SUPPORTING INFORMATION

FOR

Aromatic C-H Activation and Catalytic Hydrophenylation of Ethylene by TpRu{P(OCH$_2$)$_3$CEt}(NCMe)R

Nicholas A. Foley,[†] Zhuofeng Ke,[§, §, ⊥] T. Brent Gunnoe,[†] Thomas R. Cundari,[§*] and Jeffrey L. Petersen[‡]*

[†]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204; [‡]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, West Virginia 26506-6045; [§]Center for Advanced Scientific Computing and Modeling (CASCaM), Department of Chemistry, University of North Texas, Box 305070, Denton, Texas 76203-5070; [⊥]School of Chemistry & Chemical Engineering, Sun Yat-sen University, Guangzhou 510275, P.R. China

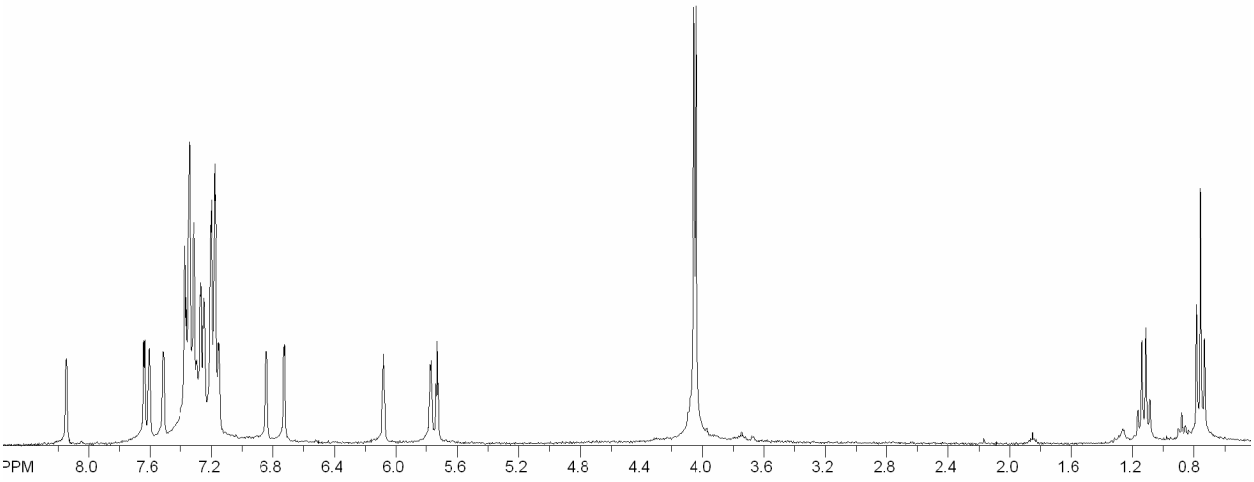

Figure S1. ^{1}H NMR spectrum of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (**1**).

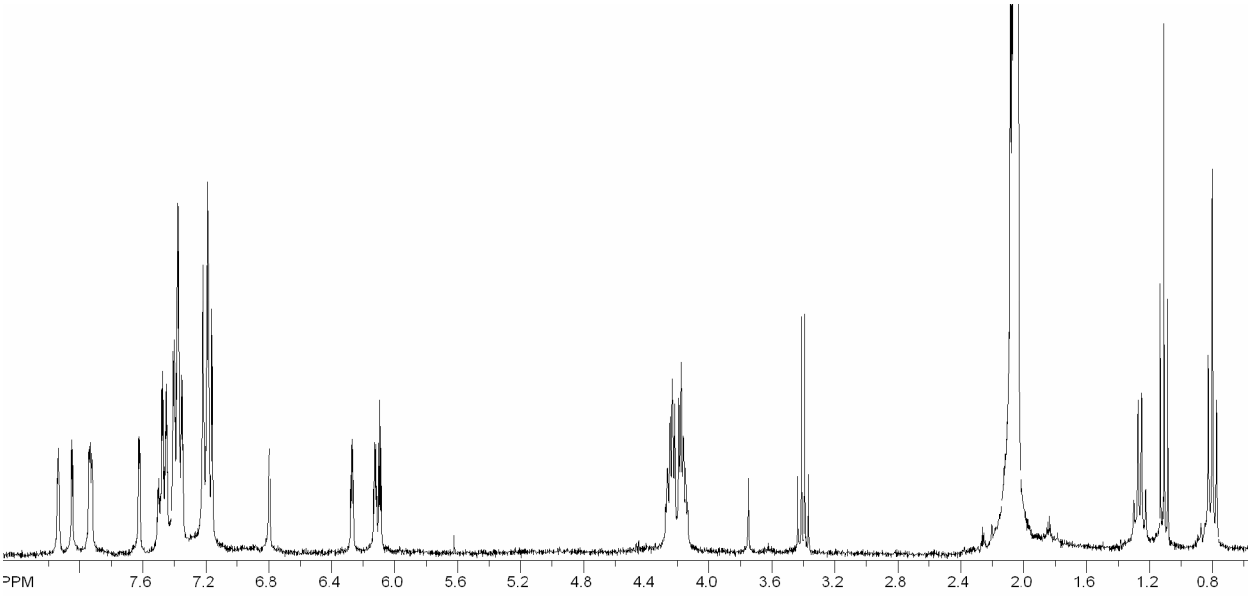

Figure S2. ^{1}H NMR spectrum of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (**2**).

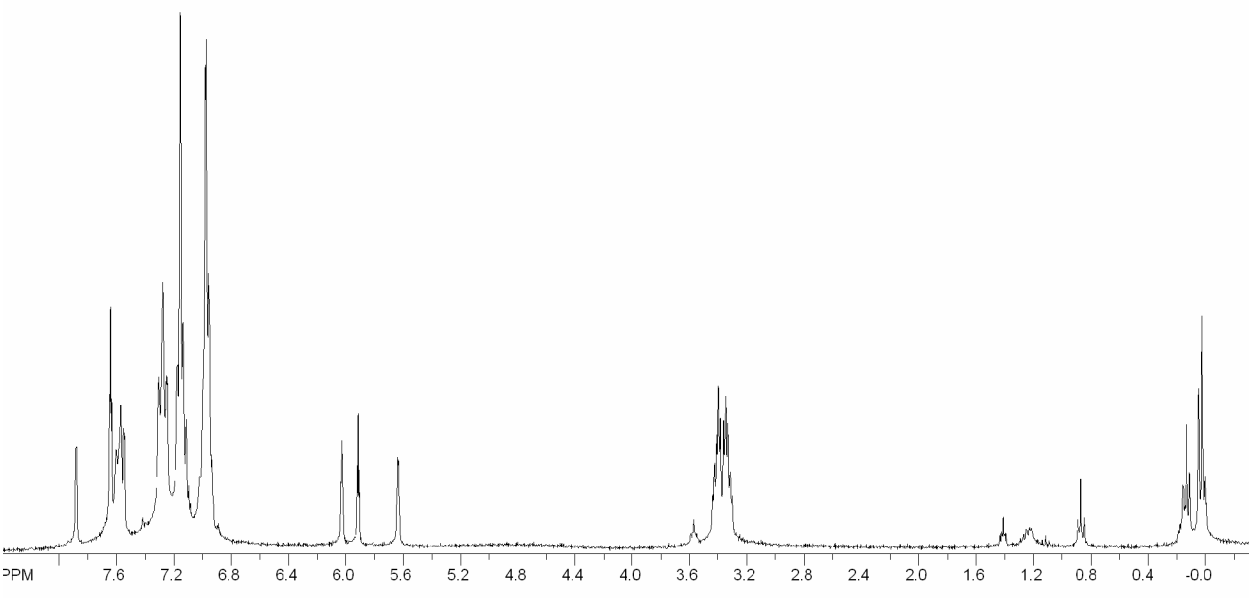

Figure S3. ^{1}H NMR spectrum of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Ph (**3**).

