Supporting Information:

Construction of Metal-Centered Chirality: Diastereoselective Addition of the Meerwein Reagent (Me_3OBF_4) to Rhodium Carbonyl Complexes Having the Cp'-P Ligand

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X-ray determination of 2b-major. Reddish-orange single crystals suitable for X-ray measurements were obtained by repeated recrystallization from THF and Et_2O. For the X-ray measurements, the crystals were fixed on the end of glass fibers with silicon grease and cooled at 100 K. Indexing was performed from 2 oscillations, which were exposed for 6.0 minutes. The camera radius was 127.40 mm. Resolution was performed in the 0.100 mm pixel mode. Cell constants and an orientation matrix for data collection were determined by the least-squares refinement, using the setting angles of 115255 reflections in the range of $1.46° < \theta < 31.51°$ on a Rigaku RAXIS-RAPID equipped with a sealed tube X-ray generator (50 kV, 40 mA) with monochromatized Mo-Kα (0.71069 Å) radiation. Crystal data: formula $C_{27}H_{27}B_1F_4O_1P_1Rh_1$, fw = 588.18, cell dimensions a = 15.14844(10) Å, b = 14.31749(13) Å, c = 15.22641(9) Å, β = 133.4424(2)°, V = 2397.78(3) Å^3, Z = 4, Dcalcd = 1.629 Mg m^{-3}, μ = 0.830 mm^{-1}. Molecules of **2b**-major are crystallized in the monoclinic system with the centrosymmetric space group $P2_1/c$ (#14). For the data collection, reflections were measured at 100(1) K to a maximum 2θ value of 63.0°. A total 270 images, corresponding to 540° oscillation angles, were collected with 3 different goniometer settings. Exposure time was 160 seconds per degree. Readout was performed in the 0.100 mm pixel mode. Intensity data were corrected for Lorentz and polarization effects. A numerical absorption correction using the program NUMABS[S1] was applied, which resulted in transmission factors ranging from 0.9672 to 0.9897. A total of 71981 measured reflections ($5.0° < 2\theta < 63.0°$), 7988 were unique (Rint = 0.0471) and used for the structure solution and refinement.

The structure were solved by direct methods (SHELXS-97)[S2] and refined on F^2 by full-matrix least-squares methods, using SHELXL-97.[S3] Non-hydrogen atoms were anisotropically refined. All H-atoms were isotropically refined. The function minimized was $[\Sigma w(Fo^2 - Fc^2)^2]$ ($w = 1 / [\sigma^2(Fo^2) + (0.0180P)^2 + 2.3638P]$), where $P = (\mathrm{Max}(Fo^2,0) + 2Fc^2) / 3$ with $\sigma^2(Fo^2)$ from counting statistics. The function $R1$ and $wR2$ were $(\Sigma||Fo| - |Fc||) / \Sigma|Fo|$ and $[\Sigma w(Fo^2-Fc^2)^2 / \Sigma(wFo^4)]^{1/2}$, respectively, and $R1$ and $wR2$ are 0.0307 and 0.0550 for 4049 reflections with $I > 2.0\sigma(I)$, respectively. Final R factors, $R1$ and $wR2$ are 0.0404 and 0.0573

for 7988 reflections (all data). The number of parameters is 424. GOF values are 1.107 for $I > 2.0\sigma(I)$ and 1.107 for all data, respectively. The maximum shift to esd ratio in the last full-matrix least-squares cycle was 0.000. The final difference Fourier map revealed the presence of a number of areas of residual electron density, the greatest of which corresponds to 0.487 e $Å^{-3}$ and the highest peak was located near the C20 atom (0.67 Å). The minimum hole of the final difference-Fourier map is –0.695 e $Å^{-3}$ (0.68 Å from Rh atom). All calculations of least-squares refinements were performed with SHELXL97 programs on Origin 3400 computer of Silicon Graphics Inc. at the Research Center for Structural Biology Institute for Protein Research, Osaka University. Text describing X-ray structure analysis, and tables containing final atomic coordinates, H-atom coordinates, thermal parameters and bond lengths and angles for **2b**-major were summarized in Table S1 ~ S6. The ORTEP-3 program[S4] was used to draw the molecule shown in Figure S1. The X-ray crystallographic files, in CIF format, are available from the Cambridge Crystallographic Data Centre on quoting the deposition numbers: CCDC 226411.

References

(S1) (a) Higashi, T. Shape - Program to obtain Crystal Shape using CCD camera. Rigaku Corporation, Tokyo, Japan, 1999. (b) Higashi, T. Numabs - Numerical Absorption Correction, Rigaku Corporation, Tokyo, Japan, 1999.

(S2) Sheldrick, G. M. SHELXS-97. Programs for Crystal Structure Analysis (Release 97-2). University of Göttingen, Germany, 1997.

(S3) Sheldrick, G. M. SHELXL-97. Programs for Crystal Structure Analysis (Release 97-2). University of Göttingen, Germany, 1997.

(S4) Farrugia, L. J. *J. Appl. Cryst.*, **1999**, *32*, 837.

