59)-C(60)-H(60B)	109.5	C(67)-C(66)-H(66B)	109.0
H(60A)-C(60)-H(60B)	109.5	C(65)-C(66)-H(66B)	109.1
C(59)-C(60)-H(60C)	109.4	H(66A)-C(66)-H(66B)	107.8
H(60A)-C(60)-H(60C)	109.5	C(68)-C(67)-C(66)	122.1(6)
H(60B)-C(60)-H(60C)	109.5	C(68)-C(67)-H(67A)	106.8
C(59)-C(61)-H(61A)	109.4	C(66)-C(67)-H(67A)	106.8
C(59)-C(61)-H(61B)	109.5	C(68)-C(67)-H(67B)	106.8
H(61A)-C(61)-H(61B)	109.5	C(66)-C(67)-H(67B)	106.8
C(59)-C(61)-H(61C)	109.5	H(67A)-C(67)-H(67B)	106.6
H(61A)-C(61)-H(61C)	109.5	C(69)-C(68)-C(67)	120.1(7)
H(61B)-C(61)-H(61C)	109.5	C(69)-C(68)-H(68A)	107.3

C(67)-C(68)-H(68A)	107.3	C(68)-C(69)-H(69B)	109.4
C(69)-C(68)-H(68B)	107.3	H(69A)-C(69)-H(69B)	109.5
C(67)-C(68)-H(68B)	107.3	C(68)-C(69)-H(69C)	109.5
H(68A)-C(68)-H(68B)	106.9	H(69A)-C(69)-H(69C)	109.5
C(68)-C(69)-H(69A)	109.5	H(69B)-C(69)-H(69C)	109.5

Figure S9. ORTEP view (30% ellipsoids) of **5b**. H atoms (except for ethylene) have been omitted for clarity.

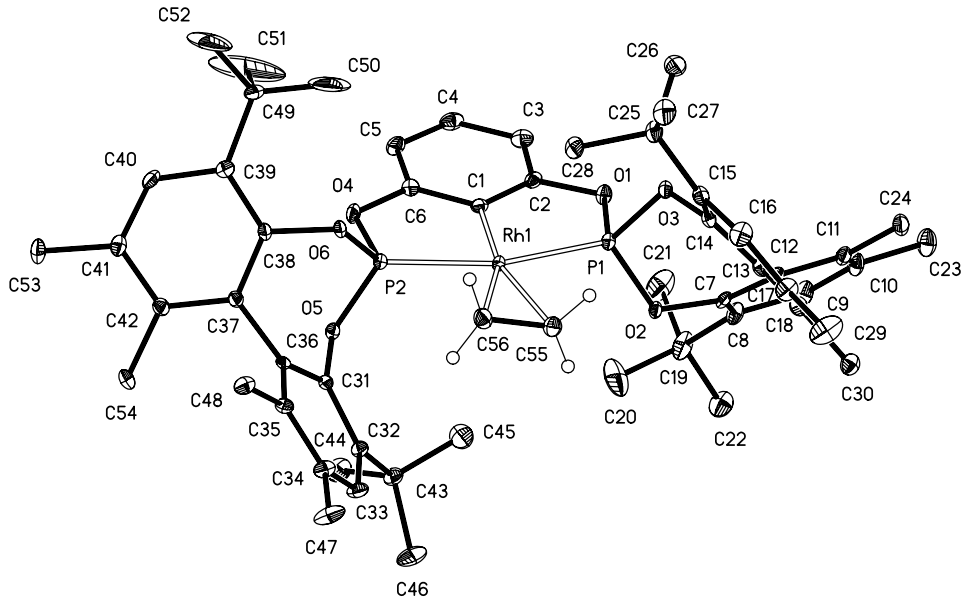


Table S6. Crystal data and structure refinement for **5b**.