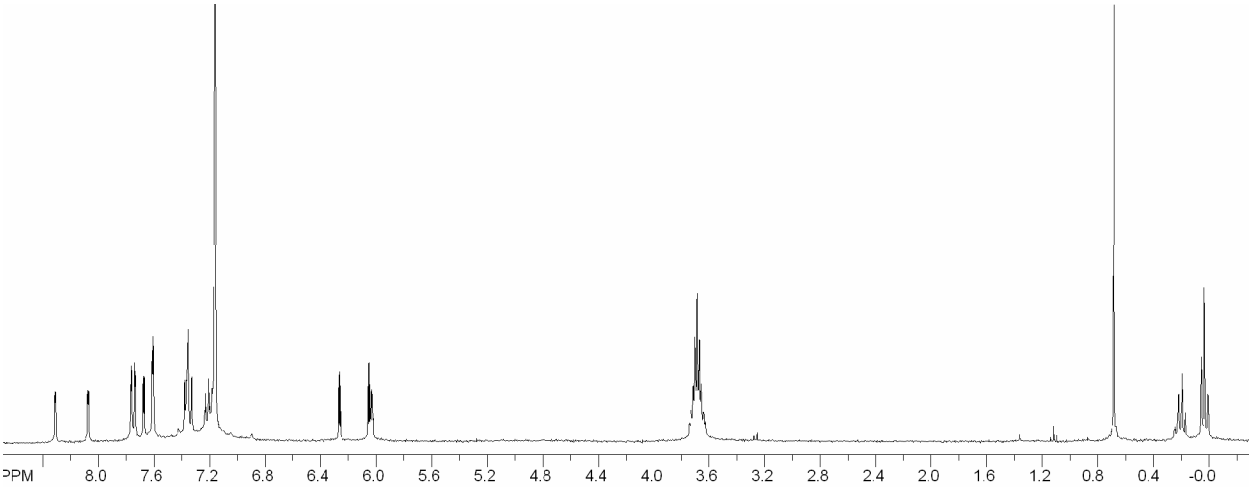

Figure S4. ^{1}H NMR spectrum of TpRu{P(OCH$_2$)$_3$CEt}(NCMe)Ph (**4**).

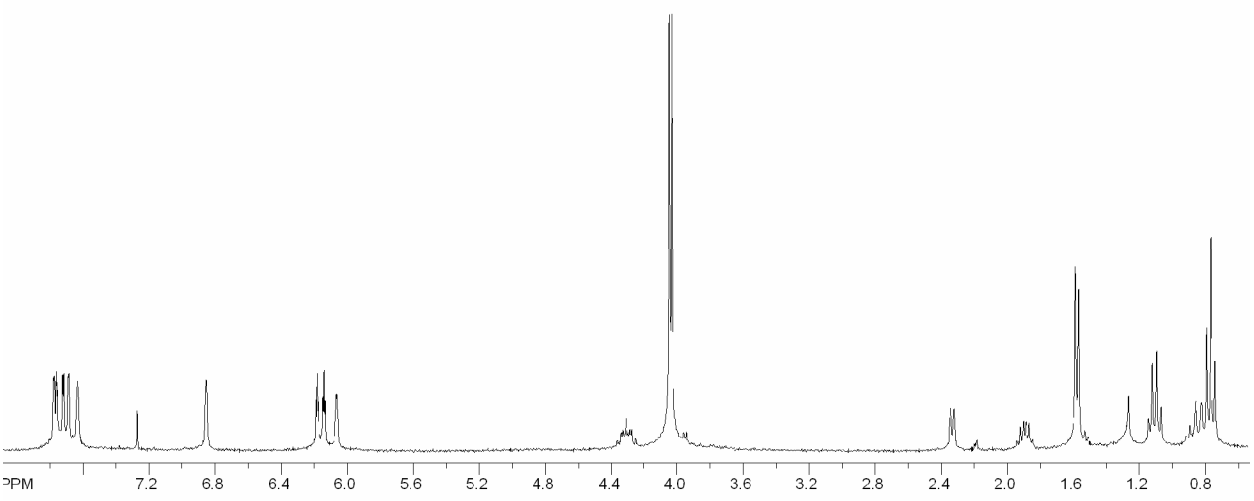

Figure S5. ^{1}H NMR spectrum of TpRu{P(OCH$_2$)$_3$CEt}}(η^3-C$_3$H$_4$Me) (**5**).

X-ray Structure Report for

TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (**1**)

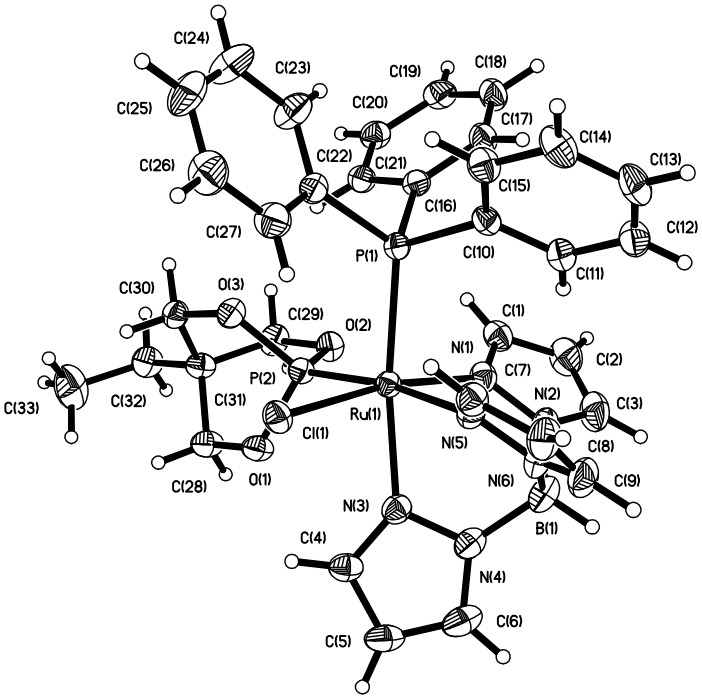

Figure S6. Perspective view of the molecular structure of the TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (**1**) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

Description of the X-ray Structural Analysis of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (1)

A yellow crystalline fragment cleaved from a large crystal of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (**1**) was washed with the perfluoropolyether PFO-XR75 (Lancaster) and sealed under nitrogen in a glass capillary. The sample was optically aligned on the four-circle of a Siemens P4 diffractometer equipped with a graphite monochromator, a monocap collimator, a Mo Kα radiation source (λ = 0.71073 Å), and a SMART CCD detector held at 5.082 cm from the crystal. Four sets of 20 frames each were collected using the ω scan

method and with a 10 s exposure time. Integration of these frames followed by reflection indexing and least-squares refinement produced a crystal orientation matrix for the tetragonal crystal lattice.

Data collection consisted of the measurement of a total of 1650 frames in five different runs covering a hemisphere of data. Frame scan parameters are summarized below:

Run	2θ	ω	ϕ	χ	Scan axis	Scan width (°)	Frames (#)	Exposure time (sec.)
1	28	43.00	0.00	280.00	2	-0.3	100	60
2	28	43.00	90.00	280.00	2	-0.3	100	60
3	28	43.00	180.00	280.00	2	-0.3	100	60
4	28	43.00	270.00	280.00	2	-0.3	100	60
5	28	28.00	0.00	30.00	3	0.3	1250	60

The program SMART (version 5.6)[1] was used for diffractometer control, frame scans, indexing, orientation matrix calculations, least-squares refinement of cell parameters, and the data collection. All 1650 crystallographic raw data frames were read by program SAINT (version 5/6.0)[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce a total of 47423 reflections and their intensities and estimated standard deviations. An semi-empirical absorption correction was applied using the SADABS routine available in SAINT.[1] The data were corrected for Lorentz and polarization effects. No evidence of crystal decomposition was observed. Data preparation was carried out by using the program XPREP,[1] which gave 7958 unique reflections (R_{int} = 3.86 %) with indices $-17 \leq h \leq 17$, $-17 \leq k \leq 17$, $-43 \leq l \leq 47$. The tetragonal space group was determined to be $P4_12_12$ (No. 92).