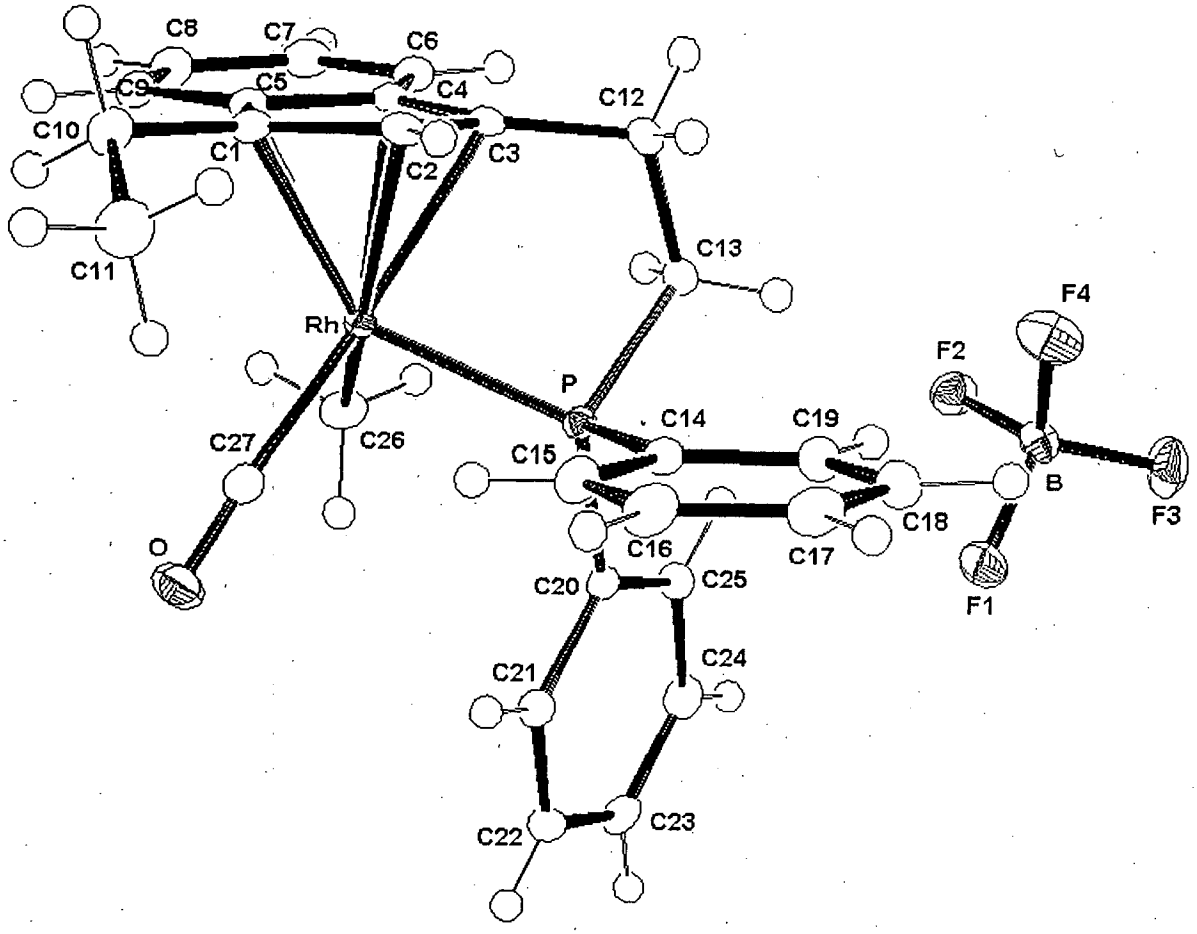

Figure S1. View of **2b**-major showing the 50% probability thermal ellipsoids.

Table S1. Crystal data and structure refinement for 2b-major.