Empirical formula	$C_{56}H_{71}O_6P_2Rh$	
Formula weight	1004.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.4092(11) Å	α= 90°.
	b = 18.8544(18) Å	β= 90°.
	c = 26.636(3) Å	γ = 90°.
Volume	5227.6(9) $Å^3$	
Z	4	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.436 mm^{-1}	
F(000)	2120	
Crystal size	0.36 x 0.16 x 0.13 mm^3	
Theta range for data collection	2.92 to 27.00°.	
Index ranges	-13<=h<=13, -16<=k<=24, -33<=l<=34	
Reflections collected	45841	
Independent reflections	11402 [R(int) = 0.0496]	
Completeness to theta = 27.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9455 and 0.8589	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11402 / 10 / 602	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0717	
R indices (all data)	R1 = 0.0421, wR2 = 0.0747	
Absolute structure parameter	-0.018(17)	
Largest diff. peak and hole	0.884 and -0.718 $e.Å^{-3}$	

Table S7. Bond lengths [Å] and angles [°] for **5b**.

Rh(1)-C(1)	2.019(3)	C(12)-C(13)	1.494(4)
Rh(1)-P(2)	2.2096(7)	C(13)-C(14)	1.388(4)
Rh(1)-P(1)	2.2237(7)	C(13)-C(18)	1.401(4)
Rh(1)-C(55)	2.228(3)	C(14)-C(15)	1.392(4)
Rh(1)-C(56)	2.230(3)	C(15)-C(16)	1.392(4)
P(1)-O(2)	1.6030(19)	C(15)-C(25)	1.534(4)
P(1)-O(1)	1.614(2)	C(16)-C(17)	1.384(5)
P(1)-O(3)	1.614(2)	C(16)-H(16)	0.9500
P(2)-O(6)	1.594(2)	C(17)-C(18)	1.391(4)
P(2)-O(4)	1.613(2)	C(17)-C(29)	1.508(4)
P(2)-O(5)	1.622(2)	C(18)-C(30)	1.503(4)
O(1)-C(2)	1.397(3)	C(19)-C(20)	1.503(5)
O(2)-C(7)	1.414(3)	C(19)-C(22)	1.533(4)
O(3)-C(14)	1.410(3)	C(19)-C(21)	1.547(5)
O(4)-C(6)	1.403(3)	C(20)-H(20A)	0.9800
O(5)-C(31)	1.401(3)	C(20)-H(20B)	0.9800
O(6)-C(38)	1.414(3)	C(20)-H(20C)	0.9800
C(1)-C(2)	1.380(4)	C(21)-H(21A)	0.9800
C(1)-C(6)	1.393(4)	C(21)-H(21B)	0.9800
C(2)-C(3)	1.386(4)	C(21)-H(21C)	0.9800
C(3)-C(4)	1.391(4)	C(22)-H(22A)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22B)	0.9800
C(4)-C(5)	1.372(4)	C(22)-H(22C)	0.9800
C(4)-H(4)	0.9500	C(23)-H(23A)	0.9800
C(5)-C(6)	1.378(4)	C(23)-H(23B)	0.9800
C(5)-H(5)	0.9500	C(23)-H(23C)	0.9800
C(7)-C(8)	1.385(4)	C(24)-H(24A)	0.9800
C(7)-C(12)	1.394(4)	C(24)-H(24B)	0.9800
C(8)-C(9)	1.409(4)	C(24)-H(24C)	0.9800
C(8)-C(19)	1.532(4)	C(25)-C(26)	1.527(4)
C(9)-C(10)	1.376(4)	C(25)-C(28)	1.531(4)
C(9)-H(9)	0.9500	C(25)-C(27)	1.540(4)
C(10)-C(11)	1.398(4)	C(26)-H(26A)	0.9800
C(10)-C(23)	1.509(4)	C(26)-H(26B)	0.9800
C(11)-C(12)	1.399(4)	C(26)-H(26C)	0.9800
C(11)-C(24)	1.502(4)	C(27)-H(27A)	0.9800

