Supporting Information

Catalytic Synthesis of Tricyclic Quinoline Derivatives from the Regioselective Hydroamination and C-H Bond Activation Reaction of Benzocyclic Amines and Alkynes

Chae S. Yi* and Sang Young Yun

Department of Chemistry, Marquette University, Milwaukee, Wisconsin 53201-1881

Ilia A. Guzei

Molecular Structure Laboratory, Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin 53706-1396

General Information. All operations were carried out in an inert-atmosphere glove box or by using standard high vacuum and Schlenk techniques unless otherwise noted. Tetrahydrofuran, benzene, hexanes and Et₂O were distilled from purple solutions of sodium and benzophenone immediately prior to use. The NMR solvents were dried from activated molecular sieves (4 Å). All amine and alkene substrates were received from commercial sources and used without further purification. The ¹H, ¹³C and ³¹P NMR spectra were recorded on a Varian Mercury 300 MHz FT-NMR spectrometer. Mass spectra were recorded from a Hewlett-Packard HP 5970 GC/MS spectrometer. High-resolution FAB mass spectra were obtained at the Center of Mass Spectrometry, Washington University, St. Louis, MO. Elemental analyses were performed at the Midwest Microlab, Indianapolis, IN.

Synthesis of [(PCy₃)₂(CO)(CH₃CN)₂RuC≡CPh]⁺BF₄⁻ (5**).** In a glove box, complex **1** (200 mg, 0.23 mmol) and phenylacetylene (120 mg, 2.3 mmol) were dissolved in 10 mL of THF in a 50 mL Schlenk tube equipped with a Teflon screw joint and a magnetic stirring bar. The tube was brought out of the box, and was stirred in an oil bath at 80 °C for 12 h. After the reaction tube was cooled to room temperature, the volatiles were removed under vacuum. A 5 mL of Et₂O was added to the concentrate, and the resulting suspension was filtered through a frit. The product **5** was isolated as a pale yellow solid after washing with Et₂O (3 × 5 mL) and drying under high vacuum (170 mg, 81% yield). Single crystals of **5** suitable for X-ray crystallographic analysis were obtained from CH₂Cl₂/Et₂O solution.

Selected spectroscopic data for **5**: ¹H NMR (CD₂Cl₂, 300 MHz) δ 7.34 – 7.05 (m, 5H, Ph), 2.55 and 2.51 (s, CH₃CN), 2.32 – 1.20 (m, PCy₃); ¹³C{¹H} NMR (CD₂Cl₂, 75 MHz) δ 203.6 (t, *J*_{PC} = 13.2 Hz, CO), 128.6, 127.1, 126.3, 125.7, 125.3, 122.8, 111.4 (C≡CPh), 103.8 (t, *J*_{PC} = 16.0 Hz, C≡CPh), 33.5 (pseudo t, *J*_{PC} = 9.6 Hz, C_{ipso} of cyclohexyl), 27.9 (C_{meta} of cyclohexyl), 26.6 (m, C_{ortho} of cyclohexyl), 25.2 (C_{para} of cyclohexyl), 4.5 (CH₃CN); ³¹P{¹H} NMR (CD₂Cl₂, 125 MHz) δ 28.8 (s, PCy₃); IR (KBr) ν_{CO} = 1892 cm⁻¹.

Catalyst Activity Survey of Selected Ruthenium Complexes.^a

Entry	Catalyst	Additive	% yield (2a:3a) ^b
1	1	none	76 : 5
2	(PCy ₃) ₂ (CO)RuHCl	none	~0
3		NH ₄ PF ₆	39 : 4
4		HBF ₄ OEt ₂	41 : 4
5	Ru ₃ (CO) ₁₂	none	~0
6		NH ₄ PF ₆	96 : 4
7		HBF ₄ OEt ₂	96 : 4
8	(PPh ₃) ₃ RuCl ₂	HBF ₄ OEt ₂	31 : 3
9	[RuCl ₂ (COD)] _x	HBF ₄ OEt ₂	45 : 4
10	(PPh ₃) ₃ (CO)RuH ₂	HBF ₄ OEt ₂	79 : 7

^aReaction conditions: indoline (0.25 mmol), propyne (10 mmol), Ru catalyst (3 mol%), additive (3 mol%), benzene (5 mL), 95 °C, 24 h. ^bDetermined by GC.

Phosphine Inhibition Study. In a glove box, complex **1** (5 mol %) and indoline (0.8 mmol) were dissolved in 5 mL of benzene in a thick-walled 25 mL Schlenk tube equipped with a magnetic stirring bar. For phosphine inhibition study, PCy₃ (5 mol %) was added to the reaction mixture. The reaction tube was brought out of the box, and cooled in a liquid nitrogen bath. Excess propyne (20 mmol) was condensed into the tube via a vacuum line transfer. The reaction tube was warmed to room temperature, and stirred in an oil bath at 95 °C. A small portion of the aliquot was drawn periodically from the reaction mixture under a nitrogen stream, and the product conversion was determined by GC.

The ^1H and ^2H NMR spectra of **2c-d:** (A) ^1H NMR spectrum of **2a**; (B) ^1H NMR spectrum of **2c-d**; (C) ^2H NMR spectrum of **2a-d**.

Isotope Effect Study. In a glove box, an equal amount of indoline and *N*-deutrated indoline (47 μL , 0.42 mmol) was added to two separate 25 mL Schlenk tubes. A predissolved $\text{Ru}_3(\text{CO})_{12}$ (1 mol %) and NH_4PF_6 (3 mol % based on amine) in THF (3 mL) was added to each Schlenk tubes. The reaction tubes were brought out of the box, and cooled in a liquid nitrogen bath. Excess propyne (20 mmol) was condensed into each tube via a vacuum line transfer. The reaction tubes were warmed to room temperature, and stirred in an oil bath at 95 $^\circ\text{C}$. A small portion of the aliquot under a nitrogen stream was drawn periodically from the reaction tube, and the product conversion was determined by GC.

General Procedure of the Catalytic Reaction. In a glove box, an amine (1.7 mmol), a terminal alkyne (10-20 mmol) and complex **1** (5 mol %) were dissolved in 5 mL benzene in a thick-walled 25 mL Schlenk tube equipped with a magnetic stirring bar. The vacuum line technique was used to transfer volatile alkynes such as propyne and 1-butyne. The reaction tube was brought out of the box, and was stirred in an oil bath at 95 °C for 16-24 h. The tube was opened to air at room temperature, and the crude product mixture was analyzed by GC. The solvent was removed from a rotary aspirator, and the organic product was isolated by column chromatography on silica gel (hexane/CH₂Cl₂).

For **2a**: ¹H NMR (C₆D₆, 300 MHz) δ 6.90 (m, 2H, Ar), 6.66 (t, *J* = 7.2 Hz, 1H, Ar), 4.99 (q, *J* = 1.2 Hz, CH₃C=CH), 3.11 (t, *J* = 8.7 Hz, NCH₂CH₂), 2.67 (t, *J* = 8.4 Hz, NCH₂CH₂), 1.85 (d, *J* = 1.5 Hz, CH₃), 1.14 (s, C(CH₃)₂); NOESY δ 4.99 ⇌ 1.85, 4.99 ⇌ 1.34, 3.11 ⇌ 1.34 (⇌ denotes NOE correlation); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 149.3, 129.0, 128.9, 126.7, 124.6, 121.4, 119.3, 117.7, 55.7 (NC(CH₃)₂), 46.4 (NCH₂CH₂), 29.1 (NCH₂CH₂), 26.9 (2CH₃), 18.1 (CH₃); GC-MS (*M*⁺ = 199); Anal. Calcd for C₁₄H₁₇N: C, 84.37; H, 8.60. Found C, 84.31; H, 8.65.

For **2b**: ¹H NMR (C₆D₆, 300 MHz) δ 6.88 (m, 2H, Ar), 6.60 (t, *J* = 7.8 Hz, 1H, Ar), 4.86 (t, *J* = 1.2 Hz, C=CH), 3.09 (m, NCH₂CH₂), 2.69 (t, *J* = 8.1 Hz, NCH₂CH₂), 2.29 (q, *J* = 7.2 Hz, CH₂), 1.59 and 1.17 (m, CH₂), 1.09 (m, 6H, 2CH₃), 0.98 (t, *J* = 7.2 Hz, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 150.1, 136.3, 126.3, 125.0, 124.5, 121.1, 117.8, 117.1, 59.1 (NC(CH₃)), 45.9 (CH₂), 33.9 (CH₂), 29.1 (CH₂), 25.7 (CH₂), 25.0 (CH₃), 14.0 (CH₃), 10.5 (CH₃); GC-MS (*M*⁺ = 227); Anal. Calcd for C₁₆H₂₁N: C, 84.53; H, 9.31. Found C, 84.36; H, 9.16.

For **2c**: ¹H NMR (C₆D₆, 300 MHz) δ 7.20 (d, *J* = 7.5 Hz, 2H, Ar), 7.03 (d, *J* = 5.4 Hz, 2H, Ar), 6.77 (m, 7H, Ar), 6.56 (d, *J* = 7.2 Hz, 1H, Ar), 6.24 (t, *J* = 7.2 Hz, 1H, Ar), 4.99 (s, C=CH), 2.77 (dt, *J* = 9.0, 8.7 Hz, 1H, NCH₂CH₂), 2.54 (dt, *J* = 8.4, 8.1 Hz, 1H, NCH₂CH₂), 2.29 (t, *J* = 7.5 Hz, NCH₂CH₂), 1.28 (s, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 149.3, 146.3, 139.4, 135.1, 130.7, 129.4, 129.0, 128.9, 128.0, 127.6, 127.4, 126.9, 125.3, 123.5, 117.7, 117.0, 61.8 (NCCH₃), 47.1 (NCH₂CH₂), 28.8 (NCH₂CH₂), 24.0 (CH₃); GC-MS (*M*⁺ = 323); Anal. Calcd for C₂₄H₂₁N: C, 89.13; H, 6.54. Found C, 88.64; H, 6.82.

For **2d**: ¹H NMR (C₆D₆, 300 MHz) δ 7.06 (d, *J* = 8.1 Hz, 2H, Ar), 6.93 (d, *J* = 7.8 Hz, 2H, Ar), 6.73 –

6.46 (m, 6H, Ar), 6.17 (t, $J = 7.5$ Hz, 1H, Ar), 4.97(s, C=CH), 2.72 (dt, $J = 9.0, 8.7$ Hz, 1H, NCH₂CH₂), 2.52 (dt, $J = 8.1, 7.5$ Hz, 1H, NCH₂CH₂), 2.23 (t, $J = 9.3$ Hz, NCH₂CH₂), 1.71 (s, CH₃), 1.70 (s, CH₃), 1.22 (s, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 149.4, 143.6, 137.4, 136.9, 136.7, 134.9, 130.6, 129.6, 129.6, 129.3, 127.4, 126.9, 125.2, 123.5, 117.6, 117.4, 61.5 (NCCH₃), 47.1 (NCH₂CH₂), 28.8 (NCH₂CH₂), 24.2 (CH₃), 21.7 (CH₃), 21.5 (CH₃); GC-MS ($M^+ = 351$).

For **2e**: ¹H NMR (C₆D₆, 300 MHz) δ 7.10 (d, $J = 7.5$ Hz, 1H, Ar), 6.90 (d, $J = 7.2$ Hz, 1H, Ar), 6.65 (t, $J = 7.5$ Hz, 1H, Ar), 5.46 (pseudo t, $J = 1.2$ Hz, C=CH), 4.11 (d, $J = 1.2$ Hz, CH₃OCH₂C=), 3.35 – 2.63 (m, 6H, NCH₂CH₂ and CH₂OCH₃), 3.10 (s, OCH₃), 2.98 (s, OCH₃), 1.21 (s, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 149.5, 131.4, 126.6, 126.2, 124.8, 121.6, 117.6, 116.6, 79.7 (CH₃OCH₂), 72.5 (CH₃OCH₂), 59.3 (OCH₃), 59.2 (OCH₃), 57.9 (NCH₂CH₂), 47.8 (NCCH₃), 29.2 (NCH₂CH₂), 21.9 (CH₃); GC-MS ($M^+ = 259$).

For **2f**: ¹H NMR (C₆D₆, 300 MHz) δ 6.85 (m, 2H, Ar), 6.67 (t, $J = 7.5$ Hz, 1H, Ar), 4.94 (q, $J = 1.2$ Hz, C=CH), 3.73 (m, NCHCH₂), 2.96 (dd, $J = 15.6, 9.6$ Hz, 1H, NCH(CH₃)CH₂), 2.38 (dd, $J = 15.6, 9.6$ Hz, 1H, NCH(CH₃)CH₂), 1.84 (d, $J = 1.5$ Hz, CH₃C=), 1.31 (s, CH₃), 1.13 (d, $J = 6.3$ Hz, CHCH₃), 1.02 (s, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 149.6, 130.6, 128.9, 125.8, 124.1, 121.2, 119.8, 118.0, 56.6 (NC(CH₃)₂), 55.9 (NCH(CH₃)CH₂), 39.5 (NCH(CH₃)CH₂), 32.3 (CH₃), 24.9 (CH₃), 23.4 (CH₃), 17.9 (CH₃); GC-MS ($M^+ = 213$).

For **2g**: ¹H NMR (C₆D₆, 300 MHz) δ 6.86 (s, 1H, Ar), 6.77 (s, 1H, Ar), 4.90 (s, CH₃C=CH), 3.03 (t, $J = 8.4$ Hz, NCH₂CH₂), 2.49 (t, $J = 8.4$ Hz, NCH₂CH₂), 1.65 (s, CH₃C=CH), 1.05 (s, C(CH₃)₂); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 147.8, 130.1, 128.3, 128.0, 124.6, 121.9, 121.2, 119.9, 55.9 (NC(CH₃)₂), 46.4 (NCH₂CH₂), 28.7 (NCH₂CH₂), 26.8 (2CH₃), 17.7 (CH₃); GC-MS ($M^+ = 233$); Anal. Calcd for C₈H₈NCl: C, 71.91; H, 6.91. Found C, 71.79; H, 6.81.