Identification code	2b-major
Empirical formula	C27 H27 B F4 O P Rh
Formula weight	588.18
Temperature	100(1) K
Wavelength	0.71069 A
Crystal system, space group	Monoclinic, P21/c (#14)
Unit cell dimensions	a = 15.14844(10) A alpha = 90 deg. b = 14.31749(13) A beta = 133.4424(2) deg. c = 15.22641(9) A gamma = 90 deg.
Volume	2397.78(3) A^3
Z, Calculated density	4, 1.629 Mg/m^3
Absorption coefficient	0.830 mm^-1
F(000)	1192
Crystal size	0.23 x 0.13 x 0.11 mm
Theta range for data collection	2.76 to 31.50 deg.
Limiting indices	-22<=h<=22, -21<=k<=21, -22<=l<=22
Reflections collected / unique	71981 / 7988 [R(int) = 0.0471]
Completeness to theta = 31.50	99.9 %
Absorption correction	Numerical
Max. and min. transmission	0.9897 and 0.9672
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7988 / 0 / 424
Goodness-of-fit on F^2	1.107
Final R indices [I>2sigma(I)]	R1 = 0.0307, wR2 = 0.0550
R indices (all data)	R1 = 0.0404, wR2 = 0.0573
Largest diff. peak and hole	0.478 and -0.695 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2b-major.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Rh	1058(1)	2516(1)	-8576(1)	10(1)
P	3064(1)	2857(1)	-7353(1)	10(1)
O	96(1)	4416(1)	-8735(1)	23(1)
C(1)	-399(1)	1980(1)	-10493(1)	13(1)
C(2)	737(2)	1988(1)	-10161(1)	13(1)
C(3)	1580(1)	1391(1)	-9124(1)	12(1)
C(4)	908(1)	928(1)	-8896(1)	12(1)
C(5)	-306(1)	1306(1)	-9720(1)	12(1)
C(6)	1249(2)	225(1)	-8050(1)	15(1)
C(7)	392(2)	-72(1)	-8047(2)	17(1)
C(8)	-798(2)	321(1)	-8840(2)	17(1)
C(9)	-1158(2)	995(1)	-9667(2)	15(1)
C(10)	-1538(1)	2490(1)	-11520(1)	17(1)
C(11)	-1332(2)	3425(1)	-11831(2)	23(1)
C(12)	2917(2)	1268(1)	-8405(2)	15(1)
C(13)	3704(1)	1697(1)	-7130(1)	14(1)
C(14)	3437(1)	3533(1)	-8072(1)	12(1)
C(15)	2580(2)	4118(1)	-9052(2)	16(1)
C(16)	2892(2)	4631(1)	-9580(2)	19(1)
C(17)	4047(2)	4553(1)	-9151(2)	19(1)
C(18)	4898(2)	3967(1)	-8180(2)	19(1)
C(19)	4605(2)	3463(1)	-7629(2)	15(1)
C(20)	3839(1)	3406(1)	-5918(1)	12(1)
C(21)	3482(1)	4311(1)	-5926(1)	14(1)
C(22)	4013(2)	4752(1)	-4848(2)	16(1)
C(23)	4898(2)	4289(1)	-3758(2)	17(1)
C(24)	5253(2)	3393(1)	-3744(1)	17(1)
C(25)	4727(1)	2946(1)	-4823(1)	14(1)
C(26)	1428(2)	2324(1)	-6974(2)	18(1)
C(27)	421(2)	3688(1)	-8687(2)	15(1)
B	7247(2)	2039(1)	-4635(2)	17(1)
F(1)	6926(1)	2956(1)	-4653(1)	23(1)
F(2)	6755(1)	1435(1)	-4340(1)	21(1)
F(3)	8504(1)	1944(1)	-3782(1)	27(1)
F(4)	6773(1)	1815(1)	-5783(1)	29(1)

Table S3. Bond lengths [A] and angles [deg] for 2b-major.

Rh-C(27)	1.8844(17)
Rh-C(26)	2.1118(16)
Rh-C(3)	2.1961(15)
Rh-C(2)	2.2405(15)
Rh-C(1)	2.2623(15)
Rh-P	2.2712(4)
Rh-C(4)	2.3041(15)
Rh-C(5)	2.3145(15)
P-C(20)	1.8013(15)
P-C(14)	1.8184(16)
P-C(13)	1.8334(16)
O-C(27)	1.133(2)
C(1)-C(2)	1.421(2)
C(1)-C(5)	1.453(2)
C(1)-C(10)	1.498(2)
C(2)-C(3)	1.441(2)
C(2)-H(2)	0.91(2)
C(3)-C(4)	1.444(2)
C(3)-C(12)	1.510(2)
C(4)-C(6)	1.422(2)
C(4)-C(5)	1.441(2)
C(5)-C(9)	1.419(2)
C(6)-C(7)	1.369(2)
C(6)-H(6)	0.92(2)
C(7)-C(8)	1.425(2)
C(7)-H(7)	0.94(2)
C(8)-C(9)	1.368(2)
C(8)-H(8)	0.93(2)
C(9)-H(9)	0.95(2)
C(10)-C(11)	1.522(3)
C(10)-H(10A)	0.95(2)
C(10)-H(10B)	0.97(2)
C(11)-H(11A)	0.92(3)
C(11)-H(11B)	0.98(3)
C(11)-H(11C)	0.96(3)
C(12)-C(13)	1.544(2)
C(12)-H(12A)	0.95(2)
C(12)-H(12B)	0.98(2)
C(13)-H(13A)	0.96(2)
C(13)-H(13B)	0.96(2)
C(14)-C(15)	1.397(2)
C(14)-C(19)	1.398(2)
C(15)-C(16)	1.389(2)
C(15)-H(15)	0.93(2)
C(16)-C(17)	1.388(3)
C(16)-H(16)	0.94(2)
C(17)-C(18)	1.389(3)
C(17)-H(17)	0.94(2)
C(18)-C(19)	1.391(2)
C(18)-H(18)	0.95(2)
C(19)-H(19)	0.91(2)
C(20)-C(25)	1.392(2)
C(20)-C(21)	1.400(2)
C(21)-C(22)	1.387(2)

C(21)-H(21)	0.92(2)
C(22)-C(23)	1.390(2)
C(22)-H(22)	0.90(2)
C(23)-C(24)	1.385(2)
C(23)-H(23)	0.93(2)
C(24)-C(25)	1.395(2)
C(24)-H(24)	0.93(2)
C(25)-H(25)	0.93(2)
C(26)-H(26A)	1.00(2)
C(26)-H(26B)	0.97(3)
C(26)-H(26C)	0.96(2)
B-F(3)	1.389(2)
B-F(1)	1.394(2)
B-F(4)	1.395(2)
B-F(2)	1.402(2)