The structure was solved by direct methods and difference Fourier analysis with the use of SHELXTL 6.1.[2] Idealized positions for the hydrogen atoms were included as fixed contributions using a riding model with isotropic temperature factors set at 1.2 (aromatic, methylene, and B-H) or 1.5 (methyl) times that of the adjacent carbon atom. The positions of the methyl hydrogen atoms were optimized by a rigid rotating group refinement with idealized tetrahedral angles. Full-matrix least-squares refinement, based upon the minimization of $\Sigma w_i |F_o^2 - F_c^2|^2$, with weighting $w_i^{-1} = [\sigma^2(F_o^2) + (0.0109\ P)^2 + 5.6513\ P]$, where $P = (\text{Max}\ (F_o^2, 0) + 2\ F_c^2)/3$, converged to give final discrepancy indices[3] of R1 = 0.0324, wR2 = 0.0765 for 7644 with $I \geq 2\ \sigma(I)$. The goodness of fit (GOF) value was 1.214.

A correction for secondary extinction was not applied. The maximum and minimum residual electron density peaks in the final difference Fourier map were 0.420 and -0.475 e/Å^3, respectively. The linear absorption coefficient, atomic scattering factors, and anomalous dispersion corrections were calculated from values found in the International Tables of X-ray Crystallography.[4]

References

1. SMART, SAINT and XPREP programs are part of Bruker crystallographic software package for single crystal data collection, reduction and preparation.
2. Sheldrick, G. M., SHELXTL6.1 (2000), Crystallographic software package, Bruker AXS, Inc. Madison, Wisconsin, USA.
3. $R_1 = \sum(||F_o| - |F_c||) / \sum|F_o|$, $wR_2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$, $R_{int.} = \sum|F_o^2 - F_o^2(\text{mean})|^2 / \sum[F_o^2]$, and $GOF = [\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$, where n is the number of

reflections and p is the total number of parameters which were varied during the last refinement cycle.

4. International Tables for X-ray Crystallography (1974). Vol. IV, p. 55. Birmingham: Kynoch Press. (Present distributor, D. Reidel, Dordrecht.).

Table S1. Crystal data and structure refinement for $TpRu\{P(OCH_2)_3CEt\}(PPh_3)Cl$ (**1**).

Identification code	bg749ccd	
Empirical formula	$C_{33}H_{36}BClN_6O_3P_2Ru$	
Formula weight	773.95	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	tetragonal	
Space group	$P4_12_12$	
Unit cell dimensions	a = 13.8513(5) Å	α= 90°
	b = 13.8513(5) Å	β= 90°
	c = 36.1727(18) Å	γ = 90°
Volume	6940.0(5) $Å^3$	
Z	8	
Density (calculated)	1.481 g/cm^3	
Absorption coefficient	6.64 cm^{-1}	
F(000)	3168	
Crystal size	0.26 x 0.36 x 0.48 mm	
θ range for data collection	1.85 to 27.50°	
Index ranges	$-17 \le h \le 17$, $-17 \le k \le 17$, $-43 \le l \le 47$	
Reflections collected	47423	
Independent reflections	7958 [R(int) = 0.0386]	
Completeness to θ = 27.50°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7958 / 0 / 425	
Goodness-of-fit on F^2	1.213	
Final R indices [I>2σ(I)]	R1 = 0.0324, wR2 = 0.0765	
R indices (all data)	R1 = 0.0345, wR2 = 0.0776	
Absolute structure parameter	0.08(3)	

Largest diff. peak and hole 0.420 and -0.475 e/Å^3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)Cl (**1**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	6922(1)	473(1)	8738(1)	33(1)
Cl(1)	7811(1)	1597(1)	8359(1)	45(1)
P(1)	5603(1)	246(1)	8339(1)	35(1)
P(2)	6290(1)	1731(1)	9021(1)	34(1)
O(1)	7073(2)	2372(2)	9240(1)	46(1)
O(2)	5501(2)	1553(2)	9341(1)	43(1)
O(3)	5765(2)	2533(2)	8776(1)	43(1)
N(1)	6376(2)	-555(2)	9106(1)	43(1)
N(2)	6949(3)	-1302(2)	9208(1)	50(1)
N(3)	8167(2)	479(2)	9095(1)	43(1)
N(4)	8505(2)	-389(2)	9222(1)	50(1)
N(5)	7725(2)	-645(2)	8470(1)	40(1)
N(6)	8113(2)	-1367(2)	8669(1)	49(1)
C(1)	5542(3)	-676(3)	9284(1)	49(1)
C(2)	5582(4)	-1493(3)	9505(1)	67(1)
C(3)	6472(4)	-1873(3)	9449(1)	68(1)
C(4)	8782(3)	1141(3)	9216(1)	47(1)
C(5)	9509(3)	723(3)	9425(1)	61(1)
C(6)	9309(3)	-237(4)	9421(1)	65(1)
C(7)	8004(3)	-785(3)	8123(1)	45(1)
C(8)	8567(3)	-1605(3)	8098(1)	59(1)
C(9)	8628(3)	-1955(3)	8446(1)	59(1)
C(10)	5706(2)	-920(2)	8092(1)	39(1)
C(11)	5913(3)	-1744(2)	8296(1)	48(1)
C(12)	6012(3)	-2630(3)	8123(1)	56(1)
C(13)	5903(3)	-2707(3)	7745(1)	58(1)
C(14)	5681(3)	-1904(3)	7543(1)	59(1)
C(15)	5583(3)	-1013(3)	7712(1)	48(1)

C(16)	4386(2)	124(2)	8540(1)	39(1)
C(17)	3847(3)	-712(3)	8509(1)	48(1)
C(18)	2923(3)	-776(3)	8659(1)	54(1)
C(19)	2533(3)	-12(3)	8844(1)	52(1)
C(20)	3055(3)	840(3)	8873(1)	48(1)
C(21)	3969(2)	917(2)	8724(1)	43(1)
C(22)	5352(3)	1087(2)	7954(1)	41(1)
C(23)	4419(3)	1334(3)	7854(1)	63(1)
C(24)	4246(4)	1922(4)	7550(1)	79(2)
C(25)	5000(4)	2263(4)	7344(1)	73(1)
C(26)	5928(4)	2007(4)	7437(1)	73(1)
C(27)	6109(3)	1420(3)	7740(1)	57(1)
C(28)	6711(3)	3185(3)	9449(1)	50(1)
C(29)	5113(3)	2415(3)	9514(1)	48(1)
C(30)	5459(3)	3403(2)	8967(1)	42(1)
C(31)	5637(2)	3312(2)	9385(1)	42(1)
C(32)	5253(3)	4210(3)	9589(1)	54(1)
C(33)	5729(4)	5161(3)	9487(2)	86(2)
B(1)	8029(4)	-1329(3)	9098(1)	56(1)

Table S3. Interatomic distances [Å] and bond angles [°] for TpRu{$P(OCH_2)_3CEt$}(PPh_3)Cl (**1**).