For **2h**: ¹H NMR (C₆D₆, 300 MHz) δ 7.51 (dd, $J = 7.5, 1.2$ Hz, 2H, Ar), 7.37 (dd, $J = 7.8, 1.5$ Hz, 2H, Ar), 7.16 – 7.04 (m, 6H, Ar), 6.87 (s, 1H, Ar), 6.65 (s, 1H, Ar), 5.31 (s, PhC=CH), 3.13 (dt, $J = 9.0, 8.7$ Hz, 1H, NCH₂CH₂), 2.92 (dt, $J = 9.3, 6.9$ Hz, 1H, NCH₂CH₂), 2.60 (t, $J = 9.0$ Hz, NCH₂CH₂), 2.08 (s, CH₃), 1.60 (s, CH₃); ¹³C{¹H} NMR (C₆D₆, 75 MHz) δ 147.4, 146.3, 139.6, 135.3, 131.1, 129.4, 128.9, 128.8, 128.0, 127.6, 127.5, 127.2, 126.5, 126.2, 123.7, 117.1, 61.8 (NCCH₃), 47.3 (NCH₂CH₂), 28.9 (NCH₂CH₂), 23.7 (CH₃), 21.8 (CH₃); GC-MS ($M^+ = 337$).

For **2i**: ¹H NMR (C₆D₆, 300 MHz) δ 6.98 (dd, $J = 7.5, 1.5$ Hz, 1H, Ar), 6.87 (dd, $J = 7.8, 1.5$ Hz, 1H,

Ar), 6.66 (t, $J = 7.5$ Hz, 1H, Ar), 5.08 (q, $J = 1.5$ Hz, $\text{CH}_3\text{C}=\text{CH}$), 2.91 (t, $J = 5.7$ Hz, NCH_2), 2.52 (t, $J = 6.6$ Hz, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.87 (d, $J = 1.5$ Hz, $\text{CH}_3\text{C}=\text{CH}$), 1.62 (m, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.15 (s, $\text{C}(\text{CH}_3)_2$); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 75 MHz) δ 142.1, 129.7, 129.6, 129.2, 123.4, 122.8, 122.2, 116.5, 56.1 ($\text{NC}(\text{CH}_3)_2$), 42.7 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 29.2 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 27.2 (2CH_3), 22.8 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 19.6 (CH_3); GC-MS ($\text{M}^+ = 213$); Anal. Calcd for $\text{C}_{15}\text{H}_{19}\text{N}$: C, 84.46; H, 8.98. Found C, 84.37; H, 8.96.

For **2j**: ^1H NMR (C_6D_6 , 300 MHz) δ 7.18 (d, $J = 7.5$ Hz, 2H, Ar), 6.99 (d, $J = 5.6$ Hz, 2H, Ar), 6.88 – 6.62 (m, 7H, Ar), 6.46 (d, $J = 7.2$ Hz, 1H, Ar), 6.32 (t, $J = 7.2$ Hz, 1H, Ar), 5.04 (s, $\text{C}=\text{CH}$), 2.58 – 2.48 (m, NCH_2CH), 2.33 (m, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.35 – 1.03 (m, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.17 (s, CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 75 MHz) δ 148.3, 142.1, 140.7, 135.1, 130.6, 130.5, 129.8, 129.5, 128.8, 127.8, 127.5, 127.3, 125.5, 121.7, 120.9, 116.4, 53.9 (NCCH_3), 44.5 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 29.2 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 23.6 (CH_3), 22.4 ($\text{NCH}_2\text{CH}_2\text{CH}_2$); GC-MS ($\text{M}^+ = 337$).

For **2k**: ^1H NMR (C_6D_6 , 300 MHz) δ 6.75 (d, $J = 3.0$ Hz, 1H, Ar), 6.55 (d, $J = 2.7$ Hz, 1H, Ar), 5.17 (q, $J = 1.5$ Hz, $\text{CH}_3\text{C}=\text{CH}$), 3.48 (s, OCH_3), 2.94 (t, $J = 5.7$ Hz, NCH_2CH_2), 2.52 (t, $J = 6.6$ Hz, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.85 (d, $J = 1.5$ Hz, $\text{CH}_3\text{C}=\text{CH}$), 1.67 (m, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.16 (s, $\text{C}(\text{CH}_3)_2$); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 75 MHz) δ 151.8, 136.5, 131.2, 129.2, 124.9, 123.5, 114.9, 109.1, 55.8 (OCH_3), 55.7 ($\text{NC}(\text{CH}_3)_2$), 42.6 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 29.4 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 26.3 (2CH_3), 23.1 ($\text{NCH}_2\text{CH}_2\text{CH}_2$), 19.5 (CH_3); EI-LRMS: M^+ (m/z) = 243.20.

For **2l**: ^1H NMR (C_6D_6 , 300 MHz) δ 6.96 (dd, $J = 8.1, 1.5$ Hz, 1H, Ar), 6.73 (dd, $J = 8.1, 1.5$ Hz, 1H, Ar), 6.60 (t, $J = 7.8$ Hz, Ar), 5.06 (q, $J = 1.2$ Hz, $\text{CH}_3\text{C}=\text{CH}$), 3.80 (t, $J = 4.5$ Hz, $\text{NCH}_2\text{CH}_2\text{O}$), 2.82 (t, $J = 4.5$ Hz, $\text{NCH}_2\text{CH}_2\text{O}$), 1.84 (d, $J = 1.2$ Hz, CH_3), 1.03 (s, 2CH_3); $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 75 MHz) δ 144.6, 131.6, 129.5, 129.2, 124.3, 117.6, 117.5, 117.1, 64.7 ($\text{NCH}_2\text{CH}_2\text{O}$), 55.5 ($\text{NC}(\text{CH}_3)_2$), 41.2 ($\text{NCH}_2\text{CH}_2\text{O}$), 26.3 (2CH_3), 19.6 (CH_3); GC-MS ($\text{M}^+ = 215$).

X-Ray Crystallographic Determination of 5.

Data Collection: A colorless crystal with approximate dimensions $0.46 \times 0.32 \times 0.20 \text{ mm}^3$ was selected under ambient conditions and attached to the tip of a nylon loop. The crystal was cooled by a stream of cold nitrogen at 100(2) K and its position was centered by using a video camera. The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α ($\lambda = 0.71073 \text{ \AA}$) radiation and the

diffractometer to crystal distance of 4.9 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° in a 6° range about ω with the exposure time of 10 seconds per frame. A total of 67 reflections was obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 9472 strong reflections from the actual data collection. The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of a full sphere to a resolution of $0.80 \text{ \AA}$. A total of 26547 data were harvested by collecting four sets of frames with 0.25° scans in ω with an exposure time 60 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Solution and Refinement: The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The E -statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement [1]. A successful solution by the direct methods provided most non-hydrogen atoms from the E -map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms (except those in the solvate molecule of ether) were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. There are two independent molecules of the complex and one solvate molecule of ether in the asymmetric unit. The crystal was found to be a non-tetrahedral twin with a 3:1 component ratio. The twin domains are related by a 180° rotation about the $[100]$ vector in direct space. The final least-squares refinement of 1104 parameters against 26548 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0574 and 0.1490, respectively. The final difference Fourier map was featureless. The ORTEP diagrams are drawn with 50% probability ellipsoids.

[1] Bruker-AXS. (2000-2003) SADABS V.2.05, SAINT V.6.22, SHELXTL V.6.10 & SMART 5.622 Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

The first symmetry independent cation.

The second symmetry independent cation.

A view with two cations superimposed.

Contents in the asymmetric unit.

Table S1. Crystal data and structure refinement for **5**.

Identification code	yi0009	
Empirical formula	C ₄₉ H ₇₇ N ₂ OP ₂ Ru . BF ₄ . ½ Et ₂ O	
Formula weight	997.01	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 13.6055(11) Å	α = 75.0160(10)°.
	b = 18.4233(15) Å	β = 83.9360(10)°.
	c = 21.0690(17) Å	γ = 89.9590(10)°.
Volume	5071.1(7) Å ³	
Z	4	
Density (calculated)	1.306 Mg/m ³	
Absorption coefficient	0.426 mm ⁻¹	
F(000)	2116	
Crystal size	0.46 x 0.32 x 0.20 mm ³	
Theta range for data collection	1.14 to 26.48°.	
Index ranges	-16<=h<=17, -21<=k<=23, 0<=l<=26	
Reflections collected	26547	
Independent reflections	26548 [R(int) = 0.0915]	
Completeness to theta = 26.48°	95.7 %	
Absorption correction	Multi-scan with SADABS	
Max. and min. transmission	0.9197 and 0.8282	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	26548 / 2 / 1104	
Goodness-of-fit on F ²	1.083	
Final R indices [I>2sigma(I)]	R1 = 0.0574, wR2 = 0.1435	
R indices (all data)	R1 = 0.0700, wR2 = 0.1490	
Largest diff. peak and hole	1.810 and -0.848 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2967(1)	1166(1)	2543(1)	10(1)
Ru(2)	7912(1)	6165(1)	2617(1)	12(1)
P(1)	1325(1)	556(1)	2774(1)	10(1)
P(2)	4632(1)	1760(1)	2309(1)	10(1)
P(3)	6327(1)	6745(1)	2364(1)	12(1)
P(4)	9486(1)	5562(1)	2828(1)	12(1)
F(1)	3706(3)	3819(2)	4188(2)	65(1)
F(2)	3472(3)	5026(2)	4204(2)	53(1)
F(3)	2962(3)	4086(2)	5095(2)	69(1)
F(4)	2161(3)	4259(2)	4188(2)	75(1)
F(5)	6618(3)	8862(2)	4159(2)	56(1)
F(6)	8145(3)	9273(2)	4267(2)	63(1)
F(7)	6945(3)	9077(2)	5116(2)	56(1)
F(8)	6835(3)	10056(2)	4229(2)	45(1)
O(1)	2320(2)	2184(2)	1316(2)	24(1)
O(2)	8985(3)	7258(2)	1435(2)	30(1)
O(3)	240(5)	7320(4)	49(3)	99(1)
N(1)	2544(3)	1836(2)	3194(2)	17(1)
N(2)	3464(3)	420(2)	3394(2)	14(1)
N(3)	8103(3)	6820(2)	3282(2)	17(1)
N(4)	7136(3)	5397(2)	3446(2)	15(1)
B(1)	3063(5)	4297(4)	4413(3)	33(2)
B(2)	7145(5)	9321(4)	4433(3)	33(2)
C(1)	1114(3)	-225(2)	3539(2)	13(1)
C(2)	1194(4)	18(3)	4174(2)	18(1)
C(3)	967(4)	-651(3)	4783(2)	23(1)
C(4)	1633(4)	-1308(3)	4747(2)	27(1)
C(5)	1537(4)	-1550(3)	4118(2)	24(1)
C(6)	1774(3)	-897(2)	3499(2)	14(1)
C(7)	975(3)	101(2)	2129(2)	14(1)
C(8)	66(3)	-444(2)	2321(2)	15(1)
C(9)	-75(4)	-834(3)	1774(2)	24(1)
C(10)	-149(4)	-275(3)	1111(2)	27(1)
C(11)	760(4)	244(3)	922(2)	26(1)
C(12)	893(4)	655(3)	1458(2)	24(1)
C(13)	357(3)	1219(2)	2948(2)	12(1)
C(14)	-710(3)	906(2)	3089(2)	17(1)
C(15)	-1410(3)	1442(3)	3346(2)	20(1)
C(16)	-1363(3)	2212(2)	2869(2)	19(1)
C(17)	-303(3)	2530(2)	2714(2)	19(1)
C(18)	397(3)	1997(2)	2454(2)	17(1)
C(19)	4840(3)	2551(2)	1552(2)	13(1)
C(20)	4783(3)	2314(2)	908(2)	15(1)
C(21)	4984(4)	2989(3)	303(2)	22(1)
C(22)	4301(4)	3634(3)	343(2)	28(1)
C(23)	4388(4)	3879(3)	971(2)	21(1)
C(24)	4164(3)	3221(2)	1589(2)	16(1)
C(25)	4968(3)	2220(2)	2956(2)	14(1)
C(26)	5909(3)	2737(3)	2769(2)	19(1)
C(27)	6073(4)	3128(3)	3315(2)	20(1)
C(28)	6105(4)	2564(3)	3984(2)	21(1)
C(29)	5152(4)	2092(3)	4166(2)	23(1)
C(30)	4991(4)	1681(3)	3639(2)	20(1)