C(27)-Rh-C(26)	86.14(7)
C(27)-Rh-C(3)	156.17(6)
C(26)-Rh-C(3)	117.69(6)
C(27)-Rh-C(2)	119.06(6)
C(26)-Rh-C(2)	152.73(6)
C(3)-Rh-C(2)	37.90(6)
C(27)-Rh-C(1)	101.60(6)
C(26)-Rh-C(1)	134.02(6)
C(3)-Rh-C(1)	63.10(6)
C(2)-Rh-C(1)	36.80(6)
C(27)-Rh-P	101.31(5)
C(26)-Rh-P	86.44(5)
C(3)-Rh-P	80.84(4)
C(2)-Rh-P	97.61(4)
C(1)-Rh-P	134.32(4)
C(27)-Rh-C(4)	152.88(6)
C(26)-Rh-C(4)	91.43(6)
C(3)-Rh-C(4)	37.33(5)
C(2)-Rh-C(4)	61.45(6)
C(1)-Rh-C(4)	61.70(6)
P-Rh-C(4)	105.50(4)
C(27)-Rh-C(5)	117.53(6)
C(26)-Rh-C(5)	99.36(6)
C(3)-Rh-C(5)	62.18(6)
C(2)-Rh-C(5)	61.07(6)
C(1)-Rh-C(5)	36.99(5)
P-Rh-C(5)	140.95(4)
C(4)-Rh-C(5)	36.35(5)
C(20)-P-C(14)	106.53(7)
C(20)-P-C(13)	110.54(7)
C(14)-P-C(13)	104.47(7)
C(20)-P-Rh	118.48(5)
C(14)-P-Rh	114.54(5)
C(13)-P-Rh	101.33(5)
C(2)-C(1)-C(5)	107.31(13)
C(2)-C(1)-C(10)	127.69(14)
C(5)-C(1)-C(10)	124.74(14)
C(2)-C(1)-Rh	70.77(9)
C(5)-C(1)-Rh	73.45(8)
C(10)-C(1)-Rh	125.69(11)
C(1)-C(2)-C(3)	109.22(13)
C(1)-C(2)-Rh	72.44(9)

C(3)-C(2)-Rh	69.38(8)
C(1)-C(2)-H(2)	124.4(14)
C(3)-C(2)-H(2)	126.3(14)
Rh-C(2)-H(2)	123.0(14)
C(2)-C(3)-C(4)	107.22(13)
C(2)-C(3)-C(12)	126.82(14)
C(4)-C(3)-C(12)	125.95(14)
C(2)-C(3)-Rh	72.72(9)
C(4)-C(3)-Rh	75.40(9)
C(12)-C(3)-Rh	117.62(10)
C(6)-C(4)-C(5)	120.41(14)
C(6)-C(4)-C(3)	131.76(14)
C(5)-C(4)-C(3)	107.83(13)
C(6)-C(4)-Rh	125.78(11)
C(5)-C(4)-Rh	72.22(8)
C(3)-C(4)-Rh	67.27(8)
C(9)-C(5)-C(4)	119.90(14)
C(9)-C(5)-C(1)	132.05(15)
C(4)-C(5)-C(1)	108.05(13)
C(9)-C(5)-Rh	124.56(11)
C(4)-C(5)-Rh	71.43(8)
C(1)-C(5)-Rh	69.55(8)
C(7)-C(6)-C(4)	117.90(15)
C(7)-C(6)-H(6)	121.5(13)
C(4)-C(6)-H(6)	120.5(13)
C(6)-C(7)-C(8)	121.63(15)
C(6)-C(7)-H(7)	119.7(14)
C(8)-C(7)-H(7)	118.7(14)
C(9)-C(8)-C(7)	122.02(15)
C(9)-C(8)-H(8)	119.5(13)
C(7)-C(8)-H(8)	118.5(13)
C(8)-C(9)-C(5)	118.10(15)
C(8)-C(9)-H(9)	120.8(13)
C(5)-C(9)-H(9)	121.1(13)
C(1)-C(10)-C(11)	114.68(14)
C(1)-C(10)-H(10A)	108.1(14)
C(11)-C(10)-H(10A)	110.4(14)
C(1)-C(10)-H(10B)	107.8(14)
C(11)-C(10)-H(10B)	109.0(14)
H(10A)-C(10)-H(10B)	106.4(19)
C(10)-C(11)-H(11A)	110.6(16)
C(10)-C(11)-H(11B)	110.1(15)
H(11A)-C(11)-H(11B)	109(2)
C(10)-C(11)-H(11C)	111.0(15)
H(11A)-C(11)-H(11C)	108(2)
H(11B)-C(11)-H(11C)	108(2)
C(3)-C(12)-C(13)	110.93(13)
C(3)-C(12)-H(12A)	108.7(13)
C(13)-C(12)-H(12A)	108.9(13)
C(3)-C(12)-H(12B)	112.0(13)
C(13)-C(12)-H(12B)	109.0(13)
H(12A)-C(12)-H(12B)	107.2(18)
C(12)-C(13)-P	105.93(11)
C(12)-C(13)-H(13A)	111.9(13)
P-C(13)-H(13A)	113.2(13)
C(12)-C(13)-H(13B)	108.7(13)
P-C(13)-H(13B)	106.3(13)
H(13A)-C(13)-H(13B)	110.4(18)