C(27)-H(27B)	0.9800	C(45)-H(45A)	0.9800
C(27)-H(27C)	0.9800	C(45)-H(45B)	0.9800
C(28)-H(28A)	0.9800	C(45)-H(45C)	0.9800
C(28)-H(28B)	0.9800	C(46)-H(46A)	0.9800
C(28)-H(28C)	0.9800	C(46)-H(46B)	0.9800
C(29)-H(29A)	0.9800	C(46)-H(46C)	0.9800
C(29)-H(29B)	0.9800	C(47)-H(47A)	0.9800
C(29)-H(29C)	0.9800	C(47)-H(47B)	0.9800
C(30)-H(30A)	0.9800	C(47)-H(47C)	0.9800
C(30)-H(30B)	0.9800	C(48)-H(48A)	0.9800
C(30)-H(30C)	0.9800	C(48)-H(48B)	0.9800
C(31)-C(36)	1.396(4)	C(48)-H(48C)	0.9800
C(31)-C(32)	1.403(4)	C(49)-C(50)	1.464(6)
C(32)-C(33)	1.389(4)	C(49)-C(52)	1.470(5)
C(32)-C(43)	1.540(4)	C(49)-C(51)	1.525(7)
C(33)-C(34)	1.386(4)	C(50)-H(50A)	0.9800
C(33)-H(33)	0.9500	C(50)-H(50B)	0.9800
C(34)-C(35)	1.400(4)	C(50)-H(50C)	0.9800
C(34)-C(47)	1.506(4)	C(51)-H(51A)	0.9800
C(35)-C(36)	1.402(4)	C(51)-H(51B)	0.9800
C(35)-C(48)	1.505(4)	C(51)-H(51C)	0.9800
C(36)-C(37)	1.488(4)	C(52)-H(52A)	0.9800
C(37)-C(38)	1.387(4)	C(52)-H(52B)	0.9800
C(37)-C(42)	1.404(4)	C(52)-H(52C)	0.9800
C(38)-C(39)	1.384(4)	C(53)-H(53A)	0.9800
C(39)-C(40)	1.398(4)	C(53)-H(53B)	0.9800
C(39)-C(49)	1.539(4)	C(53)-H(53C)	0.9800
C(40)-C(41)	1.383(4)	C(54)-H(54A)	0.9800
C(40)-H(40)	0.9500	C(54)-H(54B)	0.9800
C(41)-C(42)	1.400(4)	C(54)-H(54C)	0.9800
C(41)-C(53)	1.505(4)	C(55)-C(56)	1.353(4)
C(42)-C(54)	1.502(4)	C(55)-H(55A)	0.966(18)
C(43)-C(45)	1.519(4)	C(55)-H(55B)	0.942(18)
C(43)-C(46)	1.534(4)	C(56)-H(56A)	0.957(19)
C(43)-C(44)	1.536(5)	C(56)-H(56B)	0.939(18)
C(44)-H(44A)	0.9800		
C(44)-H(44B)	0.9800	C(1)-Rh(1)-P(2)	77.86(8)
C(44)-H(44C)	0.9800	C(1)-Rh(1)-P(1)	77.57(8)