Ru(1)-N(1)	2.092(3)
Ru(1)-N(5)	2.139(3)
Ru(1)-N(3)	2.152(3)
Ru(1)-P(2)	2.2015(8)
Ru(1)-P(1)	2.3511(8)
Ru(1)-Cl(1)	2.4117(8)
P(1)-C(16)	1.845(3)
P(1)-C(22)	1.847(3)
P(1)-C(10)	1.849(3)
P(2)-O(3)	1.595(2)
P(2)-O(1)	1.610(2)
P(2)-O(2)	1.611(2)
O(1)-C(28)	1.446(4)
O(2)-C(29)	1.452(4)
O(3)-C(30)	1.453(4)
N(1)-C(1)	1.332(5)
N(1)-N(2)	1.355(4)
N(2)-C(3)	1.349(5)
N(2)-B(1)	1.547(6)
N(3)-C(4)	1.327(5)
N(3)-N(4)	1.371(4)
N(4)-C(6)	1.344(5)
N(4)-B(1)	1.526(6)
N(5)-C(7)	1.326(4)
N(5)-N(6)	1.345(4)
N(6)-C(9)	1.350(5)
N(6)-B(1)	1.557(5)
C(1)-C(2)	1.385(5)
C(2)-C(3)	1.355(7)
C(4)-C(5)	1.385(5)
C(5)-C(6)	1.358(6)
C(7)-C(8)	1.381(5)
C(8)-C(9)	1.353(6)
C(10)-C(11)	1.389(5)

C(10)-C(15)	1.394(4)
C(11)-C(12)	1.385(5)
C(12)-C(13)	1.379(6)
C(13)-C(14)	1.367(6)
C(14)-C(15)	1.383(5)
C(16)-C(17)	1.383(5)
C(16)-C(21)	1.408(4)
C(17)-C(18)	1.392(5)
C(18)-C(19)	1.363(5)
C(19)-C(20)	1.387(5)
C(20)-C(21)	1.380(5)
C(22)-C(27)	1.382(5)
C(22)-C(23)	1.386(5)
C(23)-C(24)	1.387(5)
C(24)-C(25)	1.366(7)
C(25)-C(26)	1.375(7)
C(26)-C(27)	1.389(5)
C(28)-C(31)	1.516(5)
C(29)-C(31)	1.513(5)
C(30)-C(31)	1.539(4)
C(31)-C(32)	1.541(4)
C(32)-C(33)	1.520(6)

N(1)-Ru(1)-N(5)	89.06(11)
N(1)-Ru(1)-N(3)	84.91(11)
N(5)-Ru(1)-N(3)	81.85(10)
N(1)-Ru(1)-P(2)	95.74(8)
N(5)-Ru(1)-P(2)	172.00(8)
N(3)-Ru(1)-P(2)	92.17(8)
N(1)-Ru(1)-P(1)	91.07(8)
N(5)-Ru(1)-P(1)	91.60(8)
N(3)-Ru(1)-P(1)	172.35(8)
P(2)-Ru(1)-P(1)	94.71(3)
N(1)-Ru(1)-Cl(1)	170.43(8)
N(5)-Ru(1)-Cl(1)	86.82(8)
N(3)-Ru(1)-Cl(1)	85.96(8)

P(2)-Ru(1)-Cl(1)	87.45(3)
P(1)-Ru(1)-Cl(1)	97.67(3)
C(16)-P(1)-C(22)	100.57(15)
C(16)-P(1)-C(10)	100.46(15)
C(22)-P(1)-C(10)	101.67(14)
C(16)-P(1)-Ru(1)	118.63(10)
C(22)-P(1)-Ru(1)	121.64(12)
C(10)-P(1)-Ru(1)	110.70(11)
O(3)-P(2)-O(1)	101.39(13)
O(3)-P(2)-O(2)	101.34(13)
O(1)-P(2)-O(2)	100.81(13)
O(3)-P(2)-Ru(1)	118.33(9)
O(1)-P(2)-Ru(1)	113.34(9)
O(2)-P(2)-Ru(1)	118.79(9)
C(28)-O(1)-P(2)	116.9(2)
C(29)-O(2)-P(2)	115.8(2)
C(30)-O(3)-P(2)	116.5(2)
C(1)-N(1)-N(2)	106.3(3)
C(1)-N(1)-Ru(1)	135.0(3)
N(2)-N(1)-Ru(1)	118.7(2)
C(3)-N(2)-N(1)	109.6(4)
C(3)-N(2)-B(1)	128.7(4)
N(1)-N(2)-B(1)	121.0(3)
C(4)-N(3)-N(4)	106.0(3)
C(4)-N(3)-Ru(1)	135.7(2)
N(4)-N(3)-Ru(1)	118.1(2)
C(6)-N(4)-N(3)	109.0(3)
C(6)-N(4)-B(1)	130.5(4)
N(3)-N(4)-B(1)	120.1(3)
C(7)-N(5)-N(6)	106.4(3)
C(7)-N(5)-Ru(1)	133.3(2)
N(6)-N(5)-Ru(1)	120.2(2)
N(5)-N(6)-C(9)	109.8(3)
N(5)-N(6)-B(1)	118.6(3)
C(9)-N(6)-B(1)	131.0(3)
N(1)-C(1)-C(2)	110.2(4)

C(3)-C(2)-C(1)	105.5(4)
N(2)-C(3)-C(2)	108.3(4)
N(3)-C(4)-C(5)	111.0(4)
C(6)-C(5)-C(4)	104.9(4)
N(4)-C(6)-C(5)	109.1(4)
N(5)-C(7)-C(8)	110.4(3)
C(9)-C(8)-C(7)	105.5(3)
N(6)-C(9)-C(8)	108.0(3)
C(11)-C(10)-C(15)	118.2(3)
C(11)-C(10)-P(1)	118.5(2)
C(15)-C(10)-P(1)	123.2(3)
C(12)-C(11)-C(10)	120.6(3)
C(13)-C(12)-C(11)	120.5(4)
C(14)-C(13)-C(12)	119.4(4)
C(13)-C(14)-C(15)	120.8(3)
C(14)-C(15)-C(10)	120.5(4)
C(17)-C(16)-C(21)	118.0(3)
C(17)-C(16)-P(1)	122.6(3)
C(21)-C(16)-P(1)	119.4(2)
C(16)-C(17)-C(18)	121.2(3)
C(19)-C(18)-C(17)	120.3(3)
C(18)-C(19)-C(20)	119.4(3)
C(21)-C(20)-C(19)	121.0(3)
C(20)-C(21)-C(16)	120.0(3)
C(27)-C(22)-C(23)	118.6(3)
C(27)-C(22)-P(1)	119.3(3)
C(23)-C(22)-P(1)	121.9(3)
C(22)-C(23)-C(24)	120.9(4)
C(25)-C(24)-C(23)	120.2(4)
C(24)-C(25)-C(26)	119.5(4)
C(25)-C(26)-C(27)	120.8(4)
C(22)-C(27)-C(26)	120.1(4)
O(1)-C(28)-C(31)	110.6(3)
O(2)-C(29)-C(31)	111.4(3)
O(3)-C(30)-C(31)	110.7(3)
C(29)-C(31)-C(28)	109.1(3)

C(29)-C(31)-C(30)	107.1(3)
C(28)-C(31)-C(30)	108.4(3)
C(29)-C(31)-C(32)	110.5(3)
C(28)-C(31)-C(32)	111.1(3)
C(30)-C(31)-C(32)	110.5(3)
C(33)-C(32)-C(31)	115.6(3)
N(4)-B(1)-N(2)	108.8(3)
N(4)-B(1)-N(6)	106.8(3)
N(2)-B(1)-N(6)	109.2(3)

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $TpRu\{P(OCH_2)_3CEt\}(PPh_3)Cl$ (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	34(1)	31(1)	34(1)	-2(1)	1(1)	1(1)
Cl(1)	43(1)	41(1)	49(1)	1(1)	6(1)	-6(1)
P(1)	36(1)	32(1)	36(1)	-2(1)	-1(1)	1(1)
P(2)	34(1)	35(1)	34(1)	-3(1)	1(1)	1(1)
O(1)	34(1)	47(1)	57(1)	-20(1)	-5(1)	8(1)
O(2)	43(1)	42(1)	44(1)	-3(1)	9(1)	3(1)
O(3)	53(1)	40(1)	34(1)	-4(1)	-3(1)	7(1)
N(1)	54(2)	39(1)	38(1)	1(1)	0(1)	-3(1)
N(2)	60(2)	41(2)	49(2)	11(1)	4(2)	3(2)
N(3)	45(2)	43(2)	43(1)	-2(1)	-1(1)	6(1)
N(4)	53(2)	51(2)	45(2)	-1(1)	-6(1)	12(1)
N(5)	42(2)	36(2)	43(1)	-2(1)	-2(1)	5(1)
N(6)	56(2)	33(1)	58(2)	4(1)	0(1)	9(1)
C(1)	52(2)	48(2)	47(2)	1(2)	2(2)	-9(2)
C(2)	73(3)	64(3)	62(2)	15(2)	13(2)	-15(2)
C(3)	90(3)	50(2)	63(2)	15(2)	2(2)	-10(2)
C(4)	39(2)	57(2)	45(2)	-9(2)	-1(1)	4(2)
C(5)	43(2)	79(3)	61(2)	-16(2)	-14(2)	9(2)
C(6)	59(3)	80(3)	57(2)	-9(2)	-15(2)	23(2)