C(15)-C(14)-C(19)	119.78(15)
C(15)-C(14)-P	121.17(12)
C(19)-C(14)-P	119.05(12)
C(16)-C(15)-C(14)	119.94(15)
C(16)-C(15)-H(15)	120.3(14)
C(14)-C(15)-H(15)	119.8(14)
C(17)-C(16)-C(15)	120.34(16)
C(17)-C(16)-H(16)	119.8(15)
C(15)-C(16)-H(16)	119.9(15)
C(16)-C(17)-C(18)	119.79(16)
C(16)-C(17)-H(17)	119.0(14)
C(18)-C(17)-H(17)	121.2(14)
C(17)-C(18)-C(19)	120.48(16)
C(17)-C(18)-H(18)	119.3(14)
C(19)-C(18)-H(18)	120.1(14)
C(18)-C(19)-C(14)	119.66(15)
C(18)-C(19)-H(19)	119.7(13)
C(14)-C(19)-H(19)	120.6(14)
C(25)-C(20)-C(21)	119.90(14)
C(25)-C(20)-P	122.14(12)
C(21)-C(20)-P	117.90(12)
C(22)-C(21)-C(20)	120.29(15)
C(22)-C(21)-H(21)	120.7(14)
C(20)-C(21)-H(21)	118.9(14)
C(21)-C(22)-C(23)	119.60(15)
C(21)-C(22)-H(22)	119.1(13)
C(23)-C(22)-H(22)	121.2(13)
C(24)-C(23)-C(22)	120.35(15)
C(24)-C(23)-H(23)	120.0(14)
C(22)-C(23)-H(23)	119.6(14)
C(23)-C(24)-C(25)	120.43(15)
C(23)-C(24)-H(24)	118.6(14)
C(25)-C(24)-H(24)	120.9(14)
C(20)-C(25)-C(24)	119.42(15)
C(20)-C(25)-H(25)	119.6(13)
C(24)-C(25)-H(25)	120.9(13)
Rh-C(26)-H(26A)	112.4(13)
Rh-C(26)-H(26B)	103.6(15)
H(26A)-C(26)-H(26B)	111.7(19)
Rh-C(26)-H(26C)	110.5(14)
H(26A)-C(26)-H(26C)	110.1(19)
H(26B)-C(26)-H(26C)	108(2)
O-C(27)-Rh	176.01(15)
F(3)-B-F(1)	110.22(15)
F(3)-B-F(4)	110.08(15)
F(1)-B-F(4)	108.63(14)
F(3)-B-F(2)	109.20(14)
F(1)-B-F(2)	109.35(14)
F(4)-B-F(2)	109.35(15)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2b-major.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Rh	10(1)	10(1)	10(1)	-1(1)	7(1)	-1(1)
P	10(1)	10(1)	10(1)	0(1)	7(1)	0(1)
O	27(1)	15(1)	33(1)	-1(1)	23(1)	2(1)
C(1)	15(1)	13(1)	10(1)	-2(1)	8(1)	-2(1)
C(2)	17(1)	12(1)	13(1)	-2(1)	12(1)	-1(1)
C(3)	14(1)	11(1)	14(1)	-3(1)	11(1)	-1(1)
C(4)	14(1)	10(1)	13(1)	-3(1)	10(1)	-2(1)
C(5)	13(1)	11(1)	11(1)	-2(1)	8(1)	-2(1)
C(6)	16(1)	12(1)	13(1)	-1(1)	9(1)	0(1)
C(7)	24(1)	13(1)	17(1)	-1(1)	14(1)	-3(1)
C(8)	19(1)	18(1)	20(1)	-4(1)	15(1)	-6(1)
C(9)	14(1)	16(1)	15(1)	-4(1)	10(1)	-3(1)
C(10)	15(1)	18(1)	13(1)	1(1)	7(1)	0(1)
C(11)	23(1)	19(1)	18(1)	6(1)	11(1)	3(1)
C(12)	15(1)	13(1)	19(1)	-2(1)	13(1)	0(1)
C(13)	13(1)	12(1)	16(1)	0(1)	10(1)	1(1)
C(14)	14(1)	11(1)	12(1)	-1(1)	9(1)	-1(1)
C(15)	14(1)	16(1)	14(1)	2(1)	8(1)	0(1)
C(16)	20(1)	17(1)	14(1)	3(1)	10(1)	-1(1)
C(17)	25(1)	17(1)	19(1)	-2(1)	17(1)	-5(1)
C(18)	21(1)	16(1)	26(1)	-1(1)	19(1)	-1(1)
C(19)	15(1)	13(1)	17(1)	1(1)	11(1)	1(1)
C(20)	11(1)	12(1)	12(1)	-2(1)	8(1)	-2(1)
C(21)	12(1)	13(1)	14(1)	0(1)	8(1)	0(1)
C(22)	17(1)	14(1)	20(1)	-5(1)	13(1)	-3(1)
C(23)	16(1)	21(1)	15(1)	-6(1)	11(1)	-7(1)
C(24)	14(1)	22(1)	11(1)	1(1)	7(1)	-1(1)
C(25)	14(1)	13(1)	14(1)	1(1)	9(1)	1(1)
C(26)	23(1)	19(1)	16(1)	-3(1)	15(1)	-5(1)
C(27)	15(1)	17(1)	16(1)	-3(1)	11(1)	-3(1)
B	16(1)	17(1)	17(1)	1(1)	11(1)	3(1)
F(1)	23(1)	17(1)	28(1)	2(1)	18(1)	5(1)
F(2)	25(1)	19(1)	23(1)	-2(1)	18(1)	-4(1)
F(3)	15(1)	28(1)	32(1)	9(1)	14(1)	6(1)
F(4)	40(1)	29(1)	21(1)	3(1)	22(1)	5(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2b-major.