C(31)	5590(3)	1094(2)	2125(2)	13(1)
C(32)	6666(3)	1418(3)	1958(3)	22(1)
C(33)	7353(4)	867(3)	1706(3)	26(1)
C(34)	7330(3)	113(3)	2211(3)	23(1)
C(35)	6279(4)	-213(3)	2396(2)	21(1)
C(36)	5588(3)	332(2)	2641(2)	18(1)
C(37)	3366(3)	447(3)	1996(2)	19(1)
C(38)	3530(4)	80(4)	1611(3)	39(2)
C(39)	3609(4)	-457(3)	1221(3)	29(1)
C(40)	3890(4)	-258(3)	540(3)	37(1)
C(41)	3934(5)	-790(3)	175(3)	45(2)
C(42)	3710(5)	-1522(4)	481(3)	53(2)
C(43)	3417(5)	-1731(4)	1153(3)	52(2)
C(44)	3358(5)	-1225(3)	1523(3)	40(2)
C(45)	2575(3)	1803(3)	1790(2)	16(1)
C(46)	2331(4)	2120(3)	3606(3)	27(1)
C(47)	2071(5)	2460(4)	4153(3)	48(2)
C(48)	3817(3)	62(2)	3837(2)	16(1)
C(49)	4309(4)	-378(3)	4377(2)	25(1)
C(50)	5442(3)	6091(2)	2156(2)	15(1)
C(51)	5231(4)	5335(2)	2677(2)	20(1)
C(52)	4652(4)	4794(3)	2401(3)	22(1)
C(53)	3701(4)	5125(3)	2158(3)	25(1)
C(54)	3907(4)	5871(3)	1641(3)	26(1)
C(55)	4477(4)	6424(3)	1914(3)	26(1)
C(56)	5756(3)	7200(2)	3011(2)	14(1)
C(57)	5529(4)	6660(2)	3700(2)	18(1)
C(58)	5201(4)	7094(3)	4219(2)	20(1)
C(59)	4294(4)	7550(3)	4042(2)	22(1)
C(60)	4518(4)	8097(3)	3356(2)	20(1)
C(61)	4853(4)	7688(3)	2832(2)	21(1)
C(62)	6400(3)	7548(2)	1606(2)	14(1)
C(63)	7004(4)	8224(2)	1671(2)	18(1)
C(64)	7021(4)	8875(3)	1049(2)	25(1)
C(65)	7419(4)	8621(3)	436(2)	27(1)
C(66)	6785(4)	7986(3)	357(2)	24(1)
C(67)	6724(3)	7309(3)	971(2)	17(1)
C(68)	10401(3)	6209(2)	3026(2)	15(1)
C(69)	10476(4)	7004(2)	2563(2)	21(1)
C(70)	11127(4)	7514(2)	2823(2)	21(1)
C(71)	12151(4)	7205(3)	2930(3)	21(1)
C(72)	12075(4)	6419(3)	3379(2)	22(1)
C(73)	11436(3)	5896(3)	3129(2)	17(1)
C(74)	10052(3)	5156(3)	2158(2)	16(1)
C(75)	10386(4)	5744(3)	1518(2)	27(1)
C(76)	10686(4)	5373(3)	956(2)	32(1)
C(77)	11526(4)	4829(3)	1134(3)	30(1)
C(78)	11207(4)	4238(3)	1755(3)	28(1)
C(79)	10887(3)	4582(3)	2334(2)	18(1)
C(80)	9444(4)	4746(2)	3566(2)	16(1)
C(81)	9145(4)	4950(3)	4216(2)	22(1)
C(82)	9186(5)	4262(3)	4807(2)	33(1)
C(83)	8549(5)	3603(3)	4736(3)	35(1)
C(84)	8850(4)	3406(3)	4092(2)	26(1)
C(85)	8812(3)	4086(2)	3499(2)	16(1)
C(86)	7702(3)	5472(3)	2052(2)	22(1)
C(87)	7612(4)	5062(3)	1709(3)	31(1)
C(88)	7591(4)	4541(3)	1300(3)	27(1)

C(89)	7987(4)	3832(3)	1504(3)	33(1)
C(90)	7981(5)	3340(3)	1114(3)	41(2)
C(91)	7599(5)	3524(4)	531(3)	47(2)
C(92)	7179(4)	4219(3)	322(3)	39(1)
C(93)	7183(4)	4724(3)	698(3)	36(1)
C(94)	8569(3)	6834(3)	1887(2)	17(1)
C(95)	8170(4)	7109(3)	3691(3)	25(1)
C(96)	8250(5)	7471(4)	4228(3)	52(2)
C(97)	6641(3)	5036(3)	3879(2)	18(1)
C(98)	5957(4)	4578(3)	4416(3)	28(1)
C(99)	-984(7)	6530(5)	-151(5)	99(1)
C(100)	-517(7)	7308(5)	-333(5)	99(1)
C(101)	595(7)	8035(5)	1(5)	99(1)
C(102)	1302(7)	8014(5)	510(5)	99(1)

Table S3. Bond lengths [Å] and angles [°] for **5**.

Ru(1)-C(45)	1.844(5)	C(6)-H(6B)	0.9900
Ru(1)-C(37)	2.008(5)	C(7)-C(12)	1.530(6)
Ru(1)-N(1)	2.108(4)	C(7)-C(8)	1.545(6)
Ru(1)-N(2)	2.130(4)	C(7)-H(7)	1.0000
Ru(1)-P(1)	2.4469(12)	C(8)-C(9)	1.535(6)
Ru(1)-P(2)	2.4609(12)	C(8)-H(8A)	0.9900
Ru(2)-C(94)	1.847(5)	C(8)-H(8B)	0.9900
Ru(2)-C(86)	1.997(5)	C(9)-C(10)	1.520(7)
Ru(2)-N(3)	2.106(4)	C(9)-H(9A)	0.9900
Ru(2)-N(4)	2.121(4)	C(9)-H(9B)	0.9900
Ru(2)-P(4)	2.4407(12)	C(10)-C(11)	1.517(7)
Ru(2)-P(3)	2.4537(12)	C(10)-H(10A)	0.9900
P(1)-C(1)	1.859(4)	C(10)-H(10B)	0.9900
P(1)-C(13)	1.868(4)	C(11)-C(12)	1.541(6)
P(1)-C(7)	1.871(4)	C(11)-H(11A)	0.9900
P(2)-C(19)	1.858(4)	C(11)-H(11B)	0.9900
P(2)-C(31)	1.869(4)	C(12)-H(12A)	0.9900
P(2)-C(25)	1.875(4)	C(12)-H(12B)	0.9900
P(3)-C(50)	1.866(4)	C(13)-C(14)	1.533(6)
P(3)-C(62)	1.869(4)	C(13)-C(18)	1.536(6)
P(3)-C(56)	1.879(4)	C(13)-H(13)	1.0000
P(4)-C(80)	1.859(4)	C(14)-C(15)	1.531(6)
P(4)-C(74)	1.860(4)	C(14)-H(14A)	0.9900
P(4)-C(68)	1.874(4)	C(14)-H(14B)	0.9900
F(1)-B(1)	1.375(7)	C(15)-C(16)	1.508(6)
F(2)-B(1)	1.397(7)	C(15)-H(15A)	0.9900
F(3)-B(1)	1.381(7)	C(15)-H(15B)	0.9900
F(4)-B(1)	1.369(8)	C(16)-C(17)	1.527(6)
F(5)-B(2)	1.378(7)	C(16)-H(16A)	0.9900
F(6)-B(2)	1.377(8)	C(16)-H(16B)	0.9900
F(7)-B(2)	1.390(7)	C(17)-C(18)	1.529(6)
F(8)-B(2)	1.391(7)	C(17)-H(17A)	0.9900
O(1)-C(45)	1.149(5)	C(17)-H(17B)	0.9900
O(2)-C(94)	1.158(5)	C(18)-H(18A)	0.9900
O(3)-C(100)	1.377(7)	C(18)-H(18B)	0.9900
O(3)-C(101)	1.378(7)	C(19)-C(20)	1.538(6)
N(1)-C(46)	1.138(6)	C(19)-C(24)	1.553(6)
N(2)-C(48)	1.147(6)	C(19)-H(19)	1.0000
N(3)-C(95)	1.135(6)	C(20)-C(21)	1.534(6)
N(4)-C(97)	1.134(6)	C(20)-H(20A)	0.9900
C(1)-C(2)	1.531(6)	C(20)-H(20B)	0.9900
C(1)-C(6)	1.542(6)	C(21)-C(22)	1.522(7)
C(1)-H(1)	1.0000	C(21)-H(21A)	0.9900
C(2)-C(3)	1.536(6)	C(21)-H(21B)	0.9900
C(2)-H(2A)	0.9900	C(22)-C(23)	1.520(7)
C(2)-H(2B)	0.9900	C(22)-H(22A)	0.9900
C(3)-C(4)	1.524(7)	C(22)-H(22B)	0.9900
C(3)-H(3A)	0.9900	C(23)-C(24)	1.535(6)
C(3)-H(3B)	0.9900	C(23)-H(23A)	0.9900
C(4)-C(5)	1.520(7)	C(23)-H(23B)	0.9900
C(4)-H(4A)	0.9900	C(24)-H(24A)	0.9900
C(4)-H(4B)	0.9900	C(24)-H(24B)	0.9900
C(5)-C(6)	1.534(6)	C(25)-C(30)	1.526(6)
C(5)-H(5A)	0.9900	C(25)-C(26)	1.551(6)
C(5)-H(5B)	0.9900	C(25)-H(25)	1.0000
C(6)-H(6A)	0.9900	C(26)-C(27)	1.541(6)

C(26)-H(26A)	0.9900	C(52)-H(52A)	0.9900
C(26)-H(26B)	0.9900	C(52)-H(52B)	0.9900
C(27)-C(28)	1.523(6)	C(53)-C(54)	1.522(7)
C(27)-H(27A)	0.9900	C(53)-H(53A)	0.9900
C(27)-H(27B)	0.9900	C(53)-H(53B)	0.9900
C(28)-C(29)	1.519(7)	C(54)-C(55)	1.539(6)
C(28)-H(28A)	0.9900	C(54)-H(54A)	0.9900
C(28)-H(28B)	0.9900	C(54)-H(54B)	0.9900
C(29)-C(30)	1.532(6)	C(55)-H(55A)	0.9900
C(29)-H(29A)	0.9900	C(55)-H(55B)	0.9900
C(29)-H(29B)	0.9900	C(56)-C(57)	1.534(6)
C(30)-H(30A)	0.9900	C(56)-C(61)	1.543(6)
C(30)-H(30B)	0.9900	C(56)-H(56)	1.0000
C(31)-C(36)	1.537(6)	C(57)-C(58)	1.544(6)
C(31)-C(32)	1.551(6)	C(57)-H(57A)	0.9900
C(31)-H(31)	1.0000	C(57)-H(57B)	0.9900
C(32)-C(33)	1.535(6)	C(58)-C(59)	1.517(7)
C(32)-H(32A)	0.9900	C(58)-H(58A)	0.9900
C(32)-H(32B)	0.9900	C(58)-H(58B)	0.9900
C(33)-C(34)	1.514(7)	C(59)-C(60)	1.533(6)
C(33)-H(33A)	0.9900	C(59)-H(59A)	0.9900
C(33)-H(33B)	0.9900	C(59)-H(59B)	0.9900
C(34)-C(35)	1.522(7)	C(60)-C(61)	1.522(6)
C(34)-H(34A)	0.9900	C(60)-H(60A)	0.9900
C(34)-H(34B)	0.9900	C(60)-H(60B)	0.9900
C(35)-C(36)	1.524(6)	C(61)-H(61A)	0.9900
C(35)-H(35A)	0.9900	C(61)-H(61B)	0.9900
C(35)-H(35B)	0.9900	C(62)-C(67)	1.535(6)
C(36)-H(36A)	0.9900	C(62)-C(63)	1.537(6)
C(36)-H(36B)	0.9900	C(62)-H(62)	1.0000
C(37)-C(38)	1.188(7)	C(63)-C(64)	1.529(6)
C(38)-C(39)	1.437(7)	C(63)-H(63A)	0.9900
C(39)-C(40)	1.396(7)	C(63)-H(63B)	0.9900
C(39)-C(44)	1.419(8)	C(64)-C(65)	1.532(7)
C(40)-C(41)	1.391(7)	C(64)-H(64A)	0.9900
C(40)-H(40)	0.9500	C(64)-H(64B)	0.9900
C(41)-C(42)	1.357(8)	C(65)-C(66)	1.507(7)
C(41)-H(41)	0.9500	C(65)-H(65A)	0.9900
C(42)-C(43)	1.384(9)	C(65)-H(65B)	0.9900
C(42)-H(42)	0.9500	C(66)-C(67)	1.543(6)
C(43)-C(44)	1.358(8)	C(66)-H(66A)	0.9900
C(43)-H(43)	0.9500	C(66)-H(66B)	0.9900
C(44)-H(44)	0.9500	C(67)-H(67A)	0.9900
C(46)-C(47)	1.460(7)	C(67)-H(67B)	0.9900
C(47)-H(47A)	0.9800	C(68)-C(69)	1.532(6)
C(47)-H(47B)	0.9800	C(68)-C(73)	1.538(6)
C(47)-H(47C)	0.9800	C(68)-H(68)	1.0000
C(48)-C(49)	1.443(6)	C(69)-C(70)	1.529(6)
C(49)-H(49A)	0.9800	C(69)-H(69A)	0.9900
C(49)-H(49B)	0.9800	C(69)-H(69B)	0.9900
C(49)-H(49C)	0.9800	C(70)-C(71)	1.521(7)
C(50)-C(55)	1.529(6)	C(70)-H(70A)	0.9900
C(50)-C(51)	1.539(6)	C(70)-H(70B)	0.9900
C(50)-H(50)	1.0000	C(71)-C(72)	1.509(6)
C(51)-C(52)	1.533(6)	C(71)-H(71A)	0.9900
C(51)-H(51A)	0.9900	C(71)-H(71B)	0.9900
C(51)-H(51B)	0.9900	C(72)-C(73)	1.522(6)
C(52)-C(53)	1.512(7)	C(72)-H(72A)	0.9900