C(7)	45(2)	43(2)	48(2)	-4(1)	3(2)	2(2)
C(8)	66(3)	47(2)	62(2)	-11(2)	12(2)	13(2)
C(9)	61(2)	40(2)	76(3)	-4(2)	6(2)	15(2)
C(10)	38(2)	36(2)	42(2)	-7(1)	2(1)	-3(1)
C(11)	52(2)	39(2)	52(2)	-3(2)	-3(2)	-2(2)
C(12)	57(2)	41(2)	71(2)	-3(2)	-1(2)	-1(2)
C(13)	60(2)	43(2)	70(2)	-20(2)	14(2)	-9(2)
C(14)	70(3)	57(2)	49(2)	-17(2)	14(2)	-15(2)
C(15)	56(2)	46(2)	43(2)	-6(1)	4(2)	-2(2)
C(16)	36(2)	41(2)	40(2)	1(1)	-3(1)	2(1)
C(17)	39(2)	39(2)	67(2)	-4(2)	6(2)	0(1)
C(18)	43(2)	44(2)	76(3)	4(2)	4(2)	-8(2)
C(19)	34(2)	66(2)	56(2)	10(2)	6(2)	-1(2)
C(20)	45(2)	51(2)	47(2)	-5(1)	-2(2)	7(2)
C(21)	40(2)	40(2)	51(2)	-5(2)	-4(2)	3(1)
C(22)	51(2)	37(2)	35(1)	-3(1)	-3(1)	3(1)
C(23)	54(2)	76(3)	58(2)	22(2)	4(2)	14(2)
C(24)	70(3)	101(4)	66(2)	26(3)	-4(2)	32(3)
C(25)	100(4)	74(3)	46(2)	17(2)	-1(2)	21(3)
C(26)	89(3)	78(3)	50(2)	16(2)	7(2)	-11(3)
C(27)	59(2)	65(3)	48(2)	8(2)	-1(2)	-6(2)
C(28)	42(2)	51(2)	58(2)	-23(2)	-7(2)	11(2)
C(29)	50(2)	50(2)	42(2)	-1(2)	12(2)	9(2)
C(30)	43(2)	38(2)	45(2)	0(1)	0(1)	4(1)
C(31)	35(2)	49(2)	42(2)	-9(1)	2(1)	4(1)
C(32)	51(2)	50(2)	60(2)	-17(2)	6(2)	13(2)
C(33)	95(4)	51(3)	113(4)	-27(3)	29(3)	6(3)
B(1)	65(3)	49(2)	54(2)	10(2)	0(2)	17(2)

Table S5. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for TpRu{$P(OCH_2)_3CEt$}(PPh_3)Cl (**1**).

	x	y	z	U(eq)
H(1)	5010	-270	9264	59
H(2)	5100	-1731	9658	80
H(3)	6712	-2431	9557	81
H(4)	8733	1799	9167	57
H(5)	10021	1032	9541	73
H(6)	9672	-713	9538	78
H(7)	7843	-387	7926	54
H(8)	8845	-1863	7886	70
H(9)	8965	-2503	8519	71
H(11)	5986	-1701	8551	57
H(12)	6152	-3176	8262	68
H(13)	5979	-3302	7629	69
H(14)	5595	-1957	7289	71
H(15)	5433	-473	7570	58
H(17)	4105	-1241	8386	58
H(18)	2571	-1343	8633	65
H(19)	1923	-60	8949	63
H(20)	2785	1366	8994	57
H(21)	4310	1493	8746	52
H(23)	3901	1104	7992	75
H(24)	3616	2084	7487	95
H(25)	4885	2666	7143	88
H(26)	6441	2230	7294	87
H(27)	6740	1252	7800	69
H(28A)	7049	3766	9374	60
H(28B)	6832	3082	9710	60
H(29A)	5174	2358	9781	57
H(29B)	4432	2471	9455	57
H(30A)	4778	3513	8921	50
H(30B)	5814	3953	8871	50

H(32A)	4566	4264	9541	64
H(32B)	5334	4109	9853	64
H(33A)	5642	5280	9227	129
H(33B)	6407	5128	9541	129
H(33C)	5441	5675	9626	129
H(1A)	8351	-1886	9211	67

X-ray Structure Report for

TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (**2**)

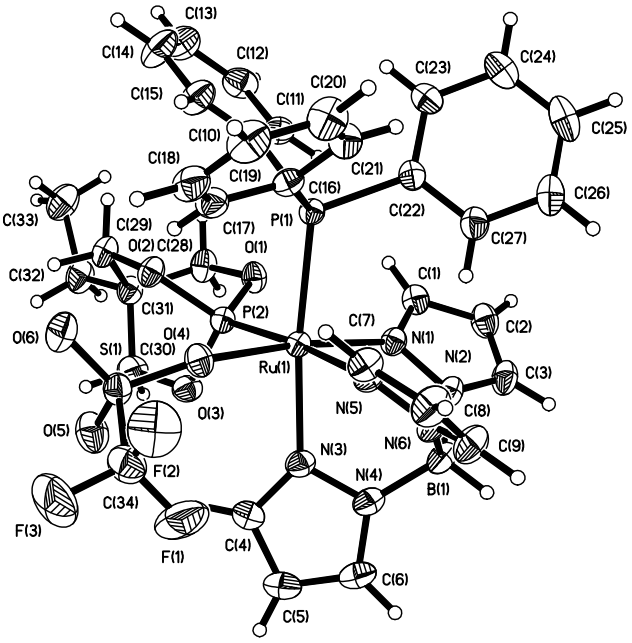

Figure S7. Perspective view of the molecular structure of the TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (**2**) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

Description of the X-ray Structural Analysis of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (2).

A yellow crystal of TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (**2**) was washed with the perfluoropolyether PFO-XR75 (Lancaster) and sealed under nitrogen in a glass capillary. The sample was optically aligned on the four-circle of a Siemens P4 diffractometer equipped with a graphite monochromator, a monocap collimator, a Mo Kα radiation source (λ = 0.71073 Å), and a SMART CCD detector held at 5.082 cm from the crystal. Four sets of 20 frames each were collected using the ω scan method and with a 10 s exposure time. Integration of these frames followed by reflection indexing and least-squares refinement produced a crystal orientation matrix for the monoclinic crystal lattice.

Data collection consisted of the measurement of a total of 1650 frames in five different runs covering a hemisphere of data. Frame scan parameters are summarized below:

Run	2θ	ω	ϕ	χ	Scan axis	Scan width (°)	Frames (#)	Exposure time (sec.)
1	28	43.00	0.00	280.00	2	-0.3	100	30
2	28	43.00	90.00	280.00	2	-0.3	100	30
3	28	43.00	180.00	280.00	2	-0.3	100	30
4	28	43.00	270.00	280.00	2	-0.3	100	30
5	28	28.00	0.00	30.00	3	0.3	1250	30

The program SMART (version 5.6)[1] was used for diffractometer control, frame scans, indexing, orientation matrix calculations, least-squares refinement of cell parameters, and the data collection. All 1650 crystallographic raw data frames were read by program SAINT (version 5/6.0)[1] and integrated using 3D profiling algorithms. The resulting data were reduced to produce a total of 27318 reflections and their intensities and estimated standard deviations. An absorption correction was applied using the SADABS routine available in SAINT.[1] The data were corrected for Lorentz and polarization effects. No evidence of crystal decomposition was observed. Data preparation was carried out by using the program XPREP,[1] which gave 9323 unique reflections (R_{int} = 3.18 %) with indices $-19 \leq h \leq 20$, $-19 \leq k \leq 19$, $-22 \leq l \leq 23$. The monoclinic space group was determined to be $P2_1/c$ (No. 14).

The structure was solved by a combination of direct methods and difference Fourier analysis with the use of SHELXTL 6.1.[2] The hydrogen atoms were included as fixed contributions using a riding model with isotropic temperature factors set at 1.2 (methylene protons, aromatic protons, and B-H) or 1.5 (methyl protons) times that of the adjacent non-

hydrogen atom. The positions of the methyl hydrogen atoms were optimized by a rigid rotating group refinement with idealized tetrahedral angles. The crystallographic asymmetric unit also contains a badly disordered molecule of methylene chloride. Its presence was confirmed by the observation of a sharp resonance at δ 4.25 in the NMR spectrum measured following the addition of crystals to benzene-d_6. The methylene chloride was treated as a diffuse electron density contribution with the aid of the SQUEEZE routine in the program PLATON.[3] Although specific positions for the independent carbon, hydrogen, and chlorine atoms of the methylene chloride molecule were not determined, the calculated density, absorption coefficient and empirical formula weight reflect their presence within the crystal lattice. Full-matrix least-squares refinement, based upon the minimization of $\Sigma w_i |F_o^2 - F_c^2|^2$, with weighting $w_i^{-1} = [\sigma^2(F_o^2) + (0.0709\ P)^2 + 0.2115\ P]$, where $P = (\text{Max}\ (F_o^2, 0) + 2\ F_c^2)/3$, converged to give final discrepancy indices[4] of R1 = 0.0354, wR2 = 0.1055 for 8063 with $I > 2\ \sigma(I)$. The goodness of fit (GOF) value was 1.068.

A correction for secondary extinction was not applied. The maximum and minimum residual electron density peaks in the final difference Fourier map were 0.757 and -0.443 e/Å^3, respectively. The linear absorption coefficient, atomic scattering factors, and anomalous dispersion corrections were calculated from values found in the International Tables of X-ray Crystallography.[5]

References

1. SMART, SAINT and XPREP programs are part of Bruker crystallographic software package for single crystal data collection, reduction and preparation.

2. Sheldrick, G. M., SHELXTL6.1 (2000), Crystallographic software package, Bruker AXS, Inc. Madison, Wisconsin, USA.

3. PLATON, written by Professor Anthony L. Spek, Bijvoet Centre for Biomolecular Research, Utrecht University. Current versions of PLATON for Windows are available from Professor Louis J. Farrugia, Department of Chemistry, University of Glasgow at www.chem.gla.ac.uk/~louis/software/.

4. $R_1 = \sum(||F_o| - |F_c||) / \sum|F_o|$, $wR_2 = [\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]]^{1/2}$, $R_{int.} = \sum|F_o^2 - F_o^2(mean)|^2 / \sum[F_o^2]$, and GOF = $[\sum[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$, where n is the number of reflections and p is the total number of parameters which were varied during the last refinement cycle.

5. International Tables for X-ray Crystallography (1974). Vol. IV, p. 55. Birmingham: Kynoch Press. (Present distributor, D. Reidel, Dordrecht.).

Table S6. Crystal data and structure refinement for TpRu{$P(OCH_2)_3CEt$}(PPh_3)OTf (**2**).

Identification code	bg750plt	
Empirical formula*	$C_{35}H_{38}BCl_2F_3N_6O_6P_2Ru$ S	
Formula weight	972.49	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.8186(8) Å	α= 90°
	b = 14.9763(8) Å	β= 104.532(1)°
	c = 18.0713(9) Å	γ = 90°
Volume	4144.2(4) $Å^3$	
Z	4	
Density (calculated)	1.559 g/cm^3	
Absorption coefficient	7.00 cm^{-1}	
F(000)	1976	

Crystal size	0.26 x 0.40 x 0.68 mm
θ range for data collection	1.33 to 27.51°
Index ranges	$-19 \leq h \leq 20$, $-19 \leq k \leq 19$, $-22 \leq l \leq 23$
Reflections collected	27318
Independent reflections	9323 [R(int) = 0.0318]
Completeness to θ = 27.51°	97.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9323 / 0 / 488
Goodness-of-fit on F^2	1.068
Final R indices [I>2σ(I)]	R1 = 0.0354, wR2 = 0.1055
R indices (all data)	R1 = 0.0400, wR2 = 0.1092
Largest diff. peak and hole	0.757 and -0.443 e/Å^3

*The crystallographic asymmetric contains a badly disordered of CH_2Cl_2 which was treated with PLATON.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for TpRu{P(OCH$_2$)$_3$CEt}(PPh$_3$)OTf (**2**). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2357(1)	4518(1)	1948(1)	33(1)
S(1)	1629(1)	5528(1)	3402(1)	46(1)
P(1)	3597(1)	5399(1)	1948(1)	34(1)
P(2)	1437(1)	5506(1)	1277(1)	35(1)
F(1)	1511(2)	3938(1)	3958(1)	111(1)
F(2)	2578(2)	4707(2)	4600(1)	106(1)
F(3)	1279(2)	5021(2)	4673(1)	131(1)
O(1)	1450(1)	5709(1)	407(1)	44(1)
O(2)	1548(1)	6476(1)	1656(1)	43(1)
O(3)	414(1)	5315(1)	1166(1)	47(1)
O(4)	2213(1)	5101(1)	3001(1)	48(1)
O(5)	722(1)	5511(1)	3018(1)	70(1)
O(6)	1956(1)	6348(1)	3765(1)	74(1)
N(1)	2484(1)	3805(1)	1007(1)	39(1)

N(2)	2551(1)	2894(1)	1066(1)	45(1)
N(3)	1360(1)	3573(1)	1987(1)	44(1)
N(4)	1529(1)	2686(1)	1900(1)	49(1)
N(5)	3177(1)	3567(1)	2691(1)	41(1)
N(6)	3123(1)	2691(1)	2482(1)	47(1)
C(1)	2560(1)	4017(2)	310(1)	45(1)
C(2)	2686(2)	3247(2)	-83(1)	55(1)
C(3)	2671(1)	2566(2)	409(1)	54(1)
C(4)	550(1)	3619(2)	2100(1)	52(1)
C(5)	199(2)	2764(2)	2083(2)	62(1)
C(6)	835(2)	2200(2)	1961(1)	58(1)
C(7)	3752(1)	3611(2)	3371(1)	49(1)
C(8)	4075(2)	2766(2)	3600(1)	63(1)
C(9)	3661(2)	2206(2)	3026(1)	60(1)
C(10)	3480(1)	6510(1)	1502(1)	40(1)
C(11)	3191(1)	6579(2)	702(1)	47(1)
C(12)	3061(2)	7406(2)	348(2)	60(1)
C(13)	3217(2)	8167(2)	772(2)	71(1)
C(14)	3504(2)	8116(2)	1552(2)	79(1)
C(15)	3636(2)	7293(2)	1913(2)	61(1)
C(16)	4311(1)	5634(1)	2906(1)	40(1)
C(17)	3959(2)	6025(2)	3463(1)	49(1)
C(18)	4481(2)	6160(2)	4201(1)	60(1)
C(19)	5346(2)	5924(2)	4386(1)	65(1)
C(20)	5711(2)	5557(2)	3836(2)	64(1)
C(21)	5190(2)	5406(2)	3097(1)	51(1)
C(22)	4386(1)	4861(1)	1492(1)	40(1)
C(23)	4937(1)	5361(2)	1160(1)	50(1)
C(24)	5587(2)	4957(2)	895(2)	68(1)
C(25)	5687(2)	4032(2)	946(2)	75(1)
C(26)	5142(2)	3534(2)	1265(2)	62(1)
C(27)	4503(1)	3942(2)	1548(1)	49(1)
C(28)	822(2)	6375(2)	8(1)	49(1)
C(29)	1004(1)	7178(1)	1230(1)	47(1)
C(30)	-162(1)	6051(2)	844(2)	55(1)
C(31)	334(1)	6791(1)	545(1)	44(1)

C(32)	-312(2)	7507(2)	135(2)	58(1)
C(33)	91(2)	8355(2)	-71(2)	74(1)
C(34)	1745(2)	4756(2)	4205(2)	71(1)
B(1)	2411(2)	2404(2)	1768(2)	50(1)

Table S8. Interatomic distances [Å] and bond angles [°] for TpRu{$P(OCH_2)_3CEt$}(PPh_3)OTf (**2**).

Ru(1)-N(1)	2.061(2)
Ru(1)-N(3)	2.133(2)
Ru(1)-N(5)	2.153(2)
Ru(1)-O(4)	2.158(1)
Ru(1)-P(2)	2.2124(5)
Ru(1)-P(1)	2.3642(5)
S(1)-O(6)	1.427(2)
S(1)-O(5)	1.428(2)
S(1)-O(4)	1.457(2)
S(1)-C(34)	1.828(3)
P(1)-C(10)	1.839(2)
P(1)-C(22)	1.843(2)
P(1)-C(16)	1.847(2)
P(2)-O(2)	1.597(2)
P(2)-O(3)	1.606(2)
P(2)-O(1)	1.607(2)
F(1)-C(34)	1.325(4)
F(2)-C(34)	1.334(4)
F(3)-C(34)	1.316(4)
O(1)-C(28)	1.464(2)
O(2)-C(29)	1.452(2)
O(3)-C(30)	1.455(3)
N(1)-C(1)	1.332(3)
N(1)-N(2)	1.370(2)
N(2)-C(3)	1.343(3)
N(2)-B(1)	1.529(3)

N(3)-C(4)	1.348(3)
N(3)-N(4)	1.373(3)
N(4)-C(6)	1.345(3)
N(4)-B(1)	1.532(3)
N(5)-C(7)	1.335(2)
N(5)-N(6)	1.362(2)
N(6)-C(9)	1.342(3)
N(6)-B(1)	1.546(3)
C(1)-C(2)	1.395(3)
C(2)-C(3)	1.357(4)
C(4)-C(5)	1.394(3)
C(5)-C(6)	1.373(4)
C(7)-C(8)	1.389(3)
C(8)-C(9)	1.367(4)
C(10)-C(15)	1.377(3)
C(10)-C(11)	1.406(3)
C(11)-C(12)	1.385(3)
C(12)-C(13)	1.362(4)
C(13)-C(14)	1.370(4)
C(14)-C(15)	1.387(4)
C(16)-C(21)	1.389(3)
C(16)-C(17)	1.396(3)
C(17)-C(18)	1.397(3)
C(18)-C(19)	1.371(4)
C(19)-C(20)	1.383(4)
C(20)-C(21)	1.401(3)
C(22)-C(27)	1.390(3)
C(22)-C(23)	1.394(3)
C(23)-C(24)	1.378(4)
C(24)-C(25)	1.395(5)
C(25)-C(26)	1.372(4)
C(26)-C(27)	1.384(3)
C(28)-C(31)	1.517(3)
C(29)-C(31)	1.528(3)
C(30)-C(31)	1.531(3)
C(31)-C(32)	1.537(3)

C(32)-C(33)	1.509(4)
N(1)-Ru(1)-N(3)	84.81(7)
N(1)-Ru(1)-N(5)	90.22(6)
N(3)-Ru(1)-N(5)	82.88(6)
N(1)-Ru(1)-O(4)	172.68(6)
N(3)-Ru(1)-O(4)	89.82(6)
N(5)-Ru(1)-O(4)	84.17(6)
N(1)-Ru(1)-P(2)	94.64(4)
N(3)-Ru(1)-P(2)	94.08(5)
N(5)-Ru(1)-P(2)	174.02(5)
O(4)-Ru(1)-P(2)	90.69(4)
N(1)-Ru(1)-P(1)	92.06(5)
N(3)-Ru(1)-P(1)	172.13(5)
N(5)-Ru(1)-P(1)	89.93(5)
O(4)-Ru(1)-P(1)	92.63(4)
P(2)-Ru(1)-P(1)	93.36(2)
O(6)-S(1)-O(5)	116.3(1)
O(6)-S(1)-O(4)	113.8(1)
O(5)-S(1)-O(4)	115.9(1)
O(6)-S(1)-C(34)	103.1(1)
O(5)-S(1)-C(34)	105.2(1)
O(4)-S(1)-C(34)	99.6(1)
C(10)-P(1)-C(22)	101.79(9)
C(10)-P(1)-C(16)	102.07(9)
C(22)-P(1)-C(16)	100.32(9)
C(10)-P(1)-Ru(1)	120.84(6)
C(22)-P(1)-Ru(1)	114.26(7)
C(16)-P(1)-Ru(1)	114.73(7)
O(2)-P(2)-O(3)	102.43(8)
O(2)-P(2)-O(1)	102.78(8)
O(3)-P(2)-O(1)	99.88(8)
O(2)-P(2)-Ru(1)	112.74(5)
O(3)-P(2)-Ru(1)	116.94(6)
O(1)-P(2)-Ru(1)	119.63(6)
C(28)-O(1)-P(2)	115.8(1)

C(29)-O(2)-P(2)	116.4(1)
C(30)-O(3)-P(2)	115.1(1)
S(1)-O(4)-Ru(1)	146.8(9)
C(1)-N(1)-N(2)	106.8(2)
C(1)-N(1)-Ru(1)	135.0(1)
N(2)-N(1)-Ru(1)	118.2(1)
C(3)-N(2)-N(1)	108.7(2)
C(3)-N(2)-B(1)	129.8(2)
N(1)-N(2)-B(1)	121.3(2)
C(4)-N(3)-N(4)	106.7(2)
C(4)-N(3)-Ru(1)	135.2(2)
N(4)-N(3)-Ru(1)	118.1(2)
C(6)-N(4)-N(3)	109.1(2)
C(6)-N(4)-B(1)	131.1(2)
N(3)-N(4)-B(1)	119.8(2)
C(7)-N(5)-N(6)	106.5(2)
C(7)-N(5)-Ru(1)	134.9(2)
N(6)-N(5)-Ru(1)	118.6(1)
C(9)-N(6)-N(5)	109.5(2)
C(9)-N(6)-B(1)	131.0(2)
N(5)-N(6)-B(1)	118.8(2)
N(1)-C(1)-C(2)	110.0(2)
C(3)-C(2)-C(1)	105.0(2)
N(2)-C(3)-C(2)	109.5(2)
N(3)-C(4)-C(5)	109.8(2)
C(6)-C(5)-C(4)	105.3(2)
N(4)-C(6)-C(5)	109.1(2)
N(5)-C(7)-C(8)	110.1(2)
C(9)-C(8)-C(7)	105.2(2)
N(6)-C(9)-C(8)	108.6(2)
C(15)-C(10)-C(11)	117.5(2)
C(15)-C(10)-P(1)	123.3(2)
C(11)-C(10)-P(1)	119.2(2)
C(12)-C(11)-C(10)	120.8(2)
C(13)-C(12)-C(11)	120.2(2)
C(12)-C(13)-C(14)	119.9(2)

C(13)-C(14)-C(15)	120.4(3)
C(10)-C(15)-C(14)	121.1(2)
C(21)-C(16)-C(17)	118.6(2)
C(21)-C(16)-P(1)	121.6(2)
C(17)-C(16)-P(1)	119.7(2)
C(16)-C(17)-C(18)	120.2(2)
C(19)-C(18)-C(17)	120.7(2)
C(18)-C(19)-C(20)	120.0(2)
C(19)-C(20)-C(21)	119.8(2)
C(16)-C(21)-C(20)	120.7(2)
C(27)-C(22)-C(23)	118.5(2)
C(27)-C(22)-P(1)	119.6(2)
C(23)-C(22)-P(1)	121.6(2)
C(24)-C(23)-C(22)	121.0(2)
C(23)-C(24)-C(25)	119.7(3)
C(26)-C(25)-C(24)	119.6(2)
C(25)-C(26)-C(27)	120.7(3)
C(26)-C(27)-C(22)	120.4(2)
O(1)-C(28)-C(31)	110.9(2)
O(2)-C(29)-C(31)	110.7(2)
O(3)-C(30)-C(31)	111.4(2)
C(28)-C(31)-C(29)	108.2(2)
C(28)-C(31)-C(30)	108.4(2)
C(29)-C(31)-C(30)	107.6(2)
C(28)-C(31)-C(32)	111.2(2)
C(29)-C(31)-C(32)	111.6(2)
C(30)-C(31)-C(32)	109.7(2)
C(33)-C(32)-C(31)	115.8(2)
F(3)-C(34)-F(1)	109.9(3)
F(3)-C(34)-F(2)	108.1(3)
F(1)-C(34)-F(2)	106.5(3)
F(3)-C(34)-S(1)	111.0(2)
F(1)-C(34)-S(1)	110.7(2)
F(2)-C(34)-S(1)	110.5(2)
N(2)-B(1)-N(4)	108.9(2)
N(2)-B(1)-N(6)	109.4(2)

N(4)-B(1)-N(6)	107.1(2)

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for TpRu{$P(OCH_2)_3CEt$}(PPh_3)OTf (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	33(1)	32(1)	32(1)	-1(1)	5(1)	0(1)
S(1)	51(1)	46(1)	44(1)	-3(1)	15(1)	4(1)
P(1)	34(1)	34(1)	33(1)	-2(1)	6(1)	0(1)
P(2)	33(1)	36(1)	35(1)	-2(1)	4(1)	1(1)
F(1)	160(2)	70(1)	106(2)	24(1)	40(1)	-24(1)
F(2)	113(2)	125(2)	62(1)	21(1)	-9(1)	20(1)
F(3)	183(3)	146(2)	99(2)	20(2)	100(2)	26(2)
O(1)	48(1)	47(1)	37(1)	2(1)	10(1)	13(1)
O(2)	45(1)	38(1)	41(1)	-6(1)	0(1)	3(1)
O(3)	35(1)	45(1)	58(1)	7(1)	5(1)	-1(1)
O(4)	50(1)	55(1)	39(1)	-5(1)	13(1)	3(1)
O(5)	50(1)	83(1)	74(1)	-9(1)	11(1)	14(1)
O(6)	85(1)	55(1)	85(1)	-22(1)	29(1)	-1(1)
N(1)	39(1)	37(1)	39(1)	-4(1)	5(1)	1(1)
N(2)	47(1)	36(1)	47(1)	-8(1)	4(1)	3(1)
N(3)	41(1)	41(1)	48(1)	1(1)	8(1)	-4(1)
N(4)	50(1)	39(1)	54(1)	0(1)	7(1)	-7(1)
N(5)	44(1)	36(1)	42(1)	4(1)	7(1)	1(1)
N(6)	52(1)	35(1)	50(1)	2(1)	4(1)	4(1)
C(1)	43(1)	50(1)	41(1)	-4(1)	8(1)	3(1)
C(2)	57(1)	64(1)	45(1)	-14(1)	14(1)	6(1)
C(3)	54(1)	48(1)	57(1)	-19(1)	8(1)	4(1)
C(4)	45(1)	57(1)	53(1)	2(1)	14(1)	-5(1)
C(5)	57(1)	67(2)	65(1)	5(1)	19(1)	-18(1)
C(6)	64(1)	47(1)	59(1)	2(1)	12(1)	-19(1)
C(7)	52(1)	48(1)	42(1)	5(1)	4(1)	1(1)
C(8)	66(1)	57(1)	53(1)	13(1)	-6(1)	10(1)

C(9)	66(1)	43(1)	65(1)	11(1)	2(1)	12(1)
C(10)	38(1)	37(1)	45(1)	4(1)	11(1)	0(1)
C(11)	48(1)	49(1)	44(1)	6(1)	11(1)	-3(1)
C(12)	58(1)	64(2)	57(1)	21(1)	14(1)	2(1)
C(13)	86(2)	47(1)	83(2)	25(1)	28(1)	9(1)
C(14)	113(2)	36(1)	85(2)	0(1)	22(2)	-2(1)
C(15)	83(2)	44(1)	55(1)	2(1)	13(1)	-3(1)
C(16)	44(1)	36(1)	37(1)	0(1)	6(1)	-6(1)
C(17)	53(1)	47(1)	46(1)	-7(1)	14(1)	-10(1)
C(18)	84(2)	55(1)	43(1)	-12(1)	21(1)	-17(1)
C(19)	79(2)	68(2)	39(1)	-5(1)	-5(1)	-7(1)
C(20)	55(1)	70(2)	52(1)	-4(1)	-13(1)	5(1)
C(21)	46(1)	56(1)	43(1)	-6(1)	1(1)	2(1)
C(22)	35(1)	45(1)	37(1)	-7(1)	4(1)	2(1)
C(23)	43(1)	62(1)	47(1)	-2(1)	14(1)	-3(1)
C(24)	56(1)	87(2)	67(2)	0(2)	29(1)	6(1)
C(25)	62(2)	104(2)	65(2)	-9(2)	25(1)	26(2)
C(26)	62(1)	61(2)	61(1)	-8(1)	12(1)	20(1)
C(27)	45(1)	48(1)	51(1)	-4(1)	9(1)	6(1)
C(28)	54(1)	50(1)	39(1)	3(1)	3(1)	15(1)
C(29)	52(1)	37(1)	49(1)	-4(1)	5(1)	7(1)
C(30)	35(1)	54(1)	73(1)	8(1)	7(1)	6(1)
C(31)	37(1)	42(1)	48(1)	-1(1)	4(1)	6(1)
C(32)	52(1)	50(1)	65(1)	4(1)	3(1)	16(1)
C(33)	85(2)	49(1)	81(2)	10(1)	8(1)	15(1)
C(34)	86(2)	80(2)	56(2)	6(1)	33(1)	1(2)
B(1)	55(1)	33(1)	59(1)	-3(1)	5(1)	0(1)

Table S10. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for TpRu{$P(OCH_2)_3CEt$}(PPh_3)OTf (**2**).

	x	y	z	U(eq)
H(1)	2532	4594	115	54
H(2)	2764	3209	-575	66

H(3)	2734	1964	306	65
H(4)	268	4143	2177	62
H(5)	-349	2608	2143	75
H(6)	792	1581	1926	69
H(7)	3914	4132	3650	59
H(8)	4484	2614	4048	75
H(9)	3739	1591	3015	73
H(11)	3085	6063	407	57
H(12)	2867	7441	-182	72
H(13)	3129	8721	532	85
H(14)	3611	8637	1841	94
H(15)	3834	7268	2443	73
H(17)	3375	6196	3342	58
H(18)	4240	6413	4572	72
H(19)	5687	6010	4881	78
H(20)	6302	5410	3956	77
H(21)	5436	5151	2730	61
H(23)	4864	5976	1117	60
H(24)	5957	5300	683	81
H(25)	6122	3754	765	90
H(26)	5202	2916	1291	74
H(27)	4150	3598	1777	58
H(28A)	408	6095	-416	59
H(28B)	1127	6838	-197	59
H(29A)	1369	7608	1053	57
H(29B)	705	7487	1562	57
H(30A)	-422	6294	1232	66
H(30B)	-629	5831	428	66
H(32A)	-672	7249	-330	69
H(32B)	-694	7661	460	69
H(33A)	387	8661	388	111
H(33B)	-359	8732	-367	111
H(33C)	501	8211	-364	111
H(1A)	2427	1756	1695	61