	x	y	z	U(eq)
H(2)	900(20)	2334(15)	-10540(20)	19(5)
H(6)	2019(18)	-34(14)	-7540(18)	11(5)
H(7)	590(20)	-537(16)	-7500(20)	23(6)
H(8)	-1338(19)	118(15)	-8775(19)	17(5)
H(9)	-1950(20)	1255(15)	-10179(19)	19(5)
H(10A)	-2020(20)	2571(16)	-11330(20)	27(6)
H(10B)	-2000(20)	2090(16)	-12220(20)	23(6)
H(11A)	-2060(20)	3698(18)	-12470(20)	33(7)
H(11B)	-840(20)	3338(18)	-12030(20)	35(7)
H(11C)	-900(20)	3848(18)	-11160(20)	34(7)
H(12A)	3098(19)	1573(15)	-8817(19)	18(5)
H(12B)	3140(20)	611(16)	-8330(20)	21(6)
H(13A)	4550(20)	1713(15)	-6710(19)	18(5)
H(13B)	3589(19)	1341(15)	-6684(19)	15(5)
H(15)	1810(20)	4173(16)	-9340(20)	21(5)
H(16)	2320(20)	5035(18)	-10230(20)	32(6)
H(17)	4240(20)	4912(16)	-9510(20)	23(6)
H(18)	5680(20)	3894(16)	-7910(20)	25(6)
H(19)	5163(19)	3074(15)	-7006(19)	17(5)
H(21)	2910(20)	4616(15)	-6660(20)	19(5)
H(22)	3800(19)	5345(15)	-4867(18)	15(5)
H(23)	5260(20)	4586(15)	-3040(20)	20(5)
H(24)	5850(20)	3099(15)	-3000(20)	19(5)
H(25)	4985(19)	2352(14)	-4821(19)	13(5)
H(26A)	1640(20)	2922(16)	-6530(20)	20(5)
H(26B)	680(20)	2053(18)	-7260(20)	34(7)
H(26C)	2070(20)	1879(18)	-6460(20)	29(6)

Table S6. Torsion angles [deg] for 2b-major.

C(27)-Rh-P-C(20)	53.93(8)
C(26)-Rh-P-C(20)	-31.41(7)
C(3)-Rh-P-C(20)	-150.19(7)
C(2)-Rh-P-C(20)	175.70(7)
C(1)-Rh-P-C(20)	172.74(8)
C(4)-Rh-P-C(20)	-121.90(7)
C(5)-Rh-P-C(20)	-131.89(8)
C(27)-Rh-P-C(14)	-73.19(7)
C(26)-Rh-P-C(14)	-158.53(7)
C(3)-Rh-P-C(14)	82.68(7)
C(2)-Rh-P-C(14)	48.57(7)
C(1)-Rh-P-C(14)	45.62(8)
C(4)-Rh-P-C(14)	110.97(7)
C(5)-Rh-P-C(14)	100.99(8)
C(27)-Rh-P-C(13)	174.99(7)
C(26)-Rh-P-C(13)	89.65(7)
C(3)-Rh-P-C(13)	-29.14(7)
C(2)-Rh-P-C(13)	-63.25(7)
C(1)-Rh-P-C(13)	-66.21(8)
C(4)-Rh-P-C(13)	-0.85(7)
C(5)-Rh-P-C(13)	-10.84(8)
C(27)-Rh-C(1)-C(2)	123.59(10)
C(26)-Rh-C(1)-C(2)	-140.51(10)
C(3)-Rh-C(1)-C(2)	-36.96(9)
P-Rh-C(1)-C(2)	4.89(11)
C(4)-Rh-C(1)-C(2)	-79.27(10)
C(5)-Rh-C(1)-C(2)	-115.62(13)
C(27)-Rh-C(1)-C(5)	-120.78(9)
C(26)-Rh-C(1)-C(5)	-24.88(13)
C(3)-Rh-C(1)-C(5)	78.67(9)
C(2)-Rh-C(1)-C(5)	115.62(13)
P-Rh-C(1)-C(5)	120.52(8)
C(4)-Rh-C(1)-C(5)	36.36(8)
C(27)-Rh-C(1)-C(10)	0.46(14)
C(26)-Rh-C(1)-C(10)	96.35(15)
C(3)-Rh-C(1)-C(10)	-160.09(15)
C(2)-Rh-C(1)-C(10)	-123.14(17)
P-Rh-C(1)-C(10)	-118.24(12)
C(4)-Rh-C(1)-C(10)	157.59(15)
C(5)-Rh-C(1)-C(10)	121.24(17)
C(5)-C(1)-C(2)-C(3)	-4.97(17)
C(10)-C(1)-C(2)-C(3)	-179.34(15)
Rh-C(1)-C(2)-C(3)	59.90(11)
C(5)-C(1)-C(2)-Rh	-64.87(10)
C(10)-C(1)-C(2)-Rh	120.75(16)
C(27)-Rh-C(2)-C(1)	-68.98(11)
C(26)-Rh-C(2)-C(1)	86.48(16)
C(3)-Rh-C(2)-C(1)	119.20(13)
P-Rh-C(2)-C(1)	-176.47(8)
C(4)-Rh-C(2)-C(1)	79.99(10)
C(5)-Rh-C(2)-C(1)	38.31(9)
C(27)-Rh-C(2)-C(3)	171.82(9)
C(26)-Rh-C(2)-C(3)	-32.73(18)
C(1)-Rh-C(2)-C(3)	-119.20(13)