C(72)-H(72B)	0.9900	C(86)-C(87)	1.187(7)
C(73)-H(73A)	0.9900	C(87)-C(88)	1.448(7)
C(73)-H(73B)	0.9900	C(88)-C(89)	1.392(7)
C(74)-C(75)	1.522(6)	C(88)-C(93)	1.399(7)
C(74)-C(79)	1.559(6)	C(89)-C(90)	1.373(7)
C(74)-H(74)	1.0000	C(89)-H(89)	0.9500
C(75)-C(76)	1.532(7)	C(90)-C(91)	1.347(9)
C(75)-H(75A)	0.9900	C(90)-H(90)	0.9500
C(75)-H(75B)	0.9900	C(91)-C(92)	1.385(9)
C(76)-C(77)	1.533(7)	C(91)-H(91)	0.9500
C(76)-H(76A)	0.9900	C(92)-C(93)	1.370(7)
C(76)-H(76B)	0.9900	C(92)-H(92)	0.9500
C(77)-C(78)	1.492(7)	C(93)-H(93)	0.9500
C(77)-H(77A)	0.9900	C(95)-C(96)	1.467(7)
C(77)-H(77B)	0.9900	C(96)-H(96A)	0.9800
C(78)-C(79)	1.539(6)	C(96)-H(96B)	0.9800
C(78)-H(78A)	0.9900	C(96)-H(96C)	0.9800
C(78)-H(78B)	0.9900	C(96)-H(96D)	0.9800
C(79)-H(79A)	0.9900	C(96)-H(96E)	0.9800
C(79)-H(79B)	0.9900	C(96)-H(96F)	0.9800
C(80)-C(81)	1.526(6)	C(97)-C(98)	1.464(6)
C(80)-C(85)	1.535(6)	C(98)-H(98A)	0.9800
C(80)-H(80)	1.0000	C(98)-H(98B)	0.9800
C(81)-C(82)	1.537(7)	C(98)-H(98C)	0.9800
C(81)-H(81A)	0.9900	C(99)-C(100)	1.507(8)
C(81)-H(81B)	0.9900	C(99)-H(99A)	0.9800
C(82)-C(83)	1.539(7)	C(99)-H(99B)	0.9800
C(82)-H(82A)	0.9900	C(99)-H(99C)	0.9800
C(82)-H(82B)	0.9900	C(100)-H(10C)	0.9900
C(83)-C(84)	1.510(7)	C(100)-H(10D)	0.9900
C(83)-H(83A)	0.9900	C(101)-C(102)	1.506(8)
C(83)-H(83B)	0.9900	C(101)-H(10E)	0.9900
C(84)-C(85)	1.530(6)	C(101)-H(10F)	0.9900
C(84)-H(84A)	0.9900	C(102)-H(10G)	0.9800
C(84)-H(84B)	0.9900	C(102)-H(10H)	0.9800
C(85)-H(85A)	0.9900	C(102)-H(10I)	0.9800
C(85)-H(85B)	0.9900		
C(45)-Ru(1)-C(37)	87.6(2)	N(3)-Ru(2)-N(4)	85.04(14)
C(45)-Ru(1)-N(1)	97.25(17)	C(94)-Ru(2)-P(4)	88.21(14)
C(37)-Ru(1)-N(1)	174.81(17)	C(86)-Ru(2)-P(4)	87.77(14)
C(45)-Ru(1)-N(2)	178.04(17)	N(3)-Ru(2)-P(4)	91.06(11)
C(37)-Ru(1)-N(2)	90.91(17)	N(4)-Ru(2)-P(4)	92.64(10)
N(1)-Ru(1)-N(2)	84.29(14)	C(94)-Ru(2)-P(3)	91.09(14)
C(45)-Ru(1)-P(1)	89.26(14)	C(86)-Ru(2)-P(3)	89.71(14)
C(37)-Ru(1)-P(1)	87.84(13)	N(3)-Ru(2)-P(3)	91.50(11)
N(1)-Ru(1)-P(1)	90.36(10)	N(4)-Ru(2)-P(3)	88.03(10)
N(2)-Ru(1)-P(1)	91.95(10)	P(4)-Ru(2)-P(3)	177.39(4)
C(45)-Ru(1)-P(2)	91.12(14)	C(1)-P(1)-C(13)	100.78(19)
C(37)-Ru(1)-P(2)	91.31(13)	C(1)-P(1)-C(7)	102.2(2)
N(1)-Ru(1)-P(2)	90.45(10)	C(13)-P(1)-C(7)	110.7(2)
N(2)-Ru(1)-P(2)	87.65(10)	C(1)-P(1)-Ru(1)	116.03(15)
P(1)-Ru(1)-P(2)	179.06(4)	C(13)-P(1)-Ru(1)	111.03(14)
C(94)-Ru(2)-C(86)	89.0(2)	C(7)-P(1)-Ru(1)	114.98(14)
C(94)-Ru(2)-N(3)	95.60(18)	C(19)-P(2)-C(31)	101.14(19)
C(86)-Ru(2)-N(3)	175.22(18)	C(19)-P(2)-C(25)	101.26(19)
C(94)-Ru(2)-N(4)	178.93(17)	C(31)-P(2)-C(25)	112.1(2)
C(86)-Ru(2)-N(4)	90.39(17)	C(19)-P(2)-Ru(1)	115.86(15)

C(31)-P(2)-Ru(1)	111.52(14)	C(4)-C(5)-H(5B)	109.3
C(25)-P(2)-Ru(1)	113.93(14)	C(6)-C(5)-H(5B)	109.3
C(50)-P(3)-C(62)	101.2(2)	H(5A)-C(5)-H(5B)	108.0
C(50)-P(3)-C(56)	112.3(2)	C(5)-C(6)-C(1)	110.4(4)
C(62)-P(3)-C(56)	101.36(19)	C(5)-C(6)-H(6A)	109.6
C(50)-P(3)-Ru(2)	112.59(14)	C(1)-C(6)-H(6A)	109.6
C(62)-P(3)-Ru(2)	114.86(15)	C(5)-C(6)-H(6B)	109.6
C(56)-P(3)-Ru(2)	113.47(15)	C(1)-C(6)-H(6B)	109.6
C(80)-P(4)-C(74)	102.2(2)	H(6A)-C(6)-H(6B)	108.1
C(80)-P(4)-C(68)	101.5(2)	C(12)-C(7)-C(8)	109.9(4)
C(74)-P(4)-C(68)	110.0(2)	C(12)-C(7)-P(1)	113.7(3)
C(80)-P(4)-Ru(2)	115.67(16)	C(8)-C(7)-P(1)	116.8(3)
C(74)-P(4)-Ru(2)	114.60(15)	C(12)-C(7)-H(7)	105.1
C(68)-P(4)-Ru(2)	111.77(14)	C(8)-C(7)-H(7)	105.1
C(100)-O(3)-C(101)	113.3(8)	P(1)-C(7)-H(7)	105.1
C(46)-N(1)-Ru(1)	171.5(4)	C(9)-C(8)-C(7)	111.3(4)
C(48)-N(2)-Ru(1)	173.1(4)	C(9)-C(8)-H(8A)	109.4
C(95)-N(3)-Ru(2)	172.9(4)	C(7)-C(8)-H(8A)	109.4
C(97)-N(4)-Ru(2)	172.9(4)	C(9)-C(8)-H(8B)	109.4
F(4)-B(1)-F(1)	110.3(5)	C(7)-C(8)-H(8B)	109.4
F(4)-B(1)-F(3)	109.9(6)	H(8A)-C(8)-H(8B)	108.0
F(1)-B(1)-F(3)	108.4(5)	C(10)-C(9)-C(8)	112.2(4)
F(4)-B(1)-F(2)	111.4(5)	C(10)-C(9)-H(9A)	109.2
F(1)-B(1)-F(2)	108.8(5)	C(8)-C(9)-H(9A)	109.2
F(3)-B(1)-F(2)	108.0(5)	C(10)-C(9)-H(9B)	109.2
F(6)-B(2)-F(5)	110.6(5)	C(8)-C(9)-H(9B)	109.2
F(6)-B(2)-F(7)	108.5(5)	H(9A)-C(9)-H(9B)	107.9
F(5)-B(2)-F(7)	108.1(5)	C(11)-C(10)-C(9)	110.0(4)
F(6)-B(2)-F(8)	111.4(5)	C(11)-C(10)-H(10A)	109.7
F(5)-B(2)-F(8)	109.6(5)	C(9)-C(10)-H(10A)	109.7
F(7)-B(2)-F(8)	108.4(5)	C(11)-C(10)-H(10B)	109.7
C(2)-C(1)-C(6)	111.9(4)	C(9)-C(10)-H(10B)	109.7
C(2)-C(1)-P(1)	113.9(3)	H(10A)-C(10)-H(10B)	108.2
C(6)-C(1)-P(1)	111.7(3)	C(10)-C(11)-C(12)	111.0(4)
C(2)-C(1)-H(1)	106.3	C(10)-C(11)-H(11A)	109.4
C(6)-C(1)-H(1)	106.3	C(12)-C(11)-H(11A)	109.4
P(1)-C(1)-H(1)	106.3	C(10)-C(11)-H(11B)	109.4
C(1)-C(2)-C(3)	110.6(4)	C(12)-C(11)-H(11B)	109.4
C(1)-C(2)-H(2A)	109.5	H(11A)-C(11)-H(11B)	108.0
C(3)-C(2)-H(2A)	109.5	C(7)-C(12)-C(11)	111.5(4)
C(1)-C(2)-H(2B)	109.5	C(7)-C(12)-H(12A)	109.3
C(3)-C(2)-H(2B)	109.5	C(11)-C(12)-H(12A)	109.3
H(2A)-C(2)-H(2B)	108.1	C(7)-C(12)-H(12B)	109.3
C(4)-C(3)-C(2)	111.6(4)	C(11)-C(12)-H(12B)	109.3
C(4)-C(3)-H(3A)	109.3	H(12A)-C(12)-H(12B)	108.0
C(2)-C(3)-H(3A)	109.3	C(14)-C(13)-C(18)	109.6(4)
C(4)-C(3)-H(3B)	109.3	C(14)-C(13)-P(1)	116.0(3)
C(2)-C(3)-H(3B)	109.3	C(18)-C(13)-P(1)	115.8(3)
H(3A)-C(3)-H(3B)	108.0	C(14)-C(13)-H(13)	104.7
C(5)-C(4)-C(3)	110.8(4)	C(18)-C(13)-H(13)	104.7
C(5)-C(4)-H(4A)	109.5	P(1)-C(13)-H(13)	104.7
C(3)-C(4)-H(4A)	109.5	C(15)-C(14)-C(13)	111.4(4)
C(5)-C(4)-H(4B)	109.5	C(15)-C(14)-H(14A)	109.4
C(3)-C(4)-H(4B)	109.5	C(13)-C(14)-H(14A)	109.4
H(4A)-C(4)-H(4B)	108.1	C(15)-C(14)-H(14B)	109.4
C(4)-C(5)-C(6)	111.6(4)	C(13)-C(14)-H(14B)	109.4
C(4)-C(5)-H(5A)	109.3	H(14A)-C(14)-H(14B)	108.0
C(6)-C(5)-H(5A)	109.3	C(16)-C(15)-C(14)	111.3(4)

C(16)-C(15)-H(15A)	109.4	H(24A)-C(24)-H(24B)	108.0
C(14)-C(15)-H(15A)	109.4	C(30)-C(25)-C(26)	110.4(4)
C(16)-C(15)-H(15B)	109.4	C(30)-C(25)-P(2)	114.2(3)
C(14)-C(15)-H(15B)	109.4	C(26)-C(25)-P(2)	116.0(3)
H(15A)-C(15)-H(15B)	108.0	C(30)-C(25)-H(25)	105.0
C(15)-C(16)-C(17)	111.0(4)	C(26)-C(25)-H(25)	105.0
C(15)-C(16)-H(16A)	109.4	P(2)-C(25)-H(25)	105.0
C(17)-C(16)-H(16A)	109.4	C(27)-C(26)-C(25)	111.5(4)
C(15)-C(16)-H(16B)	109.4	C(27)-C(26)-H(26A)	109.3
C(17)-C(16)-H(16B)	109.4	C(25)-C(26)-H(26A)	109.3
H(16A)-C(16)-H(16B)	108.0	C(27)-C(26)-H(26B)	109.3
C(16)-C(17)-C(18)	111.6(4)	C(25)-C(26)-H(26B)	109.3
C(16)-C(17)-H(17A)	109.3	H(26A)-C(26)-H(26B)	108.0
C(18)-C(17)-H(17A)	109.3	C(28)-C(27)-C(26)	111.9(4)
C(16)-C(17)-H(17B)	109.3	C(28)-C(27)-H(27A)	109.2
C(18)-C(17)-H(17B)	109.3	C(26)-C(27)-H(27A)	109.2
H(17A)-C(17)-H(17B)	108.0	C(28)-C(27)-H(27B)	109.2
C(17)-C(18)-C(13)	110.7(4)	C(26)-C(27)-H(27B)	109.2
C(17)-C(18)-H(18A)	109.5	H(27A)-C(27)-H(27B)	107.9
C(13)-C(18)-H(18A)	109.5	C(29)-C(28)-C(27)	109.7(4)
C(17)-C(18)-H(18B)	109.5	C(29)-C(28)-H(28A)	109.7
C(13)-C(18)-H(18B)	109.5	C(27)-C(28)-H(28A)	109.7
H(18A)-C(18)-H(18B)	108.1	C(29)-C(28)-H(28B)	109.7
C(20)-C(19)-C(24)	111.7(4)	C(27)-C(28)-H(28B)	109.7
C(20)-C(19)-P(2)	113.7(3)	H(28A)-C(28)-H(28B)	108.2
C(24)-C(19)-P(2)	112.3(3)	C(28)-C(29)-C(30)	111.0(4)
C(20)-C(19)-H(19)	106.2	C(28)-C(29)-H(29A)	109.4
C(24)-C(19)-H(19)	106.2	C(30)-C(29)-H(29A)	109.4
P(2)-C(19)-H(19)	106.2	C(28)-C(29)-H(29B)	109.4
C(21)-C(20)-C(19)	111.0(4)	C(30)-C(29)-H(29B)	109.4
C(21)-C(20)-H(20A)	109.4	H(29A)-C(29)-H(29B)	108.0
C(19)-C(20)-H(20A)	109.4	C(25)-C(30)-C(29)	112.3(4)
C(21)-C(20)-H(20B)	109.4	C(25)-C(30)-H(30A)	109.1
C(19)-C(20)-H(20B)	109.4	C(29)-C(30)-H(30A)	109.1
H(20A)-C(20)-H(20B)	108.0	C(25)-C(30)-H(30B)	109.1
C(22)-C(21)-C(20)	112.2(4)	C(29)-C(30)-H(30B)	109.1
C(22)-C(21)-H(21A)	109.2	H(30A)-C(30)-H(30B)	107.9
C(20)-C(21)-H(21A)	109.2	C(36)-C(31)-C(32)	108.6(4)
C(22)-C(21)-H(21B)	109.2	C(36)-C(31)-P(2)	115.6(3)
C(20)-C(21)-H(21B)	109.2	C(32)-C(31)-P(2)	115.7(3)
H(21A)-C(21)-H(21B)	107.9	C(36)-C(31)-H(31)	105.3
C(23)-C(22)-C(21)	110.9(4)	C(32)-C(31)-H(31)	105.3
C(23)-C(22)-H(22A)	109.5	P(2)-C(31)-H(31)	105.3
C(21)-C(22)-H(22A)	109.5	C(33)-C(32)-C(31)	110.7(4)
C(23)-C(22)-H(22B)	109.5	C(33)-C(32)-H(32A)	109.5
C(21)-C(22)-H(22B)	109.5	C(31)-C(32)-H(32A)	109.5
H(22A)-C(22)-H(22B)	108.1	C(33)-C(32)-H(32B)	109.5
C(22)-C(23)-C(24)	111.4(4)	C(31)-C(32)-H(32B)	109.5
C(22)-C(23)-H(23A)	109.4	H(32A)-C(32)-H(32B)	108.1
C(24)-C(23)-H(23A)	109.4	C(34)-C(33)-C(32)	111.0(4)
C(22)-C(23)-H(23B)	109.4	C(34)-C(33)-H(33A)	109.4
C(24)-C(23)-H(23B)	109.4	C(32)-C(33)-H(33A)	109.4
H(23A)-C(23)-H(23B)	108.0	C(34)-C(33)-H(33B)	109.4
C(23)-C(24)-C(19)	111.0(4)	C(32)-C(33)-H(33B)	109.4
C(23)-C(24)-H(24A)	109.4	H(33A)-C(33)-H(33B)	108.0
C(19)-C(24)-H(24A)	109.4	C(33)-C(34)-C(35)	111.0(4)
C(23)-C(24)-H(24B)	109.4	C(33)-C(34)-H(34A)	109.4
C(19)-C(24)-H(24B)	109.4	C(35)-C(34)-H(34A)	109.4

C(33)-C(34)-H(34B)	109.4	C(50)-C(51)-H(51A)	109.5
C(35)-C(34)-H(34B)	109.4	C(52)-C(51)-H(51B)	109.5
H(34A)-C(34)-H(34B)	108.0	C(50)-C(51)-H(51B)	109.5
C(34)-C(35)-C(36)	111.3(4)	H(51A)-C(51)-H(51B)	108.1
C(34)-C(35)-H(35A)	109.4	C(53)-C(52)-C(51)	112.1(4)
C(36)-C(35)-H(35A)	109.4	C(53)-C(52)-H(52A)	109.2
C(34)-C(35)-H(35B)	109.4	C(51)-C(52)-H(52A)	109.2
C(36)-C(35)-H(35B)	109.4	C(53)-C(52)-H(52B)	109.2
H(35A)-C(35)-H(35B)	108.0	C(51)-C(52)-H(52B)	109.2
C(35)-C(36)-C(31)	111.5(4)	H(52A)-C(52)-H(52B)	107.9
C(35)-C(36)-H(36A)	109.3	C(52)-C(53)-C(54)	110.7(4)
C(31)-C(36)-H(36A)	109.3	C(52)-C(53)-H(53A)	109.5
C(35)-C(36)-H(36B)	109.3	C(54)-C(53)-H(53A)	109.5
C(31)-C(36)-H(36B)	109.3	C(52)-C(53)-H(53B)	109.5
H(36A)-C(36)-H(36B)	108.0	C(54)-C(53)-H(53B)	109.5
C(38)-C(37)-Ru(1)	171.2(5)	H(53A)-C(53)-H(53B)	108.1
C(37)-C(38)-C(39)	170.2(6)	C(53)-C(54)-C(55)	110.9(4)
C(40)-C(39)-C(44)	117.0(5)	C(53)-C(54)-H(54A)	109.5
C(40)-C(39)-C(38)	123.2(5)	C(55)-C(54)-H(54A)	109.5
C(44)-C(39)-C(38)	119.8(5)	C(53)-C(54)-H(54B)	109.5
C(41)-C(40)-C(39)	121.6(5)	C(55)-C(54)-H(54B)	109.5
C(41)-C(40)-H(40)	119.2	H(54A)-C(54)-H(54B)	108.0
C(39)-C(40)-H(40)	119.2	C(50)-C(55)-C(54)	111.2(4)
C(42)-C(41)-C(40)	119.9(6)	C(50)-C(55)-H(55A)	109.4
C(42)-C(41)-H(41)	120.0	C(54)-C(55)-H(55A)	109.4
C(40)-C(41)-H(41)	120.0	C(50)-C(55)-H(55B)	109.4
C(41)-C(42)-C(43)	119.4(6)	C(54)-C(55)-H(55B)	109.4
C(41)-C(42)-H(42)	120.3	H(55A)-C(55)-H(55B)	108.0
C(43)-C(42)-H(42)	120.3	C(57)-C(56)-C(61)	109.8(4)
C(44)-C(43)-C(42)	122.0(6)	C(57)-C(56)-P(3)	114.3(3)
C(44)-C(43)-H(43)	119.0	C(61)-C(56)-P(3)	116.3(3)
C(42)-C(43)-H(43)	119.0	C(57)-C(56)-H(56)	105.1
C(43)-C(44)-C(39)	120.0(5)	C(61)-C(56)-H(56)	105.1
C(43)-C(44)-H(44)	120.0	P(3)-C(56)-H(56)	105.1
C(39)-C(44)-H(44)	120.0	C(56)-C(57)-C(58)	110.9(4)
O(1)-C(45)-Ru(1)	178.1(4)	C(56)-C(57)-H(57A)	109.5
N(1)-C(46)-C(47)	177.9(6)	C(58)-C(57)-H(57A)	109.5
C(46)-C(47)-H(47A)	109.5	C(56)-C(57)-H(57B)	109.5
C(46)-C(47)-H(47B)	109.5	C(58)-C(57)-H(57B)	109.5
H(47A)-C(47)-H(47B)	109.5	H(57A)-C(57)-H(57B)	108.1
C(46)-C(47)-H(47C)	109.5	C(59)-C(58)-C(57)	111.2(4)
H(47A)-C(47)-H(47C)	109.5	C(59)-C(58)-H(58A)	109.4
H(47B)-C(47)-H(47C)	109.5	C(57)-C(58)-H(58A)	109.4
N(2)-C(48)-C(49)	177.1(5)	C(59)-C(58)-H(58B)	109.4
C(48)-C(49)-H(49A)	109.5	C(57)-C(58)-H(58B)	109.4
C(48)-C(49)-H(49B)	109.5	H(58A)-C(58)-H(58B)	108.0
H(49A)-C(49)-H(49B)	109.5	C(58)-C(59)-C(60)	109.5(4)
C(48)-C(49)-H(49C)	109.5	C(58)-C(59)-H(59A)	109.8
H(49A)-C(49)-H(49C)	109.5	C(60)-C(59)-H(59A)	109.8
H(49B)-C(49)-H(49C)	109.5	C(58)-C(59)-H(59B)	109.8
C(55)-C(50)-C(51)	110.2(4)	C(60)-C(59)-H(59B)	109.8
C(55)-C(50)-P(3)	116.7(3)	H(59A)-C(59)-H(59B)	108.2
C(51)-C(50)-P(3)	115.4(3)	C(61)-C(60)-C(59)	111.7(4)
C(55)-C(50)-H(50)	104.3	C(61)-C(60)-H(60A)	109.3
C(51)-C(50)-H(50)	104.3	C(59)-C(60)-H(60A)	109.3
P(3)-C(50)-H(50)	104.3	C(61)-C(60)-H(60B)	109.3
C(52)-C(51)-C(50)	110.6(4)	C(59)-C(60)-H(60B)	109.3
C(52)-C(51)-H(51A)	109.5	H(60A)-C(60)-H(60B)	107.9

C(60)-C(61)-C(56)	112.0(4)	C(69)-C(70)-H(70B)	109.0
C(60)-C(61)-H(61A)	109.2	H(70A)-C(70)-H(70B)	107.8
C(56)-C(61)-H(61A)	109.2	C(72)-C(71)-C(70)	110.5(4)
C(60)-C(61)-H(61B)	109.2	C(72)-C(71)-H(71A)	109.5
C(56)-C(61)-H(61B)	109.2	C(70)-C(71)-H(71A)	109.5
H(61A)-C(61)-H(61B)	107.9	C(72)-C(71)-H(71B)	109.5
C(67)-C(62)-C(63)	113.1(4)	C(70)-C(71)-H(71B)	109.5
C(67)-C(62)-P(3)	112.8(3)	H(71A)-C(71)-H(71B)	108.1
C(63)-C(62)-P(3)	112.7(3)	C(71)-C(72)-C(73)	112.3(4)
C(67)-C(62)-H(62)	105.8	C(71)-C(72)-H(72A)	109.2
C(63)-C(62)-H(62)	105.8	C(73)-C(72)-H(72A)	109.2
P(3)-C(62)-H(62)	105.8	C(71)-C(72)-H(72B)	109.2
C(64)-C(63)-C(62)	111.0(4)	C(73)-C(72)-H(72B)	109.2
C(64)-C(63)-H(63A)	109.4	H(72A)-C(72)-H(72B)	107.9
C(62)-C(63)-H(63A)	109.4	C(72)-C(73)-C(68)	111.5(4)
C(64)-C(63)-H(63B)	109.4	C(72)-C(73)-H(73A)	109.3
C(62)-C(63)-H(63B)	109.4	C(68)-C(73)-H(73A)	109.3
H(63A)-C(63)-H(63B)	108.0	C(72)-C(73)-H(73B)	109.3
C(63)-C(64)-C(65)	110.6(4)	C(68)-C(73)-H(73B)	109.3
C(63)-C(64)-H(64A)	109.5	H(73A)-C(73)-H(73B)	108.0
C(65)-C(64)-H(64A)	109.5	C(75)-C(74)-C(79)	109.7(4)
C(63)-C(64)-H(64B)	109.5	C(75)-C(74)-P(4)	113.6(3)
C(65)-C(64)-H(64B)	109.5	C(79)-C(74)-P(4)	117.0(3)
H(64A)-C(64)-H(64B)	108.1	C(75)-C(74)-H(74)	105.1
C(66)-C(65)-C(64)	110.7(4)	C(79)-C(74)-H(74)	105.1
C(66)-C(65)-H(65A)	109.5	P(4)-C(74)-H(74)	105.1
C(64)-C(65)-H(65A)	109.5	C(74)-C(75)-C(76)	111.0(4)
C(66)-C(65)-H(65B)	109.5	C(74)-C(75)-H(75A)	109.4
C(64)-C(65)-H(65B)	109.5	C(76)-C(75)-H(75A)	109.4
H(65A)-C(65)-H(65B)	108.1	C(74)-C(75)-H(75B)	109.4
C(65)-C(66)-C(67)	111.8(4)	C(76)-C(75)-H(75B)	109.4
C(65)-C(66)-H(66A)	109.3	H(75A)-C(75)-H(75B)	108.0
C(67)-C(66)-H(66A)	109.3	C(75)-C(76)-C(77)	110.4(4)
C(65)-C(66)-H(66B)	109.3	C(75)-C(76)-H(76A)	109.6
C(67)-C(66)-H(66B)	109.3	C(77)-C(76)-H(76A)	109.6
H(66A)-C(66)-H(66B)	107.9	C(75)-C(76)-H(76B)	109.6
C(62)-C(67)-C(66)	111.3(4)	C(77)-C(76)-H(76B)	109.6
C(62)-C(67)-H(67A)	109.4	H(76A)-C(76)-H(76B)	108.1
C(66)-C(67)-H(67A)	109.4	C(78)-C(77)-C(76)	110.0(4)
C(62)-C(67)-H(67B)	109.4	C(78)-C(77)-H(77A)	109.7
C(66)-C(67)-H(67B)	109.4	C(76)-C(77)-H(77A)	109.7
H(67A)-C(67)-H(67B)	108.0	C(78)-C(77)-H(77B)	109.7
C(69)-C(68)-C(73)	110.5(4)	C(76)-C(77)-H(77B)	109.7
C(69)-C(68)-P(4)	114.7(3)	H(77A)-C(77)-H(77B)	108.2
C(73)-C(68)-P(4)	115.8(3)	C(77)-C(78)-C(79)	111.7(4)
C(69)-C(68)-H(68)	104.8	C(77)-C(78)-H(78A)	109.3
C(73)-C(68)-H(68)	104.8	C(79)-C(78)-H(78A)	109.3
P(4)-C(68)-H(68)	104.8	C(77)-C(78)-H(78B)	109.3
C(70)-C(69)-C(68)	110.5(4)	C(79)-C(78)-H(78B)	109.3
C(70)-C(69)-H(69A)	109.6	H(78A)-C(78)-H(78B)	107.9
C(68)-C(69)-H(69A)	109.6	C(78)-C(79)-C(74)	110.8(4)
C(70)-C(69)-H(69B)	109.6	C(78)-C(79)-H(79A)	109.5
C(68)-C(69)-H(69B)	109.6	C(74)-C(79)-H(79A)	109.5
H(69A)-C(69)-H(69B)	108.1	C(78)-C(79)-H(79B)	109.5
C(71)-C(70)-C(69)	112.7(4)	C(74)-C(79)-H(79B)	109.5
C(71)-C(70)-H(70A)	109.0	H(79A)-C(79)-H(79B)	108.1
C(69)-C(70)-H(70A)	109.0	C(81)-C(80)-C(85)	111.6(4)
C(71)-C(70)-H(70B)	109.0	C(81)-C(80)-P(4)	113.5(3)

C(85)-C(80)-P(4)	112.3(3)	O(2)-C(94)-Ru(2)	179.1(5)
C(81)-C(80)-H(80)	106.3	N(3)-C(95)-C(96)	179.0(6)
C(85)-C(80)-H(80)	106.3	C(95)-C(96)-H(96A)	109.5
P(4)-C(80)-H(80)	106.3	C(95)-C(96)-H(96B)	109.5
C(80)-C(81)-C(82)	110.8(4)	H(96A)-C(96)-H(96B)	109.5
C(80)-C(81)-H(81A)	109.5	C(95)-C(96)-H(96C)	109.5
C(82)-C(81)-H(81A)	109.5	H(96A)-C(96)-H(96C)	109.5
C(80)-C(81)-H(81B)	109.5	H(96B)-C(96)-H(96C)	109.5
C(82)-C(81)-H(81B)	109.5	C(95)-C(96)-H(96D)	109.5
H(81A)-C(81)-H(81B)	108.1	H(96A)-C(96)-H(96D)	141.1
C(81)-C(82)-C(83)	111.0(4)	H(96B)-C(96)-H(96D)	56.3
C(81)-C(82)-H(82A)	109.4	H(96C)-C(96)-H(96D)	56.3
C(83)-C(82)-H(82A)	109.4	C(95)-C(96)-H(96E)	109.5
C(81)-C(82)-H(82B)	109.4	H(96A)-C(96)-H(96E)	56.3
C(83)-C(82)-H(82B)	109.4	H(96B)-C(96)-H(96E)	141.1
H(82A)-C(82)-H(82B)	108.0	H(96C)-C(96)-H(96E)	56.3
C(84)-C(83)-C(82)	111.4(4)	H(96D)-C(96)-H(96E)	109.5
C(84)-C(83)-H(83A)	109.4	C(95)-C(96)-H(96F)	109.5
C(82)-C(83)-H(83A)	109.4	H(96A)-C(96)-H(96F)	56.3
C(84)-C(83)-H(83B)	109.4	H(96B)-C(96)-H(96F)	56.3
C(82)-C(83)-H(83B)	109.4	H(96C)-C(96)-H(96F)	141.1
H(83A)-C(83)-H(83B)	108.0	H(96D)-C(96)-H(96F)	109.5
C(83)-C(84)-C(85)	111.6(4)	H(96E)-C(96)-H(96F)	109.5
C(83)-C(84)-H(84A)	109.3	N(4)-C(97)-C(98)	176.9(6)
C(85)-C(84)-H(84A)	109.3	C(97)-C(98)-H(98A)	109.5
C(83)-C(84)-H(84B)	109.3	C(97)-C(98)-H(98B)	109.5
C(85)-C(84)-H(84B)	109.3	H(98A)-C(98)-H(98B)	109.5
H(84A)-C(84)-H(84B)	108.0	C(97)-C(98)-H(98C)	109.5
C(84)-C(85)-C(80)	111.0(4)	H(98A)-C(98)-H(98C)	109.5
C(84)-C(85)-H(85A)	109.4	H(98B)-C(98)-H(98C)	109.5
C(80)-C(85)-H(85A)	109.4	C(100)-C(99)-H(99A)	109.5
C(84)-C(85)-H(85B)	109.4	C(100)-C(99)-H(99B)	109.5
C(80)-C(85)-H(85B)	109.4	H(99A)-C(99)-H(99B)	109.5
H(85A)-C(85)-H(85B)	108.0	C(100)-C(99)-H(99C)	109.5
C(87)-C(86)-Ru(2)	177.7(5)	H(99A)-C(99)-H(99C)	109.5
C(86)-C(87)-C(88)	174.9(6)	H(99B)-C(99)-H(99C)	109.5
C(89)-C(88)-C(93)	118.0(5)	O(3)-C(100)-C(99)	109.4(8)
C(89)-C(88)-C(87)	119.8(5)	O(3)-C(100)-H(10C)	109.8
C(93)-C(88)-C(87)	122.2(5)	C(99)-C(100)-H(10C)	109.8
C(90)-C(89)-C(88)	120.0(5)	O(3)-C(100)-H(10D)	109.8
C(90)-C(89)-H(89)	120.0	C(99)-C(100)-H(10D)	109.8
C(88)-C(89)-H(89)	120.0	H(10C)-C(100)-H(10D)	108.3
C(91)-C(90)-C(89)	121.6(6)	O(3)-C(101)-C(102)	110.2(8)
C(91)-C(90)-H(90)	119.2	O(3)-C(101)-H(10E)	109.6
C(89)-C(90)-H(90)	119.2	C(102)-C(101)-H(10E)	109.6
C(90)-C(91)-C(92)	119.7(6)	O(3)-C(101)-H(10F)	109.6
C(90)-C(91)-H(91)	120.1	C(102)-C(101)-H(10F)	109.6
C(92)-C(91)-H(91)	120.1	H(10E)-C(101)-H(10F)	108.1
C(93)-C(92)-C(91)	119.9(6)	C(101)-C(102)-H(10G)	109.5
C(93)-C(92)-H(92)	120.1	C(101)-C(102)-H(10H)	109.5
C(91)-C(92)-H(92)	120.1	H(10G)-C(102)-H(10H)	109.5
C(92)-C(93)-C(88)	120.7(5)	C(101)-C(102)-H(10I)	109.5
C(92)-C(93)-H(93)	119.6	H(10G)-C(102)-H(10I)	109.5
C(88)-C(93)-H(93)	119.6	H(10H)-C(102)-H(10I)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	8(1)	13(1)	10(1)	-3(1)	-2(1)	0(1)
Ru(2)	9(1)	16(1)	11(1)	-4(1)	-2(1)	1(1)
P(1)	8(1)	10(1)	12(1)	-2(1)	-3(1)	0(1)
P(2)	9(1)	12(1)	10(1)	-4(1)	-3(1)	1(1)
P(3)	10(1)	13(1)	12(1)	-4(1)	-3(1)	0(1)
P(4)	10(1)	12(1)	12(1)	-2(1)	-2(1)	-1(1)
F(1)	55(3)	72(3)	78(3)	-40(2)	-6(2)	13(2)
F(2)	62(3)	45(2)	46(2)	1(2)	-16(2)	-6(2)
F(3)	99(4)	65(3)	35(2)	1(2)	-2(2)	-1(2)
F(4)	55(3)	50(2)	123(4)	-11(2)	-56(3)	10(2)
F(5)	53(2)	59(2)	72(3)	-38(2)	-24(2)	-2(2)
F(6)	32(2)	53(2)	104(4)	-24(2)	7(2)	-5(2)
F(7)	81(3)	51(2)	29(2)	1(2)	-8(2)	1(2)
F(8)	54(2)	33(2)	42(2)	-1(2)	-1(2)	5(2)
O(1)	20(2)	29(2)	17(2)	4(1)	-7(1)	-1(2)
O(2)	22(2)	32(2)	27(2)	7(2)	0(2)	0(2)
N(1)	9(2)	19(2)	22(2)	-7(2)	-1(2)	-1(2)
N(2)	7(2)	15(2)	19(2)	-5(2)	2(2)	-4(2)
N(3)	12(2)	18(2)	23(2)	-8(2)	-5(2)	2(2)
N(4)	10(2)	13(2)	23(2)	-6(2)	-2(2)	-1(2)
B(1)	43(4)	26(4)	31(3)	-6(3)	-11(3)	7(3)
B(2)	38(4)	30(4)	29(3)	-5(3)	-3(3)	-7(3)
C(1)	12(2)	15(2)	11(2)	1(2)	-2(2)	0(2)
C(2)	18(3)	17(2)	15(2)	0(2)	2(2)	4(2)
C(3)	34(3)	20(3)	12(2)	2(2)	-1(2)	0(2)
C(4)	38(3)	20(3)	18(3)	6(2)	-3(2)	2(2)
C(5)	37(3)	13(2)	19(3)	0(2)	-1(2)	7(2)
C(6)	18(2)	9(2)	14(2)	0(2)	-5(2)	2(2)
C(7)	11(2)	14(2)	18(2)	-6(2)	-4(2)	3(2)
C(8)	12(2)	15(2)	18(2)	-4(2)	-3(2)	-2(2)
C(9)	30(3)	20(3)	24(3)	-8(2)	-6(2)	-5(2)
C(10)	37(3)	28(3)	20(3)	-10(2)	-9(2)	2(2)
C(11)	34(3)	32(3)	15(2)	-7(2)	-9(2)	-6(2)
C(12)	29(3)	21(3)	22(3)	-7(2)	-6(2)	-7(2)
C(13)	11(2)	12(2)	11(2)	-2(2)	-1(2)	2(2)
C(14)	13(2)	10(2)	28(3)	-5(2)	-6(2)	-2(2)
C(15)	11(2)	18(3)	28(3)	-3(2)	2(2)	-1(2)
C(16)	14(3)	15(2)	28(3)	-6(2)	-4(2)	3(2)
C(17)	12(2)	12(2)	29(3)	-1(2)	-2(2)	2(2)
C(18)	12(2)	13(2)	24(2)	0(2)	-2(2)	-1(2)
C(19)	11(2)	15(2)	13(2)	-5(2)	0(2)	-1(2)
C(20)	16(2)	13(2)	14(2)	-4(2)	-2(2)	0(2)
C(21)	23(3)	28(3)	12(2)	-2(2)	-2(2)	-5(2)
C(22)	33(3)	32(3)	15(2)	1(2)	-7(2)	3(2)
C(23)	27(3)	13(2)	21(3)	0(2)	-3(2)	4(2)
C(24)	15(2)	16(2)	17(2)	-5(2)	-6(2)	3(2)
C(25)	11(2)	16(2)	16(2)	-6(2)	-5(2)	3(2)
C(26)	14(3)	23(3)	22(2)	-12(2)	-4(2)	-3(2)
C(27)	18(3)	21(3)	22(2)	-9(2)	-4(2)	-5(2)
C(28)	25(3)	21(3)	24(3)	-13(2)	-15(2)	2(2)
C(29)	33(3)	23(3)	13(2)	-3(2)	-9(2)	-1(2)
C(30)	27(3)	17(3)	17(2)	-4(2)	-9(2)	-3(2)
C(31)	9(2)	16(2)	16(2)	-6(2)	-5(2)	6(2)

C(32)	11(2)	17(3)	36(3)	-7(2)	1(2)	2(2)
C(33)	13(3)	26(3)	39(3)	-14(2)	4(2)	-1(2)
C(34)	11(2)	25(3)	38(3)	-16(2)	-5(2)	5(2)
C(35)	17(3)	17(2)	31(3)	-9(2)	-4(2)	5(2)
C(36)	16(3)	16(2)	21(2)	-3(2)	-2(2)	1(2)
C(37)	12(2)	21(3)	24(3)	-9(2)	-2(2)	-2(2)
C(38)	24(3)	58(4)	44(4)	-34(3)	4(3)	-5(3)
C(39)	22(3)	43(3)	28(3)	-19(2)	-3(2)	9(2)
C(40)	44(4)	36(3)	31(3)	-14(3)	2(3)	-1(3)
C(41)	62(4)	46(4)	29(3)	-17(3)	7(3)	7(3)
C(42)	78(5)	38(4)	48(4)	-25(3)	4(4)	8(4)
C(43)	72(5)	32(3)	48(4)	-9(3)	-1(3)	26(3)
C(44)	46(4)	44(4)	27(3)	-5(3)	-6(3)	14(3)
C(45)	13(2)	17(2)	18(2)	-4(2)	-1(2)	-2(2)
C(46)	18(3)	34(3)	35(3)	-19(3)	-3(2)	-1(2)
C(47)	50(4)	64(4)	42(4)	-37(3)	-6(3)	12(3)
C(48)	18(3)	14(2)	18(2)	-6(2)	-3(2)	0(2)
C(49)	27(3)	25(3)	24(3)	-3(2)	-14(2)	7(2)
C(50)	13(2)	16(2)	20(2)	-9(2)	-11(2)	1(2)
C(51)	18(3)	15(2)	28(3)	-5(2)	-12(2)	1(2)
C(52)	15(3)	17(2)	38(3)	-10(2)	-10(2)	0(2)
C(53)	18(3)	23(3)	39(3)	-14(2)	-7(2)	-3(2)
C(54)	22(3)	23(3)	40(3)	-11(2)	-21(2)	1(2)
C(55)	21(3)	15(3)	48(3)	-13(2)	-13(2)	0(2)
C(56)	16(2)	15(2)	13(2)	-6(2)	-1(2)	0(2)
C(57)	24(3)	15(2)	14(2)	-3(2)	2(2)	3(2)
C(58)	26(3)	18(3)	15(2)	-3(2)	1(2)	2(2)
C(59)	21(3)	22(3)	23(3)	-10(2)	6(2)	-1(2)
C(60)	18(3)	22(3)	21(2)	-7(2)	-1(2)	5(2)
C(61)	18(3)	23(3)	24(3)	-9(2)	-3(2)	6(2)
C(62)	14(2)	14(2)	13(2)	0(2)	-3(2)	0(2)
C(63)	21(3)	17(2)	15(2)	-3(2)	-3(2)	-7(2)
C(64)	27(3)	21(3)	24(3)	-3(2)	-4(2)	-6(2)
C(65)	31(3)	23(3)	22(3)	1(2)	0(2)	-11(2)
C(66)	27(3)	32(3)	12(2)	-4(2)	-4(2)	-2(2)
C(67)	19(3)	19(2)	15(2)	-5(2)	-5(2)	0(2)
C(68)	14(2)	11(2)	21(2)	-4(2)	-5(2)	0(2)
C(69)	15(3)	15(2)	31(3)	-4(2)	-7(2)	0(2)
C(70)	18(3)	11(2)	32(3)	-4(2)	-5(2)	5(2)
C(71)	16(3)	19(3)	32(3)	-10(2)	-7(2)	-2(2)
C(72)	18(3)	19(3)	28(3)	-2(2)	-12(2)	3(2)
C(73)	15(2)	17(2)	22(2)	-7(2)	-9(2)	5(2)
C(74)	15(2)	17(2)	18(2)	-7(2)	-2(2)	5(2)
C(75)	29(3)	24(3)	23(3)	-1(2)	4(2)	7(2)
C(76)	36(3)	40(3)	19(3)	-6(2)	0(2)	7(3)
C(77)	28(3)	31(3)	34(3)	-15(2)	4(2)	0(2)
C(78)	26(3)	23(3)	36(3)	-12(2)	1(2)	5(2)
C(79)	14(2)	18(2)	22(2)	-4(2)	-3(2)	3(2)
C(80)	18(3)	12(2)	15(2)	-1(2)	-5(2)	0(2)
C(81)	23(3)	20(3)	22(3)	-5(2)	-5(2)	-4(2)
C(82)	48(4)	29(3)	20(3)	1(2)	-10(3)	-16(3)
C(83)	54(4)	23(3)	23(3)	3(2)	-4(3)	-12(3)
C(84)	35(3)	14(3)	25(3)	3(2)	-2(2)	-5(2)
C(85)	14(2)	13(2)	20(2)	-3(2)	-4(2)	-1(2)
C(86)	12(3)	28(3)	29(3)	-10(2)	-5(2)	5(2)
C(87)	21(3)	38(3)	44(3)	-26(3)	-14(2)	9(2)
C(88)	18(3)	36(3)	32(3)	-19(2)	-1(2)	3(2)
C(89)	34(3)	36(3)	31(3)	-9(2)	-9(3)	2(3)

C(90)	41(4)	26(3)	59(4)	-17(3)	-7(3)	-6(3)
C(91)	41(4)	49(4)	60(4)	-37(3)	7(3)	-16(3)
C(92)	44(4)	48(4)	27(3)	-16(3)	-5(3)	-17(3)
C(93)	41(4)	28(3)	41(3)	-8(3)	-19(3)	1(3)
C(94)	6(2)	22(3)	21(2)	-1(2)	-4(2)	3(2)
C(95)	17(3)	31(3)	33(3)	-18(2)	-11(2)	4(2)
C(96)	56(4)	64(5)	54(4)	-44(4)	-18(3)	6(4)
C(97)	14(2)	14(2)	28(3)	-7(2)	-2(2)	3(2)
C(98)	28(3)	21(3)	30(3)	-3(2)	11(2)	-6(2)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **5**.

	x	y	z	U(eq)
H(1)	417	-409	3564	16
H(2A)	722	421	4199	21
H(2B)	1869	220	4168	21
H(3A)	1061	-490	5187	28
H(3B)	267	-817	4815	28
H(4A)	2329	-1158	4756	32
H(4B)	1449	-1736	5136	32
H(5A)	854	-1743	4130	29
H(5B)	1994	-1964	4097	29
H(6A)	1662	-1064	3102	16
H(6B)	2478	-740	3460	16
H(7)	1546	-219	2051	16
H(8A)	152	-828	2735	18
H(8B)	-533	-161	2401	18
H(9A)	490	-1164	1731	29
H(9B)	-684	-1155	1900	29
H(10A)	-206	-548	768	33
H(10B)	-749	25	1138	33
H(11A)	694	618	497	32
H(11B)	1352	-53	860	32
H(12A)	1498	981	1327	28
H(12B)	322	981	1497	28
H(13)	506	1320	3373	14
H(14A)	-930	826	2678	20
H(14B)	-738	413	3420	20
H(15A)	-2095	1234	3415	24
H(15B)	-1228	1484	3779	24
H(16A)	-1786	2554	3063	22
H(16B)	-1621	2179	2455	22
H(17A)	-74	2617	3119	22
H(17B)	-288	3019	2379	22
H(18A)	1081	2208	2379	20
H(18B)	209	1947	2026	20
H(19)	5533	2740	1535	15
H(20A)	5276	1925	878	17
H(20B)	4119	2093	912	17
H(21A)	5679	3167	268	26
H(21B)	4894	2829	-101	26
H(22A)	4474	4065	-46	33
H(22B)	3609	3473	336	33
H(23A)	3920	4286	994	26
H(23B)	5065	4081	960	26
H(24A)	3463	3056	1628	19
H(24B)	4269	3390	1987	19
H(25)	4412	2562	3010	16
H(26A)	6491	2434	2695	22
H(26B)	5845	3123	2351	22
H(27A)	6703	3424	3194	24
H(27B)	5532	3480	3349	24
H(28A)	6675	2234	3964	25
H(28B)	6187	2834	4325	25
H(29A)	4587	2421	4213	28
H(29B)	5180	1720	4597	28

H(30A)	5530	1323	3619	24
H(30B)	4359	1388	3766	24
H(31)	5418	973	1713	16
H(32A)	6681	1901	1615	26
H(32B)	6902	1514	2357	26
H(33A)	7144	798	1289	31
H(33B)	8038	1078	1612	31
H(34A)	7602	173	2613	28
H(34B)	7751	-240	2029	28
H(35A)	6280	-690	2745	25
H(35B)	6034	-326	2005	25
H(36A)	5798	409	3055	22
H(36B)	4908	112	2740	22
H(40)	4054	253	321	44
H(41)	4122	-639	-289	54
H(42)	3755	-1889	235	64
H(43)	3251	-2244	1363	62
H(44)	3150	-1385	1983	48
H(47A)	1534	2163	4456	72
H(47B)	1853	2974	3979	72
H(47C)	2649	2472	4391	72
H(49A)	4372	-894	4336	37
H(49B)	3922	-381	4797	37
H(49C)	4968	-157	4364	37
H(50)	5795	5951	1765	18
H(51A)	5863	5109	2808	24
H(51B)	4845	5421	3075	24
H(52A)	5069	4669	2031	27
H(52B)	4497	4321	2751	27
H(53A)	3253	5203	2535	30
H(53B)	3367	4769	1964	30
H(54A)	3273	6092	1507	32
H(54B)	4299	5784	1245	32
H(55A)	4626	6896	1564	32
H(55B)	4060	6546	2285	32
H(56)	6278	7557	3060	17
H(57A)	6125	6373	3825	22
H(57B)	4997	6297	3691	22
H(58A)	5052	6734	4658	24
H(58B)	5749	7435	4246	24
H(59A)	4109	7834	4374	26
H(59B)	3732	7209	4041	26
H(60A)	3917	8380	3234	24
H(60B)	5042	8464	3370	24
H(61A)	5025	8061	2403	25
H(61B)	4301	7364	2783	25
H(62)	5708	7723	1567	17
H(63A)	6711	8391	2058	21
H(63B)	7689	8072	1745	21
H(64A)	7445	9293	1092	29
H(64B)	6344	9062	1000	29
H(65A)	7426	9049	39	32
H(65B)	8106	8454	477	32
H(66A)	7064	7824	-36	28
H(66B)	6111	8167	282	28
H(67A)	6246	6928	922	21
H(67B)	7379	7076	1005	21
H(68)	10128	6277	3466	18

H(69A)	10761	6984	2115	25
H(69B)	9807	7213	2528	25
H(70A)	11196	8016	2504	25
H(70B)	10799	7578	3246	25
H(71A)	12517	7201	2499	25
H(71B)	12524	7535	3130	25
H(72A)	11789	6437	3826	26
H(72B)	12746	6215	3414	26
H(73A)	11374	5397	3452	21
H(73B)	11762	5830	2706	21
H(74)	9504	4863	2050	20
H(75A)	10955	6041	1584	32
H(75B)	9842	6092	1396	32
H(76A)	10904	5765	546	39
H(76B)	10108	5097	874	39
H(77A)	11709	4590	770	36
H(77B)	12114	5108	1196	36
H(78A)	11759	3896	1870	33
H(78B)	10648	3938	1680	33
H(79A)	11463	4839	2440	21
H(79B)	10647	4177	2730	21
H(80)	10136	4565	3587	19
H(81A)	8465	5143	4216	26
H(81B)	9595	5353	4257	26
H(82A)	8946	4397	5220	40
H(82B)	9880	4105	4836	40
H(83A)	8619	3159	5109	42
H(83B)	7845	3741	4756	42
H(84A)	8402	3001	4051	31
H(84B)	9530	3214	4094	31
H(85A)	8119	4242	3465	19
H(85B)	9057	3945	3088	19
H(89)	8262	3689	1914	40
H(90)	8254	2858	1259	49
H(91)	7617	3179	264	56
H(92)	6889	4345	-82	46
H(93)	6906	5203	549	43
H(96A)	7587	7559	4419	77
H(96B)	8615	7952	4053	77
H(96C)	8602	7143	4570	77
H(96D)	8949	7544	4276	77
H(96E)	7921	7151	4642	77
H(96F)	7934	7959	4125	77
H(98A)	5282	4750	4362	42
H(98B)	6139	4628	4840	42
H(98C)	5992	4050	4404	42
H(99A)	-490	6171	-240	149
H(99B)	-1535	6523	-414	149
H(99C)	-1230	6389	320	149
H(10C)	-257	7450	-806	119
H(10D)	-1019	7675	-259	119
H(10E)	37	8361	72	119
H(10F)	939	8250	-447	119
H(10G)	927	7977	941	149
H(10H)	1716	8475	380	149
H(10I)	1722	7577	538	149

Table S6. Torsion angles [°] for **5**.

C(45)-Ru(1)-P(1)-C(1)	-179.5(2)	C(86)-Ru(2)-P(4)-C(68)	153.3(2)
C(37)-Ru(1)-P(1)-C(1)	92.9(2)	N(3)-Ru(2)-P(4)-C(68)	-31.29(19)
N(1)-Ru(1)-P(1)-C(1)	-82.23(19)	N(4)-Ru(2)-P(4)-C(68)	-116.37(19)
N(2)-Ru(1)-P(1)-C(1)	2.06(18)	P(3)-Ru(2)-P(4)-C(68)	138.8(9)
P(2)-Ru(1)-P(1)-C(1)	66(2)	C(45)-Ru(1)-N(1)-C(46)	167(3)
C(45)-Ru(1)-P(1)-C(13)	-65.2(2)	C(37)-Ru(1)-N(1)-C(46)	8(4)
C(37)-Ru(1)-P(1)-C(13)	-152.8(2)	N(2)-Ru(1)-N(1)-C(46)	-14(3)
N(1)-Ru(1)-P(1)-C(13)	32.02(18)	P(1)-Ru(1)-N(1)-C(46)	77(3)
N(2)-Ru(1)-P(1)-C(13)	116.31(17)	P(2)-Ru(1)-N(1)-C(46)	-102(3)
P(2)-Ru(1)-P(1)-C(13)	-179(100)	C(45)-Ru(1)-N(2)-C(48)	57(7)
C(45)-Ru(1)-P(1)-C(7)	61.4(2)	C(37)-Ru(1)-N(2)-C(48)	97(3)
C(37)-Ru(1)-P(1)-C(7)	-26.2(2)	N(1)-Ru(1)-N(2)-C(48)	-85(3)
N(1)-Ru(1)-P(1)-C(7)	158.67(19)	P(1)-Ru(1)-N(2)-C(48)	-175(3)
N(2)-Ru(1)-P(1)-C(7)	-117.03(18)	P(2)-Ru(1)-N(2)-C(48)	6(3)
P(2)-Ru(1)-P(1)-C(7)	-53(2)	C(94)-Ru(2)-N(3)-C(95)	-170(3)
C(45)-Ru(1)-P(2)-C(19)	0.9(2)	C(86)-Ru(2)-N(3)-C(95)	-6(4)
C(37)-Ru(1)-P(2)-C(19)	88.5(2)	N(4)-Ru(2)-N(3)-C(95)	11(3)
N(1)-Ru(1)-P(2)-C(19)	-96.37(18)	P(4)-Ru(2)-N(3)-C(95)	-82(3)
N(2)-Ru(1)-P(2)-C(19)	179.36(18)	P(3)-Ru(2)-N(3)-C(95)	99(3)
P(1)-Ru(1)-P(2)-C(19)	115(2)	C(94)-Ru(2)-N(4)-C(97)	-49(11)
C(45)-Ru(1)-P(2)-C(31)	-114.1(2)	C(86)-Ru(2)-N(4)-C(97)	-104(3)
C(37)-Ru(1)-P(2)-C(31)	-26.5(2)	N(3)-Ru(2)-N(4)-C(97)	78(3)
N(1)-Ru(1)-P(2)-C(31)	148.67(18)	P(4)-Ru(2)-N(4)-C(97)	169(3)
N(2)-Ru(1)-P(2)-C(31)	64.40(18)	P(3)-Ru(2)-N(4)-C(97)	-14(3)
P(1)-Ru(1)-P(2)-C(31)	0(2)	C(13)-P(1)-C(1)-C(2)	-57.1(4)
C(45)-Ru(1)-P(2)-C(25)	117.8(2)	C(7)-P(1)-C(1)-C(2)	-171.2(3)
C(37)-Ru(1)-P(2)-C(25)	-154.6(2)	Ru(1)-P(1)-C(1)-C(2)	62.9(3)
N(1)-Ru(1)-P(2)-C(25)	20.53(19)	C(13)-P(1)-C(1)-C(6)	175.0(3)
N(2)-Ru(1)-P(2)-C(25)	-63.74(18)	C(7)-P(1)-C(1)-C(6)	60.8(3)
P(1)-Ru(1)-P(2)-C(25)	-128(2)	Ru(1)-P(1)-C(1)-C(6)	-65.0(3)
C(94)-Ru(2)-P(3)-C(50)	115.4(2)	C(6)-C(1)-C(2)-C(3)	-54.7(5)
C(86)-Ru(2)-P(3)-C(50)	26.5(2)	P(1)-C(1)-C(2)-C(3)	177.6(3)
N(3)-Ru(2)-P(3)-C(50)	-148.92(19)	C(1)-C(2)-C(3)-C(4)	55.6(6)
N(4)-Ru(2)-P(3)-C(50)	-63.94(19)	C(2)-C(3)-C(4)-C(5)	-56.8(6)
P(4)-Ru(2)-P(3)-C(50)	41.0(9)	C(3)-C(4)-C(5)-C(6)	56.9(6)
C(94)-Ru(2)-P(3)-C(62)	0.4(2)	C(4)-C(5)-C(6)-C(1)	-55.5(5)
C(86)-Ru(2)-P(3)-C(62)	-88.6(2)	C(2)-C(1)-C(6)-C(5)	54.6(5)
N(3)-Ru(2)-P(3)-C(62)	96.00(18)	P(1)-C(1)-C(6)-C(5)	-176.4(3)
N(4)-Ru(2)-P(3)-C(62)	-179.02(18)	C(1)-P(1)-C(7)-C(12)	169.3(3)
P(4)-Ru(2)-P(3)-C(62)	-74.1(9)	C(13)-P(1)-C(7)-C(12)	62.7(4)
C(94)-Ru(2)-P(3)-C(56)	-115.6(2)	Ru(1)-P(1)-C(7)-C(12)	-64.1(4)
C(86)-Ru(2)-P(3)-C(56)	155.4(2)	C(1)-P(1)-C(7)-C(8)	39.6(4)
N(3)-Ru(2)-P(3)-C(56)	-19.97(19)	C(13)-P(1)-C(7)-C(8)	-67.0(4)
N(4)-Ru(2)-P(3)-C(56)	65.01(18)	Ru(1)-P(1)-C(7)-C(8)	166.1(3)
P(4)-Ru(2)-P(3)-C(56)	170.0(9)	C(12)-C(7)-C(8)-C(9)	54.1(5)
C(94)-Ru(2)-P(4)-C(80)	179.8(2)	P(1)-C(7)-C(8)-C(9)	-174.4(3)
C(86)-Ru(2)-P(4)-C(80)	-91.2(2)	C(7)-C(8)-C(9)-C(10)	-55.5(5)
N(3)-Ru(2)-P(4)-C(80)	84.20(19)	C(8)-C(9)-C(10)-C(11)	56.5(6)
N(4)-Ru(2)-P(4)-C(80)	-0.88(19)	C(9)-C(10)-C(11)-C(12)	-57.1(6)
P(3)-Ru(2)-P(4)-C(80)	-105.7(9)	C(8)-C(7)-C(12)-C(11)	-55.5(5)
C(94)-Ru(2)-P(4)-C(74)	-61.7(2)	P(1)-C(7)-C(12)-C(11)	171.4(3)
C(86)-Ru(2)-P(4)-C(74)	27.4(2)	C(10)-C(11)-C(12)-C(7)	57.8(6)
N(3)-Ru(2)-P(4)-C(74)	-157.25(19)	C(1)-P(1)-C(13)-C(14)	-57.5(4)
N(4)-Ru(2)-P(4)-C(74)	117.67(19)	C(7)-P(1)-C(13)-C(14)	50.0(4)
P(3)-Ru(2)-P(4)-C(74)	12.8(9)	Ru(1)-P(1)-C(13)-C(14)	179.0(3)
C(94)-Ru(2)-P(4)-C(68)	64.3(2)	C(1)-P(1)-C(13)-C(18)	171.9(3)

C(7)-P(1)-C(13)-C(18)	-80.6(4)	C(37)-C(38)-C(39)-C(40)	155(4)
Ru(1)-P(1)-C(13)-C(18)	48.4(4)	C(37)-C(38)-C(39)-C(44)	-23(4)
C(18)-C(13)-C(14)-C(15)	-56.9(5)	C(44)-C(39)-C(40)-C(41)	-0.8(9)
P(1)-C(13)-C(14)-C(15)	169.6(3)	C(38)-C(39)-C(40)-C(41)	-178.3(6)
C(13)-C(14)-C(15)-C(16)	56.7(5)	C(39)-C(40)-C(41)-C(42)	-0.6(10)
C(14)-C(15)-C(16)-C(17)	-55.1(5)	C(40)-C(41)-C(42)-C(43)	1.5(11)
C(15)-C(16)-C(17)-C(18)	55.4(5)	C(41)-C(42)-C(43)-C(44)	-1.0(11)
C(16)-C(17)-C(18)-C(13)	-56.4(5)	C(42)-C(43)-C(44)-C(39)	-0.4(10)
C(14)-C(13)-C(18)-C(17)	56.6(5)	C(40)-C(39)-C(44)-C(43)	1.3(9)
P(1)-C(13)-C(18)-C(17)	-169.8(3)	C(38)-C(39)-C(44)-C(43)	178.9(6)
C(31)-P(2)-C(19)-C(20)	55.2(4)	C(37)-Ru(1)-C(45)-O(1)	41(13)
C(25)-P(2)-C(19)-C(20)	170.7(3)	N(1)-Ru(1)-C(45)-O(1)	-137(13)
Ru(1)-P(2)-C(19)-C(20)	-65.5(3)	N(2)-Ru(1)-C(45)-O(1)	81(15)
C(31)-P(2)-C(19)-C(24)	-176.7(3)	P(1)-Ru(1)-C(45)-O(1)	-47(13)
C(25)-P(2)-C(19)-C(24)	-61.2(3)	P(2)-Ru(1)-C(45)-O(1)	132(13)
Ru(1)-P(2)-C(19)-C(24)	62.6(3)	Ru(1)-N(1)-C(46)-C(47)	9(18)
C(24)-C(19)-C(20)-C(21)	52.9(5)	Ru(1)-N(2)-C(48)-C(49)	-26(12)
P(2)-C(19)-C(20)-C(21)	-178.8(3)	C(62)-P(3)-C(50)-C(55)	-50.2(4)
C(19)-C(20)-C(21)-C(22)	-54.7(5)	C(56)-P(3)-C(50)-C(55)	57.2(4)
C(20)-C(21)-C(22)-C(23)	56.8(6)	Ru(2)-P(3)-C(50)-C(55)	-173.3(3)
C(21)-C(22)-C(23)-C(24)	-57.0(6)	C(62)-P(3)-C(50)-C(51)	178.0(3)
C(22)-C(23)-C(24)-C(19)	55.4(5)	C(56)-P(3)-C(50)-C(51)	-74.7(4)
C(20)-C(19)-C(24)-C(23)	-53.6(5)	Ru(2)-P(3)-C(50)-C(51)	54.9(4)
P(2)-C(19)-C(24)-C(23)	177.4(3)	C(55)-C(50)-C(51)-C(52)	55.5(5)
C(19)-P(2)-C(25)-C(30)	-173.0(3)	P(3)-C(50)-C(51)-C(52)	-169.7(3)
C(31)-P(2)-C(25)-C(30)	-66.0(4)	C(50)-C(51)-C(52)-C(53)	-56.2(6)
Ru(1)-P(2)-C(25)-C(30)	61.9(4)	C(51)-C(52)-C(53)-C(54)	56.3(6)
C(19)-P(2)-C(25)-C(26)	-43.0(4)	C(52)-C(53)-C(54)-C(55)	-56.0(6)
C(31)-P(2)-C(25)-C(26)	64.1(4)	C(51)-C(50)-C(55)-C(54)	-56.2(6)
Ru(1)-P(2)-C(25)-C(26)	-168.1(3)	P(3)-C(50)-C(55)-C(54)	169.6(4)
C(30)-C(25)-C(26)-C(27)	-52.2(5)	C(53)-C(54)-C(55)-C(50)	56.7(6)
P(2)-C(25)-C(26)-C(27)	176.0(3)	C(50)-P(3)-C(56)-C(57)	68.8(4)
C(25)-C(26)-C(27)-C(28)	54.9(5)	C(62)-P(3)-C(56)-C(57)	176.0(3)
C(26)-C(27)-C(28)-C(29)	-57.4(5)	Ru(2)-P(3)-C(56)-C(57)	-60.3(4)
C(27)-C(28)-C(29)-C(30)	58.1(5)	C(50)-P(3)-C(56)-C(61)	-60.8(4)
C(26)-C(25)-C(30)-C(29)	53.8(5)	C(62)-P(3)-C(56)-C(61)	46.4(4)
P(2)-C(25)-C(30)-C(29)	-173.4(3)	Ru(2)-P(3)-C(56)-C(61)	170.1(3)
C(28)-C(29)-C(30)-C(25)	-57.6(5)	C(61)-C(56)-C(57)-C(58)	-55.2(5)
C(19)-P(2)-C(31)-C(36)	-176.2(3)	P(3)-C(56)-C(57)-C(58)	172.0(3)
C(25)-P(2)-C(31)-C(36)	76.7(4)	C(56)-C(57)-C(58)-C(59)	58.5(5)
Ru(1)-P(2)-C(31)-C(36)	-52.4(4)	C(57)-C(58)-C(59)-C(60)	-57.9(5)
C(19)-P(2)-C(31)-C(32)	55.2(4)	C(58)-C(59)-C(60)-C(61)	56.8(5)
C(25)-P(2)-C(31)-C(32)	-51.9(4)	C(59)-C(60)-C(61)-C(56)	-55.8(5)
Ru(1)-P(2)-C(31)-C(32)	179.0(3)	C(57)-C(56)-C(61)-C(60)	54.5(5)
C(36)-C(31)-C(32)-C(33)	57.4(5)	P(3)-C(56)-C(61)-C(60)	-173.8(3)
P(2)-C(31)-C(32)-C(33)	-170.6(3)	C(50)-P(3)-C(62)-C(67)	-56.8(4)
C(31)-C(32)-C(33)-C(34)	-57.8(6)	C(56)-P(3)-C(62)-C(67)	-172.6(3)
C(32)-C(33)-C(34)-C(35)	56.2(6)	Ru(2)-P(3)-C(62)-C(67)	64.7(3)
C(33)-C(34)-C(35)-C(36)	-55.6(5)	C(50)-P(3)-C(62)-C(63)	173.6(3)
C(34)-C(35)-C(36)-C(31)	56.9(5)	C(56)-P(3)-C(62)-C(63)	57.9(4)
C(32)-C(31)-C(36)-C(35)	-57.1(5)	Ru(2)-P(3)-C(62)-C(63)	-64.9(3)
P(2)-C(31)-C(36)-C(35)	170.9(3)	C(67)-C(62)-C(63)-C(64)	52.2(5)
C(45)-Ru(1)-C(37)-C(38)	-15(3)	P(3)-C(62)-C(63)-C(64)	-178.4(3)
N(1)-Ru(1)-C(37)-C(38)	145(3)	C(62)-C(63)-C(64)-C(65)	-56.0(5)
N(2)-Ru(1)-C(37)-C(38)	167(3)	C(63)-C(64)-C(65)-C(66)	59.3(6)
P(1)-Ru(1)-C(37)-C(38)	75(3)	C(64)-C(65)-C(66)-C(67)	-57.7(6)
P(2)-Ru(1)-C(37)-C(38)	-106(3)	C(63)-C(62)-C(67)-C(66)	-50.1(5)
Ru(1)-C(37)-C(38)-C(39)	-105(5)	P(3)-C(62)-C(67)-C(66)	-179.5(3)

C(65)-C(66)-C(67)-C(62)	52.9(5)	C(87)-C(88)-C(93)-C(92)	179.7(5)
C(80)-P(4)-C(68)-C(69)	-170.0(3)	C(86)-Ru(2)-C(94)-O(2)	-169(100)
C(74)-P(4)-C(68)-C(69)	82.3(4)	N(3)-Ru(2)-C(94)-O(2)	10(29)
Ru(2)-P(4)-C(68)-C(69)	-46.2(4)	N(4)-Ru(2)-C(94)-O(2)	137(25)
C(80)-P(4)-C(68)-C(73)	59.4(4)	P(4)-Ru(2)-C(94)-O(2)	-81(29)
C(74)-P(4)-C(68)-C(73)	-48.3(4)	P(3)-Ru(2)-C(94)-O(2)	102(29)
Ru(2)-P(4)-C(68)-C(73)	-176.8(3)	Ru(2)-N(3)-C(95)-C(96)	3(36)
C(73)-C(68)-C(69)-C(70)	-54.9(5)	Ru(2)-N(4)-C(97)-C(98)	40(11)
P(4)-C(68)-C(69)-C(70)	172.0(3)	C(101)-O(3)-C(100)-C(99)	-169.2(8)
C(68)-C(69)-C(70)-C(71)	55.6(5)	C(100)-O(3)-C(101)-C(102)	171.0(8)
C(69)-C(70)-C(71)-C(72)	-55.0(6)		
C(70)-C(71)-C(72)-C(73)	54.5(5)		
C(71)-C(72)-C(73)-C(68)	-55.5(5)		
C(69)-C(68)-C(73)-C(72)	55.2(5)		
P(4)-C(68)-C(73)-C(72)	-172.2(3)		
C(80)-P(4)-C(74)-C(75)	-167.2(4)		
C(68)-P(4)-C(74)-C(75)	-60.0(4)		
Ru(2)-P(4)-C(74)-C(75)	66.9(4)		
C(80)-P(4)-C(74)-C(79)	-37.8(4)		
C(68)-P(4)-C(74)-C(79)	69.4(4)		
Ru(2)-P(4)-C(74)-C(79)	-163.7(3)		
C(79)-C(74)-C(75)-C(76)	56.3(6)		
P(4)-C(74)-C(75)-C(76)	-170.7(4)		
C(74)-C(75)-C(76)-C(77)	-58.9(6)		
C(75)-C(76)-C(77)-C(78)	58.9(6)		
C(76)-C(77)-C(78)-C(79)	-57.8(6)		
C(77)-C(78)-C(79)-C(74)	56.1(6)		
C(75)-C(74)-C(79)-C(78)	-54.4(5)		
P(4)-C(74)-C(79)-C(78)	174.3(3)		
C(74)-P(4)-C(80)-C(81)	171.6(3)		
C(68)-P(4)-C(80)-C(81)	57.9(4)		
Ru(2)-P(4)-C(80)-C(81)	-63.2(4)		
C(74)-P(4)-C(80)-C(85)	-60.7(4)		
C(68)-P(4)-C(80)-C(85)	-174.3(3)		
Ru(2)-P(4)-C(80)-C(85)	64.5(3)		
C(85)-C(80)-C(81)-C(82)	55.3(5)		
P(4)-C(80)-C(81)-C(82)	-176.6(4)		
C(80)-C(81)-C(82)-C(83)	-55.3(6)		
C(81)-C(82)-C(83)-C(84)	55.8(7)		
C(82)-C(83)-C(84)-C(85)	-55.8(6)		
C(83)-C(84)-C(85)-C(80)	55.2(6)		
C(81)-C(80)-C(85)-C(84)	-55.1(5)		
P(4)-C(80)-C(85)-C(84)	176.1(3)		
C(94)-Ru(2)-C(86)-C(87)	51(12)		
N(3)-Ru(2)-C(86)-C(87)	-114(12)		
N(4)-Ru(2)-C(86)-C(87)	-130(12)		
P(4)-Ru(2)-C(86)-C(87)	-38(12)		
P(3)-Ru(2)-C(86)-C(87)	142(12)		
Ru(2)-C(86)-C(87)-C(88)	32(18)		
C(86)-C(87)-C(88)-C(89)	42(7)		
C(86)-C(87)-C(88)-C(93)	-138(7)		
C(93)-C(88)-C(89)-C(90)	0.9(8)		
C(87)-C(88)-C(89)-C(90)	-179.1(5)		
C(88)-C(89)-C(90)-C(91)	0.0(9)		
C(89)-C(90)-C(91)-C(92)	-1.5(9)		
C(90)-C(91)-C(92)-C(93)	2.1(9)		
C(91)-C(92)-C(93)-C(88)	-1.2(9)		
C(89)-C(88)-C(93)-C(92)	-0.3(8)		