P(2)-Rh(1)-P(1)	155.37(3)	C(4)-C(5)-C(6)	118.5(3)
C(1)-Rh(1)-C(55)	163.13(11)	C(4)-C(5)-H(5)	120.7
P(2)-Rh(1)-C(55)	118.68(8)	C(6)-C(5)-H(5)	120.8
P(1)-Rh(1)-C(55)	85.76(8)	C(5)-C(6)-C(1)	124.0(3)
C(1)-Rh(1)-C(56)	161.50(11)	C(5)-C(6)-O(4)	118.8(3)
P(2)-Rh(1)-C(56)	84.39(8)	C(1)-C(6)-O(4)	117.2(3)
P(1)-Rh(1)-C(56)	120.24(8)	C(8)-C(7)-C(12)	124.1(2)
C(55)-Rh(1)-C(56)	35.32(11)	C(8)-C(7)-O(2)	120.7(2)
O(2)-P(1)-O(1)	104.53(10)	C(12)-C(7)-O(2)	115.2(2)
O(2)-P(1)-O(3)	103.44(10)	C(7)-C(8)-C(9)	113.9(3)
O(1)-P(1)-O(3)	95.29(10)	C(7)-C(8)-C(19)	128.2(3)
O(2)-P(1)-Rh(1)	116.10(8)	C(9)-C(8)-C(19)	117.9(3)
O(1)-P(1)-Rh(1)	109.60(7)	C(10)-C(9)-C(8)	124.2(3)
O(3)-P(1)-Rh(1)	124.49(7)	C(10)-C(9)-H(9)	117.9
O(6)-P(2)-O(4)	104.45(11)	C(8)-C(9)-H(9)	117.9
O(6)-P(2)-O(5)	103.38(11)	C(9)-C(10)-C(11)	119.7(3)
O(4)-P(2)-O(5)	95.60(11)	C(9)-C(10)-C(23)	119.8(3)
O(6)-P(2)-Rh(1)	117.07(8)	C(11)-C(10)-C(23)	120.5(3)
O(4)-P(2)-Rh(1)	110.11(8)	C(10)-C(11)-C(12)	118.2(3)
O(5)-P(2)-Rh(1)	122.90(7)	C(10)-C(11)-C(24)	120.0(3)
C(2)-O(1)-P(1)	112.41(17)	C(12)-C(11)-C(24)	121.8(3)
C(7)-O(2)-P(1)	119.31(17)	C(7)-C(12)-C(11)	119.5(2)
C(14)-O(3)-P(1)	118.37(18)	C(7)-C(12)-C(13)	119.9(2)
C(6)-O(4)-P(2)	112.21(17)	C(11)-C(12)-C(13)	120.6(2)
C(31)-O(5)-P(2)	115.33(17)	C(14)-C(13)-C(18)	119.3(3)
C(38)-O(6)-P(2)	122.50(18)	C(14)-C(13)-C(12)	119.2(2)
C(2)-C(1)-C(6)	114.5(2)	C(18)-C(13)-C(12)	121.4(2)
C(2)-C(1)-Rh(1)	122.9(2)	C(13)-C(14)-C(15)	123.4(3)
C(6)-C(1)-Rh(1)	122.5(2)	C(13)-C(14)-O(3)	116.3(2)
C(1)-C(2)-C(3)	124.5(3)	C(15)-C(14)-O(3)	120.2(2)
C(1)-C(2)-O(1)	117.5(2)	C(14)-C(15)-C(16)	114.4(3)
C(3)-C(2)-O(1)	118.0(3)	C(14)-C(15)-C(25)	123.0(3)
C(2)-C(3)-C(4)	117.5(3)	C(16)-C(15)-C(25)	122.6(2)
C(2)-C(3)-H(3)	121.3	C(17)-C(16)-C(15)	123.9(3)
C(4)-C(3)-H(3)	121.3	C(17)-C(16)-H(16)	118.1
C(5)-C(4)-C(3)	121.0(3)	C(15)-C(16)-H(16)	118.1
C(5)-C(4)-H(4)	119.5	C(16)-C(17)-C(18)	119.7(3)
C(3)-C(4)-H(4)	119.5	C(16)-C(17)-C(29)	120.4(3)

C(18)-C(17)-C(29)	119.9(3)	H(24A)-C(24)-H(24C)	109.5
C(17)-C(18)-C(13)	118.3(3)	H(24B)-C(24)-H(24C)	109.5
C(17)-C(18)-C(30)	120.1(3)	C(26)-C(25)-C(28)	109.7(3)
C(13)-C(18)-C(30)	121.7(3)	C(26)-C(25)-C(15)	110.4(2)
C(20)-C(19)-C(8)	115.3(3)	C(28)-C(25)-C(15)	111.5(2)
C(20)-C(19)-C(22)	107.9(3)	C(26)-C(25)-C(27)	106.8(3)
C(8)-C(19)-C(22)	109.1(3)	C(28)-C(25)-C(27)	107.2(2)
C(20)-C(19)-C(21)	108.0(3)	C(15)-C(25)-C(27)	111.2(2)
C(8)-C(19)-C(21)	108.2(3)	C(25)-C(26)-H(26A)	109.5
C(22)-C(19)-C(21)	108.3(3)	C(25)-C(26)-H(26B)	109.5
C(19)-C(20)-H(20A)	109.4	H(26A)-C(26)-H(26B)	109.5
C(19)-C(20)-H(20B)	109.4	C(25)-C(26)-H(26C)	109.4
H(20A)-C(20)-H(20B)	109.5	H(26A)-C(26)-H(26C)	109.5
C(19)-C(20)-H(20C)	109.6	H(26B)-C(26)-H(26C)	109.5
H(20A)-C(20)-H(20C)	109.5	C(25)-C(27)-H(27A)	109.4
H(20B)-C(20)-H(20C)	109.5	C(25)-C(27)-H(27B)	109.5
C(19)-C(21)-H(21A)	109.4	H(27A)-C(27)-H(27B)	109.5
C(19)-C(21)-H(21B)	109.4	C(25)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21B)	109.5	H(27A)-C(27)-H(27C)	109.5
C(19)-C(21)-H(21C)	109.6	H(27B)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21C)	109.5	C(25)-C(28)-H(28A)	109.4
H(21B)-C(21)-H(21C)	109.5	C(25)-C(28)-H(28B)	109.5
C(19)-C(22)-H(22A)	109.6	H(28A)-C(28)-H(28B)	109.5
C(19)-C(22)-H(22B)	109.3	C(25)-C(28)-H(28C)	109.5
H(22A)-C(22)-H(22B)	109.5	H(28A)-C(28)-H(28C)	109.5
C(19)-C(22)-H(22C)	109.5	H(28B)-C(28)-H(28C)	109.5
H(22A)-C(22)-H(22C)	109.5	C(17)-C(29)-H(29A)	109.4
H(22B)-C(22)-H(22C)	109.5	C(17)-C(29)-H(29B)	109.5
C(10)-C(23)-H(23A)	109.5	H(29A)-C(29)-H(29B)	109.5
C(10)-C(23)-H(23B)	109.5	C(17)-C(29)-H(29C)	109.5
H(23A)-C(23)-H(23B)	109.5	H(29A)-C(29)-H(29C)	109.5
C(10)-C(23)-H(23C)	109.5	H(29B)-C(29)-H(29C)	109.5
H(23A)-C(23)-H(23C)	109.5	C(18)-C(30)-H(30A)	109.5
H(23B)-C(23)-H(23C)	109.5	C(18)-C(30)-H(30B)	109.4
C(11)-C(24)-H(24A)	109.5	H(30A)-C(30)-H(30B)	109.5
C(11)-C(24)-H(24B)	109.4	C(18)-C(30)-H(30C)	109.5
H(24A)-C(24)-H(24B)	109.5	H(30A)-C(30)-H(30C)	109.5
C(11)-C(24)-H(24C)	109.5	H(30B)-C(30)-H(30C)	109.5

C(36)-C(31)-O(5)	116.1(2)	C(46)-C(43)-C(44)	106.7(3)
C(36)-C(31)-C(32)	123.3(3)	C(45)-C(43)-C(32)	112.1(3)
O(5)-C(31)-C(32)	120.6(2)	C(46)-C(43)-C(32)	110.3(3)
C(33)-C(32)-C(31)	114.7(3)	C(44)-C(43)-C(32)	109.8(3)
C(33)-C(32)-C(43)	122.2(3)	C(43)-C(44)-H(44A)	109.5
C(31)-C(32)-C(43)	123.0(3)	C(43)-C(44)-H(44B)	109.5
C(34)-C(33)-C(32)	124.0(3)	H(44A)-C(44)-H(44B)	109.5
C(34)-C(33)-H(33)	118.0	C(43)-C(44)-H(44C)	109.5
C(32)-C(33)-H(33)	118.0	H(44A)-C(44)-H(44C)	109.5
C(33)-C(34)-C(35)	119.1(3)	H(44B)-C(44)-H(44C)	109.5
C(33)-C(34)-C(47)	120.3(3)	C(43)-C(45)-H(45A)	109.5
C(35)-C(34)-C(47)	120.6(3)	C(43)-C(45)-H(45B)	109.5
C(34)-C(35)-C(36)	119.2(3)	H(45A)-C(45)-H(45B)	109.5
C(34)-C(35)-C(48)	118.9(3)	C(43)-C(45)-H(45C)	109.5
C(36)-C(35)-C(48)	121.9(3)	H(45A)-C(45)-H(45C)	109.5
C(31)-C(36)-C(35)	118.6(2)	H(45B)-C(45)-H(45C)	109.5
C(31)-C(36)-C(37)	119.2(2)	C(43)-C(46)-H(46A)	109.5
C(35)-C(36)-C(37)	122.1(2)	C(43)-C(46)-H(46B)	109.5
C(38)-C(37)-C(42)	119.3(3)	H(46A)-C(46)-H(46B)	109.5
C(38)-C(37)-C(36)	120.3(2)	C(43)-C(46)-H(46C)	109.4
C(42)-C(37)-C(36)	120.4(2)	H(46A)-C(46)-H(46C)	109.5
C(39)-C(38)-C(37)	124.1(3)	H(46B)-C(46)-H(46C)	109.5
C(39)-C(38)-O(6)	120.0(2)	C(34)-C(47)-H(47A)	109.5
C(37)-C(38)-O(6)	115.8(2)	C(34)-C(47)-H(47B)	109.4
C(38)-C(39)-C(40)	114.4(3)	H(47A)-C(47)-H(47B)	109.5
C(38)-C(39)-C(49)	126.9(3)	C(34)-C(47)-H(47C)	109.5
C(40)-C(39)-C(49)	118.7(3)	H(47A)-C(47)-H(47C)	109.5
C(41)-C(40)-C(39)	124.3(3)	H(47B)-C(47)-H(47C)	109.5
C(41)-C(40)-H(40)	117.9	C(35)-C(48)-H(48A)	109.6
C(39)-C(40)-H(40)	117.8	C(35)-C(48)-H(48B)	109.4
C(40)-C(41)-C(42)	119.2(3)	H(48A)-C(48)-H(48B)	109.5
C(40)-C(41)-C(53)	120.2(3)	C(35)-C(48)-H(48C)	109.5
C(42)-C(41)-C(53)	120.6(3)	H(48A)-C(48)-H(48C)	109.5
C(41)-C(42)-C(37)	118.5(3)	H(48B)-C(48)-H(48C)	109.5
C(41)-C(42)-C(54)	120.1(3)	C(50)-C(49)-C(52)	110.1(5)
C(37)-C(42)-C(54)	121.3(3)	C(50)-C(49)-C(51)	107.9(6)
C(45)-C(43)-C(46)	108.0(3)	C(52)-C(49)-C(51)	104.7(5)
C(45)-C(43)-C(44)	109.9(3)	C(50)-C(49)-C(39)	114.6(3)

C(52)-C(49)-C(39)	111.5(3)
C(51)-C(49)-C(39)	107.5(3)
C(49)-C(50)-H(50A)	109.4
C(49)-C(50)-H(50B)	109.3
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.8
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.4
C(49)-C(51)-H(51B)	109.6
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.4
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.4
H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(41)-C(53)-H(53A)	109.4
C(41)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(41)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(42)-C(54)-H(54A)	109.6
C(42)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(42)-C(54)-H(54C)	109.4
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(56)-C(55)-Rh(1)	72.41(18)
C(56)-C(55)-H(55A)	121.6(19)
Rh(1)-C(55)-H(55A)	104.7(17)
C(56)-C(55)-H(55B)	122(2)
Rh(1)-C(55)-H(55B)	99.9(18)
H(55A)-C(55)-H(55B)	116(3)
C(55)-C(56)-Rh(1)	72.27(18)
C(55)-C(56)-H(56A)	119(2)
Rh(1)-C(56)-H(56A)	101(2)
C(55)-C(56)-H(56B)	116(2)
Rh(1)-C(56)-H(56B)	106(2)
H(56A)-C(56)-H(56B)	123(3)