P-Rh-C(2)-C(3)	64.33(9)
C(4)-Rh-C(2)-C(3)	-39.22(9)
C(5)-Rh-C(2)-C(3)	-80.90(9)
C(1)-C(2)-C(3)-C(4)	6.31(17)
Rh-C(2)-C(3)-C(4)	68.11(10)
C(1)-C(2)-C(3)-C(12)	-173.73(14)
Rh-C(2)-C(3)-C(12)	-111.93(15)
C(1)-C(2)-C(3)-Rh	-61.80(11)
C(27)-Rh-C(3)-C(2)	-17.9(2)
C(26)-Rh-C(3)-C(2)	163.76(9)
C(1)-Rh-C(3)-C(2)	35.89(9)
P-Rh-C(3)-C(2)	-115.19(9)
C(4)-Rh-C(3)-C(2)	113.67(13)
C(5)-Rh-C(3)-C(2)	77.73(9)
C(27)-Rh-C(3)-C(4)	-131.61(15)
C(26)-Rh-C(3)-C(4)	50.09(11)
C(2)-Rh-C(3)-C(4)	-113.67(13)
C(1)-Rh-C(3)-C(4)	-77.78(9)
P-Rh-C(3)-C(4)	131.14(9)
C(5)-Rh-C(3)-C(4)	-35.94(8)
C(27)-Rh-C(3)-C(12)	105.13(18)
C(26)-Rh-C(3)-C(12)	-73.18(13)
C(2)-Rh-C(3)-C(12)	123.07(16)
C(1)-Rh-C(3)-C(12)	158.96(14)
P-Rh-C(3)-C(12)	7.87(11)
C(4)-Rh-C(3)-C(12)	-123.26(16)
C(5)-Rh-C(3)-C(12)	-159.20(14)
C(2)-C(3)-C(4)-C(6)	175.30(16)
C(12)-C(3)-C(4)-C(6)	-4.7(3)
Rh-C(3)-C(4)-C(6)	-118.41(17)
C(2)-C(3)-C(4)-C(5)	-5.14(16)
C(12)-C(3)-C(4)-C(5)	174.90(14)
Rh-C(3)-C(4)-C(5)	61.15(10)
C(2)-C(3)-C(4)-Rh	-66.29(10)
C(12)-C(3)-C(4)-Rh	113.75(15)
C(27)-Rh-C(4)-C(6)	-95.48(18)
C(26)-Rh-C(4)-C(6)	-11.17(14)
C(3)-Rh-C(4)-C(6)	126.03(17)
C(2)-Rh-C(4)-C(6)	165.86(16)
C(1)-Rh-C(4)-C(6)	-152.08(15)
P-Rh-C(4)-C(6)	75.53(14)
C(5)-Rh-C(4)-C(6)	-115.09(17)
C(27)-Rh-C(4)-C(5)	19.61(18)
C(26)-Rh-C(4)-C(5)	103.91(10)
C(3)-Rh-C(4)-C(5)	-118.88(13)
C(2)-Rh-C(4)-C(5)	-79.06(10)
C(1)-Rh-C(4)-C(5)	-36.99(9)
P-Rh-C(4)-C(5)	-169.38(8)
C(27)-Rh-C(4)-C(3)	138.49(14)
C(26)-Rh-C(4)-C(3)	-137.20(10)
C(2)-Rh-C(4)-C(3)	39.83(9)
C(1)-Rh-C(4)-C(3)	81.89(10)
P-Rh-C(4)-C(3)	-50.50(9)
C(5)-Rh-C(4)-C(3)	118.88(13)
C(6)-C(4)-C(5)-C(9)	1.8(2)
C(3)-C(4)-C(5)-C(9)	-177.85(14)
Rh-C(4)-C(5)-C(9)	-119.82(14)
C(6)-C(4)-C(5)-C(1)	-178.23(14)

C(3)-C(4)-C(5)-C(1)	2.16(16)
Rh-C(4)-C(5)-C(1)	60.19(10)
C(6)-C(4)-C(5)-Rh	121.58(14)
C(3)-C(4)-C(5)-Rh	-58.04(10)
C(2)-C(1)-C(5)-C(9)	-178.28(16)
C(10)-C(1)-C(5)-C(9)	-3.7(3)
Rh-C(1)-C(5)-C(9)	118.63(17)
C(2)-C(1)-C(5)-C(4)	1.71(17)
C(10)-C(1)-C(5)-C(4)	176.30(14)
Rh-C(1)-C(5)-C(4)	-61.38(10)
C(2)-C(1)-C(5)-Rh	63.09(10)
C(10)-C(1)-C(5)-Rh	-122.32(15)
C(27)-Rh-C(5)-C(9)	-56.04(15)
C(26)-Rh-C(5)-C(9)	34.47(14)
C(3)-Rh-C(5)-C(9)	150.92(15)
C(2)-Rh-C(5)-C(9)	-165.77(15)
C(1)-Rh-C(5)-C(9)	-127.67(17)
P-Rh-C(5)-C(9)	130.40(12)
C(4)-Rh-C(5)-C(9)	114.03(17)
C(27)-Rh-C(5)-C(4)	-170.07(9)
C(26)-Rh-C(5)-C(4)	-79.56(10)
C(3)-Rh-C(5)-C(4)	36.90(9)
C(2)-Rh-C(5)-C(4)	80.20(9)
C(1)-Rh-C(5)-C(4)	118.30(13)
P-Rh-C(5)-C(4)	16.37(12)
C(27)-Rh-C(5)-C(1)	71.63(10)
C(26)-Rh-C(5)-C(1)	162.14(9)
C(3)-Rh-C(5)-C(1)	-81.40(10)
C(2)-Rh-C(5)-C(1)	-38.10(9)
P-Rh-C(5)-C(1)	-101.93(9)
C(4)-Rh-C(5)-C(1)	-118.30(13)
C(5)-C(4)-C(6)-C(7)	-0.2(2)
C(3)-C(4)-C(6)-C(7)	179.35(16)
Rh-C(4)-C(6)-C(7)	89.06(17)
C(4)-C(6)-C(7)-C(8)	-1.6(2)
C(6)-C(7)-C(8)-C(9)	1.8(3)
C(7)-C(8)-C(9)-C(5)	-0.1(2)
C(4)-C(5)-C(9)-C(8)	-1.6(2)
C(1)-C(5)-C(9)-C(8)	178.41(16)
Rh-C(5)-C(9)-C(8)	-88.72(17)
C(2)-C(1)-C(10)-C(11)	-32.3(2)
C(5)-C(1)-C(10)-C(11)	154.26(15)
Rh-C(1)-C(10)-C(11)	60.16(19)
C(2)-C(3)-C(12)-C(13)	110.67(17)
C(4)-C(3)-C(12)-C(13)	-69.38(19)
Rh-C(3)-C(12)-C(13)	22.23(17)
C(3)-C(12)-C(13)-P	-46.96(15)
C(20)-P-C(13)-C(12)	176.01(10)
C(14)-P-C(13)-C(12)	-69.75(11)
Rh-P-C(13)-C(12)	49.53(11)
C(20)-P-C(14)-C(15)	-106.92(14)
C(13)-P-C(14)-C(15)	136.04(13)
Rh-P-C(14)-C(15)	26.11(15)
C(20)-P-C(14)-C(19)	73.08(14)
C(13)-P-C(14)-C(19)	-43.96(14)
Rh-P-C(14)-C(19)	-153.90(11)
C(19)-C(14)-C(15)-C(16)	-0.3(2)
P-C(14)-C(15)-C(16)	179.66(13)

C(14)-C(15)-C(16)-C(17)	1.1(3)
C(15)-C(16)-C(17)-C(18)	-0.7(3)
C(16)-C(17)-C(18)-C(19)	-0.4(3)
C(17)-C(18)-C(19)-C(14)	1.2(3)
C(15)-C(14)-C(19)-C(18)	-0.8(2)
P-C(14)-C(19)-C(18)	179.18(13)
C(14)-P-C(20)-C(25)	-117.60(13)
C(13)-P-C(20)-C(25)	-4.67(15)
Rh-P-C(20)-C(25)	111.57(12)
C(14)-P-C(20)-C(21)	65.34(14)
C(13)-P-C(20)-C(21)	178.27(12)
Rh-P-C(20)-C(21)	-65.49(13)
C(25)-C(20)-C(21)-C(22)	0.1(2)
P-C(20)-C(21)-C(22)	177.28(12)
C(20)-C(21)-C(22)-C(23)	-0.2(2)
C(21)-C(22)-C(23)-C(24)	0.1(2)
C(22)-C(23)-C(24)-C(25)	0.1(2)
C(21)-C(20)-C(25)-C(24)	0.1(2)
P-C(20)-C(25)-C(24)	-176.92(12)
C(23)-C(24)-C(25)-C(20)	-0.2(2)
C(26)-Rh-C(27)-O	107(2)
C(3)-Rh-C(27)-O	-71(2)
C(2)-Rh-C(27)-O	-84(2)
C(1)-Rh-C(27)-O	-119(2)
P-Rh-C(27)-O	22(2)
C(4)-Rh-C(27)-O	-167(2)
C(5)-Rh-C(27)-O	-154(2)

Symmetry transformations used to generate equivalent atoms: