Supporting Information

Scope and Mechanistic Analysis for Chemoselective Hydrogenolysis of Carbonyl Compounds Catalyzed by a Cationic Ruthenium-Hydride Complex with Tunable Phenol Ligand

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1. General Information. All operations were carried out in a nitrogen-filled glove box or by using standard high vacuum and Schlenk techniques unless otherwise noted. Solvents were freshly distilled over appropriate drying reagents. Benzene, toluene, and hexanes were distilled from purple solutions of sodium and benzophenone, and dichloromethane was dried over calcium hydride prior to use. All organic substrates were received from commercial sources and were used without further purification. The ^{1}H, ^{2}H, ^{13}C and ^{31}P NMR spectra were recorded on a Varian 300 or 400 MHz FT-NMR spectrometer, and the data are reported as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad, app = apparent; coupling constant(s) in Hz; integration. FT-IR spectra were recorded on Perkin Elmer Spectrum 100 spectrometer. Mass spectra were recorded from Agilent 6850 GC-MS spectrometer with a HP-5 (5% phenylmethylpolysiloxane) column (30 m, 0.32 mm, 0.25 μm). High resolution mass spectra were obtained at the Mass Spectrometry Facility, Washington University, St. Louis, MO and at the Mass Spectrometry Facility, University of Wisconsin-Milwaukee, Milwaukee, WI. Elemental analyses were performed at the Midwest Microlab, Indianapolis, IN.

2. Experimental Procedure

General Procedure for the Catalytic Hydrogenolysis Reaction. Method A: In a glove box, a carbonyl substrate (1.0 mmol), complex **1** (18 mg, 3 mol %) and phenol (10 mg, 10 mol %) were dissolved in 1,4-dioxane (2 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and cooled in a liquid N_2 bath and evacuated *in vacuo*. {**Procedure for the In-situ Generation of the Cationic Ru-H Catalyst:** Complex **3** (17 mg, 1 mol %) and phenol (4 mg, 4 mol %) were dissolved in CH_2Cl_2 (1 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. $HBF_4{\cdot}OEt_2$ (7 μL, 4 mol %) was added under a stream of N_2 gas, and the mixture was stirred about 15 min at room temperature.} The tube was filled with H_2 (2 atm) via a vacuum line, and was stirred in an oil bath set at 110-130 °C for 8-16 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the solution was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the filtrate was analyzed by GC-MS. Analytically pure product was isolated by a simple column chromatography on silica gel (280-400 mesh, hexanes/EtOAc).

Method B: In a glove box, a carbonyl substrate (1.0 mmol), complex **1** (18 mg, 3 mol %) and phenol (10 mg, 10 mol %) were dissolved in 2-propanol/1,4-dioxane (2 mL, 1:1 v/v) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and stirred in an oil bath set at 130 °C for 8-16 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the solution was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the filtrate was analyzed by GC-MS. Analytically pure product was isolated by a simple column chromatography on silica gel (280-400 mesh, hexanes/EtOAc).

Ligand Screening and Optimization Study. In a glove box, 4-methoxyacetophenone (160 mg, 1.0 mmol), complex **1** (18 mg, 3 mol %) and ligand (10 mol %) were dissolved in 1,4-dioxane (2 mL) in a 25 mL

Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and was cooled in liquid N_2 bath. The tube was evacuated under a high vacuum, and was filled with H_2 (2 atm) via a vacuum line. The tube was stirred in an oil bath set at 130 °C for 12 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the solution was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the filtrate was analyzed by ^1H NMR.

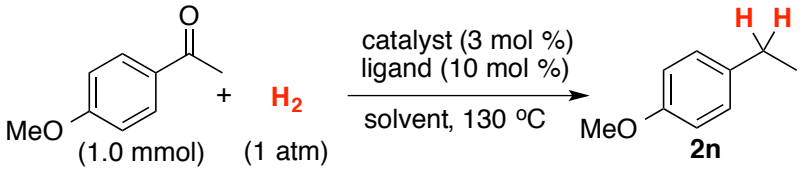
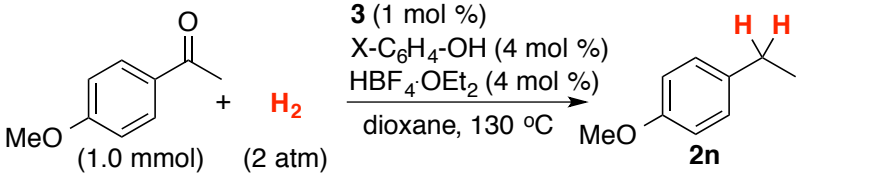


Table S1. Screening for the Hydrogenolysis Reaction of 4-Methoxyacetophenone.[a]

	catalyst	ligand	solvent	yield
1	**1**	phenol	dioxane	95
2	**1**	phenol	PhCl	89
3	**1**	aniline	PhCl	<5
4	**1**	2-NH_2PhCOMe	PhCl	35
5	**1**	benzamide	PhCl	<5
6	**1**	1,2-catechol	toluene	73
7	**1**	1,1'-BINOL	toluene	54
8	**1**	1,2-$C_6H_4(NH_2)_2$	toluene	<5
9	**3**	phenol	dioxane	<5
10	**3**/$HBF_4{\cdot}OEt_2$	phenol	dioxane	95
11	$[Ru(cod)Cl_2]_x$	phenol	dioxane	0
12	$RuCl_3{\cdot}3H_2O$	phenol	dioxane	0
13	$Ru_3(CO)_{12}$	phenol	dioxane	0
14	$(PPh_3)_3(CO)RuH_2$	phenol	dioxane	0
15	**1**	CH_3CO_2H	dioxane	<5
16	**1**	*p*-Me-$C_6H_4SO_3H$	dioxane	0
17	**1**	C_6H_5COOH	dioxane	0
18	$HBF_4{\cdot}OEt_2$	phenol	dioxane	0

[a] Reaction conditions: 4-methoxyacetophenone (1.0 mmol), solvent (2 mL), catalyst (3 mol %), ligand (10 mol %), H_2 (1 atm), 130 °C, 12 h. [b] The product yield was determined by ^1H NMR using methyl benzoate as an internal standard.



X = OMe, CH_3, Et, t-Bu, H, F, Cl, CF_3

3. Hammett Study. In a glove box, complex **3** (40 mg, 1 mol %) and *p*-X-C_6H_4OH (4 mol %) were dissolved in CH_2Cl_2 (2 mL) in 25 mL Schlenk tube equipped with a Teflon screw cap stopcock. The tube was brought out of the box, and $HBF_4 \cdot OEt_2$ (15 μL, 4 mol %) was added under N_2 stream. After the mixture was stirred 15 min at room temperature, the solvent was removed *in vacuo*. 4-Methoxyacetophenone (240 mg) was added, and the residue was dissolved in 1,4-dioxane (8 mL). The resulting solution was divided into four equal portions, and each portion was transferred into four separate 25 mL Schlenk tubes. The tubes were cooled in liquid N_2 bath, evacuated under high vacuum, and were filled with H_2 (1 atm) via a vacuum line. The tubes were stirred in an oil bath set at 130 °C. Each tube was taken out from the oil bath at 30 min intervals. The tube was cooled in ice-water bath, and the solvent was removed *in vacuo*. Methyl benzoate (10 mg, internal standard) in $CDCl_3$ (1 mL) was added, and the conversion of the product **2n** was analyzed by ^1H NMR. The reaction rate was measured by monitoring the appearance of the product signals on ^1H NMR, which was normalized against the internal standard peak. The k_{obs} was determined from a first-order plot of $-ln[(\text{4-methoxyacetophenone})_t/(\text{4-methoxyacetophenone})_0]$ vs time. The Hammett plot of $\log(k_X/k_H)$ vs σ_p is shown in Figure S1.

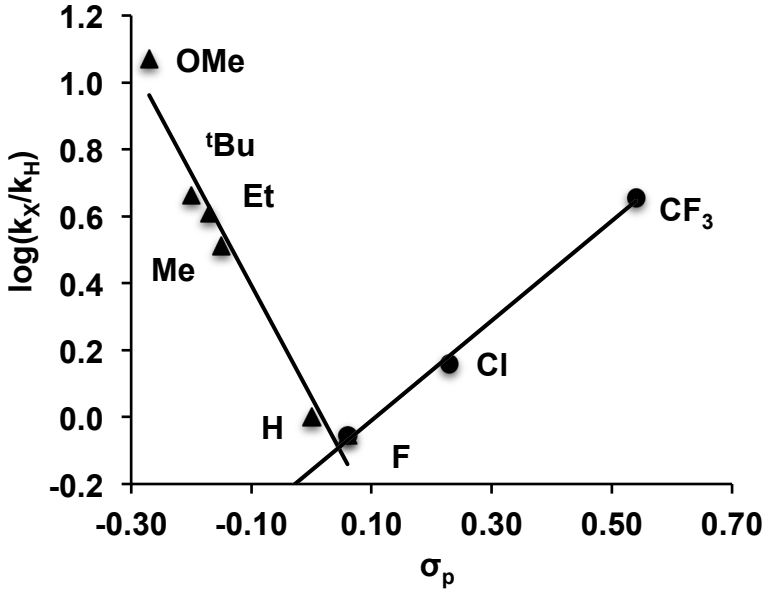


Figure S1. Hammett Plot of the Hydrogenolysis of 4-Methoxyacetophenone Catalyzed by **3**/$HBF_4 \cdot OEt_2$/*p*-X-C_6H_4OH (X = OMe, *t*-Bu, Me, Et, H, F, Cl, CF_3).

4. Deuterium Isotope Effect Study. In a glove box, **3** (50 mg, 1 mol %) and *p*-X-C_6H_4OH (4 mol %) (X = OMe, Et, F, Cl, CF_3) were dissolved in CH_2Cl_2 (2 mL) 25 mL Schlenk tubes equipped with a Teflon screw cap stopcock. The tubes were brought out of the box, and $HBF_4 \cdot OEt_2$ (20 μL, 4 mol %) was added under a N_2 stream. After the mixture was stirred for 15 min at room temperature, solvent was removed *in vacuo*. The tube was brought into the glove box, and 4-methoxyacetophenone (300 mg) was dissolved in dioxane (8 mL). The

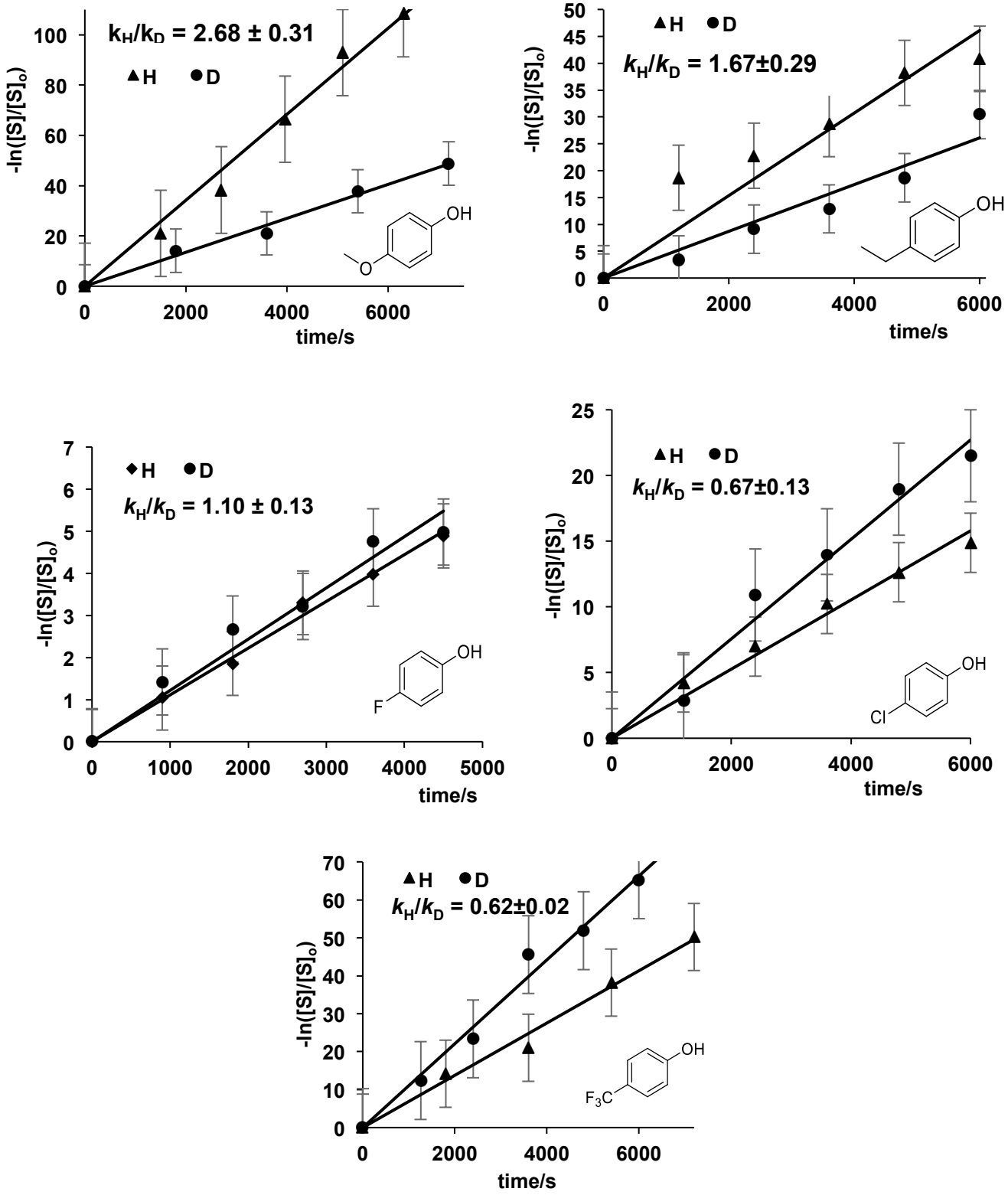


Figure S2. First Order Plots from the Hydrogenolysis Reaction of 4-Methoxyacetophenone with H_2 and D_2 Catalyzed by **3**/$HBF_4{\cdot}OEt_2$/*p*-X-C_6H_4OH (X = OMe, Et, Cl, F, CF_3).

resulting solution was divided into five equal portions, and each portion was placed into five separate 25 mL Schlenk tubes. The tubes were brought out of the glove box, cooled in liquid nitrogen bath, and was evacuated under high vacuum. The tubes were filled with H_2 or D_2 (2 atm) via a vacuum line, and were stirred in an oil bath set at 130 °C. Each tube was taken out from the oil bath in 30 min intervals, and was cooled to room temperature. After the solvent was removed *in vacuo*, methyl benzoate (10 mg, internal standard) dissolved in $CDCl_3$ (1 mL) was added, and the resulting solution was analyzed by ^1H and ^2H NMR. The reaction rate was measured by monitoring the appearance of the product signals on ^1H NMR, which were normalized against an internal standard (methyl benzoate). The k_{obs} was determined from a first-order plot of $-ln$[(4-methoxyacetophenone)$_t$/(4-methoxyacetophenone)$_0$] vs time. The k_H/k_D was calculated from the ratio of slope for each phenol ligands (Figure S2).

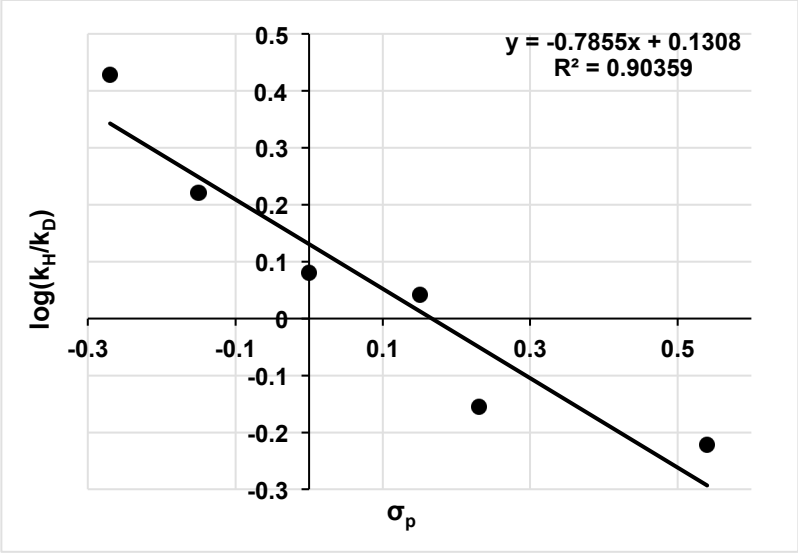
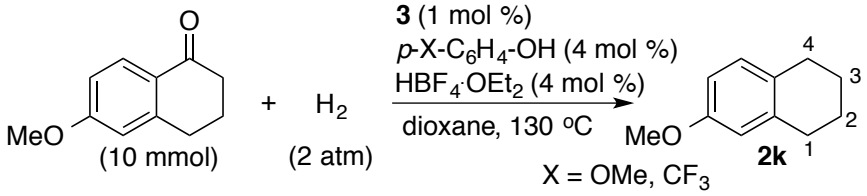


Figure S3. Plot of log(k_H/k_D) vs σ_p from the Hydrogenolysis Reaction of 4-Methoxyacetophenone with H_2 and D_2 Catalyzed by **3**/$HBF_4{\cdot}OEt_2$/*p*-X-C_6H_4OH (X = OMe, Et, Cl, F, CF_3).



5. Carbon Isotope Effect Study. In a glove box, **3** (400 mg, 1 mol %) and *p*-X-C_6H_4OH (4 mol %, X = OMe or CF_3) were dissolved in CH_2Cl_2 (5 mL) in a 100 mL Schlenk tube equipped with a Teflon screw cap stopcock. The tube was brought out of the box, and $HBF_4{\cdot}OEt_2$ (60 μL, 4 mol %) was added under a nitrogen stream. After the mixture was stirred for 15 min at room temperature, the solvent was removed *in vacuo*. After the tube was brought into the glove box, 6-methoxy-1-tetralone (1.76 g, 10 mmol) was added, and the mixture

was dissolved in dioxane (8 mL). The tube was brought out of the glove box, was cooled in liquid nitrogen, was evacuated under high vacuum, and was filled with H_2 (1 atm) via a vacuum line. The tube was stirred in an oil bath set at 130 °C for 2 h (2.5 h and 3 h for the repeated runs). The conversion was determined separately by GC after filtering a small sample of the crude mixture through a short silica gel column and eluting with CH_2Cl_2 (20 mL) (15, 18 and 20% conversions). The product **2k** was isolated by a column chromatography on silica gel (hexanes/Et_2O = 40:1). The experiment was repeated by using 1-(4-methoxyphenyl)ethanol.

The $^{13}C\{^1H\}$ NMR analysis of the isolated product **2k** was performed by following Singleton's NMR method (ref. 22 of the main text). The sample was prepared identically by dissolving 200 mg of the isolated **2k** in $CDCl_3$ (0.5 mL) in a 5 mm high precision NMR tube. The $^{13}C\{^1H\}$ NMR spectra were recorded with H-decoupling and 45 degree pulses. A 120 s delay between pulses was imposed to minimize T_1 variations (d1 = 120 s, at = 5.0 s, np = 245098, nt = 736). The data are summarized in Tables S2 and S3.

Table S2: Average ^{13}C Integration of the Product **2k** Obtained from 6-Methoxy-1-tetralone at High Conversion (Virgin, R_0; 95% conversion), at Low Conversion (R; avg 18% conversion) and the Calculated ^{13}C KIE using **3**/$HBF_4 \cdot OEt_2$/4-OMe-C_6H_4OH.

	OMe	**C1**	**C2**	**C3**	**C4**
R_0	1.0000	1.0051	0.9968	1.0000	1.0223
R1	1.0000	0.9991	0.9868	0.9999	0.9801
R2	1.0000	1.0050	0.9980	1.0006	0.9811
R3	1.0000	1.0050	0.9979	1.0005	0.9811
R	1.0000	1.0030	0.9942	1.0004	0.9807
R_0/R	1.0000	1.0021	1.0026	0.9996	**1.0424**

Table S3: Average ^{13}C Integration of the Product **2k** Obtained from 6-Methoxy-1-tetralone at High Conversion (Virgin , R_0; 95% conversion), at Low Conversion (R; avg 18% conversion) and the Calculated ^{13}C KIE using **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH.

	OMe	**C1**	**C2**	**C3**	**C4**
R_0	1.0000	1.0051	0.9968	1.0000	1.0223
R1	1.0000	0.9989	0.9972	0.9990	0.9615
R2	1.0000	0.9999	0.9969	0.9996	0.9617
R3	1.0000	0.9990	0.9970	0.9998	0.9627
R	1.0000	0.9993	0.9971	0.9995	0.9620
R_0/R	1.0000	1.0058	0.9997	1.0005	**1.0627**

6. Deuterium Labeling Study. In a glove box, complex **3** (17 mg, 1 mol %) and 4-methoxyphenol (8 mg, 4 mol %) were dissolved in CH_2Cl_2 (1 mL) in a 25 mL Schlenk tube equipped with a Teflon stopcock and a magnetic stirring bar. The tube was brought out of the glove box, and $HBF_4 \cdot OEt_2$ (7 μL, 4 mol %) was added via a syringe under a stream of N_2. After the mixture was stirred for 15 min at room temperature, the solvent was removed *in vacuo*. The tube was brought into the glove box, and 4-methoxyacetophenone (150 mg, 1.0 mmol) and dioxane (2 mL) were added. The tube was brought out of the glove box, was cooled in liquid nitrogen, and was evacuated under high vacuum. The tube was filled with D_2 (2 atm) via a vacuum line. The tube was stirred in an oil bath set at 130 °C for 4 h. The reaction tube was taken out of the oil bath, and was cooled to room temperature. After the tube was open to air, the crude product mixture was filtered through a short silica gel column by eluting with CH_2Cl_2 (10 mL), and the resulting solution was analyzed by GC-MS (50% conversion). The product was isolated by a simple column chromatography on silica gel (280-400 mesh, hexanes/EtOAc = 100:1). The products were analyzed by ^1H and ^2H NMR (Figure S4). The procedure was repeated for the hydrogenolysis of 1-(4-methoxyphenyl)ethanol with D_2 by using **3**/$HBF_4 \cdot OEt_2$/*p*-OMe-C_6H_4OH. The same procedure was used for the hydrogenolysis of 4-methoxyacetophenone and 1-(4-methoxyphenyl)ethanol with D_2 by using **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH (Figure S5).

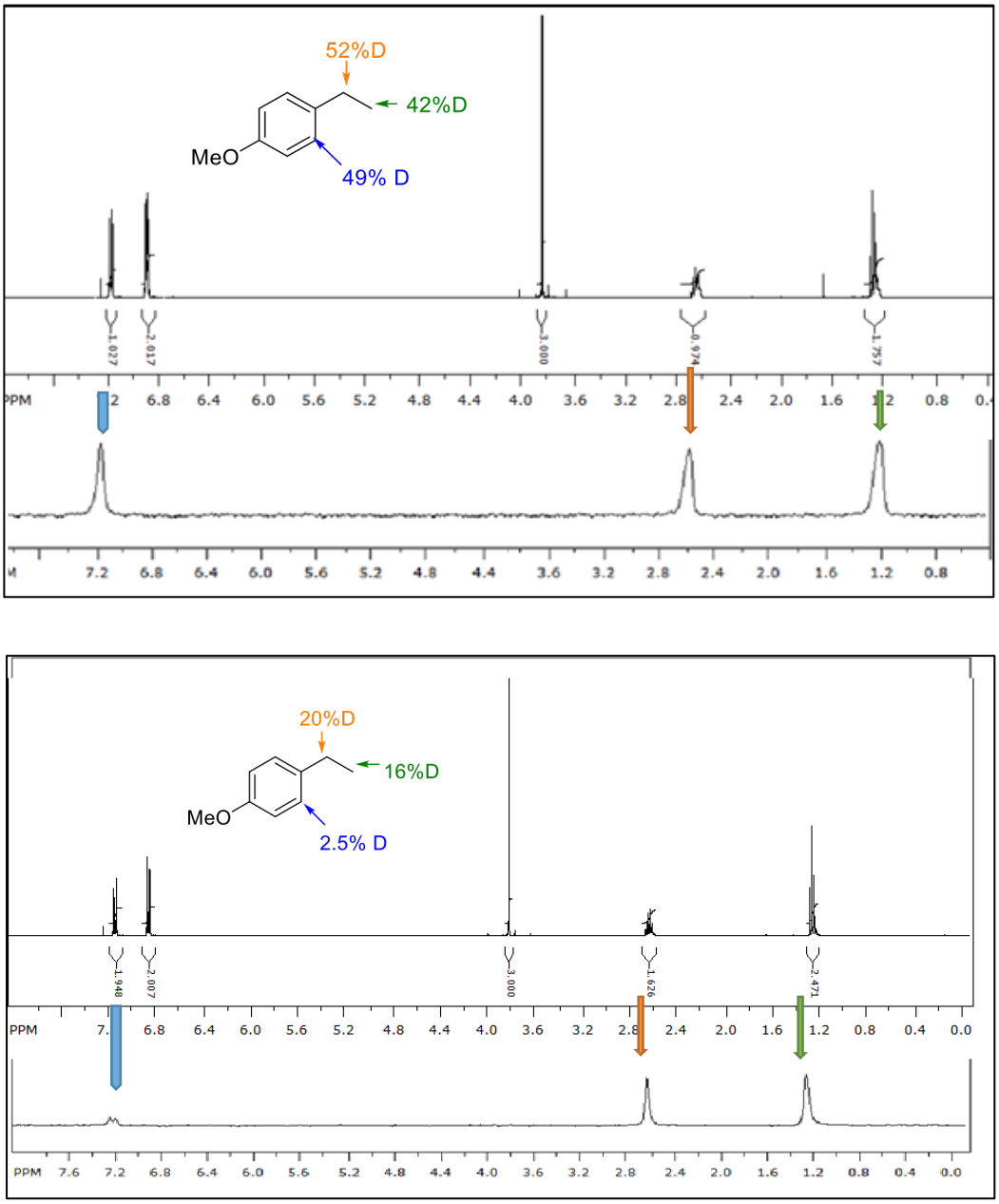


Figure S4. ^{1}H and ^{2}H NMR spectra for the Hydrogenolysis of 4-Methoxyacetophenone (Top) and 1-(4-Methoxyphenyl)ethanol (Bottom) with D_2 Catalyzed by **3**/$HBF_4 \cdot OEt_2$/*p*-OMe-C_6H_4OH.

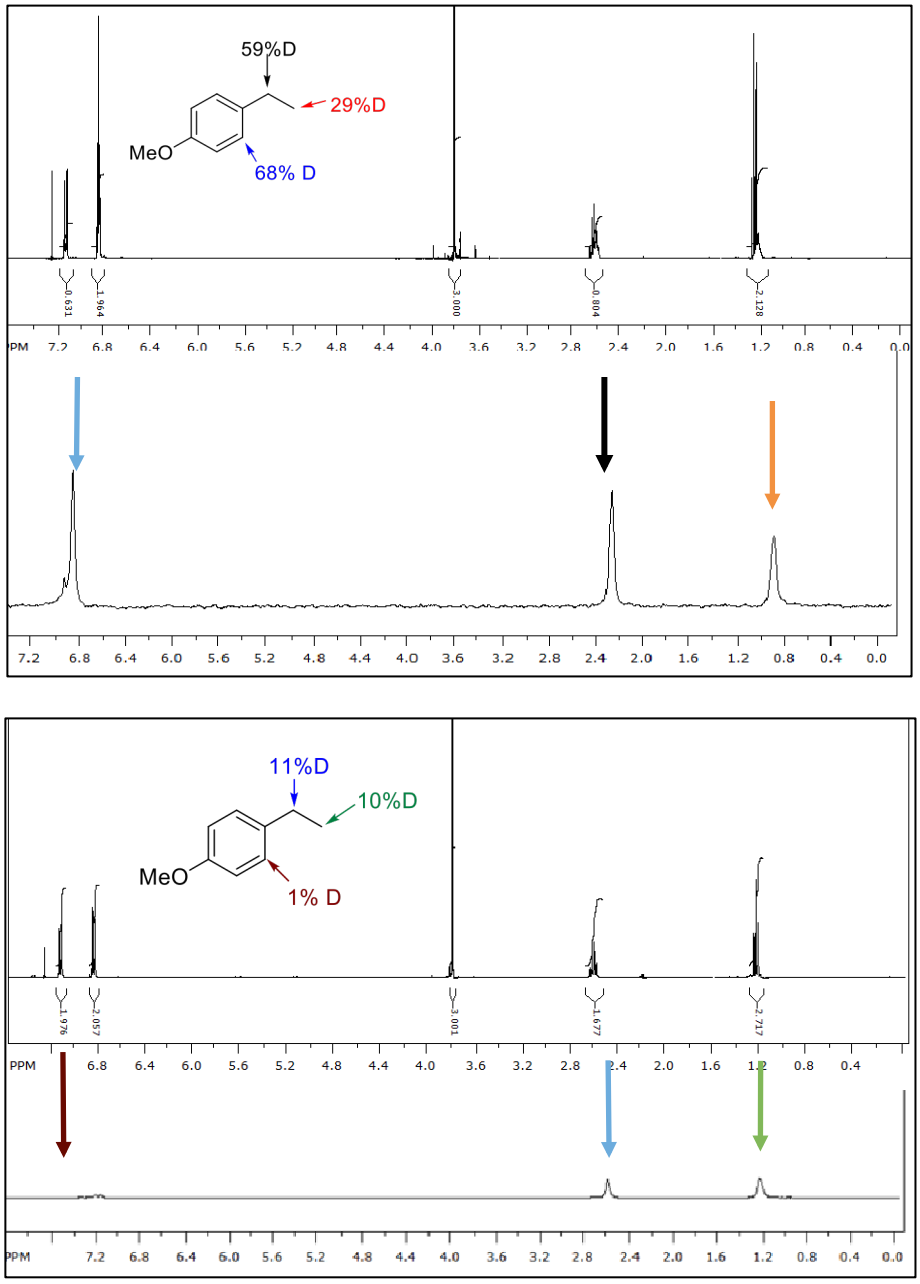


Figure S5. ^{1}H and ^{2}H NMR spectra for the Hydrogenolysis of 4-Methoxyacetophenone (Top) and 1-(4-Methoxyphenyl)ethanol (Bottom) with D_2 Catalyzed by **3**/$HBF_4{\cdot}OEt_2$/*p*-CF_3-C_6H_4OH.

7. Empirical Rate Measurements: Catalyst Concentration Dependence Study. In a glove box, Complex **3** (20 mg, 0.01 mmol) and *p*-OMe-C_6H_4OH (4 equiv, 0.04 mmol) were dissolved in CH_2Cl_2 (2.0 mL) in a 25 mL Schlenk tubes equipped with a Teflon screw cap stopcock. The tubes were brought out of the box, and $HBF_4{\cdot}OEt_2$ (15 µL, 0.04 mmol) was added under a nitrogen stream. The mixture was stirred for 15 min at room temperature, and the solvent was removed *in vacuo*. The tube was brought into the glove box, and 4-methoxyacetophenone (300 mg, 2 mmol) and 1,4-dioxane (4 mL) were added. The resulting solution was divided into equal portions, and each portion was transferred into four separate 25 mL Schlenk tubes. The tubes were brought out of the glove box, were cooled in liquid nitrogen bath, and was evacuated under high vacuum. Each tube was filled with H_2 (2 atm) via a high vacuum line, and was stirred in an oil bath set at 130 °C. Each

tube was taken out from the oil bath at 20 min intervals, was cooled in a liquid N_2 bath, and the solvent was removed *in vacuo*. Methyl benzoate (internal standard, 10 μL) in $CDCl_3$ (1 mL) was added, and the product conversion was analyzed by ^1H NMR. The reaction rate was measured by monitoring the appearance of the product signals on ^1H NMR, which was normalized against the internal standard peak. The initial rate of the reaction was determined from a first-order plot of [1-ethyl-4-methoxybenzene] vs time. This procedure was repeated for 5 different catalyst concentrations (0.011-0.034 mM) for the plot of initial rate vs [catalyst] (Figure S6). The same procedure was repeated by using **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH (Figure S7).

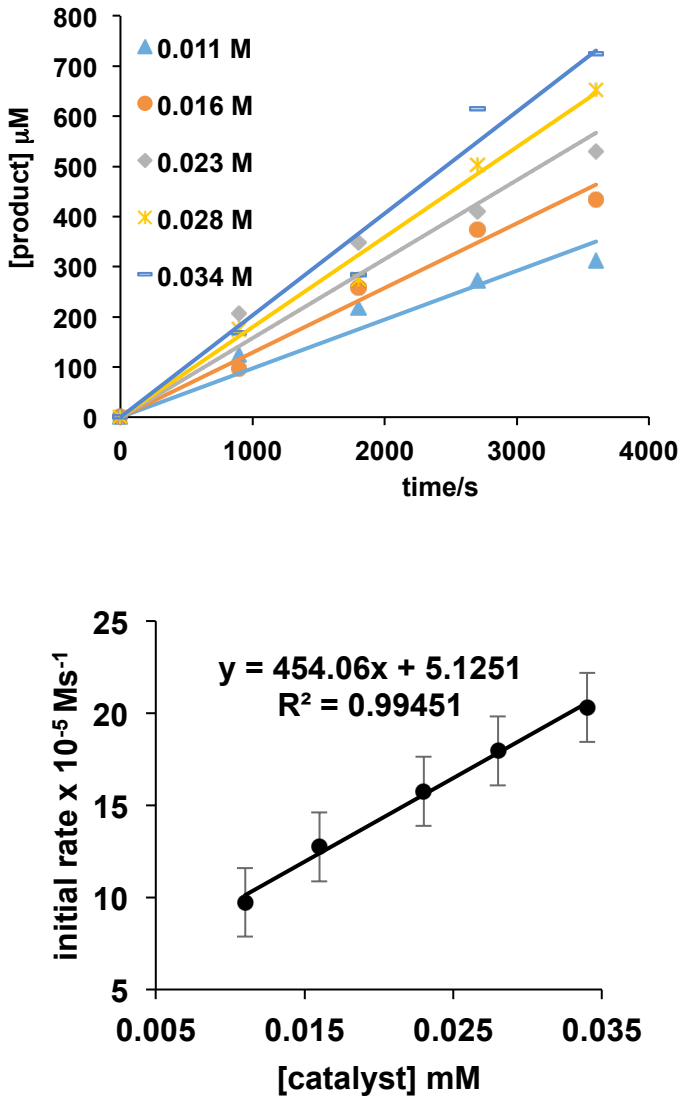


Figure S6. Plot of the Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs Catalyst Concentration (Bottom) by **3**/$HBF_4 \cdot OEt_2$/*p*-OMe-C_6H_4OH.

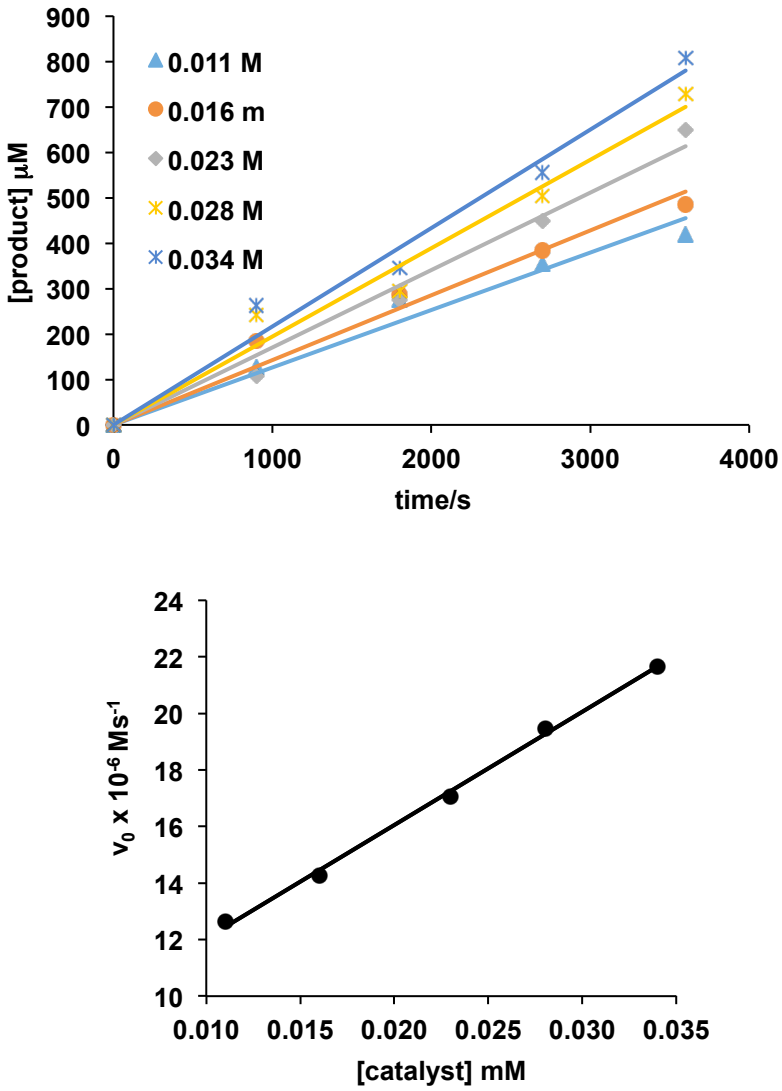


Figure S7. Plot of the Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs Catalyst Concentration (Bottom) by **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH.

Ketone Substrate Dependence Study. In a glove box, Complex **3** (20 mg, 0.01 mmol) and *p*-OMe-C_6H_4OH (4 equiv, 0.04 mmol) were dissolved in CH_2Cl_2 (2.0 mL) in a 25 mL Schlenk tubes equipped with a Teflon screw cap stopcock. The tubes were brought out of the box, and $HBF_4 \cdot OEt_2$ (15 µL, 0.04 mmol) was added under a nitrogen stream. The mixture was stirred for 15 min at room temperature, and the solvent was removed *in vacuo*. The tube was brought into the glove box, and 4-methoxyacetophenone (300 mg, 2 mmol) and 1,4-dioxane (4 mL) were added. The resulting solution was divided into equal portions, and each portion was transferred into four separate 25 mL Schlenk tubes. The tubes were brought out of the glove box, were cooled in liquid nitrogen bath, and were evacuated under high vacuum. Each tube was filled with H_2 (2 atm) via vacuum line, and was stirred in an oil bath set at 130 °C. Each tube was taken out from the oil bath at 20 min intervals, was cooled in a liquid N_2 bath, and the solvent was removed *in vacuo*. Methyl benzoate (internal standard, 10 µL) in $CDCl_3$ (1 mL) was added, and the product conversion was analyzed by ^1H NMR. The initial

rate of the reaction was determined from a first-order plot of [1-ethyl-4-methoxybenzene] vs time. This procedure was repeated at 5 different 4-methoxyacetophenone substrate concentrations (0.33 M-2.0 M) for the plot of initial rate vs [4-methoxyacetophenone] (Figure S8). The same procedure was used for **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH (Figure S9).

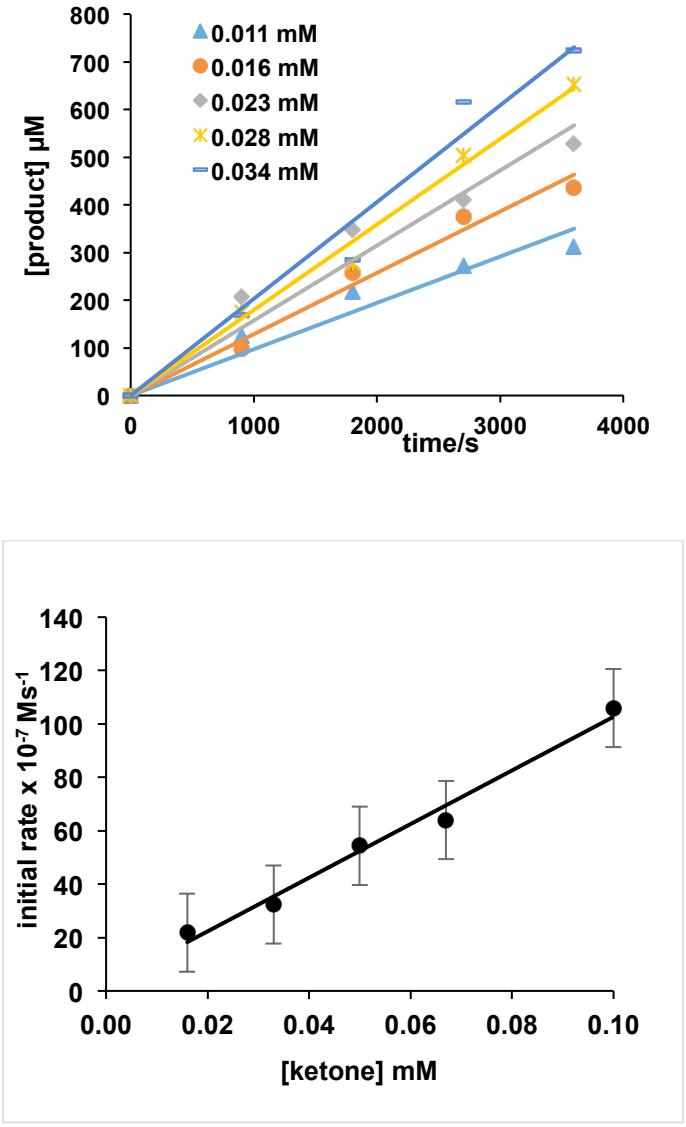


Figure S8. Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs [4-Methoxyacetophenone] (Bottom) Catalyzed by **3**/$HBF_4 \cdot OEt_2$/*p*-OMe-C_6H_4OH.

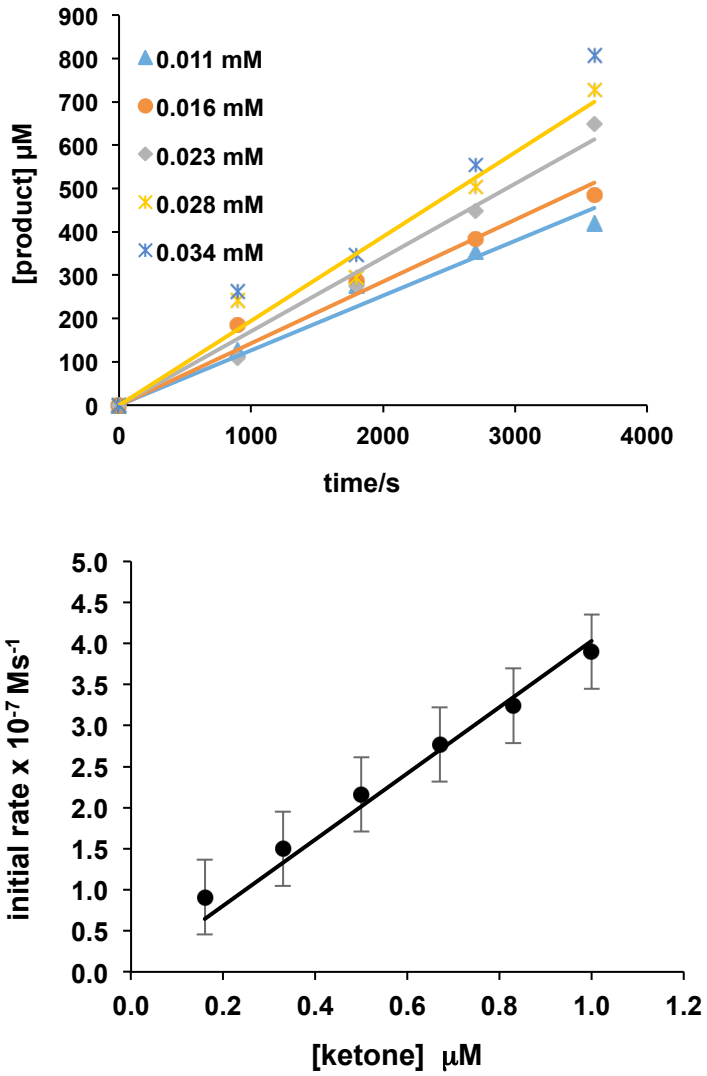
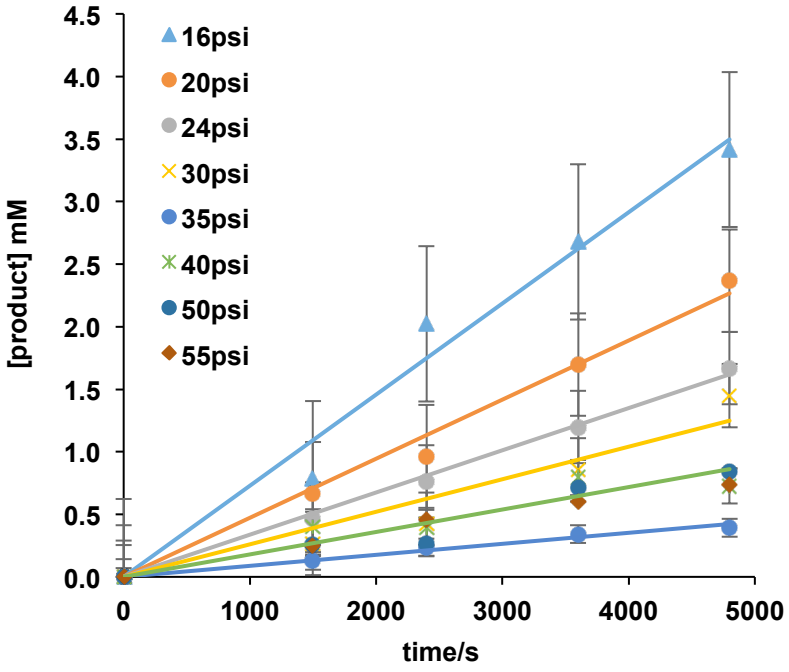


Figure S9. The Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs [4-Methoxyacetophenone] (Bottom) Catalyzed by **3**/$HBF_4{\cdot}OEt_2$/*p*-CF_3-C_6H_4OH.

Hydrogen Pressure Dependence Study. In a glove box, **3** (20 mg, 0.01 mol) and *p*-OMe-C_6H_4OH (4.0 equiv, 0.04 mmol) were dissolved in CH_2Cl_2 (2 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock. The tube was brought out of the box, and $HBF_4{\cdot}OEt_2$ (15 µL, 4 equiv) was added under a nitrogen stream. The resulting mixture was stirred about 15 min at room temperature, and the solvent was removed *in vacuo*. After 4-methoxyacetophenone (300 mg, 2.0 mmol) in 1,4-dioxane (4 mL) was added, the resulting solution was divided into four equal portions, and each portion was transferred into four separate 100 mL Fisher-Porter tubes. The tube was cooled in liquid nitrogen bath, and was evacuated under high vacuum. Each tube was filled with H_2 (1-5 atm). The tube was stirred in an oil bath set at 130 °C. Each tube was taken out from the oil bath at 20 min intervals, cooled in a liquid N_2 bath and the solvent was removed *in vacuo*. Methyl benzoate (10 µL, internal standard) in $CDCl_3$ (1 mL) was added, and the product conversion was analyzed by ^1H NMR. The same procedure was repeated at six different H_2 pressure (16-55 psi) for the plot of initial rate vs

H_2 pressure (Figure S10). The same procedure was repeated by using the catalyst **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH (Figure S11).



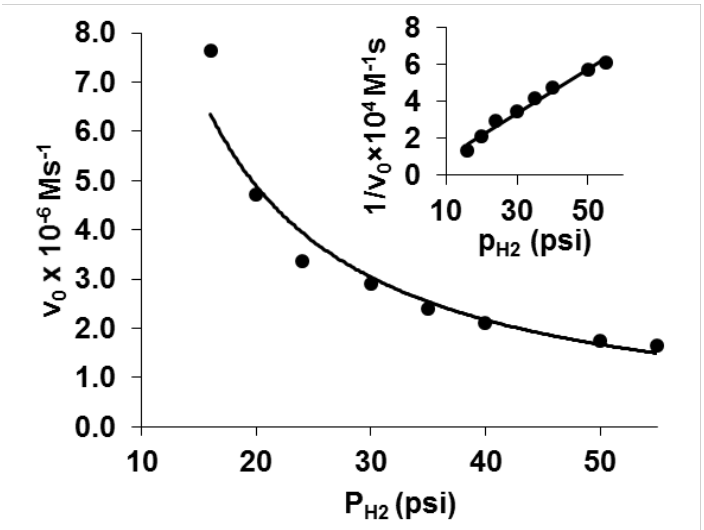


Figure S10. The Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs Hydrogen Pressure (Bottom) for the Reaction Catalyzed by **3**/$HBF_4 \cdot OEt_2$/*p*-OMe-C_6H_4OH. (Inset) Plot of $1/v_0$ vs P_{H2}.

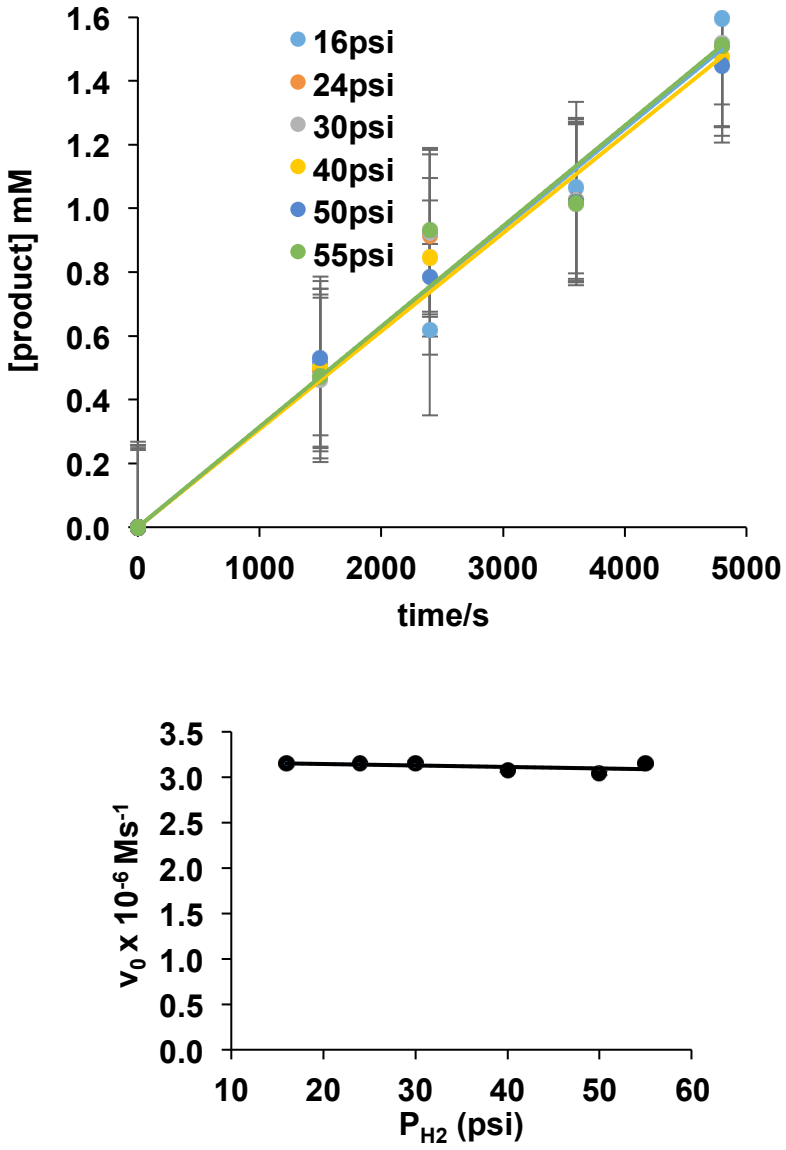


Figure S11. The Formation of 1-Ethyl-4-methoxybenzene vs Time (Top) and Initial Rate vs Hydrogen Pressure (Bottom) Catalyzed by **3**/$HBF_4 \cdot OEt_2$/*p*-CF_3-C_6H_4OH.

8. X-Ray Crystallographic Determination of 4a, 4b, 4c, 5 and 6.

For **4a**: Colorless single crystals of **4a** were grown in acetone/*n*-pentane at room temperature. A suitable crystal with the dimension of 0.2975 × 0.1164 × 0.0395 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 30380 reflection data were collected by using MoKα (λ = 0.71073) radiation while the crystal sample was cooled at 100.00(10 K) K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The molecular structure of **4a** is shown in Figure S12.

For **4b**: Colorless single crystals of **4b** were grown in acetone/*n*-pentane at room temperature. A suitable crystal with the dimension of 0.376 × 0.2569 × 0.1911 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 35933 reflection data were collected by using MoKα (λ = 0.71073) radiation while the crystal sample was cooled at 100.00(10 K) K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The molecular structure of **4b** is shown in Figure S13.

For **4c**: Colorless single crystals of **4c** were grown in acetone/*n*-pentane at room temperature. A suitable crystal with the dimension of 0.3138 × 0.2705 × 0.1982 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 30380 reflection data were collected by using CuKα (λ = 1.54184) radiation while the crystal sample was cooled at 100.00(10 K) K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The molecular structure of **4c** is shown in Figure S14.

For **5**: Colorless single crystals of **5** were grown in acetone/*n*-pentane at room temperature. A suitable crystal with the dimension of 0.6545 × 0.082 × 0.0667mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 32469 reflection data were collected by using MoKα (λ = 0.71073) radiation while the crystal sample was cooled at 100.00(10 K) K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The molecular structure of **5** is shown in Figure S15.

For **6**: Colorless single crystals of **6** were grown in acetone/*n*-pentane at room temperature. A suitable crystal with the dimension of 0.2265 × 0.1198 × 0.0692 mm^3 was selected and mounted on an Oxford SuperNova diffractometer equipped with dual microfocus Cu/Mo X-ray sources, X-ray mirror optics, and Atlas CCD area detector. A total of 22228 reflection data were collected by using MoKα (λ = 0.71073) radiation while the crystal sample was cooled at 100.00(10 K) K during the data collection. Using Olex2, the molecular structure was solved with the ShelXS structure solution program by using Direct Methods, and the data was refined with the XL refinement package using Least Squares minimization. The hydrogen atom of bridging OH group could not be located due to twining disorder of the data. The molecular structure of **6** is shown in Figure S16.

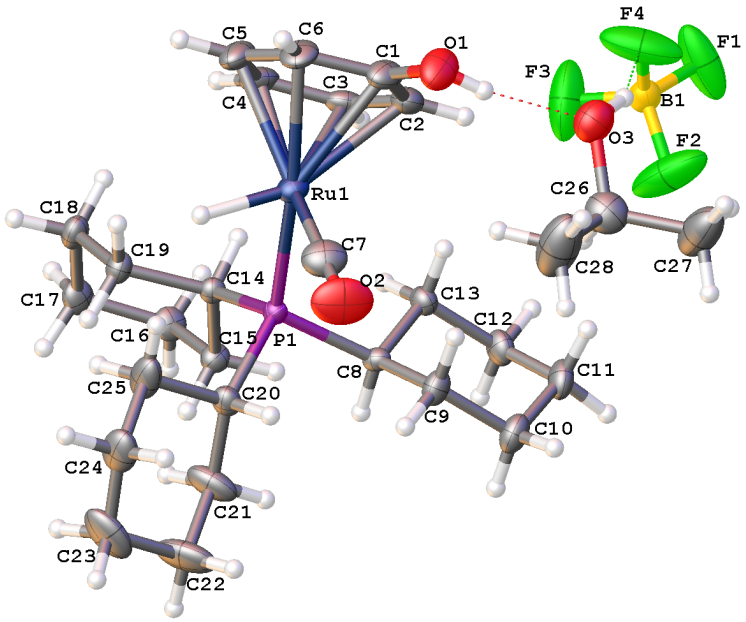


Figure S12. Molecular Structure of **4a.**

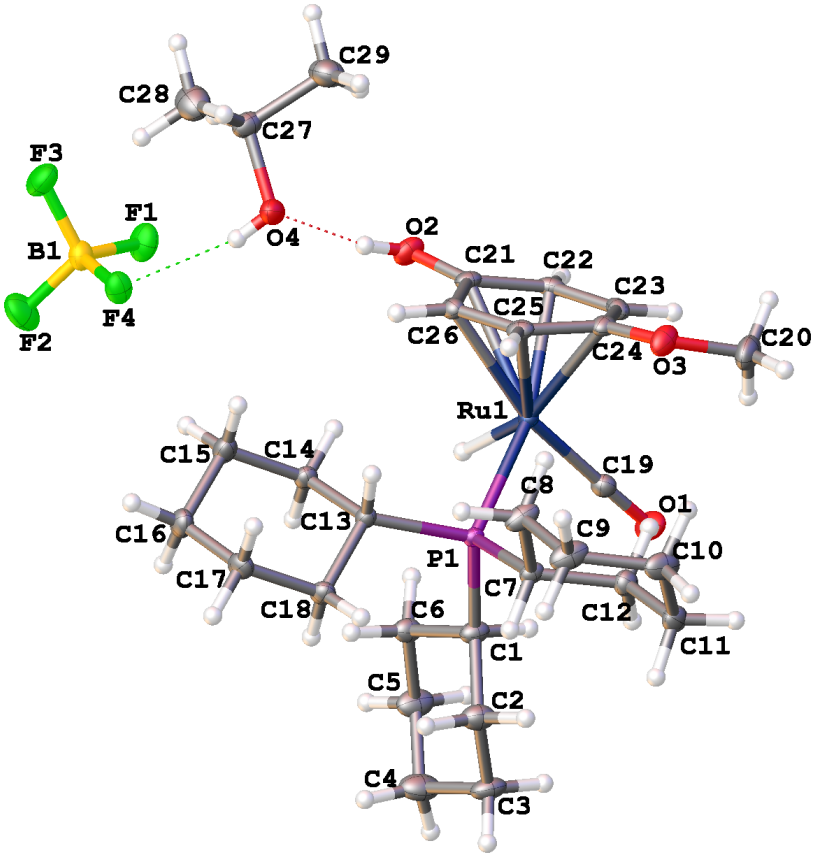


Figure S13. Molecular Structure of **4b**.

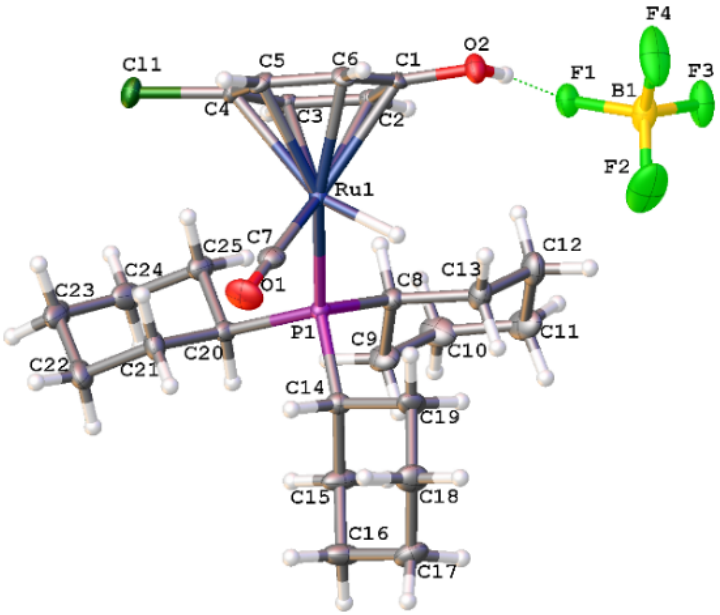


Figure S14. Molecular Structure of **4c**.

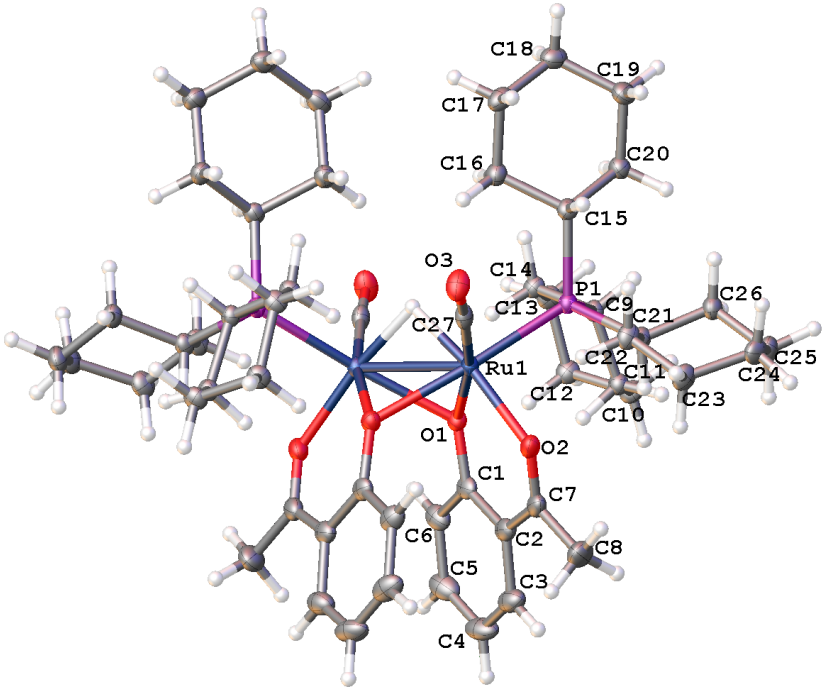


Figure S15. Molecular Structure of **5**.

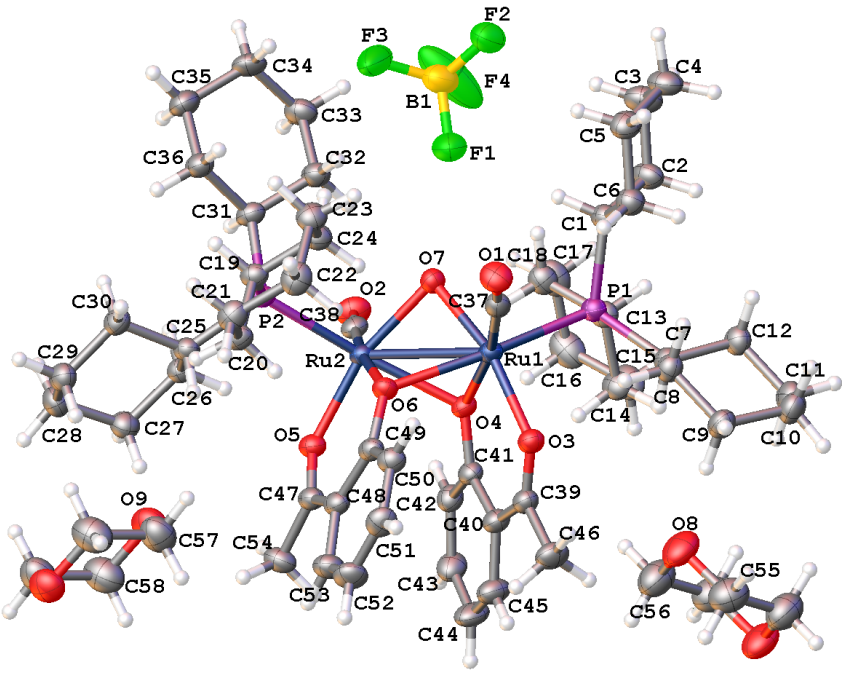
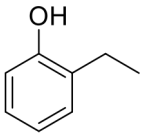


Figure S16. Molecular Structure of **6**.

9. Characterization Data of the Products.



2a

Table 2, compound 2a. Method A at 130 °C for 8 h. The product **2a** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). Yellow oil, Yield: 122 mg, 94 %. Data for **2a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 7.2 Hz, 1H), 7.83 (t, *J* = 7.9 Hz, 1H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 4.76 (br s, 1H), 2.75 (q, *J* = 7.2 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 129.4, 127.1, 121.0, 115.2, 23.0, 14.1 ppm; GC-MS *m/z* = 122 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S1]

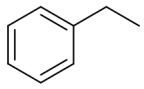
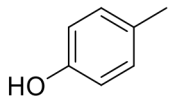
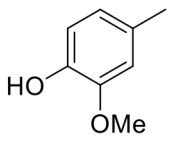

2b

Table 2, Compound 2b. Method A at 130 °C for 12 h. The product **2b** was isolated by a column chromatography on silica gel (hexanes). Colorless liquid, Yield: 101 mg, 79 %. Data for **2b**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.27 (m, 2H), 7.13-7.18 (m, 3H), 2.60-2.65 (q, 2H), 1.20-1.24 (t, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 144.4, 128.4, 128.0, 125.7, 29.0,16.0 ppm; GC-MS *m/z* = 128 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S2]



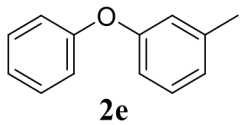
2c

Table 2, compound 2c. Method A at 130 °C for 12 h. The product **2c** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). While solid, Yield: 97 mg, 90 %. Data for **2c**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (d, *J* = 7.9 Hz, 2H), 6.72 (d, *J* = 7.9 Hz, 2H), 5.0 (br s, 1H), 2.31 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 153.2, 130.2, 130.1, 115.2, 20.6 ppm; GC-MS *m/z* = 108 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S3]



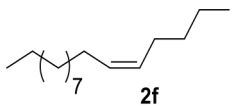
2d

Table 2, compound 2d. Method A at 130 °C for 12 h. The product **2d** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). White solid, Yield: 131 mg, 95 %. Data for **2d**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.85 (d, *J* = 7.4 Hz, 1H), 6.77-6.62 (m, 2H), 5.55 (s, 1H), 3.84 (s, 3H), 2.34 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 146.2, 143.3, 129.6, 121.5, 114.2, 111.7, 55.8, 21.0 ppm; GC-MS *m/z* = 138 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S4]



2e

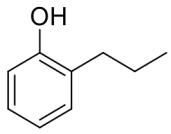
Table 2, compound 2e. Method A at 130 °C for 8 h. The product **2e** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). Colorless oil, Yield: 169 mg, 92 %. Data for **2e**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 8.5, 7.3 Hz, 2H), 7.21 (dd, *J* = 7.8, 7.6 Hz, 1H), 7.09 (t, *J* = 7.3 Hz, 1H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.83 (s, 1H), 6.81 (d, *J* = 7.8 Hz, 1H), 2.33 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) 157.6, 157.4, 140.2, 129.9, 129.7, 124.3, 123.3, 119.8, 119.1, 116.1, 21.6 ppm; GC-MS *m/z* = 184 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S5]



2f

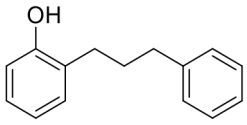
Table 2, compound 2f. Method A at 130 °C for 12 h. The product **2f** was isolated by a column chromatography on silica gel (hexanes). Colorless liquid, Yield: 161 mg, 72 %. Data for **2f**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.58-5.27 (m, 2H), 2.12-1.89 (m, 4H), 1.31-1.22 (m, 20H),

0.89 (t, J = 7.0 Hz, 6H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 130.4, 129.9, 77.4, 32.6, 32.3, 31.9, 31.6, 29.7, 29.7, 29.5, 29.4, 29.2, 29.2, 29.1, 22.7, 14.1 ppm; GC-MS m/z = 224 (M^+); ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.[S5]



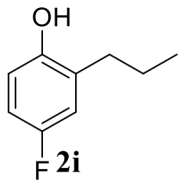
2g

Table 2, compound 2g. Method A at 130 °C for 8 h. The product **2g** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 10:1). Colorless liquid, Yield: 151 mg, 91 %. Data for **2g**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.84-7.24 (m, 4H), 5.73 (s, 1H), 2.71 (m, 2H), 1.70-1.82 (m, 2H), 1.08 (t, J = 9.0 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 154.0, 130.8, 129.2, 127.5, 115.8, 121.1, 32.5, 23.4, 14.5 ppm; GC-MS m/z = 136 (M^+); ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.[S6]



2h

Table 2, compound 2h. Method A at 130 °C for 8 h. The product **2h** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 20:1). White solid, Yield: 196 mg, 92 %. Data for **2h**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.28-7.19 (m, 3H), 7.38-7.28 (m, 2H), 7.19-7.09 (m, 2H), 6.95-6.87 (m, 1H), 6.77 (d, J = 8.2 Hz, 1H), 4.82 (s, 1H), 2.71 (dt, J = 15.7, 7.8 Hz, 4H), 2.00 (quintet, J = 7.8 Hz, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 153.4, 142.2, 130.1, 128.4, 128.3, 128.1, 127.1, 125.7, 120.7, 115.2, 35.5, 31.2, 29.4 ppm; GC-MS m/z = 212 (M^+); ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.[S7]



2i

Table 2, compound 2i. Method A at 130 °C for 8 h. The product **2i** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 20:1). Colorless liquid, Yield: 140 mg, 91 %. Data for **2i**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.86-6.67 (m, 3H), 5.18 (s, 1H), 2.53 (t, J = 7.7 Hz, 2H), 1.62 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 157.2 (d, $J_{C\text{-}F}$ = 236.0 Hz), 149.5, 130.3 (d, $J_{C\text{-}F}$ = 7.6 Hz), 116.4 (d, $J_{C\text{-}F}$ = 22.9 Hz), 115.7 (d, $J_{C\text{-}F}$ = 25.0 Hz), 112.9 (d, $J_{C\text{-}F}$ = 25.0 Hz), 32.0, 22.7, 13.9 ppm; GC-MS m/z = 154 (M^+); ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.[S8]

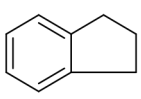
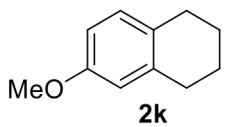

2j

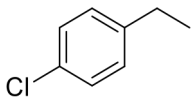
Table 2, compound 2j. Method A at 130 °C for 16 h. The product **2j** was isolated by a column chromatography on silica gel (hexanes). Colorless liquid, Yield: 165 mg, 90 %. Data for **2j**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.29-7.24 (m, 2H), 7.18-7.15 (m, 2H), 2.95 (t, J = 7.5 Hz, 4H), 2.10 (quintet, J = 7.4 Hz, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 144.1, 125.9, 124.3, 32.8, 25.3 ppm; GC-MS m/z = 118 (M^+); ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.[S9]



2k

Table 2, compound 2k. Method A at 130 °C for 16 h. The product **2k** was isolated by a column chromatography on silica gel (hexanes/Et_2O = 100:1). White solid, Yield: 142 mg, 88 %. Data for **2k**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.98 (d, J = 8.4 Hz, 1H), 6.68 (dd,

J = 8.4, 2.8 Hz, 1H), 6.61 (d, J = 2.8 Hz, 1H), 3.75 (s, 3H), 2.68 - 2.78 (m, 4H), 1.76-1.80 (m, 4H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 157.5, 138.3, 130.1, 129.4, 113.8, 111.9, 55.4, 29.9, 28.7, 23.6, 23.3 ppm; GC-MS m/z = 162 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S10]



2l

Table 2, compound 2l. Method A at 130 °C for 12 h. The product **2l** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). Colorless liquid, Yield: 113 mg, 82 %. Data for **2l**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, J = 8.8 Hz, 2H), 7.13 (d, J = 8.6 Hz, 2H), 2.63 (q, J = 7.6 Hz, 2H), 1.23 (t, J = 7.6 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 142.7, 131.3, 129.8, 128.5, 28.4, 15.7 ppm; GC-MS m/z = 140 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S11]

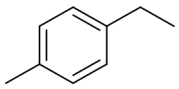
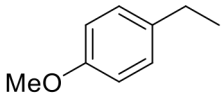

2m

Table 2, compound 2m. Method A 130 °C for 12 h. The product **2m** was isolated by a column chromatography on silica gel (hexanes/Et_2O = 100:1). Colorless liquid, Yield: 110 mg, 92 %. Data for **2m**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08-6.98 (m, 4H); 3.40 (q, J = 7.0 Hz, 2H), 2.15 (s, 3H), 1.13 (t, J = 7.0 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 141.2, 138.1, 131.2, 127.4, 29.1, 21.2, 16.9 ppm; GC-MS m/z = 120 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S12]



2n

Table 2, compound 2n. Method A at 130 °C for 12 h. The product **2n** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 40:1). Colorless liquid, Yield: 132 mg, 95 %. Data for **2n**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, J = 8.7 Hz, 2H), 6.85 (d, J = 8.7 Hz, 2H), 3.81 (s, 3H), 2.61 (q, J = 7.5 Hz, 2H), 1.23 (t, J = 7.5 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 157.5, 136.3, 128.7, 113.7, 55.2, 27.9, 15.9 ppm; GC-MS m/z = 136 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S13]

Table 2, compound 2o. Method A at 130 °C for 24 h. The product **2o** was isolated by a column chromatography on silica gel (hexanes). Colorless liquid, Yield: 65 % (GC). Data for **2o**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21-1.44 (m, 18H), 0.91 (t, J = 6.8 Hz, 6H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 32.0, 29.8, 29.8, 29.5, 22.8, 14.1 ppm; GC-MS m/z = 156 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S14]

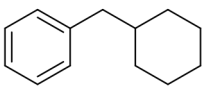
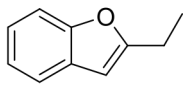

2p

Table 2, compound 2p. Method A at 130 °C for 24 h. The product **2p** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 20:1). Colorless liquid, Yield: 94 mg, 54 %. Data for **2p**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.20 (m, 3H), 7.05-6.92 (m, 2H), 2.39 (d, J = 6.2 Hz, 2H), 1.80-1.66 (m, 5H), 1.46-1.33 (m, 1H), 1.21-1.12 (m, 3H), 0.88-0.71 (m, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 138.7, 128.6, 128.2, 126.0, 41.0, 38.9, 33.2, 28.3, 25.8 ppm; GC-MS m/z = 174 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S15]



2q

Table 2, compound 2q. Method A at 130 °C for 12 h. The product **2q** was isolated by

a column chromatography on silica gel (hexanes/EtOAc = 20:1). Colorless liquid, Yield: 144 mg, 95 %. Data for **2q**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (m, 1H), 7.40 (m, 1H), 7.18 (m, 2H), 6.37 (d, *J* = 1.2 Hz, 1H), 2.81 (q, *J* = 7.6 Hz, 2H), 1.34 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.5, 154.9, 129.0, 123.0, 122.3, 120.2, 110.7, 101.1, 21.9, 11.9 ppm; GC-MS *m/z* = 146 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S16]

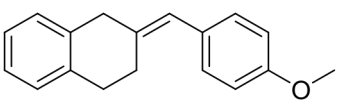

2r

Table 2, compound 2r. Method B at 130 °C for 12 h. Analytically pure product **2r** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). White solid, Yield: 212 mg, 85 %; Data for **2r**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18-7.10 (m, 3H), 7.10-7.07 (m, 2H), 7.00 (d, *J* = 7.0 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.25 (s, 1H), 3.81 (s, 3H) 3.46 (s, 1H), 2.78 (t, *J* = 8.2 Hz, 2H), 2.19 (t, *J* = 8.2 Hz, 2H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.1, 141.2, 134.8, 134.4, 131.4, 130.0, 127.2, 126.4, 126.3, 125.6, 123.6, 113.8, 55.3, 42.9, 28.2, 27.0 ppm; GC-MS *m/z* = 250 (M^+); Anal. Calcd for $C_{18}H_{18}O$: C, 86.36; H, 7.25. Found: C, 86.29; H, 7.19.

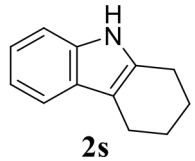

2s

Table 2, compound 2s. Method A at 130 °C for 24 h. The product **2s** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 20:1). White solid, Yield: 94 mg, 55 %. Data for **2s**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (br s, 1H), 7.46 (d, *J* = 7.0 Hz, 1H), 7.29-7.27 (m, 1H), 7.13-7.05 (m, 2H), 2.75-2.70 (m, 4H), 1.95-1.84 (m, 4H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 135.6, 134.0, 127.8, 120.9, 119.1, 117.7, 110.3 (2C), 23.3, 23.2, 23.2, 20.9 ppm; GC-MS *m/z* = 171 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S17]

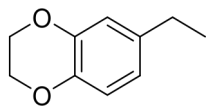

2t

Table 2, compound 2t. Method A at 130 °C for 12 h. Analytically pure product **2t** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 20:1). Colorless liquid Yield: 147 mg, 90 %. Data for **2t**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.81-6.67 (m, 1H), 6.74-6.66 (m, 2H), 4.25 (s, 4H), 2.56 (q, *J* = 7.6 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 143.2, 141.4, 137.6, 120.1, 116.9, 116.4, 64.4, 64.3, 28.1, 15.7 ppm; GC-MS *m/z* = 164 (M^+); Anal. Calcd for $C_{10}H_{12}O_2$: C, 73.15; H, 7.37. Found: C, 73.20; H, 7.34.

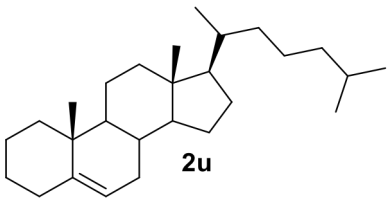
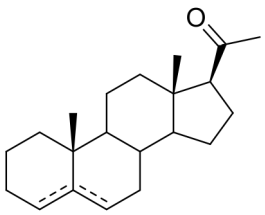
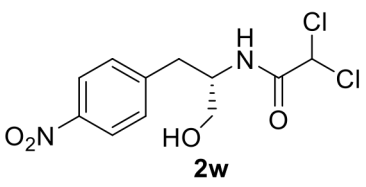

2u

Table 3, compound 2u. Method B at 130 °C for 12 h. Analytically pure product **2u** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). White solid, Yield: 206 mg, 56 %. Data for **2u**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.30-5.28 (m, 1H), 2.32-2.18 (m, 1H), 2.10-1.93 (m, 3H), 1.90-1.81 (m, 2H), 1.79-1.69 (m, 1H), 1.63-0.92 (m, 23H), 1.00 (s, 3H), 0.92 (d, *J* = 6.4 Hz, 3H), 0.90 (d, *J* = 1.3 Hz, 3H), 0.88 (d, *J* = 1.3 Hz, 3H), 0.70 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 143.7, 119.0, 56.8, 56.1, 50.6, 42.31, 39.9, 39.8, 39.5, 37.5, 36.2, 35.8, 32.9, 31.9, 31.8, 28.2, 28.0, 28.0, 24.3, 23.8, 22.8, 22.5, 20.7, 19.5, 18.7, 11.8 ppm; GC-MS *m/z* = 370 (M^+); ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S18]



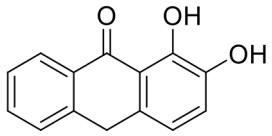
2v

Table 3, compound 2v. Method B at 130 °C for 12 h. Analytically pure product was isolated by a column chromatography on silica gel (hexanes/EtOAc = 100:1). White solid, Yield: 156 mg, 52 %. (isomers were not separated) Data for **2v**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.28 (br s, 1H), 5.24 (dt, *J* = 5.4, 1.9 Hz, 1H), 2.51 (td, *J* = 8.9, 6.5 Hz, 2H), 2.11-2.26 (m, 4H), 2.09 (s, 6H), 1.05-2.04 (m, 40 H), 0.90 (s, 3H), 0.76 (d, *J* = 0.4 Hz, 3H), 0.57 (s, 3H), 0.56 (s, 3H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 209.6, 209.6, 144.5, 143.5, 119.2, 118.6, 63.9, 63.8, 56.8, 56.77, 54.5, 46.9, 44.3, 43.5, 40.4, 39.3, 39.1, 38.6, 37.5, 36.2, 35.8, 35.4, 32.0, 28.9, 28.8, 27.3, 27.1, 26.9, 26.7, 26.5, 24.4, 24.3, 24.1, 22.8, 22.6, 22.1, 21.2, 20.7, 20.75, 13.4, 13.36, 12.1 ppm; GC-MS *m/z* = 300 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S18]



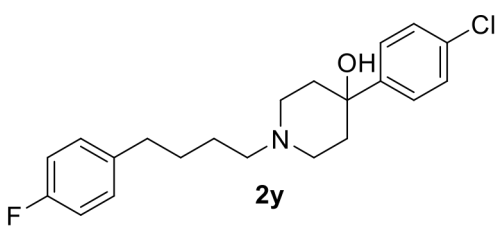
2w

Table 3, compound 2w. Method B at 150 °C for 12 h. Analytically pure product **2w** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 4:1). White solid, Yield: 137 mg, 45 %. Data for **2w**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 9.0 Hz, 1H), 5.74 (s, 1H), 5.26 (t, *J* = 3.3 Hz, 1H), 4.22 (tdd, *J* = 8.4, 8.4, 5.2, 2.9 Hz, 1H), 3.73 (dd, *J* = 11.1, 8.0 Hz, 1H), 3.57-3.51 (m, 2H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 164.4, 147.7, 126.7, 126.7, 123.7, 70.3, 65.9, 56.5, 42.7 ppm; GC-MS *m/z* = 306 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S19]



2x

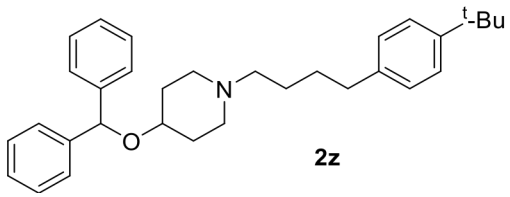
Table 3, compound 2x. Method A at 130 °C for 24 h. The product **2x** was isolated by a column chromatography on silica gel (CH_2Cl_2/methanol = 100:1). Orange solid, Yield: 151 mg, 67 %. Data for **2x**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.76 (s, 1H), 7.99 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.22-7.40 (m, 1H), 7.06-7.21 (m, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 6.53 (dt, *J* = 8.2, 1.1 Hz, 2H), 5.41 (br s, 1H), 3.97 (s, 2H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 190.1, 149.3, 142.8, 142.6, 133.7, 133.5, 132.2, 130.8, 128.5, 127.0, 120.7, 118.2, 31.8 ppm; GC-MS *m/z* = 226 (M^+). ^{1}H and ^{13}C NMR spectral data are in good agreement with the literature data.[S20]



2y

Table 2, compound 2y. Method B at 150 °C for 12 h. Analytically pure product **2y** was isolated by a column chromatography on silica gel (CH_2Cl_2/MeOH = 80:1). White solid, Yield: 245 mg, 68 %. Data for **2y**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76-7.03 (m, 8H), 3.43-3.47 (m, 1H), 2.67-2.80 (m, 2H), 2.27-2.39 (m, 2H), 2.10-2.23 (m, 1H), 2.02-2.10 (m, 2H), 1.64-1.76 (m, 2H), 1.39-1.57 (m, 3H), 1.18-1.39 (m, 4H) ppm; ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 144.8 (d, J_{C-F} = 249 Hz), 129.6 (d, J_{C-F} = 7.8 Hz), 128.4 (d, J_{C-F} = 6.9 Hz), 128.2 (d, J_{C-F} = 5.9 Hz),

126.8, 125.6, 115.0, 114.8, 58.9, 54.3, 42.1, 35.8, 33.4, 29.5, 26.9 ppm; GC-MS *m/z* = 361 (M^+); HRMS (ESI) Calcd for $[M+H]^+$ $C_{21}H_{25}ClFNO$: 362.8934 Found: 362.8938.



2z

Table 3, compound 2z. Method B at 150 °C for 12 h. Analytically pure product **2z** was isolated by a column chromatography on silica gel (hexanes/EtOAc = 4:1). White solid, Yield: 191 mg, 84 %. Data for **2z**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.11 (m, 12H), 7.02 (d, *J* = 8.1 Hz, 2H), 5.44 (s, 1H), 3.40-3.29 (m, 1H), 2.70-2.59 (m, 2H), 2.50 (t, *J* = 7.5 Hz, 2H), 2.27-2.18 (m, 2H), 2.09-1.93 (m, 2H), 1.86-1.74 (m, 2H), 1.71-1.59 (m, 2H), 1.57-1.37 (m, 5H), 1.25-1.19 (m, 9H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 148.3, 142.8, 139.4, 128.3, 128.0, 127.2, 127.1, 125.1, 79.9, 58.6, 51.19, 51.18, 51.17, 35.2, 34.3, 31.4, 29.5, 26.9 ppm; GC-MS *m/z* = 455 (M^+); HRMS (ESI) Calcd for $[M+H]^+$ $C_{32}H_{41}NO$: 456.3251 Found: 456.3266.

Synthesis of $[(C_6H_5OH)(PCy_3)(CO)RuH]^+BF_4^-$ (4a). The complex $\{[(PCy_3)(CO)RuH]_4(\mu\text{-}O)(\mu\text{-}OH)_2\}$ (**3**) (200 mg, 0.12 mmol) and phenol (44 mg, 0.48 mmol) were dissolved in CH_2Cl_2 (5 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar, and $HBF_4{\cdot}OEt_2$ (64 μL, 0.48 mmol) was added under N_2 stream. After stirring for 1 h at room temperature, the solvent was removed under vacuum, and the residue was washed with hexanes. The resulting residue was dissolved in acetone (2 mL), layered with *n*-pentane (2 mL), and stored in a glove box for 3 days for crystallization. The resulting solid was filtered through a fritted funnel to yield the product as white crystalline solids (210 mg, 76 % yield). Single crystals of **4a** suitable for X-ray crystallography were obtained from acetone/*n*-pentane solution. Data for **4a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (br s, 1H), 6.62-6.70 (m, 1H), 6.54-6.62 (m, 1H), 6.33 (d, *J* = 7.0 Hz, 1H), 5.91 (d, *J* = 5.5 Hz, 1H), 5.69 (t, *J* = 5.9 Hz, 1H), 0.76-2.45 (m, 33H), -10.86 (d, $J_{P\text{-}H}$ = 27.1 Hz, 1H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 197.6 (d, $J_{C\text{-}P}$ = 18.1 Hz), 148.8, 103.8, 103.6, 88.1, 85.4, 84.8, 38.3, 37.9, 30.7, 30.1, 30.1, 27.9, 27.7, 26.7 ppm; $^{31}P\{^1H\}$ NMR (400 MHz, $CDCl_3$) δ 70.78 ppm; FT-IR (solid) ν_{CO} = 1973 cm^{-1}; HRMS (ESI) Calcd for $[M]^+$ $C_{25}H_{40}O_2PRu$: 505.1902 Found: 505.1911.

Synthesis of $[(4\text{-}OMe\text{-}C_6H_4OH)(PCy_3)(CO)RuH]^+BF_4^-$ (4b). Followed the same procedure as **4a** by using 4-methoxyphenol (60 mg, 0.48 mmol). Stored in a glove box for 3 days for crystallization and filtered the resulting solid through a fritted funnel to yield the product as white crystals (198 mg, 76 % yield). Single crystals of **4b** suitable for X-ray crystallography were obtained from acetone/*n*-pentane solution. Data for **4b**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.44 (dd, *J* = 7.2, 2.3 Hz, 1H), 6.36 (dd, *J* = 7.4, 2.6 Hz, 1H), 3.79 (s, 3H), 6.00-6.15 (m, 2H), 1.79-2.06 (m, 15H), 2.18 (s, 2H), 1.63-1.79 (m, 3H), 1.22-1.51 (m, 16H), -10.61 (d, $J_{P\text{-}H}$ = 27.0 Hz, 1H) ppm; $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 198.6 (d, $J_{C\text{-}P}$ = 18.8 Hz) 87.6, 87.5, 85.0, 84.2, 57.8, 37.7, 37.5, 30.8, 30.1, 27.9, 27.8, 26.7 ppm; FT-IR (solid) ν_{CO} = 1963 cm^{-1}; $^{31}P\{^1H\}$ NMR (400 MHz, $CDCl_3$) δ 71.38 ppm; HRMS (ESI) Calcd for $[M]^+$ $C_{26}H_{42}O_3PRu$: 535.1912 Found: 535.1917.

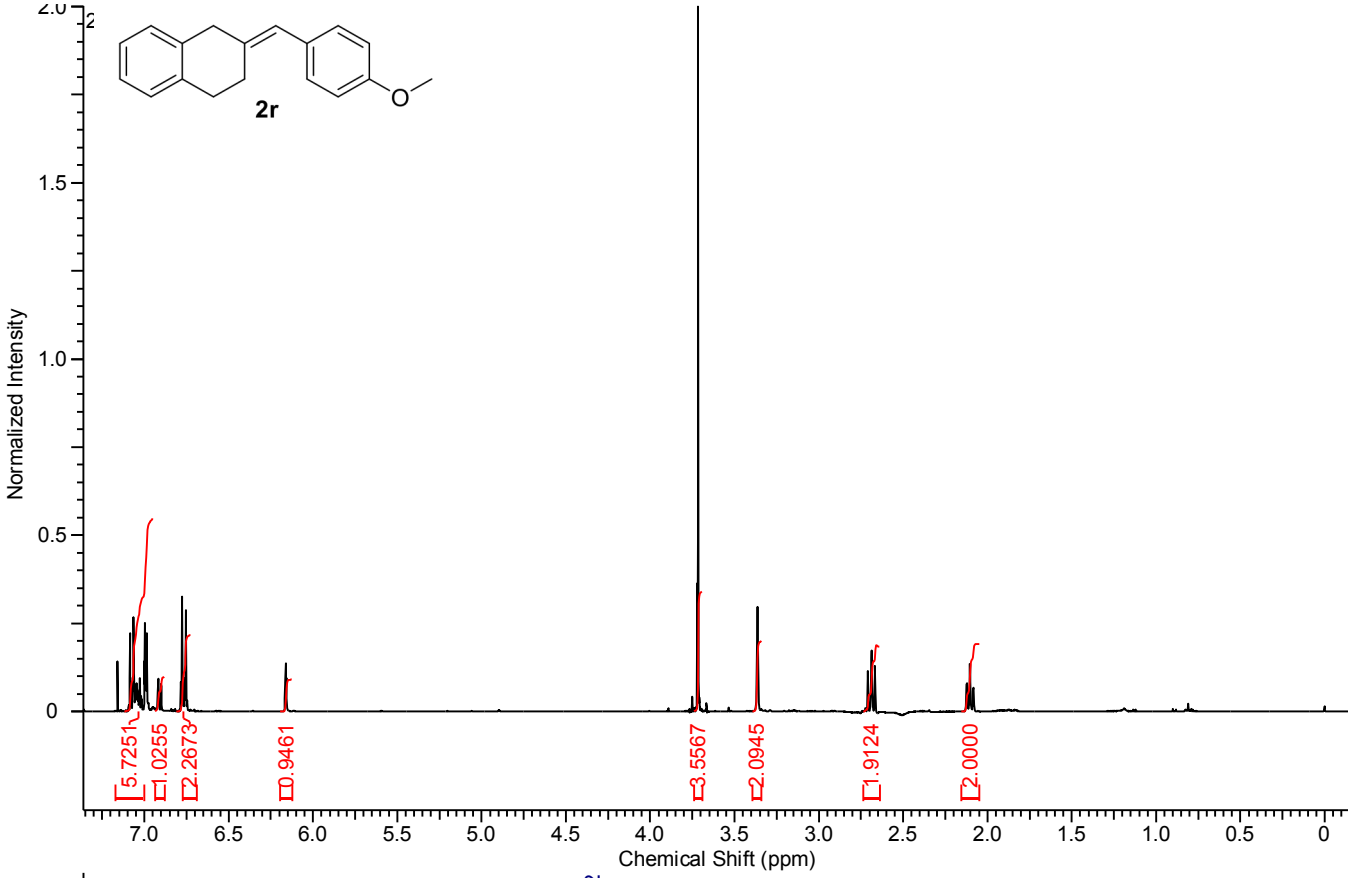
Synthesis of [(4-Cl-C_6H_4OH)(PCy_3)(CO)RuH]$^+BF_4^-$ (4c). Followed the same procedure as **4a** by using 4-chlorophenol (60 mg, 0.48 mmol). Crushed out with hexanes and filtered the resulting solid through a fritted funnel to yield the product as white solids (180 mg, ca. 72 % yield). Data for **4c**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75-6.85 (m, 1H), 6.68 (d, *J* = 7.0 Hz, 1H), 6.17 (d, *J* = 5.4 Hz, 1H), 5.98 (d, *J* = 6.7 Hz, 1H), 0.98-2.04 (m, 33H), -10.40 (d, *J* = 27.4 Hz, 1H) ppm; FT-IR (solid) ν_{CO} = 1983 cm^{-1}; ^{31}P{^{1}H} NMR (400 MHz, $CDCl_3$) δ 71.86 ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 196.2 (d, $J_{C\text{-}P}$ = 18.0 Hz), 104.1, 101.8, 85.7, 82.9, 37.9, 37.6, 30.6, 39.9, 27.8, 27.6, 26.5 ppm; HRMS (ESI) Calcd for [M]$^+$ $C_{25}H_{39}ClO_2PRu$: 539.1420 Found: 539.1417.

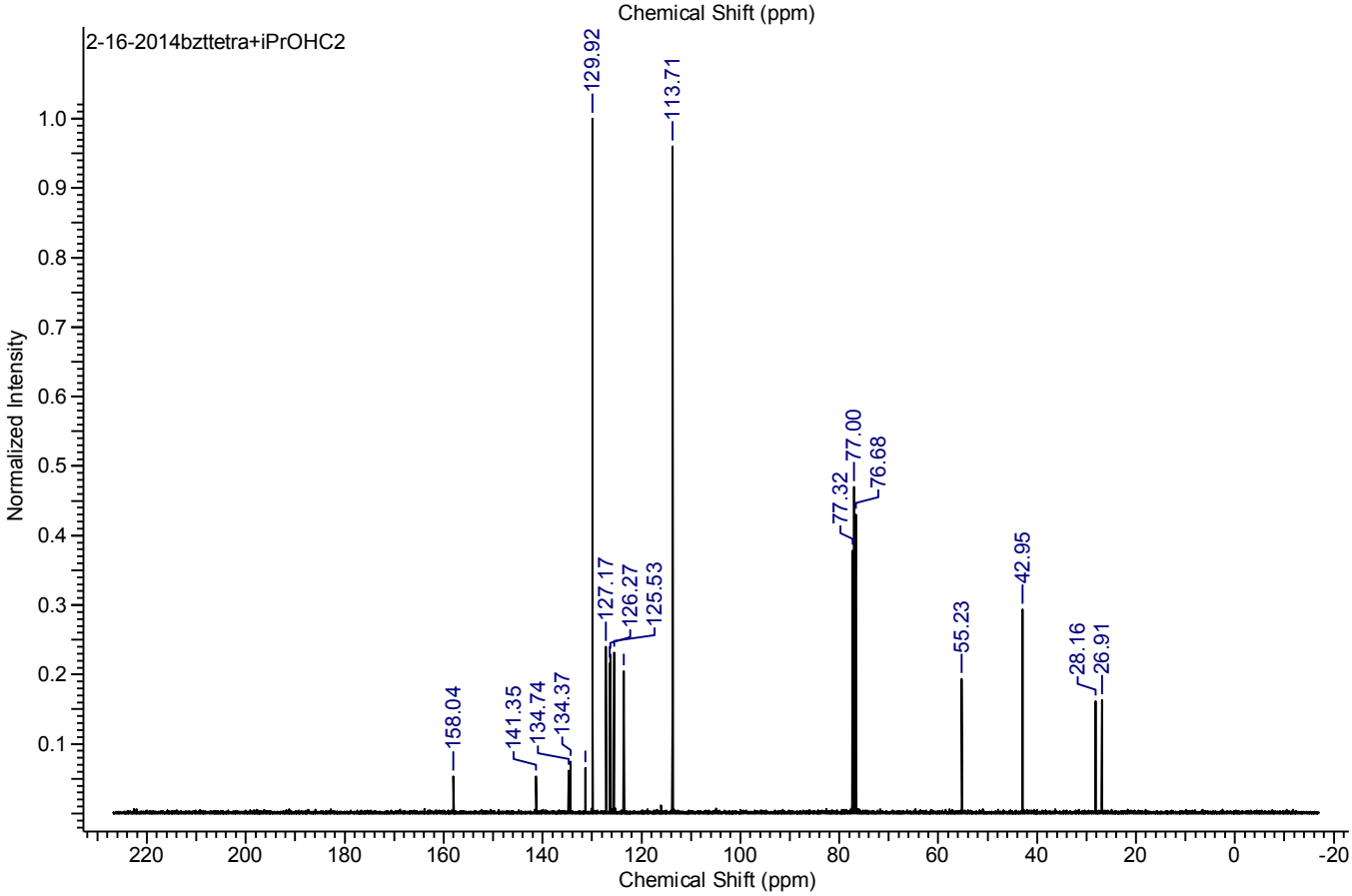
Synthesis of [(2-COMe-C_6H_4OH)(PCy_3)(CO)RuH]$^+BF_4^-$ (4d). The complex {[(PCy_3)(CO)RuH]$_4$(μ-O)(μ-OH)$_2$} (**3**) (200 mg, 0.12 mmol) and 2-hydroxyacetophenone (64 mg, 0.48 mmol) were dissolved in CH_2Cl_2 (5 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar, and $HBF_4{\cdot}OEt_2$ (64 μL, 0.48 mmol) was added under N_2 stream. The color of the solution was changed from dark red to light red immediately. After stirring for 1 h at room temperature, the solvent was removed under vacuum, and hexanes (10 mL) was added to the residue. The resulting solid was filtered through a fritted funnel, and was washed with hexanes to yield the product as orange solids (281 mg, 82 % yield). Data for **4d**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (br s, 1H), 6.57 (t, *J* = 6.4 Hz, 1H), 6.23 (d, *J* = 6.6 Hz, 1H), 5.91 (d, *J* = 6.1 Hz, 1H), 5.68 (t, *J* = 5.9 Hz, 1H), 2.07-1.61 (m, 20H), 1.46-1.14 (m, 17H), -10.87 (d, J_{PH} = 26.8 Hz, 1H) ppm; ^{31}P{^{1}H} NMR (400 MHz, $CDCl_3$) δ 70.8 ppm. The compound decomposed during the ^{13}C NMR data acquisition.

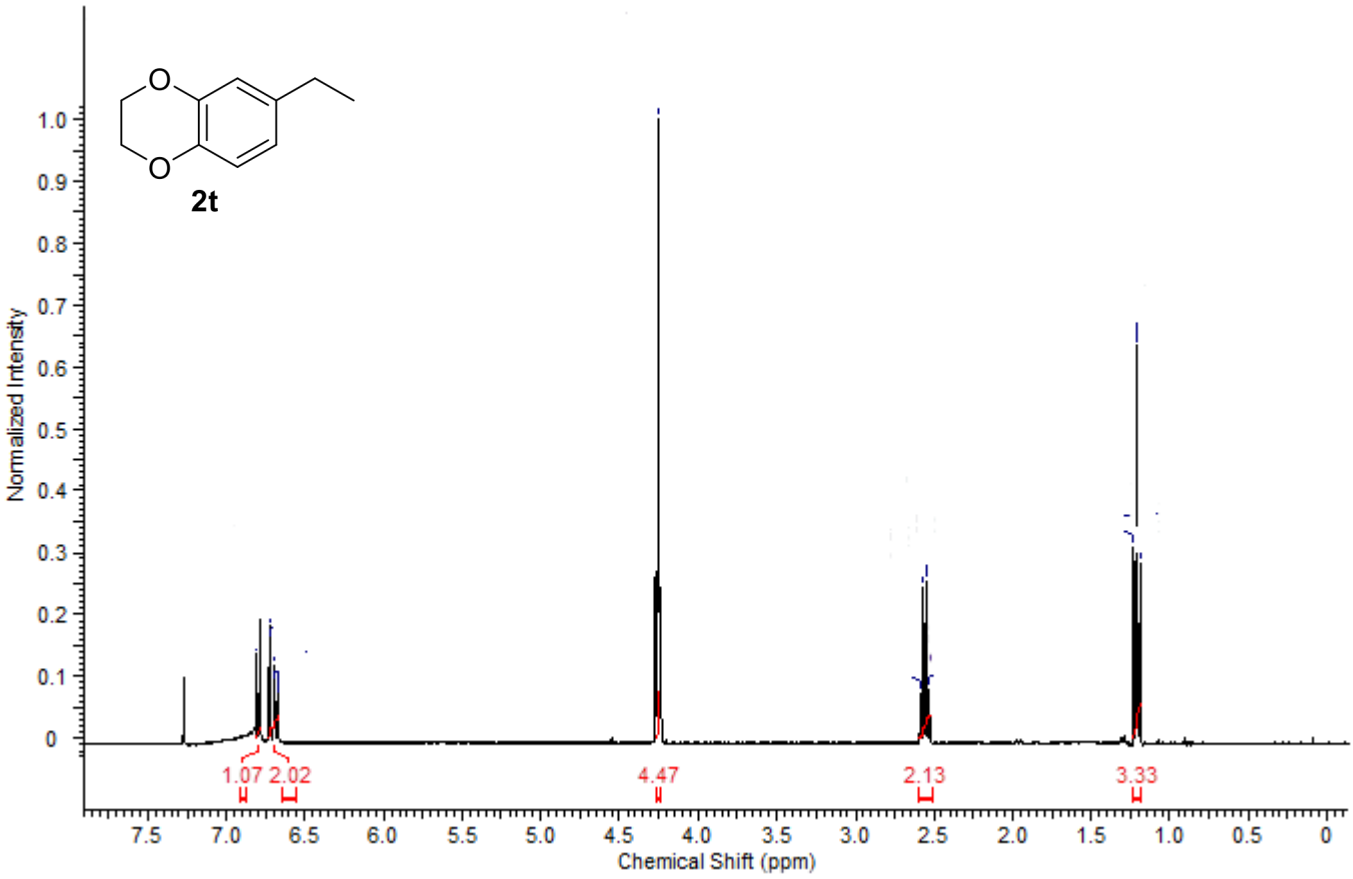
Synthesis of {[(2-COMe-C_6H_4OH)(PCy_3)(CO)Ru]$_2$(μ-H)}$^+BF_4^-$ (5). The compound **4d** (200 mg, 0.27 mmol) was dissolved in CH_2Cl_2 (2 mL), and the solution was layered with *n*-pentane (2 mL). Stored in a glove box for 3 days for crystallization, and the resulting solid was filtered through a fritted funnel to yield the product **5** as bright orange crystals (160 mg, 90 % yield). Single crystals of **5** suitable for X-ray crystallography were obtained from CH_2Cl_2/*n*-pentane solution. Data for **5**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.30 (m, 4H), 6.45-6.56 (m, 4H), 5.12-5.21 (m, 1H), 2.40 (s, 6H), 0.90-1.92 (m, 112H), -28.30 (t, $J_{P\text{-}H}$ = 9.5 Hz, 1H) ppm; selected ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 204.5, 201.1 (d, $J_{C\text{-}P}$ = 17.1 Hz) ppm; ^{31}P{^{1}H} NMR (400 MHz, $CDCl_3$) δ 70.7 ppm; FT-IR (solid) ν_{CO} = 1929, 1944 cm^{-1}; HRMS (ESI) Calcd for [M]$^+$ $C_{54}H_{81}O_6P_2Ru_2$: 1091.3595 Found: 1091.3605.

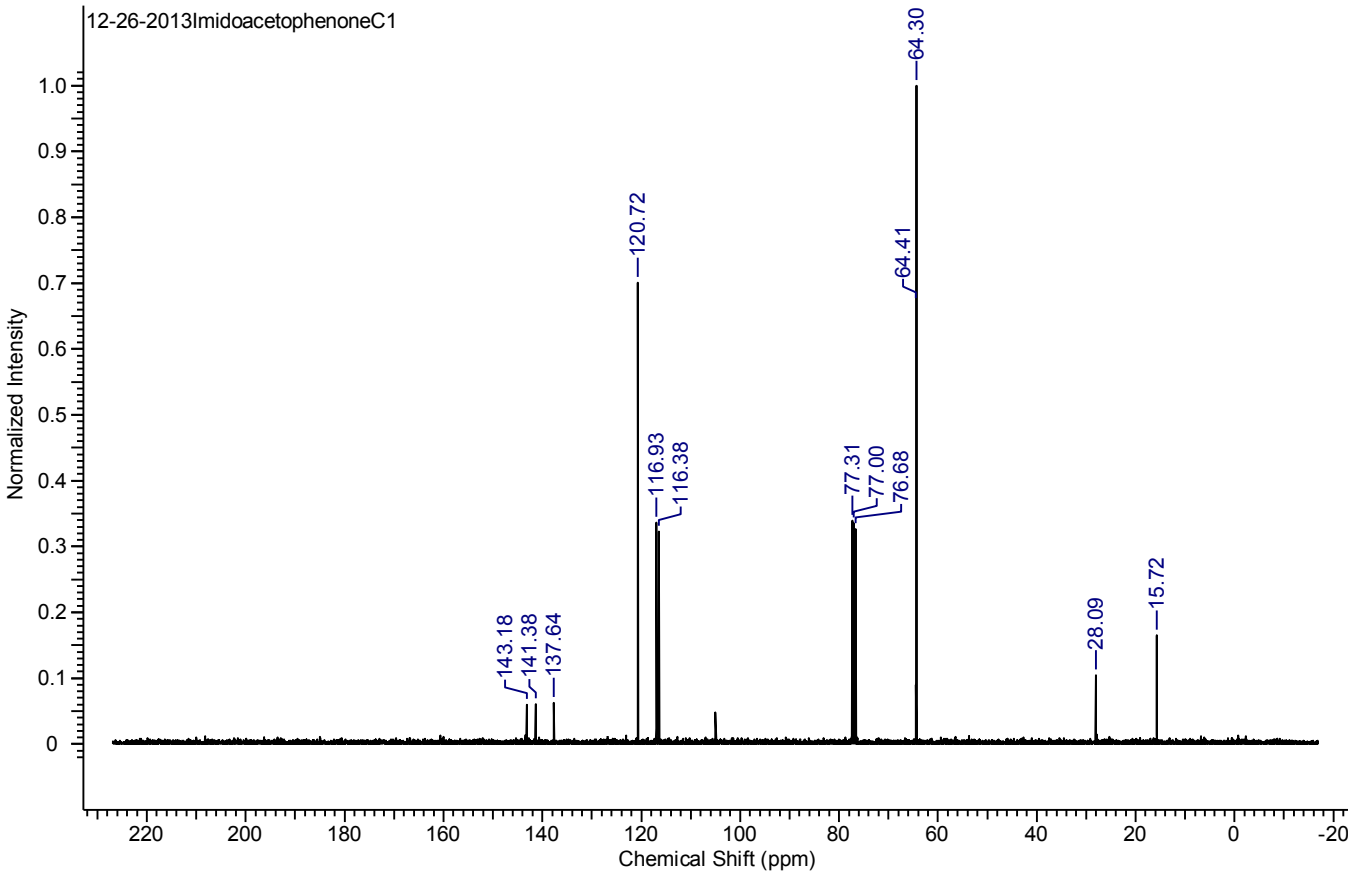
Synthesis of {[(2-COMe-C_6H_4OH)(PCy_3)(CO)Ru]$_2$(μ-OH)}$^+BF_4^-$ (6). The complex **5** (20 mg, 0.027 mmol) was dissolved in dioxane (2 mL) and H_2O (5 μL). The resulting solution was heated at 80 °C for 1 h. Stored in a glove box for one day to obtain **6** as bright orange crystalline solids (18 mg, 95 % yield). Single crystals of **6** suitable for X-ray crystallography were obtained from dioxane/*n*-pentane solution. Data for **6**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.30 (m, 4H), 7.00 (dd, *J* = 8.7, 1.1 Hz, 2H), 6.71-6.62 (m, 2H), 2.17-2.05 (m, 6H), 1.84-1.50 (m, 33H), 1.28-0.92 (m, 33H), -3.18 (s, 1H) ppm; selected ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 205.9 (d, $J_{C\text{-}P}$ = 17.8 Hz), 205.2 ppm; ^{31}P{^{1}H} NMR (400 MHz, $CDCl_3$) δ 66.5 ppm; HRMS (ESI) Calcd for [M]$^+$ $C_{54}H_{81}O_7P_2Ru_2$: 1107.3539 Found: 1107.3530.

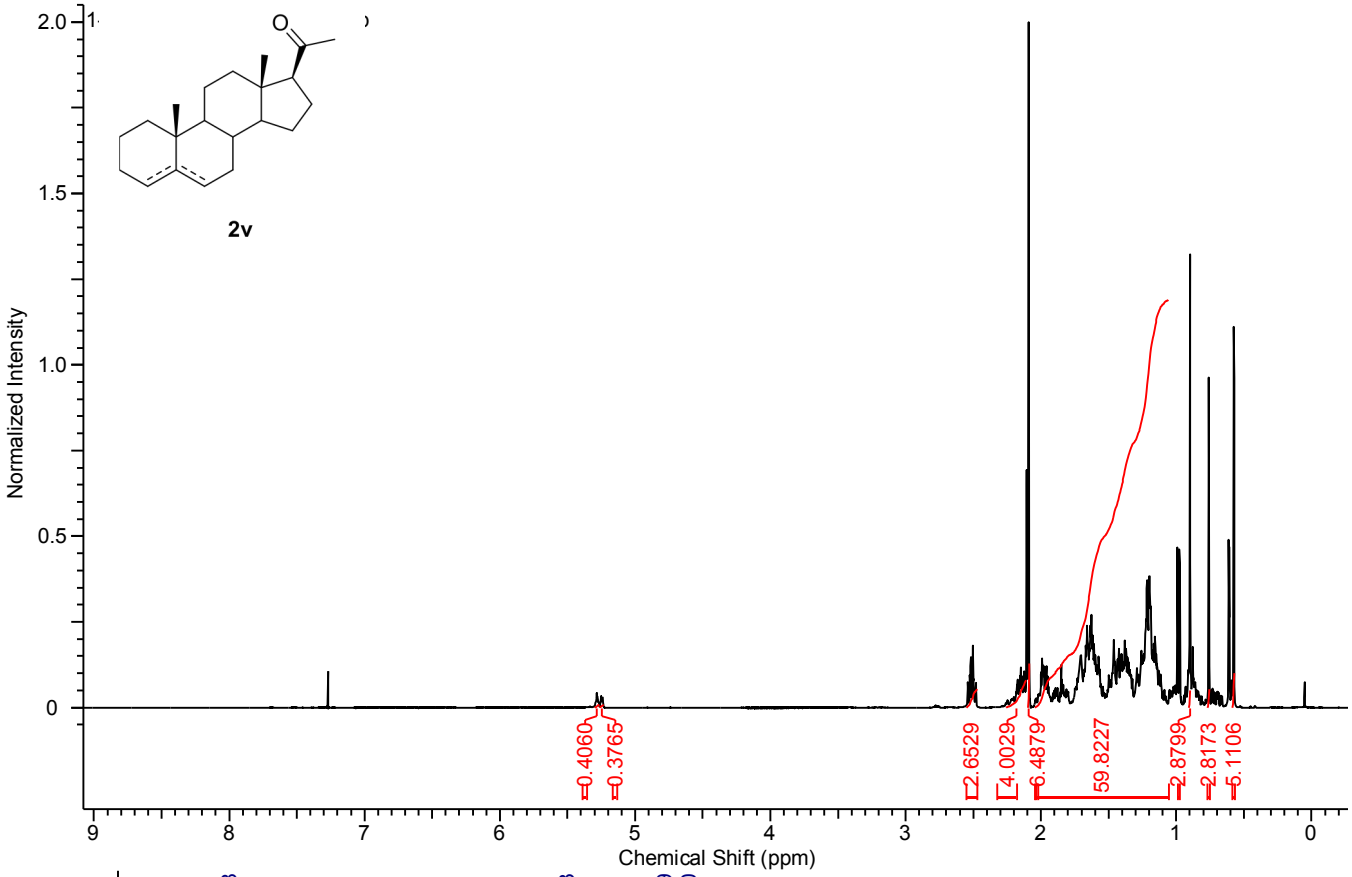
10. ^{1}H and ^{13}C NMR Spectra of the Products.

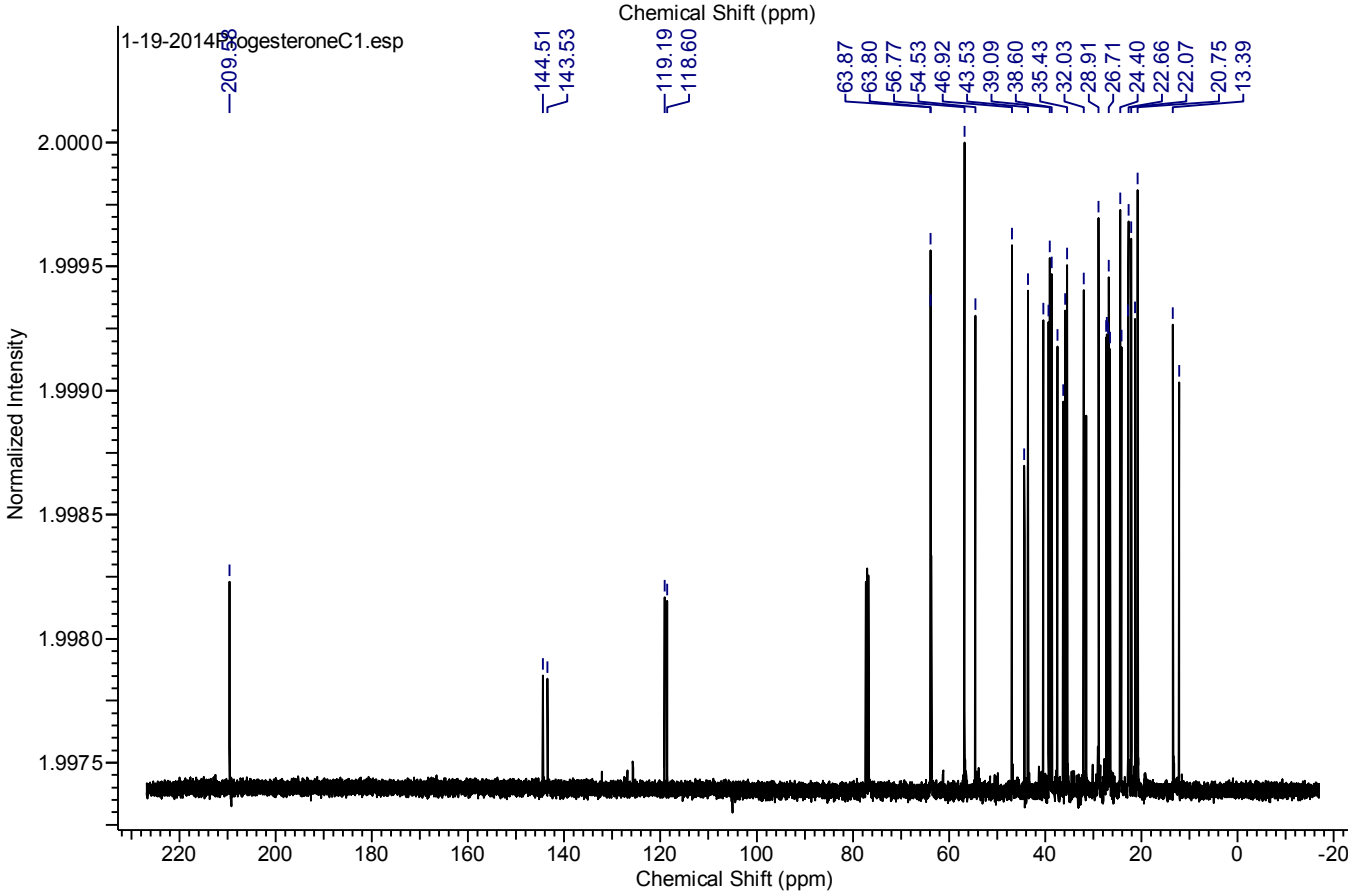


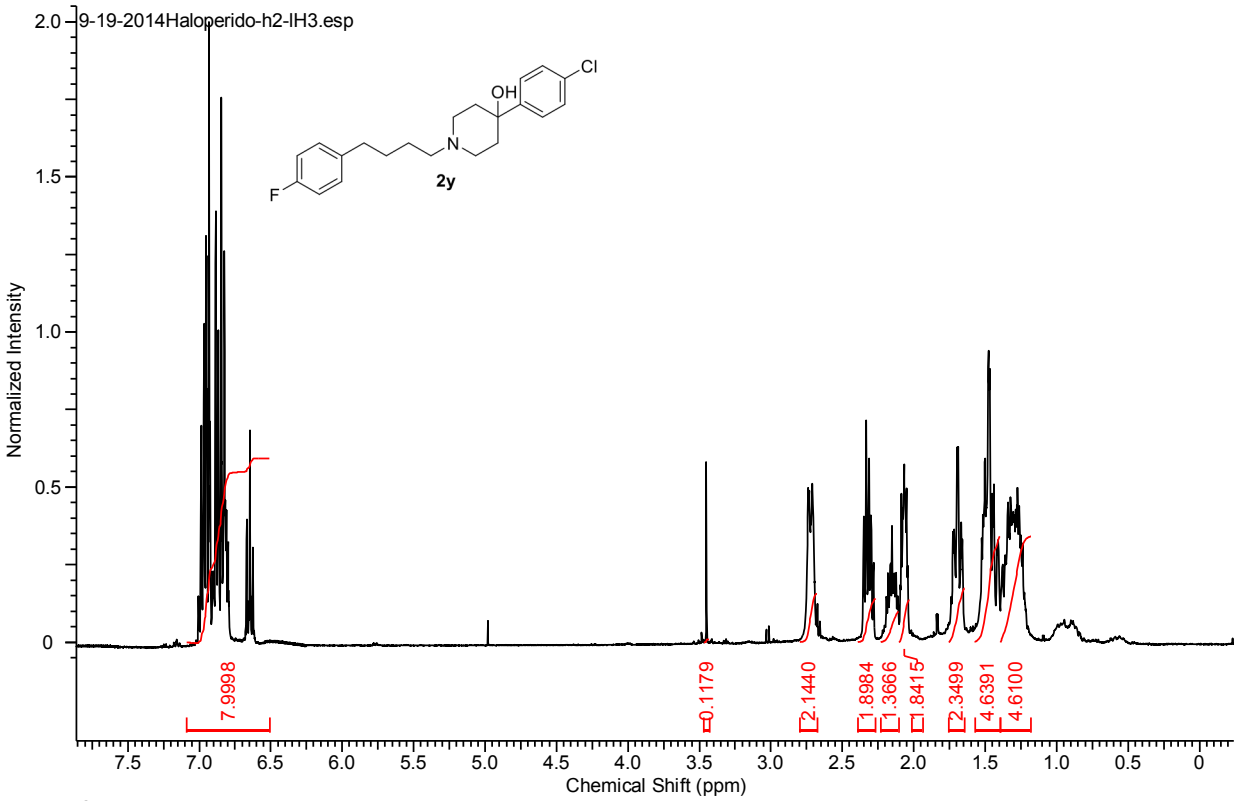


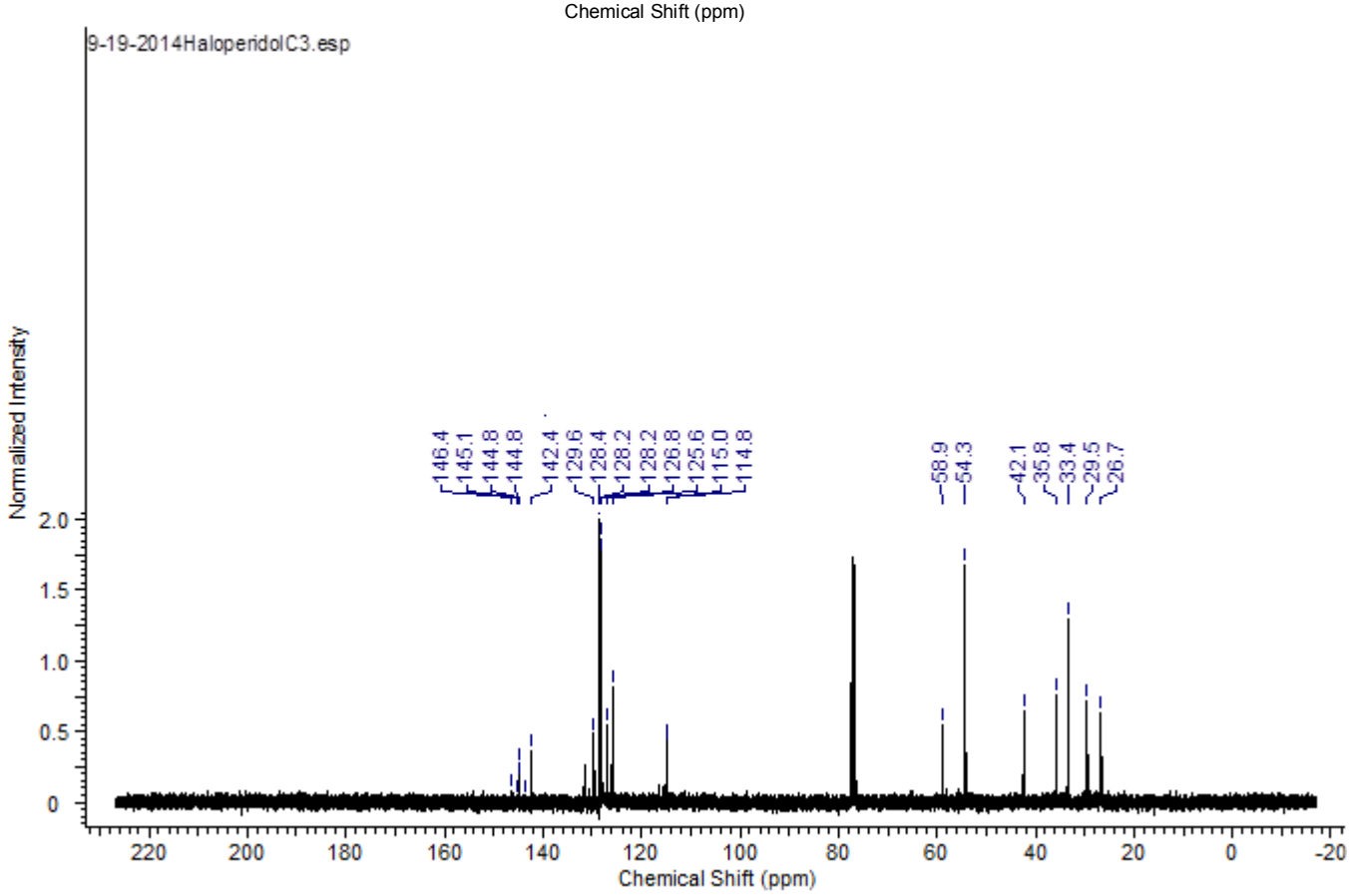

2t
Normalized Intensity
1.07
2.02
4.47
2.13
3.33
Chemical Shift (ppm)

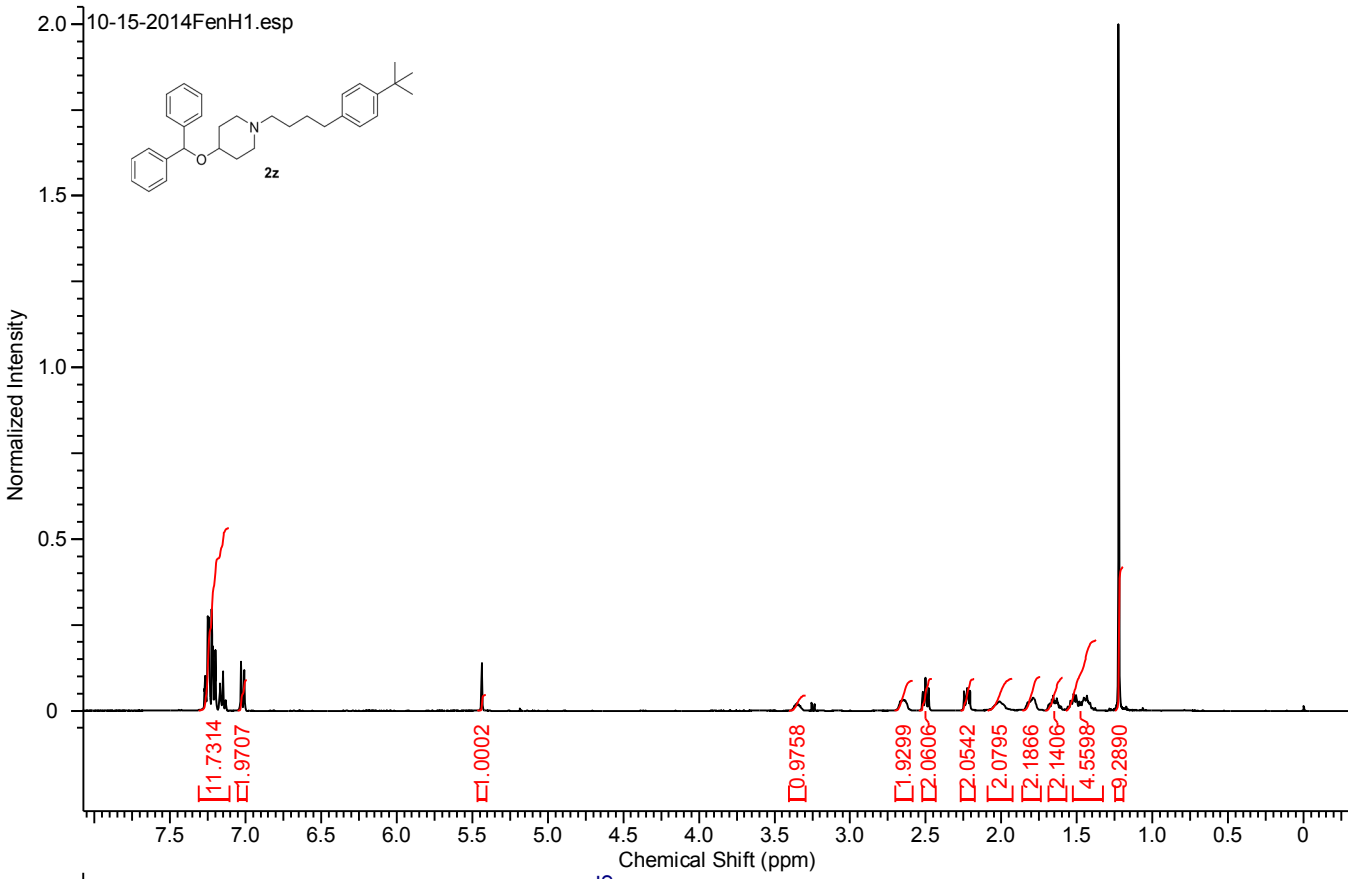

12-26-2013ImidoacetophenoneC1
Normalized Intensity
64.30
120.72
64.41
116.93
116.38
77.31
77.00
76.68
143.18
141.38
137.64
28.09
15.72
Chemical Shift (ppm)

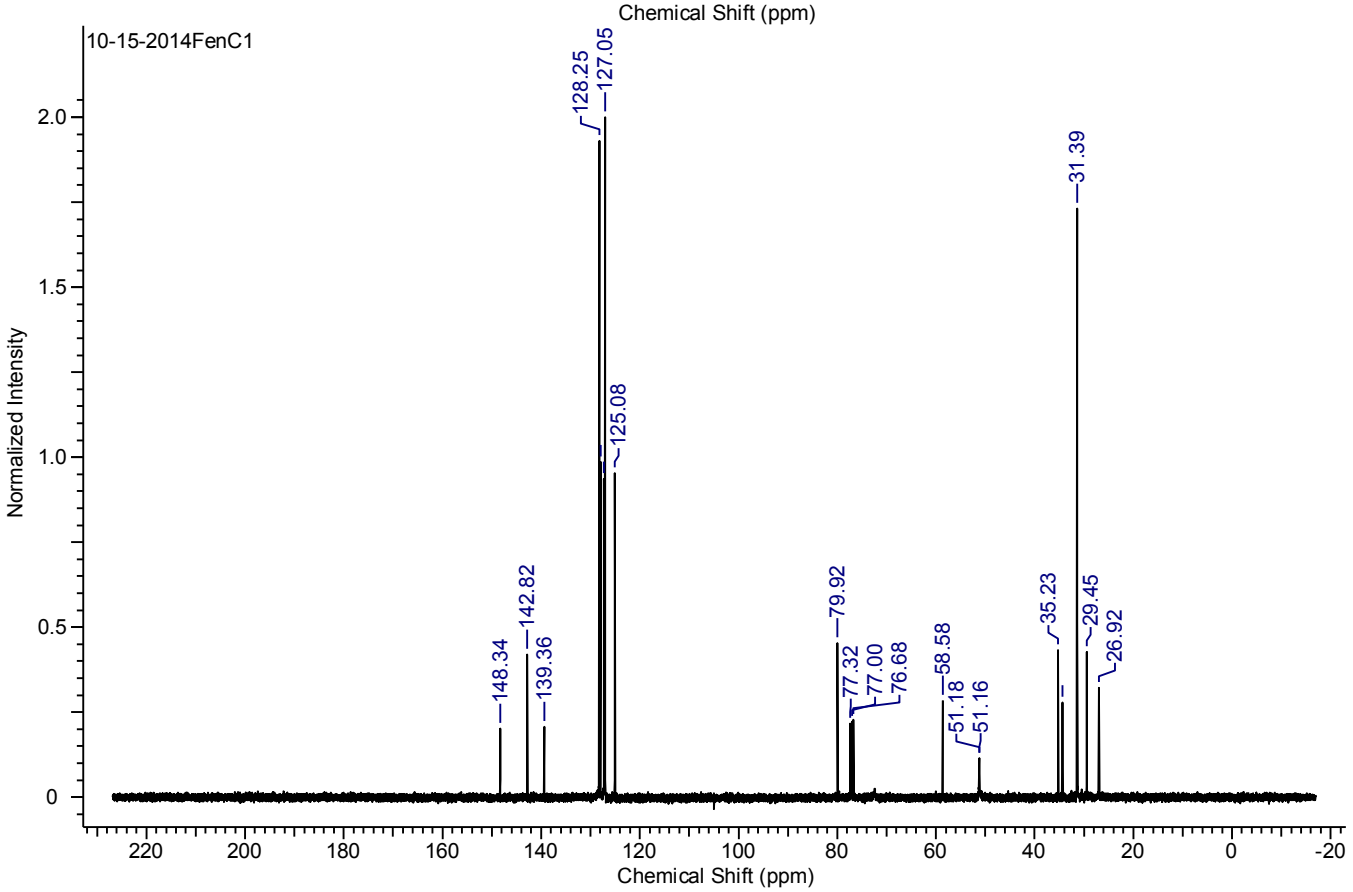

2v
Normalized Intensity
Chemical Shift (ppm)
0.4060
0.3765
2.6529
4.0029
6.4879
59.8227
2.8799
2.8173
5.1106

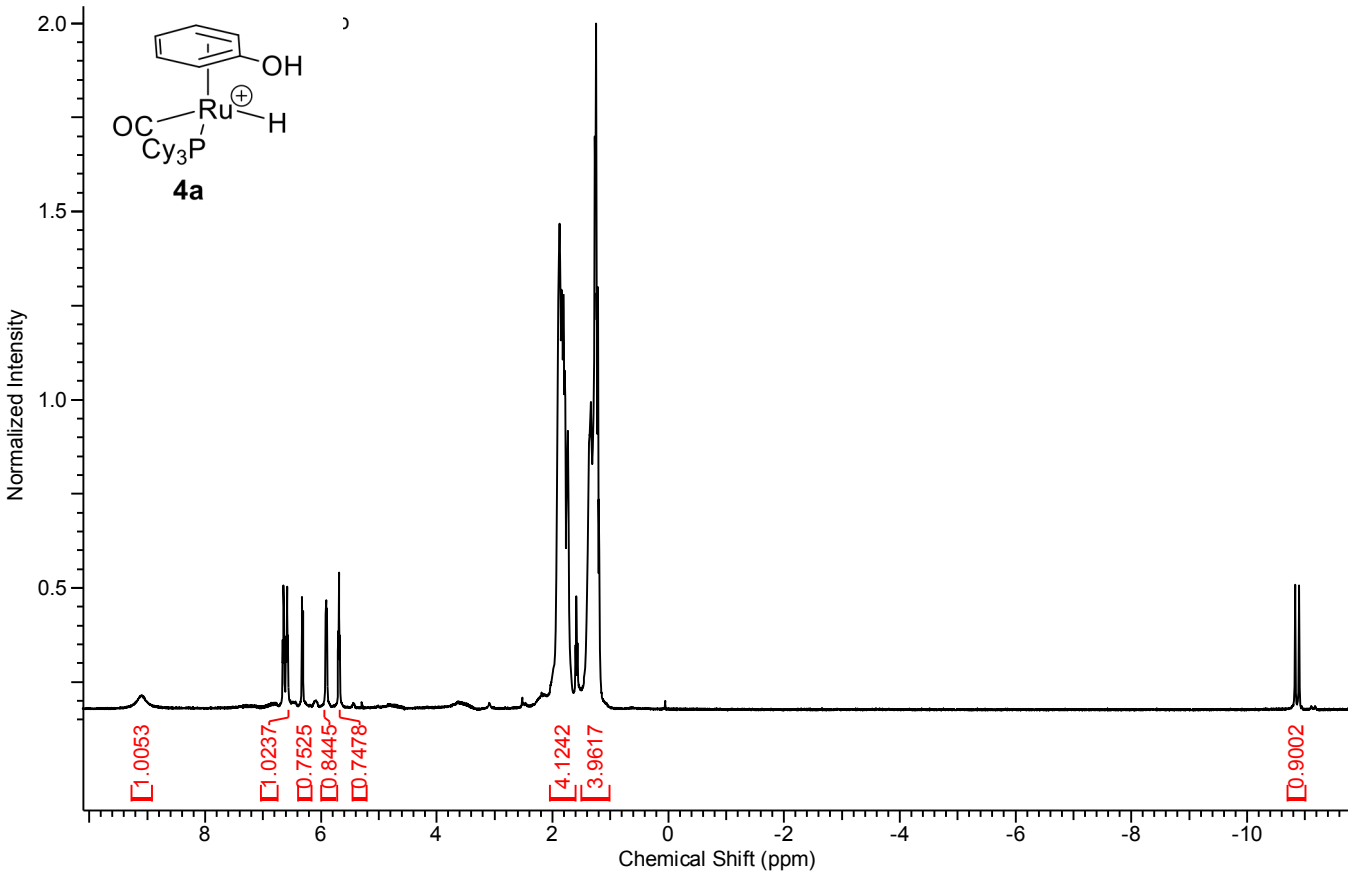

1-19-2014ProgesteroneC1.esp
209.38
144.51
143.53
119.19
118.60
63.87
63.80
56.77
54.53
46.92
43.53
39.09
38.60
35.43
32.03
28.91
26.71
24.40
22.66
22.07
20.75
13.39
Normalized Intensity
Chemical Shift (ppm)

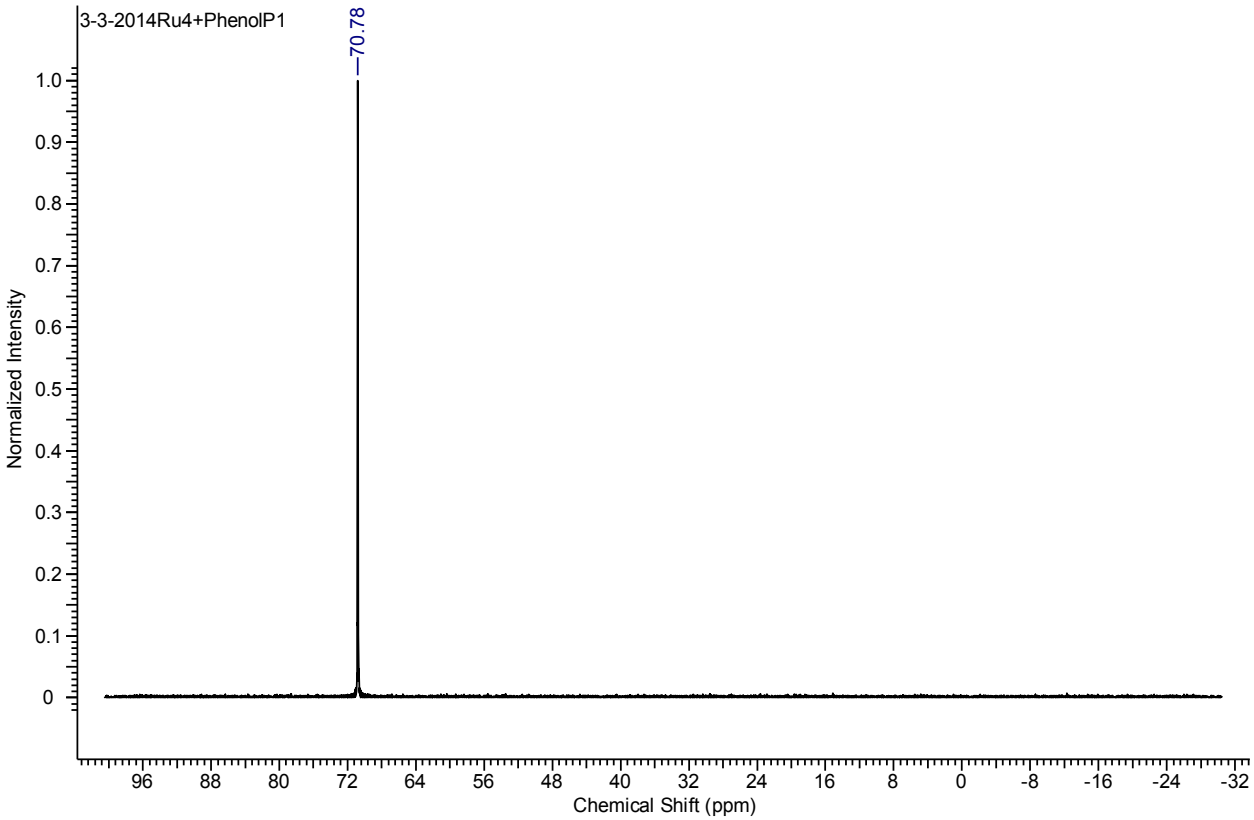

9-19-2014Haloperido-h2-IH3.esp
Cl
OH
N
F
2y
Normalized Intensity
2.0
1.5
1.0
0.5
0
7.9998
0.1179
2.1440
1.8984
1.3666
1.8415
2.3499
4.6391
4.6100
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

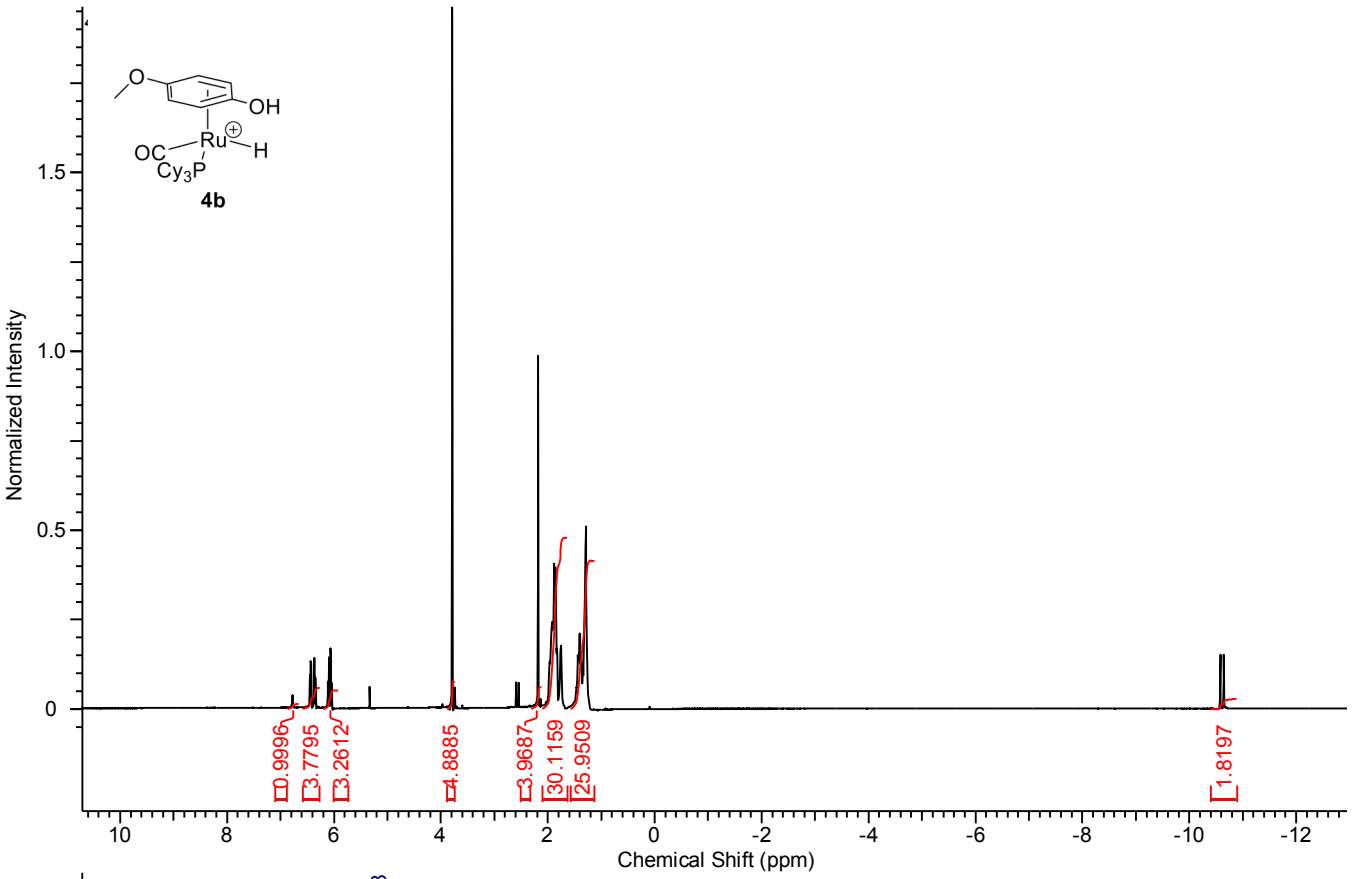

9-19-2014HaloperidolC3.esp
Normalized Intensity
146.4
145.1
144.8
144.8
142.4
129.6
128.4
128.2
128.2
126.8
125.6
115.0
114.8
58.9
54.3
42.1
35.8
33.4
29.5
26.7
2.0
1.5
1.0
0.5
0
220
200
180
160
140
120
100
80
60
40
20
0
-20
Chemical Shift (ppm)

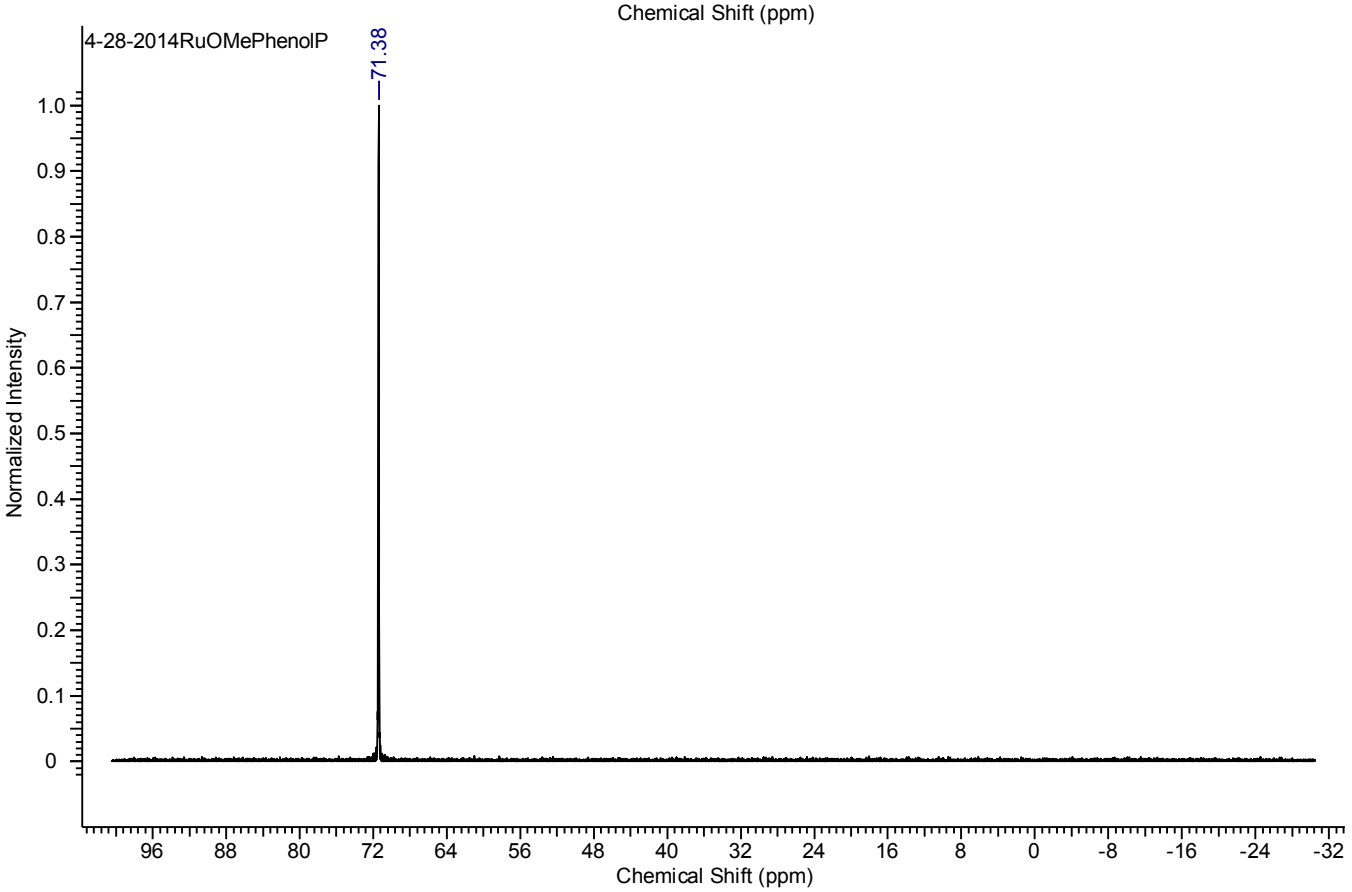

10-15-2014FenH1.esp
2z
Normalized Intensity
Chemical Shift (ppm)
11.7314
1.9707
1.0002
0.9758
1.9299
2.0606
2.0542
2.0795
2.1866
2.1406
4.5598
9.2890

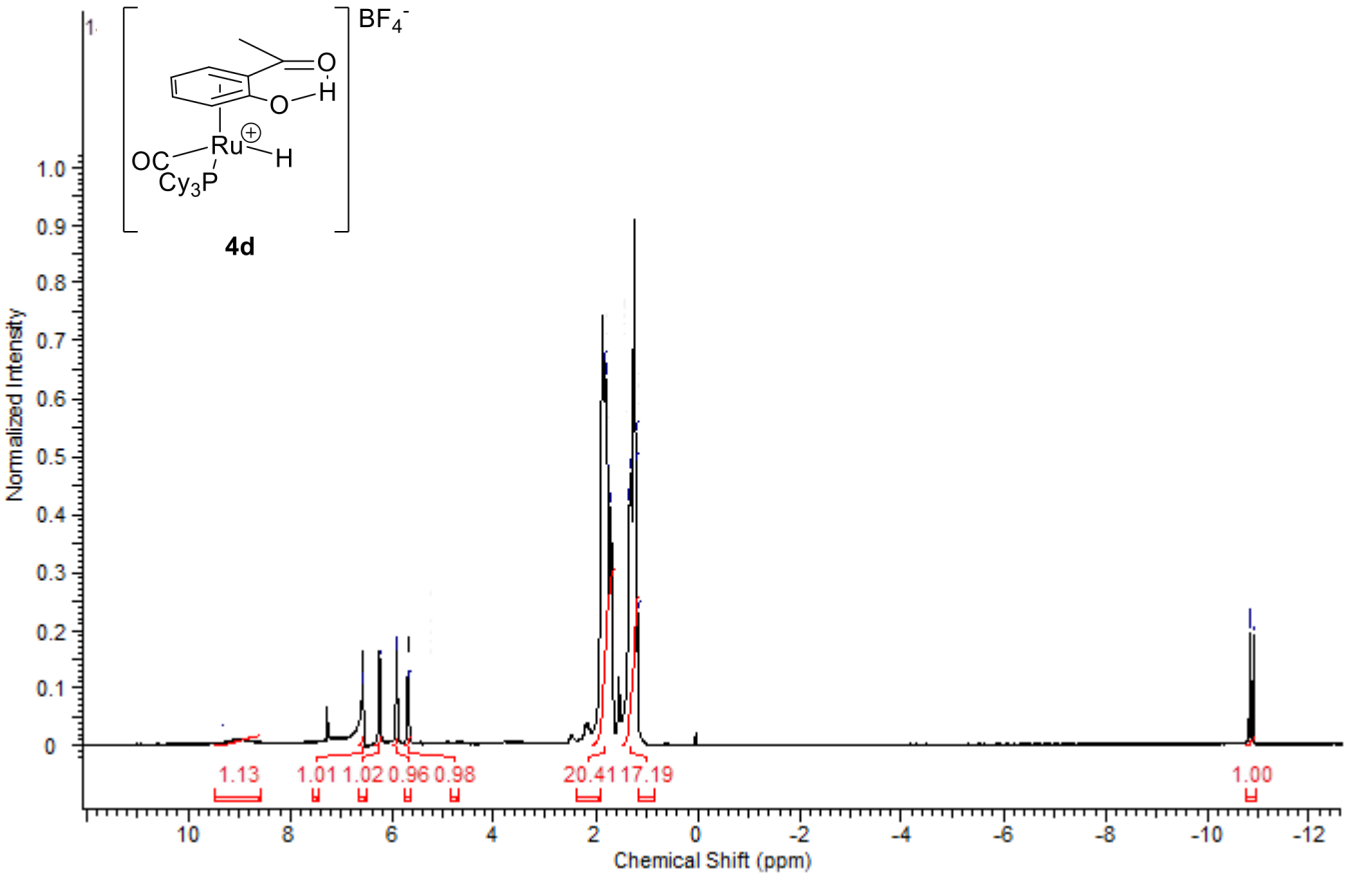

10-15-2014FenC1
Normalized Intensity
Chemical Shift (ppm)
128.25
127.05
125.08
148.34
142.82
139.36
79.92
77.32
77.00
76.68
58.58
51.18
51.16
35.23
31.39
29.45
26.92

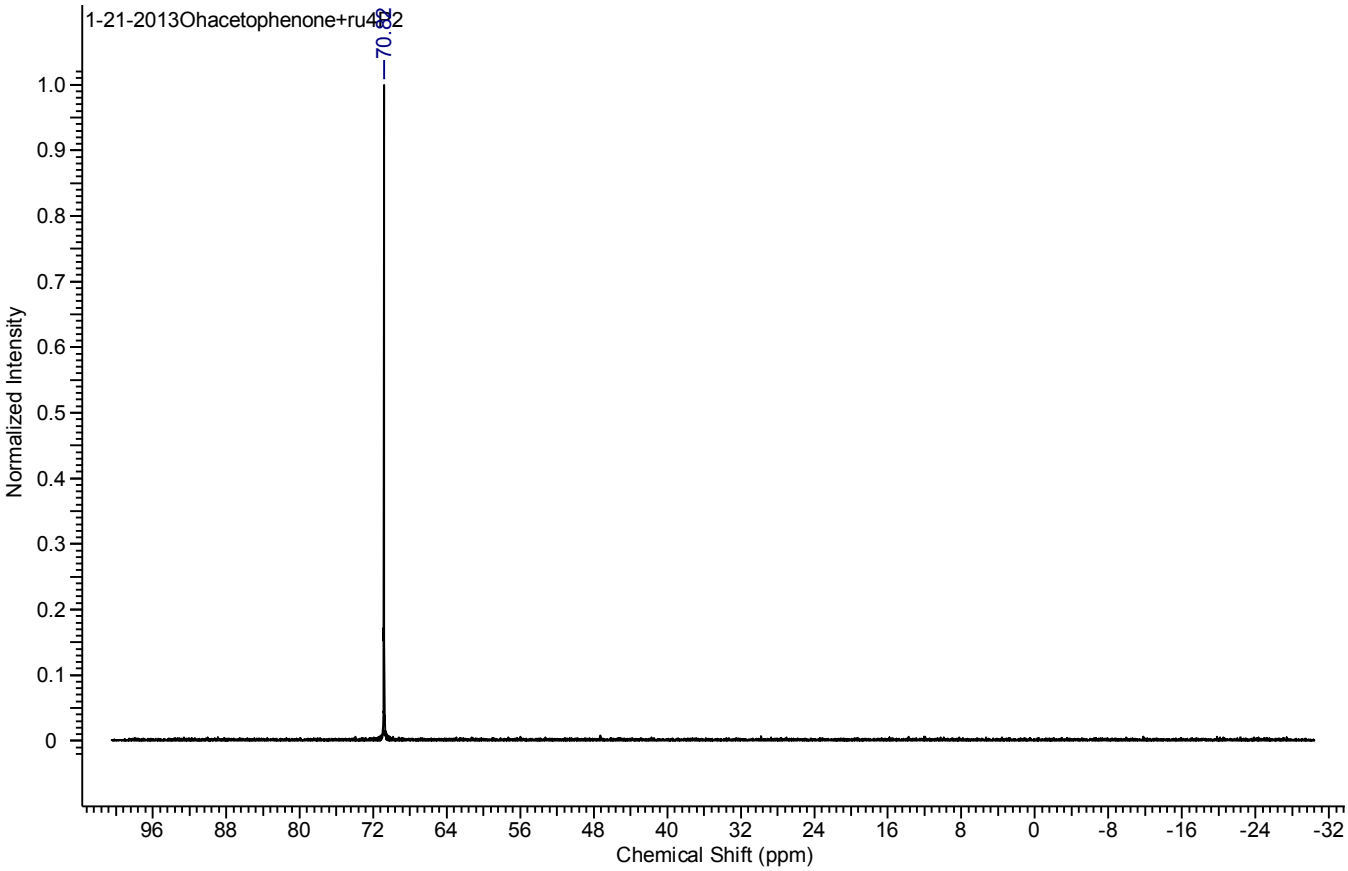

OH
Ru
H
OC
Cy3P
4a
Normalized Intensity
Chemical Shift (ppm)
1.0053
1.0237
0.7525
0.8445
0.7478
4.1242
3.9617
0.9002

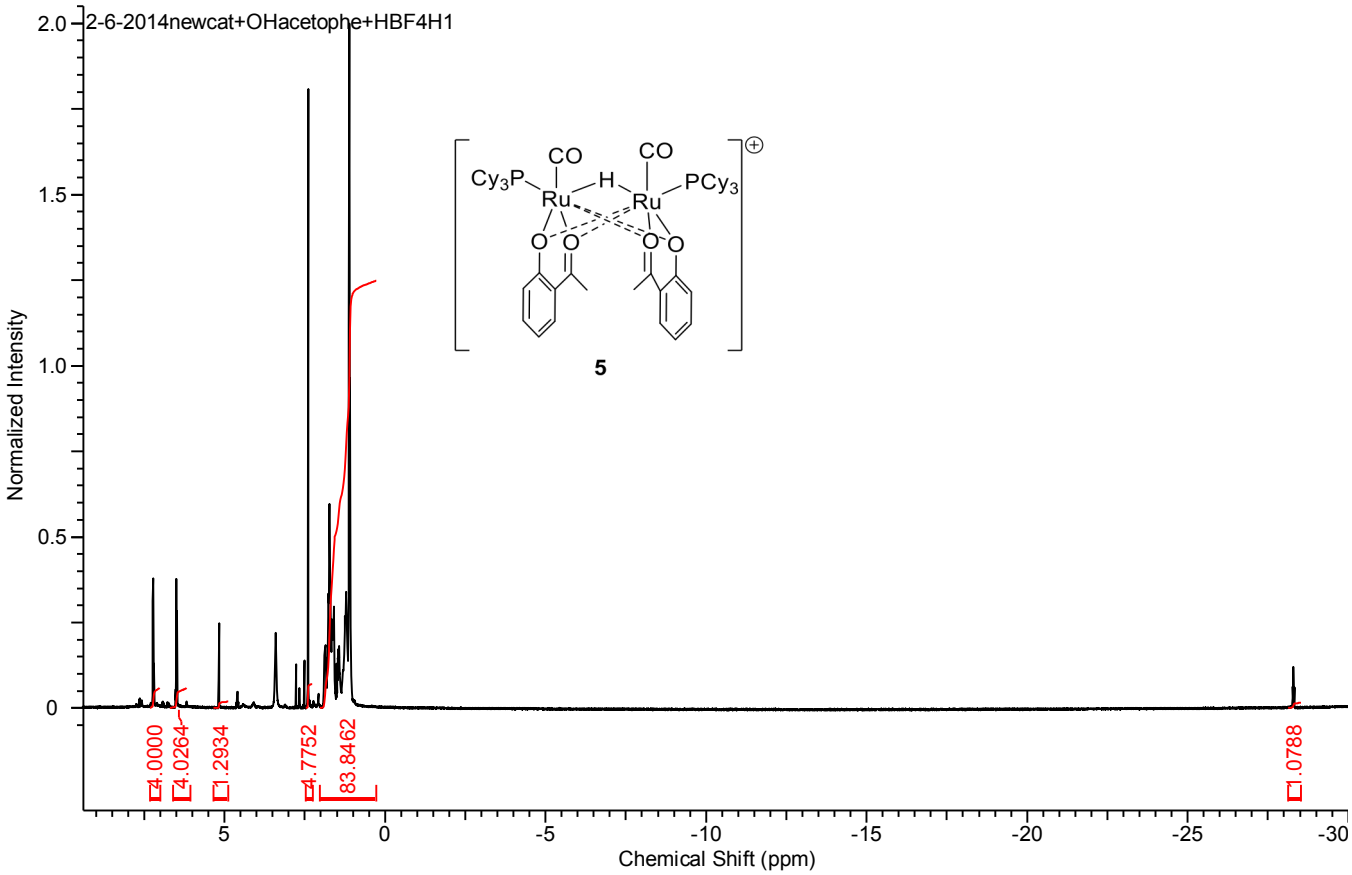

3-3-2014Ru4+PhenolP1
70.78
Normalized Intensity
Chemical Shift (ppm)

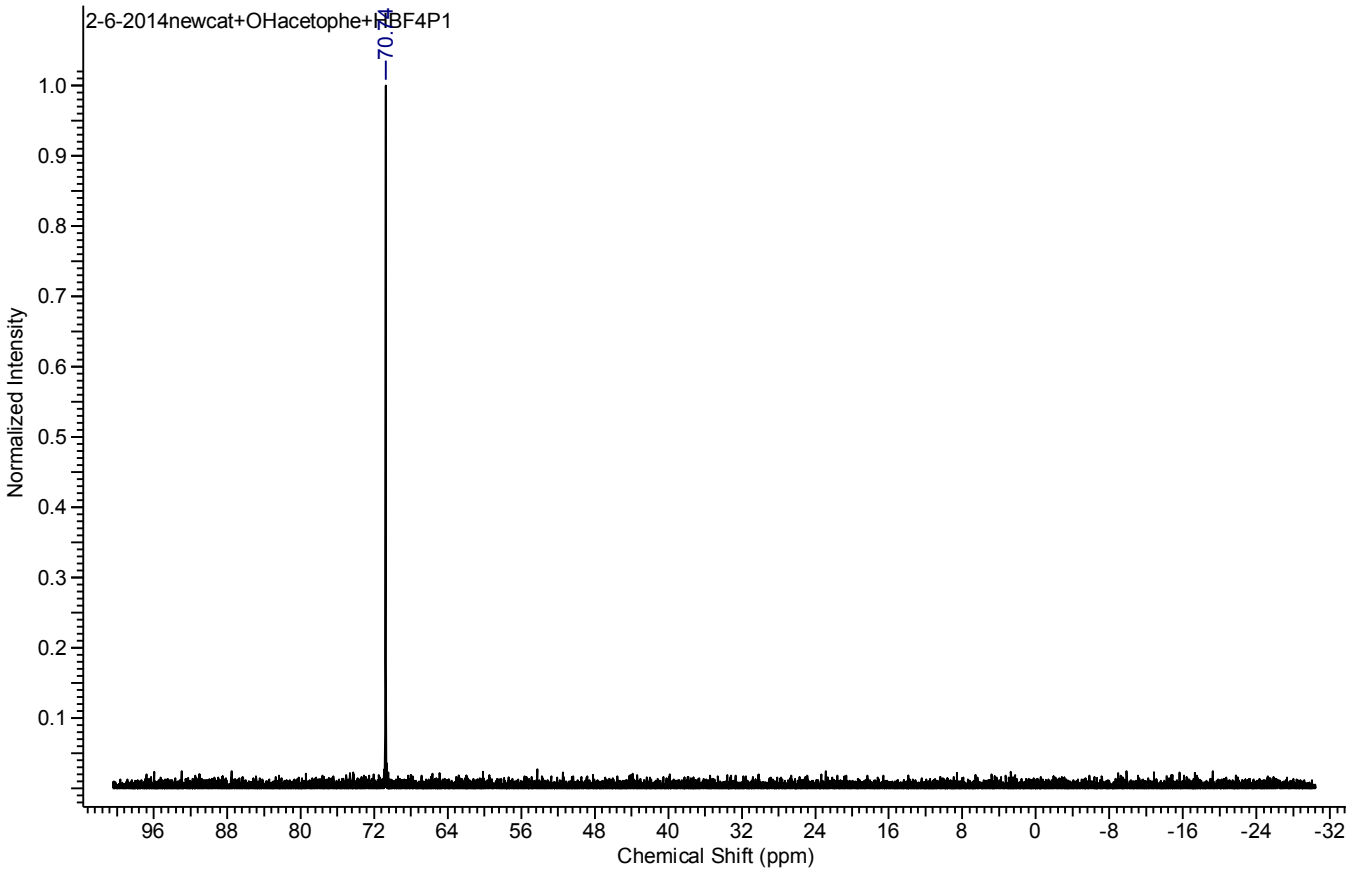

O
OH
OC
Ru
H
Cy3P
4b
Normalized Intensity
1.5
1.0
0.5
0
0.9996
3.7795
3.2612
4.8885
3.9687
30.1159
25.9509
1.8197
10
8
6
4
2
0
-2
-4
-6
-8
-10
-12
Chemical Shift (ppm)

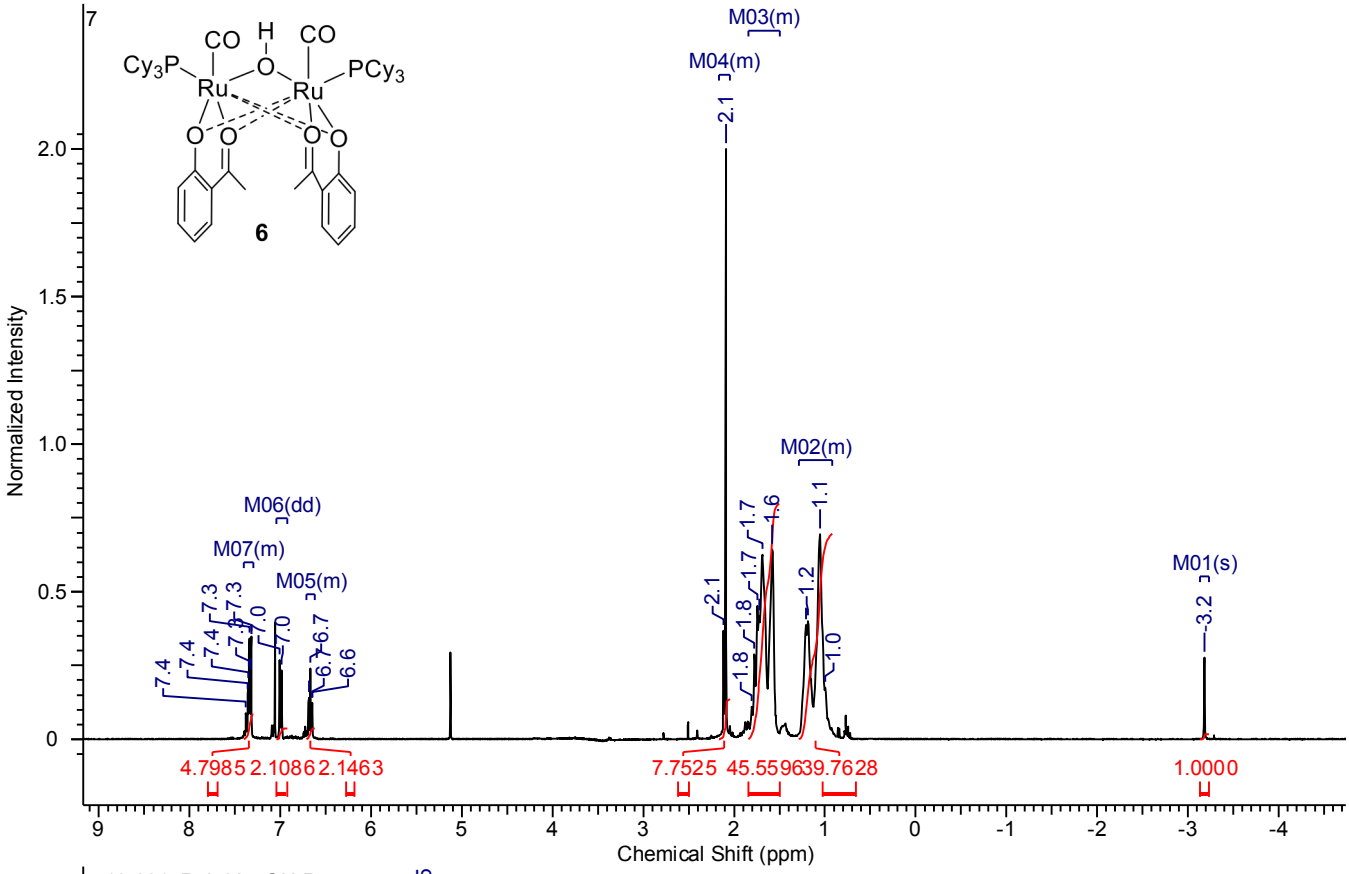

4-28-2014RuOMePhenolP
71.38
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
96
88
80
72
64
56
48
40
32
24
16
8
0
-8
-16
-24
-32
Chemical Shift (ppm)

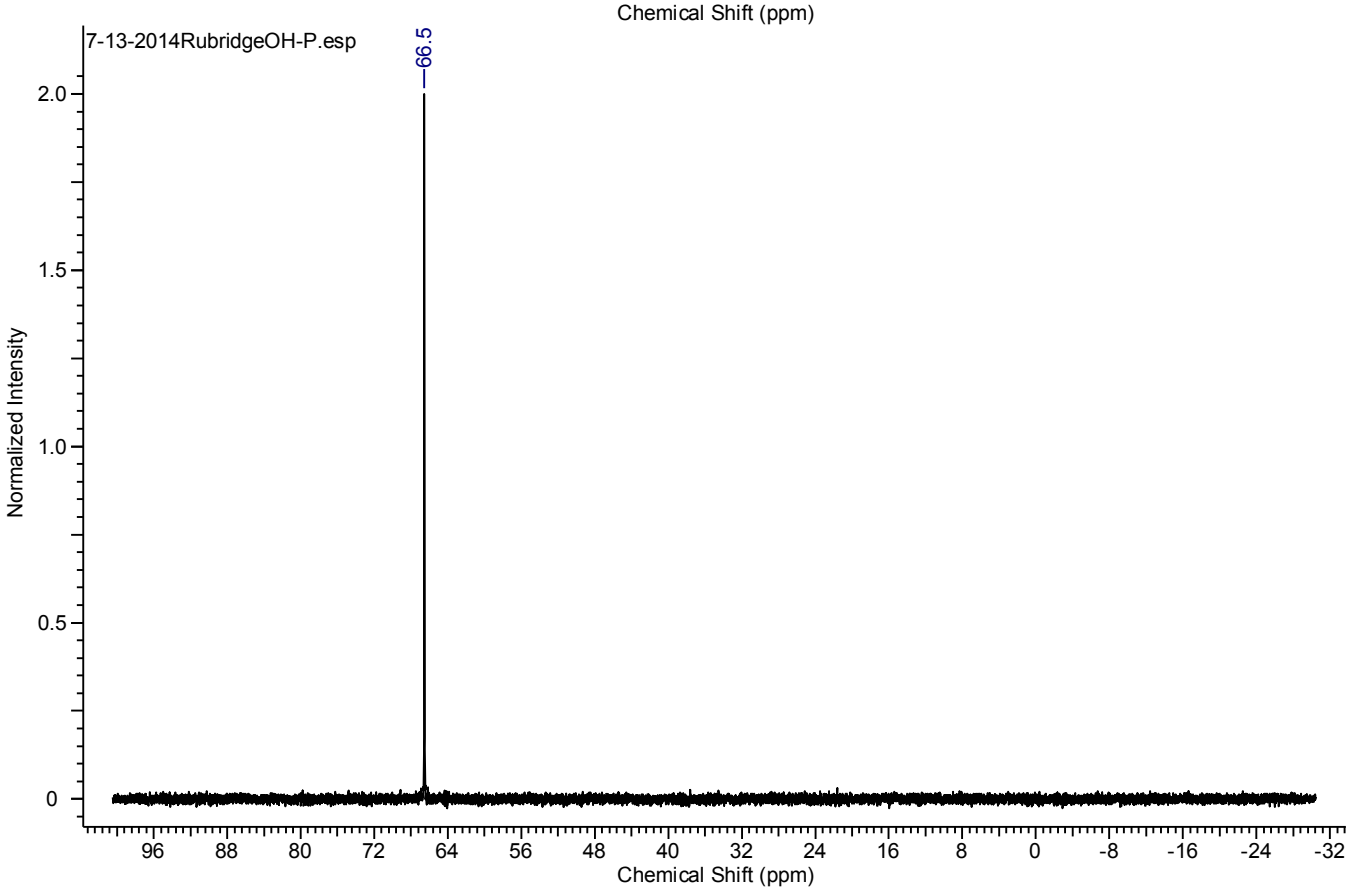

BF4-
O
H
O
OC
Ru
H
Cy3P
4d
Normalized Intensity
1.13
1.01 1.02 0.96 0.98
20.41 17.19
1.00
Chemical Shift (ppm)


1-21-2013Ohacetophenone+ru4d2
70.82
Normalized Intensity
Chemical Shift (ppm)


2-6-2014newcat+OHacetophe+HBF4H1
Normalized Intensity
Chemical Shift (ppm)
4.0000
4.0264
1.2934
4.7752
83.8462
1.0788
CO
CO
Cy3P
H
PCy3
Ru
Ru
O
O
O
O
5


2-6-2014newcat+OHacetophe+HBF4P1
70.74
Normalized Intensity
Chemical Shift (ppm)


7
CO
H
CO
Cy3P
O
PCy3
Ru
Ru
O
O
O
O
6
M03(m)
M04(m)
2.1
M02(m)
1.1
1.7
1.6
1.7
1.8
1.2
1.8
1.0
M06(dd)
M07(m)
M05(m)
7.4
7.4
7.4
7.3
7.3
7.0
7.0
6.7
6.7
6.6
M01(s)
3.2
4.79852.10862.1463
7.75255.55963.7628
1.0000
Normalized Intensity
Chemical Shift (ppm)


7-13-2014RubridgeOH-P.esp
66.5
Normalized Intensity
Chemical Shift (ppm)

11. X-Ray Crystallographic Data of 4a, 4b, 4c, 5 and 6.

Table S4. Crystal Data and Structure Refinement for 4a.

Identification code	yi2u
Empirical formula	$C_{28}H_{48}BF_4O_3PRu$
Formula weight	651.51
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	10.29093(13)
b/Å	18.5770(3)
c/Å	31.9420(4)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	6106.51(14)
Z	8
ρ_{calc}mg/mm^3	1.417
m/mm^{-1}	5.093
F(000)	2720.0
Crystal size/mm^3	0.2975 × 0.1164 × 0.0395
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	9.52 to 147.3°
Index ranges	-12 ≤ h ≤ 12, -22 ≤ k ≤ 15, -38 ≤ l ≤ 38
Reflections collected	30380
Independent reflections	6048 [R_{int} = 0.0287, R_{sigma} = 0.0198]
Data/restraints/parameters	6048/0/357
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.0943
Final R indexes [all data]	R_1 = 0.0443, wR_2 = 0.0966
Largest diff. peak/hole / e Å^{-3}	1.14/-0.69

Table S5. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ru1	4164.0(2)	2254.41(12)	3808.34(7)	22.86(8)
P1	4178.7(6)	3500.4(4)	3796.8(2)	16.24(14)
O1	6024(3)	782.5(14)	3649.7(9)	44.1(6)
O2	4662(4)	2302.3(17)	2884.3(8)	61.8(9)
C1	5356(3)	1181.3(17)	3922.1(11)	32.6(7)
C2	5909(3)	1723.6(17)	4174.9(10)	28.9(7)
C3	5120(4)	2104.3(17)	4456.6(9)	30.0(7)
C4	3774(4)	1958.1(17)	4491.2(10)	32.6(7)
C5	3235(4)	1427.6(18)	4233.1(11)	36.4(8)
C6	4014(3)	1044.7(17)	3941.4(12)	35.0(8)

C7	4489(4)	2289.0(19)	3241.4(12)	41.0(9)
C8	5829(3)	3904.3(15)	3779.1(8)	18.4(5)
C9	6584(3)	3702.0(18)	3384.7(9)	26.4(6)
C10	7878(3)	4107.8(19)	3370.9(10)	32.3(7)
C11	8681(3)	3988.2(19)	3764.5(11)	32.7(7)
C12	7904(3)	4157.5(18)	4159.9(10)	28.7(7)
C13	6631(3)	3734.3(16)	4169.4(9)	23.3(6)
C14	3442(3)	3873.4(15)	4279.2(8)	18.1(5)
C15	3700(3)	4671.7(16)	4381.1(9)	23.1(6)
C16	3168(3)	4855.7(17)	4816.4(9)	27.3(6)
C17	1725(3)	4676.4(18)	4855.9(10)	29.8(7)
C18	1463(3)	3893.5(18)	4741.4(9)	27.3(6)
C19	1974(3)	3721.4(17)	4304.3(9)	23.4(6)
C20	3379(3)	3877.3(17)	3320.5(9)	23.8(6)
C21	3340(4)	4693(2)	3296.7(12)	45.2(10)
C22	2868(5)	4945(2)	2864.7(13)	59.8(13)
C23	1566(4)	4631(3)	2754.1(13)	56.3(12)
C24	1571(4)	3827(2)	2788.3(11)	43.2(9)
C25	2031(3)	3565(2)	3217.0(11)	42.6(9)
F1	10646(3)	1851(2)	4763.5(8)	81.9(11)
F2	10064(4)	2273.3(19)	4136.0(9)	93.9(12)
F3	8601(3)	2170(2)	4638.3(11)	88.3(11)
F4	9427(4)	1199.3(13)	4315.8(8)	86.7(11)
O3	8446(3)	1097.1(15)	3540.3(9)	44.7(6)
C26	8704(4)	1694(2)	3262.1(13)	46.1(9)
C27	10120(4)	1699(3)	3145.9(15)	72.4(16)
C28	7846(5)	1621(4)	2889.2(15)	82.8(19)
B1	9688(4)	1885(2)	4468.5(11)	30.8(8)

Table S6. Anisotropic Displacement Parameters ($Å^2×10^3$) for 4a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	27.75(13)	17.50(12)	23.34(13)	-2.79(8)	1.01(8)	-4.18(9)
P1	16.1(3)	17.6(3)	15.1(3)	0.3(2)	-1.6(2)	-0.8(3)
O1	44.0(16)	28.4(13)	59.9(17)	-10.5(12)	14.8(13)	1.3(12)
O2	105(3)	58.3(19)	21.8(13)	-12.5(12)	6.6(15)	-0.6(18)
C1	39.3(18)	18.0(15)	40.4(18)	2.0(13)	9.2(15)	3.3(14)
C2	30.9(16)	24.5(15)	31.2(16)	7.1(13)	0.9(13)	2.7(13)
C3	45.7(19)	22.0(15)	22.3(14)	6.5(12)	-1.8(13)	2.8(14)
C4	47(2)	22.9(16)	27.9(15)	7.4(12)	12.5(14)	4.3(14)
C5	36.5(18)	22.9(16)	50(2)	8.1(15)	12.8(16)	-3.5(14)
C6	39.3(18)	15.2(14)	51(2)	3.0(14)	3.2(16)	-8.8(14)
C7	56(2)	28.6(18)	38(2)	-6.6(14)	-0.8(17)	-4.3(17)
C8	20.7(13)	17.5(13)	17.1(12)	1.9(10)	-3(1)	-3.3(11)
C9	21.3(14)	33.6(17)	24.4(14)	-5.4(12)	4.2(11)	-3.7(13)
C10	23.8(15)	40.8(19)	32.3(16)	-5.1(14)	6.6(13)	-6.1(14)

C11	17.2(14)	36.2(18)	44.8(19)	-5.4(15)	0.6(13)	-2.7(13)
C12	20.2(14)	33.6(17)	32.4(16)	-1.7(13)	-7.5(12)	0.4(13)
C13	20.3(13)	24.3(15)	25.3(14)	2.0(11)	-4.1(11)	1.0(12)
C14	18.9(13)	20.2(14)	15.3(12)	-0.1(10)	-0.4(10)	0.2(11)
C15	24.3(14)	20.8(14)	24.1(14)	-2.2(11)	2.4(11)	0.2(12)
C16	31.1(16)	26.4(16)	24.4(14)	-7.6(12)	1.7(12)	2.4(13)
C17	29.3(16)	36.6(18)	23.5(14)	-3.1(13)	5.0(12)	6.3(14)
C18	20.6(14)	37.5(18)	23.9(14)	2.9(13)	3.3(11)	-1.2(13)
C19	18.6(13)	27.9(15)	23.6(14)	-1.9(12)	1.1(11)	-2.3(12)
C20	22.6(14)	30.0(16)	18.6(13)	2.3(11)	-3.3(11)	1.7(12)
C21	64(3)	31.3(19)	39.9(19)	1.6(15)	-26.1(18)	10.6(18)
C22	90(4)	38(2)	51(2)	14.7(18)	-42(2)	-3(2)
C23	62(3)	70(3)	37(2)	-2.4(19)	-27.0(19)	28(2)
C24	30.3(17)	70(3)	29.1(17)	7.4(17)	-11.5(14)	-1.9(18)
C25	24.1(16)	75(3)	28.7(17)	12.5(17)	-7.4(13)	-4.8(17)
F1	70.0(18)	130(3)	45.2(14)	-39.0(16)	-29.5(13)	57.1(19)
F2	128(3)	110(3)	44.2(15)	23.2(15)	-9.3(17)	-75(2)
F3	35.2(13)	128(3)	102(2)	-59(2)	10.9(14)	0.6(16)
F4	180(4)	30.9(13)	49.3(15)	0.5(11)	-33.9(19)	10.7(17)
O3	43.8(15)	48.8(16)	41.6(14)	-3.2(12)	6.4(12)	-2.9(13)
C26	51(2)	42(2)	45(2)	-6.2(17)	-4.1(18)	0.7(19)
C27	46(3)	116(5)	55(3)	31(3)	-10(2)	-26(3)
C28	50(3)	151(6)	47(3)	12(3)	-1(2)	-19(3)
B1	28.9(18)	38(2)	25.7(17)	5.2(15)	1.7(14)	1.3(16)

Table S7. Bond Lengths for 4a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	P1	2.3150(7)	C10	C11	1.521(5)
Ru1	C1	2.369(3)	C11	C12	1.528(4)
Ru1	C2	2.359(3)	C12	C13	1.529(4)
Ru1	C3	2.309(3)	C14	C15	1.541(4)
Ru1	C4	2.285(3)	C14	C19	1.539(4)
Ru1	C5	2.262(3)	C15	C16	1.533(4)
Ru1	C6	2.292(3)	C16	C17	1.527(4)
Ru1	C7	1.842(4)	C17	C18	1.524(5)
P1	C8	1.858(3)	C18	C19	1.526(4)
P1	C14	1.852(3)	C20	C21	1.517(5)
P1	C20	1.866(3)	C20	C25	1.540(4)
O1	C1	1.334(4)	C21	C22	1.536(5)
O2	C7	1.155(5)	C22	C23	1.503(6)
C1	C2	1.411(5)	C23	C24	1.498(6)
C1	C6	1.406(5)	C24	C25	1.528(4)
C2	C3	1.403(5)	F1	B1	1.366(4)
C3	C4	1.416(5)	F2	B1	1.341(4)
C4	C5	1.399(5)	F3	B1	1.351(5)
C5	C6	1.421(5)	F4	B1	1.390(5)

C8	C9	1.527(4)	O3	C26	1.445(5)
C8	C13	1.528(4)	C26	C27	1.503(6)
C9	C10	1.531(4)	C26	C28	1.489(6)

Table S8. Bond Angles for 4a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Ru1	C1	147.19(9)	C4	C3	Ru1	71.12(19)
P1	Ru1	C2	114.89(8)	C3	C4	Ru1	72.99(17)
C2	Ru1	C1	34.72(12)	C5	C4	Ru1	71.16(19)
C3	Ru1	P1	97.60(8)	C5	C4	C3	118.5(3)
C3	Ru1	C1	62.63(12)	C4	C5	Ru1	72.99(18)
C3	Ru1	C2	34.96(11)	C4	C5	C6	121.0(3)
C4	Ru1	P1	104.90(9)	C6	C5	Ru1	73.01(19)
C4	Ru1	C1	75.04(12)	C1	C6	Ru1	75.45(18)
C4	Ru1	C2	63.86(12)	C1	C6	C5	119.5(3)
C4	Ru1	C3	35.89(13)	C5	C6	Ru1	70.65(18)
C4	Ru1	C6	64.85(13)	O2	C7	Ru1	178.2(4)
C5	Ru1	P1	133.74(9)	C9	C8	P1	113.01(19)
C5	Ru1	C1	63.60(12)	C9	C8	C13	110.4(2)
C5	Ru1	C2	74.94(12)	C13	C8	P1	112.65(19)
C5	Ru1	C3	63.90(13)	C8	C9	C10	110.2(2)
C5	Ru1	C4	35.84(13)	C11	C10	C9	112.2(3)
C5	Ru1	C6	36.34(12)	C10	C11	C12	111.6(3)
C6	Ru1	P1	169.61(10)	C11	C12	C13	111.1(3)
C6	Ru1	C1	35.05(12)	C8	C13	C12	109.9(2)
C6	Ru1	C2	63.22(12)	C15	C14	P1	117.74(19)
C6	Ru1	C3	75.17(12)	C19	C14	P1	112.12(19)
C7	Ru1	P1	87.04(11)	C19	C14	C15	109.5(2)
C7	Ru1	C1	94.94(15)	C16	C15	C14	110.2(2)
C7	Ru1	C2	111.36(15)	C17	C16	C15	111.9(2)
C7	Ru1	C3	143.92(16)	C18	C17	C16	111.1(3)
C7	Ru1	C4	168.06(14)	C17	C18	C19	111.0(3)
C7	Ru1	C5	133.63(15)	C18	C19	C14	110.3(2)
C7	Ru1	C6	103.22(15)	C21	C20	P1	115.3(2)
C8	P1	Ru1	114.23(9)	C21	C20	C25	110.0(3)
C8	P1	C20	103.12(13)	C25	C20	P1	115.5(2)
C14	P1	Ru1	110.99(9)	C20	C21	C22	111.0(3)
C14	P1	C8	104.39(12)	C23	C22	C21	112.0(4)
C14	P1	C20	110.93(13)	C24	C23	C22	111.5(3)
C20	P1	Ru1	112.66(10)	C23	C24	C25	112.5(3)
O1	C1	Ru1	129.4(2)	C24	C25	C20	110.6(3)
O1	C1	C2	124.2(3)	O3	C26	C27	109.5(4)
O1	C1	C6	115.8(3)	O3	C26	C28	108.3(4)
C2	C1	Ru1	72.27(18)	C28	C26	C27	112.2(4)
C6	C1	Ru1	69.50(19)	F1	B1	F4	109.8(3)
C6	C1	C2	120.0(3)	F2	B1	F1	111.3(4)

C1	C2	Ru1	73.01(19)	F2	B1	F3	110.3(4)
C3	C2	Ru1	70.57(18)	F2	B1	F4	105.7(3)
C3	C2	C1	119.6(3)	F3	B1	F1	109.8(3)
C2	C3	Ru1	74.47(18)	F3	B1	F4	109.9(4)
C2	C3	C4	121.3(3)				

Table S9. Hydrogen Bonds for 4a.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1	O3	0.80(5)	1.80(5)	2.584(4)	169(5)
O3	H3A	F4	1.00(6)	1.72(6)	2.682(4)	160(5)

Table S10. Torsion Angles for 4a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	P1	C8	C9	62.3(2)	C4	Ru1	C1	C2	-65.5(2)
Ru1	P1	C8	C13	-63.6(2)	C4	Ru1	C1	C6	67.4(2)
Ru1	P1	C14	C15	163.69(18)	C4	Ru1	C2	C1	101.7(2)
Ru1	P1	C14	C19	-67.9(2)	C4	Ru1	C2	C3	-29.20(19)
Ru1	P1	C20	C21	179.2(2)	C4	Ru1	C3	C2	131.7(3)
Ru1	P1	C20	C25	49.1(3)	C4	Ru1	C5	C6	-131.1(3)
Ru1	C1	C2	C3	55.0(3)	C4	Ru1	C6	C1	-99.9(2)
Ru1	C1	C6	C5	-57.3(3)	C4	Ru1	C6	C5	29.2(2)
Ru1	C2	C3	C4	55.8(3)	C4	Ru1	C7	O2	64(13)
Ru1	C3	C4	C5	56.6(3)	C4	C5	C6	Ru1	-57.3(3)
Ru1	C4	C5	C6	57.3(3)	C4	C5	C6	C1	2.4(5)
Ru1	C5	C6	C1	59.7(3)	C5	Ru1	P1	C8	126.89(17)
P1	Ru1	C1	O1	-91.2(4)	C5	Ru1	P1	C14	9.21(17)
P1	Ru1	C1	C2	28.9(3)	C5	Ru1	P1	C20	-115.88(17)
P1	Ru1	C1	C6	161.76(17)	C5	Ru1	C1	O1	137.9(4)
P1	Ru1	C2	C1	-163.20(16)	C5	Ru1	C1	C2	-101.9(2)
P1	Ru1	C2	C3	65.9(2)	C5	Ru1	C1	C6	30.9(2)
P1	Ru1	C3	C2	-123.38(18)	C5	Ru1	C2	C1	65.2(2)
P1	Ru1	C3	C4	104.97(18)	C5	Ru1	C2	C3	-65.8(2)
P1	Ru1	C4	C3	-82.28(18)	C5	Ru1	C3	C2	101.3(2)
P1	Ru1	C4	C5	148.58(19)	C5	Ru1	C3	C4	-30.38(19)
P1	Ru1	C5	C4	-44.2(3)	C5	Ru1	C4	C3	129.1(3)
P1	Ru1	C5	C6	-175.28(17)	C5	Ru1	C6	C1	-129.1(3)
P1	Ru1	C6	C1	-109.9(5)	C5	Ru1	C7	O2	39(13)
P1	Ru1	C6	C5	19.2(7)	C6	Ru1	P1	C8	111.2(5)
P1	Ru1	C7	O2	-116(13)	C6	Ru1	P1	C14	-6.5(5)
P1	C8	C9	C10	174.7(2)	C6	Ru1	P1	C20	-131.6(5)
P1	C8	C13	C12	-172.9(2)	C6	Ru1	C1	O1	107.1(4)
P1	C14	C15	C16	-172.6(2)	C6	Ru1	C1	C2	-132.8(3)
P1	C14	C19	C18	168.1(2)	C6	Ru1	C2	C1	28.2(2)
P1	C20	C21	C22	170.8(3)	C6	Ru1	C2	C3	-102.8(2)
P1	C20	C25	C24	-171.3(3)	C6	Ru1	C3	C2	64.2(2)
O1	C1	C2	Ru1	126.0(3)	C6	Ru1	C3	C4	-67.4(2)

O1	C1	C2	C3	-179.0(3)	C6	Ru1	C4	C3	99.6(2)
O1	C1	C6	Ru1	-124.9(3)	C6	Ru1	C4	C5	-29.6(2)
O1	C1	C6	C5	177.9(3)	C6	Ru1	C5	C4	131.1(3)
C1	Ru1	P1	C8	16.49(18)	C6	Ru1	C7	O2	62(13)
C1	Ru1	P1	C14	-101.20(18)	C6	C1	C2	Ru1	-52.5(3)
C1	Ru1	P1	C20	133.71(18)	C6	C1	C2	C3	2.5(5)
C1	Ru1	C2	C3	-131.0(3)	C7	Ru1	P1	C8	-78.04(16)
C1	Ru1	C3	C2	28.97(19)	C7	Ru1	P1	C14	164.28(16)
C1	Ru1	C3	C4	-102.7(2)	C7	Ru1	P1	C20	39.19(17)
C1	Ru1	C4	C3	63.73(19)	C7	Ru1	C1	O1	1.0(4)
C1	Ru1	C4	C5	-65.4(2)	C7	Ru1	C1	C2	121.1(2)
C1	Ru1	C5	C4	101.2(2)	C7	Ru1	C1	C6	-106.0(2)
C1	Ru1	C5	C6	-29.8(2)	C7	Ru1	C2	C1	-66.3(2)
C1	Ru1	C6	C5	129.1(3)	C7	Ru1	C2	C3	162.8(2)
C1	Ru1	C7	O2	97(13)	C7	Ru1	C3	C2	-28.0(3)
C1	C2	C3	Ru1	-56.2(3)	C7	Ru1	C3	C4	-159.6(2)
C1	C2	C3	C4	-0.4(5)	C7	Ru1	C4	C3	97.4(8)
C2	Ru1	P1	C8	34.18(13)	C7	Ru1	C4	C5	-31.7(9)
C2	Ru1	P1	C14	-83.51(13)	C7	Ru1	C5	C4	171.4(2)
C2	Ru1	P1	C20	151.40(13)	C7	Ru1	C5	C6	40.3(3)
C2	Ru1	C1	O1	-120.1(4)	C7	Ru1	C6	C1	79.6(3)
C2	Ru1	C1	C6	132.8(3)	C7	Ru1	C6	C5	-151.3(2)
C2	Ru1	C3	C4	-131.7(3)	C8	P1	C14	C15	40.2(2)
C2	Ru1	C4	C3	28.48(18)	C8	P1	C14	C19	168.6(2)
C2	Ru1	C4	C5	-100.7(2)	C8	P1	C20	C21	-57.2(3)
C2	Ru1	C5	C4	66.0(2)	C8	P1	C20	C25	172.7(3)
C2	Ru1	C5	C6	-65.1(2)	C8	C9	C10	C11	54.9(4)
C2	Ru1	C6	C1	-27.9(2)	C9	C8	C13	C12	59.7(3)
C2	Ru1	C6	C5	101.2(2)	C9	C10	C11	C12	-53.1(4)
C2	Ru1	C7	O2	128(13)	C10	C11	C12	C13	54.2(4)
C2	C1	C6	Ru1	53.8(3)	C11	C12	C13	C8	-57.5(3)
C2	C1	C6	C5	-3.5(5)	C13	C8	C9	C10	-58.2(3)
C2	C3	C4	Ru1	-57.4(3)	C14	P1	C8	C9	-176.3(2)
C2	C3	C4	C5	-0.8(5)	C14	P1	C8	C13	57.8(2)
C3	Ru1	P1	C8	66.01(13)	C14	P1	C20	C21	54.1(3)
C3	Ru1	P1	C14	-51.67(13)	C14	P1	C20	C25	-76.0(3)
C3	Ru1	P1	C20	-176.76(14)	C14	C15	C16	C17	-55.9(3)
C3	Ru1	C1	O1	-149.3(4)	C15	C14	C19	C18	-59.3(3)
C3	Ru1	C1	C2	-29.17(19)	C15	C16	C17	C18	54.6(3)
C3	Ru1	C1	C6	103.6(2)	C16	C17	C18	C19	-55.4(3)
C3	Ru1	C2	C1	131.0(3)	C17	C18	C19	C14	58.3(3)
C3	Ru1	C4	C5	-129.1(3)	C19	C14	C15	C16	57.8(3)
C3	Ru1	C5	C4	30.4(2)	C20	P1	C8	C9	-60.3(2)
C3	Ru1	C5	C6	-100.6(2)	C20	P1	C8	C13	173.8(2)
C3	Ru1	C6	C1	-63.2(2)	C20	P1	C14	C15	-70.3(2)
C3	Ru1	C6	C5	65.9(2)	C20	P1	C14	C19	58.2(2)

C3	Ru1	C7	O2	145(12)	C20	C21	C22	C23	55.9(5)
C3	C4	C5	Ru1	-57.5(3)	C21	C20	C25	C24	56.1(4)
C3	C4	C5	C6	-0.2(5)	C21	C22	C23	C24	-53.9(5)
C4	Ru1	P1	C8	101.89(13)	C22	C23	C24	C25	54.1(5)
C4	Ru1	P1	C14	-15.79(14)	C23	C24	C25	C20	-55.3(5)
C4	Ru1	P1	C20	-140.88(14)	C25	C20	C21	C22	-56.5(4)
C4	Ru1	C1	O1	174.4(4)					

Table S11. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4b.

Atom	*x*	*y*	*z*	U(eq)
H	2740(50)	2410(20)	3668(13)	57(13)
H1	6740(50)	930(30)	3616(15)	56(15)
H2	6809	1830	4155	35
H3	5496	2467	4627	36
H4	3248	2214	4685	39
H5	2334	1322	4253	44
H6	3631	699	3761	42
H8	5710	4438	3772	22
H9A	6063	3823	3134	32
H9B	6749	3177	3382	32
H10A	8381	3946	3124	39
H10B	7705	4629	3338	39
H11A	9462	4299	3755	39
H11B	8975	3481	3774	39
H12A	7713	4679	4170	34
H12B	8429	4034	4409	34
H13A	6819	3212	4180	28
H13B	6130	3864	4423	28
H14	3839	3596	4515	22
H15A	4646	4767	4373	28
H15B	3275	4980	4168	28
H16A	3660	4583	5030	33
H16B	3298	5375	4871	33
H17A	1437	4766	5147	36
H17B	1218	4995	4669	36
H18A	517	3800	4752	33
H18B	1890	3575	4948	33
H19A	1510	4019	4095	28
H19B	1807	3209	4239	28
H20	3947	3726	3082	29
H21A	4219	4888	3350	54
H21B	2749	4881	3516	54
H22A	2807	5476	2863	72
H22B	3511	4801	2650	72
H23A	897	4831	2944	68
H23B	1336	4771	2464	68

H24A	2147	3625	2570	52
H24B	681	3644	2737	52
H25A	2075	3033	3218	51
H25B	1400	3716	3434	51
H3A	9000(60)	1140(30)	3796(18)	90(20)
H26	8490	2153	3410	55
H27A	10648	1739	3400	109
H27B	10297	2110	2962	109
H27C	10337	1251	2999	109
H28A	8051	1172	2742	124
H28B	7986	2030	2701	124
H28C	6936	1613	2979	124

Table S12. Crystal Data and Structure Refinement for 4b.

Identification code	Yi2w
Empirical formula	$C_{29}H_{50}BO_4F_4PRu$
Formula weight	681.54
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.51406(15)
b/Å	12.03200(16)
c/Å	24.8572(3)
α/°	90.00
β/°	92.3407(12)
γ/°	90.00
Volume/Å^3	3141.94(7)
Z	4
ρ_{calc}mg/mm^3	1.441
m/mm^{-1}	0.606
F(000)	1424.0
Crystal size/mm^3	0.376 × 0.2569 × 0.1911
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.98 to 58.98°
Index ranges	$-13 \le h \le 14$, $-16 \le k \le 15$, $-33 \le l \le 33$
Reflections collected	35933
Independent reflections	7944 [R_{int} = 0.0327, R_{sigma} = 0.0301]
Data/restraints/parameters	7944/0/376
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0283, wR_2 = 0.0606
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0643
Largest diff. peak/hole / e Å^{-3}	1.07/-0.54

Table S13. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4b. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ru1	7689.97(12)	5768.65(11)	2143.73(5)	11.47(4)
P1	6765.7(4)	5746.1(3)	1281.97(16)	11.62(9)
O1	9821.6(13)	7147.4(12)	1741.7(5)	26.6(3)
O2	6013.4(14)	6064.8(11)	3304.4(5)	22.9(3)
O3	9275.5(13)	3312.6(10)	2243.5(5)	24.3(3)
C1	7017.9(18)	7053.1(14)	891.4(7)	18.7(4)
C2	6994(2)	6955.6(16)	280.7(7)	25.0(4)
C3	7364(2)	8055.2(16)	17.5(7)	25.2(4)
C4	6516(2)	9008.1(17)	189.3(8)	33.1(5)
C5	6526(2)	9109.5(15)	793.9(8)	27.5(4)
C6	6200.5(18)	8025.6(14)	1071.0(7)	18.7(4)

C7	7390.7(16)	4649.7(14)	835.7(6)	14.4(3)
C8	7001(2)	3454.0(15)	971.2(7)	23.3(4)
C9	7517(2)	2638.4(16)	559.7(8)	27.6(4)
C10	8959(2)	2705.2(16)	547.2(8)	27.3(4)
C11	9394.0(18)	3884.7(16)	431.7(7)	21.5(4)
C12	8849.2(17)	4717.5(15)	828.6(7)	18.3(4)
C13	5041.4(16)	5447.2(14)	1302.7(6)	14.1(3)
C14	4308.4(16)	6172.4(15)	1697.5(7)	17.0(3)
C15	2968.8(17)	5714.8(17)	1757.0(7)	21.5(4)
C16	2244.0(18)	5662.0(17)	1211.8(7)	22.8(4)
C17	2976.4(17)	4989.4(16)	806.4(7)	20.4(4)
C18	4326.0(17)	5427.0(16)	749.8(7)	18.1(4)
C19	9001.8(17)	6609.0(15)	1885.9(7)	17.2(3)
C20	10612.9(19)	3535.2(19)	2248.3(9)	32.8(5)
C21	6777.7(17)	5461.0(14)	3007.4(6)	15.9(3)
C22	8097.9(17)	5678.0(14)	3049.3(6)	16.2(3)
C23	8961.1(17)	4986.4(14)	2787.3(7)	16.9(3)
C24	8522.0(17)	4071.2(14)	2472.3(7)	16.2(3)
C25	7204.9(17)	3953.0(14)	2376.8(7)	15.5(3)
C26	6334.8(17)	4648.8(14)	2635.1(6)	15.6(3)
O4	3740.0(14)	5237.7(12)	3336.2(5)	24.4(3)
C27	3333.5(19)	4919.1(16)	3864.3(7)	22.4(4)
C28	2307(2)	4048.1(19)	3807.6(10)	37.3(5)
C29	4501(2)	4505.4(19)	4178.2(8)	32.4(5)
F1	2272.6(11)	7592.6(10)	3546.1(5)	29.2(3)
F2	410.6(12)	7876.8(11)	3057.6(5)	37.8(3)
F3	511.1(11)	6588.9(11)	3720.5(4)	31.6(3)
F4	1556(1)	6292.0(9)	2948.8(4)	23.8(2)
B1	1183(2)	7107.8(18)	3322.0(8)	20.2(4)

Table S14. Anisotropic Displacement Parameters ($Å^2×10^3$) for 4b. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	12.16(7)	10.89(7)	11.36(7)	0.30(5)	0.45(5)	-1.39(5)
P1	12.9(2)	11.6(2)	10.43(19)	-0.22(15)	1.56(15)	0.11(16)
O1	22.4(7)	29.1(7)	28.3(7)	5.2(6)	2.2(5)	-10.1(6)
O2	26.4(8)	21.7(7)	21.1(7)	-3.0(5)	9.3(5)	0.7(6)
O3	24.7(7)	16.5(6)	32.3(7)	2.4(5)	10.5(6)	5.3(6)
C1	25.6(10)	14.6(8)	16.1(8)	1.1(7)	4.9(7)	0.8(7)
C2	34.1(11)	21.8(9)	19.2(9)	1.0(7)	4.0(8)	1.8(8)
C3	38.0(12)	20.9(9)	17.3(9)	3.8(7)	8.8(8)	0.8(9)
C4	50.3(14)	23.6(10)	25.6(10)	6.5(8)	5.1(9)	5.5(10)
C5	42.3(13)	14.9(9)	25.9(10)	1.3(8)	8.9(9)	5.3(9)
C6	24.2(10)	15.7(8)	16.4(8)	-0.5(7)	3.2(7)	3.3(7)
C7	17.3(9)	13.2(8)	13.1(8)	-1.3(6)	3.8(6)	0.2(7)
C8	32.4(11)	14.2(8)	24.0(9)	-2.9(7)	12.0(8)	-3.9(8)

C9	42.7(13)	15.0(9)	25.9(10)	-3.6(8)	12.5(8)	-3.0(9)
C10	40.0(12)	19.8(9)	23(1)	0.1(8)	10.3(8)	11.0(9)
C11	20.6(10)	25.3(9)	18.8(9)	-1.3(7)	4.6(7)	6.3(8)
C12	17.8(9)	18.5(9)	18.8(8)	-1.2(7)	2.0(7)	2.2(7)
C13	13.0(8)	16.6(8)	12.7(8)	-0.4(6)	1.3(6)	-0.6(7)
C14	16.2(9)	21.2(9)	13.6(8)	-1.1(7)	1.5(6)	1.5(7)
C15	16.8(9)	30.5(10)	17.2(8)	-1.7(7)	2.8(7)	0.8(8)
C16	14.4(9)	32.0(11)	22.1(9)	-0.8(8)	-0.4(7)	-1.6(8)
C17	17.6(9)	26.4(10)	16.7(8)	-0.8(7)	-3.8(6)	-2.5(8)
C18	17.5(9)	23.6(9)	13.3(8)	-0.9(7)	-0.4(6)	-1.6(7)
C19	18.5(9)	17.8(8)	15.1(8)	0.4(7)	-0.3(6)	-0.2(7)
C20	22.3(11)	35.7(12)	41.3(12)	7(1)	11.4(9)	9.7(9)
C21	21.5(9)	14.9(8)	11.6(8)	3.0(6)	3.8(6)	0.8(7)
C22	24.8(9)	12.8(8)	10.8(8)	1.4(6)	-2.9(6)	-3.7(7)
C23	15.0(9)	17.5(8)	17.9(8)	6.2(7)	-2.8(6)	-1.5(7)
C24	18.9(9)	13.7(8)	16.4(8)	4.7(6)	3.8(6)	1.9(7)
C25	20.4(9)	12.5(8)	13.7(8)	2.5(6)	1.7(6)	-3.8(7)
C26	14.4(8)	17.2(8)	15.0(8)	3.0(7)	0.1(6)	-2.6(7)
O4	20.3(7)	32.6(8)	20.5(7)	5.2(6)	3.7(5)	8.1(6)
C27	26.6(10)	20.1(9)	21.2(9)	1.5(7)	7.9(7)	2.6(8)
C28	32.0(12)	34.7(12)	44.9(13)	10.4(10)	-0.9(10)	-7.3(10)
C29	35.0(12)	36.0(12)	25.9(10)	7.4(9)	-2.0(9)	-1.7(10)
F1	21.2(6)	29.5(6)	37.1(6)	-8.9(5)	1.3(5)	-7.5(5)
F2	40.2(8)	34.9(7)	37.7(7)	0.5(6)	-4.9(6)	18.5(6)
F3	25.0(6)	42.1(7)	28.4(6)	-1.1(5)	7.6(5)	-7.6(5)
F4	22.1(6)	25.2(6)	24.1(5)	-6.9(5)	0.0(4)	3.8(5)
B1	17.3(10)	19.4(10)	24(1)	-2.5(8)	0.7(8)	1.9(8)

Table S15. Bond Lengths for 4b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	P1	2.3159(4)	C8	C9	1.533(2)
Ru1	C19	1.8460(18)	C9	C10	1.519(3)
Ru1	C21	2.4154(16)	C10	C11	1.522(3)
Ru1	C22	2.2769(16)	C11	C12	1.533(2)
Ru1	C23	2.2487(16)	C13	C14	1.543(2)
Ru1	C24	2.3548(17)	C13	C18	1.540(2)
Ru1	C25	2.3221(17)	C14	C15	1.525(2)
Ru1	C26	2.3409(17)	C15	C16	1.529(2)
P1	C1	1.8726(18)	C16	C17	1.525(3)
P1	C7	1.8607(17)	C17	C18	1.525(2)
P1	C13	1.8511(17)	C21	C22	1.412(2)
O1	C19	1.147(2)	C21	C26	1.412(2)
O2	C21	1.329(2)	C22	C23	1.410(3)
O3	C20	1.431(2)	C23	C24	1.418(2)
O3	C24	1.349(2)	C24	C25	1.403(2)
C1	C2	1.522(2)	C25	C26	1.413(2)

C1	C6	1.529(2)	O4	C27	1.449(2)
C2	C3	1.533(3)	C27	C28	1.507(3)
C3	C4	1.524(3)	C27	C29	1.511(3)
C4	C5	1.507(3)	F1	B1	1.382(2)
C5	C6	1.520(2)	F2	B1	1.380(2)
C7	C8	1.537(2)	F3	B1	1.388(2)
C7	C12	1.536(2)	F4	B1	1.417(2)

Table S16. Bond Angles for 4b.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Ru1	C21	130.80(4)	C10	C9	C8	111.14(17)
P1	Ru1	C24	116.52(4)	C9	C10	C11	111.17(16)
P1	Ru1	C25	97.56(4)	C10	C11	C12	111.39(15)
P1	Ru1	C26	103.56(4)	C11	C12	C7	111.83(15)
C19	Ru1	P1	88.66(5)	C14	C13	P1	115.03(12)
C19	Ru1	C21	136.21(7)	C18	C13	P1	114.93(11)
C19	Ru1	C22	104.84(7)	C18	C13	C14	109.77(14)
C19	Ru1	C23	92.60(7)	C15	C14	C13	110.17(14)
C19	Ru1	C24	108.86(7)	C14	C15	C16	110.98(15)
C19	Ru1	C25	140.96(7)	C17	C16	C15	111.15(15)
C19	Ru1	C26	167.36(7)	C16	C17	C18	111.99(15)
C22	Ru1	P1	165.66(5)	C17	C18	C13	110.21(14)
C22	Ru1	C21	34.87(6)	O1	C19	Ru1	177.79(16)
C22	Ru1	C24	64.10(6)	O2	C21	Ru1	132.92(12)
C22	Ru1	C25	75.09(6)	O2	C21	C22	118.21(16)
C22	Ru1	C26	63.30(6)	O2	C21	C26	123.48(17)
C23	Ru1	P1	150.21(5)	C22	C21	Ru1	67.20(9)
C23	Ru1	C21	63.23(6)	C26	C21	Ru1	69.87(9)
C23	Ru1	C22	36.31(6)	C26	C21	C22	118.25(15)
C23	Ru1	C24	35.77(6)	C21	C22	Ru1	77.93(9)
C23	Ru1	C25	63.83(6)	C23	C22	Ru1	70.76(9)
C23	Ru1	C26	75.20(6)	C23	C22	C21	120.40(15)
C24	Ru1	C21	73.40(6)	C22	C23	Ru1	72.94(10)
C25	Ru1	C21	62.28(6)	C22	C23	C24	120.82(16)
C25	Ru1	C24	34.90(6)	C24	C23	Ru1	76.20(10)
C25	Ru1	C26	35.29(6)	O3	C24	Ru1	131.05(11)
C26	Ru1	C21	34.49(6)	O3	C24	C23	125.08(16)
C26	Ru1	C24	62.95(6)	O3	C24	C25	116.92(16)
C1	P1	Ru1	114.00(6)	C23	C24	Ru1	68.03(9)
C7	P1	Ru1	114.50(6)	C25	C24	Ru1	71.28(10)
C7	P1	C1	103.03(8)	C25	C24	C23	117.99(16)
C13	P1	Ru1	110.54(5)	C24	C25	Ru1	73.83(10)
C13	P1	C1	109.71(8)	C24	C25	C26	121.06(16)
C13	P1	C7	104.42(8)	C26	C25	Ru1	73.08(10)
C24	O3	C20	117.62(15)	C21	C26	Ru1	75.64(10)
C2	C1	P1	117.10(13)	C21	C26	C25	120.36(16)

C2	C1	C6	111.33(15)	C25	C26	Ru1	71.63(10)
C6	C1	P1	113.46(12)	O4	C27	C28	109.62(16)
C1	C2	C3	111.42(15)	O4	C27	C29	106.94(16)
C4	C3	C2	111.61(16)	C28	C27	C29	112.50(17)
C5	C4	C3	111.10(17)	F1	B1	F3	109.86(16)
C4	C5	C6	112.94(16)	F1	B1	F4	108.03(15)
C5	C6	C1	112.61(15)	F2	B1	F1	111.77(17)
C8	C7	P1	115.41(11)	F2	B1	F3	109.54(16)
C12	C7	P1	110.25(11)	F2	B1	F4	109.03(15)
C12	C7	C8	109.13(15)	F3	B1	F4	108.55(16)
C9	C8	C7	110.36(14)				

Table S17. Hydrogen Bonds for 4b.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O2	H2	O4	0.83(3)	1.78(3)	2.593(2)	169(3)
O4	H4	F4	0.71(2)	2.07(2)	2.7620(18)	165(3)

Table S18. Torsion Angles for 4b.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	P1	C1	C2	153.43(13)	C21	Ru1	C19	O1	-8(4)
Ru1	P1	C1	C6	-74.69(14)	C21	Ru1	C22	C23	128.52(15)
Ru1	P1	C7	C8	71.27(14)	C21	Ru1	C23	C22	-30.07(10)
Ru1	P1	C7	C12	-52.92(12)	C21	Ru1	C23	C24	98.78(11)
Ru1	P1	C13	C14	50.32(13)	C21	Ru1	C24	O3	174.91(18)
Ru1	P1	C13	C18	179.26(11)	C21	Ru1	C24	C23	-67.04(10)
Ru1	C21	C22	C23	-58.92(14)	C21	Ru1	C24	C25	65.11(10)
Ru1	C21	C26	C25	58.20(14)	C21	Ru1	C25	C24	-100.89(11)
Ru1	C22	C23	C24	-61.73(14)	C21	Ru1	C25	C26	29.62(9)
Ru1	C23	C24	O3	125.59(16)	C21	Ru1	C26	C25	-129.40(15)
Ru1	C23	C24	C25	-52.67(14)	C21	C22	C23	Ru1	62.51(14)
Ru1	C24	C25	C26	-58.11(14)	C21	C22	C23	C24	0.8(2)
Ru1	C25	C26	C21	-60.18(14)	C22	Ru1	P1	C1	126.25(19)
P1	Ru1	C19	O1	149(4)	C22	Ru1	P1	C7	-115.45(19)
P1	Ru1	C21	O2	-72.66(18)	C22	Ru1	P1	C13	2.13(19)
P1	Ru1	C21	C22	179.32(8)	C22	Ru1	C19	O1	-26(4)
P1	Ru1	C21	C26	44.81(12)	C22	Ru1	C21	O2	108.0(2)
P1	Ru1	C22	C21	-2.1(2)	C22	Ru1	C21	C26	-134.51(15)
P1	Ru1	C22	C23	126.43(17)	C22	Ru1	C23	C24	128.84(15)
P1	Ru1	C23	C22	-156.36(8)	C22	Ru1	C24	O3	-148.89(18)
P1	Ru1	C23	C24	-27.51(16)	C22	Ru1	C24	C23	-30.84(10)
P1	Ru1	C24	O3	47.08(18)	C22	Ru1	C24	C25	101.31(11)
P1	Ru1	C24	C23	165.14(9)	C22	Ru1	C25	C24	-65.90(10)
P1	Ru1	C24	C25	-62.72(10)	C22	Ru1	C25	C26	64.62(10)
P1	Ru1	C25	C24	126.66(9)	C22	Ru1	C26	C21	27.15(10)
P1	Ru1	C25	C26	-102.82(9)	C22	Ru1	C26	C25	-102.25(11)
P1	Ru1	C26	C21	-146.71(9)	C22	C21	C26	Ru1	-48.27(13)

P1	Ru1	C26	C25	83.88(9)	C22	C21	C26	C25	9.9(2)
P1	C1	C2	C3	-173.47(14)	C22	C23	C24	Ru1	60.11(14)
P1	C1	C6	C5	173.50(13)	C22	C23	C24	O3	-174.30(15)
P1	C7	C8	C9	177.17(14)	C22	C23	C24	C25	7.4(2)
P1	C7	C12	C11	-175.63(12)	C23	Ru1	P1	C1	-127.25(11)
P1	C13	C14	C15	-169.56(12)	C23	Ru1	P1	C7	-8.95(11)
P1	C13	C18	C17	170.72(12)	C23	Ru1	P1	C13	108.63(11)
O2	C21	C22	Ru1	-127.78(14)	C23	Ru1	C19	O1	-60(4)
O2	C21	C22	C23	173.29(15)	C23	Ru1	C21	O2	139.27(19)
O2	C21	C26	Ru1	128.83(16)	C23	Ru1	C21	C22	31.26(10)
O2	C21	C26	C25	-172.97(15)	C23	Ru1	C21	C26	-103.25(11)
O3	C24	C25	Ru1	-127.27(14)	C23	Ru1	C22	C21	-128.52(15)
O3	C24	C25	C26	174.63(15)	C23	Ru1	C24	O3	-118.1(2)
C1	P1	C7	C8	-164.39(14)	C23	Ru1	C24	C25	132.15(15)
C1	P1	C7	C12	71.43(13)	C23	Ru1	C25	C24	-28.88(10)
C1	P1	C13	C14	-76.24(13)	C23	Ru1	C25	C26	101.64(11)
C1	P1	C13	C18	52.71(14)	C23	Ru1	C26	C21	64.01(10)
C1	C2	C3	C4	-55.8(2)	C23	Ru1	C26	C25	-65.39(10)
C2	C1	C6	C5	-51.9(2)	C23	C24	C25	Ru1	51.13(13)
C2	C3	C4	C5	55.1(2)	C23	C24	C25	C26	-7.0(2)
C3	C4	C5	C6	-53.3(3)	C24	Ru1	P1	C1	-144.81(8)
C4	C5	C6	C1	52.1(2)	C24	Ru1	P1	C7	-26.52(8)
C6	C1	C2	C3	53.7(2)	C24	Ru1	P1	C13	91.06(8)
C7	P1	C1	C2	28.76(16)	C24	Ru1	C19	O1	-93(4)
C7	P1	C1	C6	160.64(13)	C24	Ru1	C21	O2	176.35(19)
C7	P1	C13	C14	173.93(12)	C24	Ru1	C21	C22	68.33(10)
C7	P1	C13	C18	-57.13(14)	C24	Ru1	C21	C26	-66.17(10)
C7	C8	C9	C10	58.7(2)	C24	Ru1	C22	C21	-98.11(11)
C8	C7	C12	C11	56.63(18)	C24	Ru1	C22	C23	30.41(10)
C8	C9	C10	C11	-56.2(2)	C24	Ru1	C23	C22	-128.84(15)
C9	C10	C11	C12	54.1(2)	C24	Ru1	C25	C26	130.52(15)
C10	C11	C12	C7	-55.0(2)	C24	Ru1	C26	C21	100.17(11)
C12	C7	C8	C9	-58.1(2)	C24	Ru1	C26	C25	-29.23(10)
C13	P1	C1	C2	-81.99(16)	C24	C25	C26	Ru1	58.46(14)
C13	P1	C1	C6	49.89(15)	C24	C25	C26	C21	-1.7(2)
C13	P1	C7	C8	-49.75(15)	C25	Ru1	P1	C1	-175.67(8)
C13	P1	C7	C12	-173.94(11)	C25	Ru1	P1	C7	-57.37(7)
C13	C14	C15	C16	-57.8(2)	C25	Ru1	P1	C13	60.20(7)
C14	C13	C18	C17	-57.77(19)	C25	Ru1	C19	O1	-110(4)
C14	C15	C16	C17	55.4(2)	C25	Ru1	C21	O2	-147.76(19)
C15	C16	C17	C18	-54.7(2)	C25	Ru1	C21	C22	104.22(11)
C16	C17	C18	C13	56.0(2)	C25	Ru1	C21	C26	-30.28(10)
C18	C13	C14	C15	58.98(18)	C25	Ru1	C22	C21	-62.62(10)
C19	Ru1	P1	C1	-34.35(8)	C25	Ru1	C22	C23	65.89(10)
C19	Ru1	P1	C7	83.95(8)	C25	Ru1	C23	C22	-100.64(11)
C19	Ru1	P1	C13	-158.47(8)	C25	Ru1	C23	C24	28.20(10)

C19 Ru1 C21 O2	76.2(2)	C25 Ru1 C24 O3	109.8(2)
C19 Ru1 C21 C22	-31.82(15)	C25 Ru1 C24 C23	-132.15(15)
C19 Ru1 C21 C26	-166.33(11)	C25 Ru1 C26 C21	129.40(15)
C19 Ru1 C22 C21	157.82(10)	C26 Ru1 P1 C1	148.92(8)
C19 Ru1 C22 C23	-73.66(11)	C26 Ru1 P1 C7	-92.79(7)
C19 Ru1 C23 C22	111.79(11)	C26 Ru1 P1 C13	24.79(8)
C19 Ru1 C23 C24	-119.36(11)	C26 Ru1 C19 O1	-45(4)
C19 Ru1 C24 O3	-51.13(18)	C26 Ru1 C21 O2	-117.5(2)
C19 Ru1 C24 C23	66.93(11)	C26 Ru1 C21 C22	134.51(15)
C19 Ru1 C24 C25	-160.92(10)	C26 Ru1 C22 C21	-26.88(10)
C19 Ru1 C25 C24	29.41(15)	C26 Ru1 C22 C23	101.64(11)
C19 Ru1 C25 C26	159.93(11)	C26 Ru1 C23 C22	-64.82(10)
C19 Ru1 C26 C21	48.4(4)	C26 Ru1 C23 C24	64.02(10)
C19 Ru1 C26 C25	-81.0(3)	C26 Ru1 C24 O3	139.34(18)
C20 O3 C24 Ru1	80.3(2)	C26 Ru1 C24 C23	-102.60(11)
C20 O3 C24 C23	-10.0(2)	C26 Ru1 C24 C25	29.54(9)
C20 O3 C24 C25	168.25(16)	C26 Ru1 C25 C24	-130.52(15)
C21 Ru1 P1 C1	124.68(8)	C26 C21 C22 Ru1	49.48(14)
C21 Ru1 P1 C7	-117.03(8)	C26 C21 C22 C23	-9.4(2)
C21 Ru1 P1 C13	0.55(8)		

Table S19. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4b.

Atom	*x*	*y*	*z*	U(eq)
H	6910(20)	6889(19)	2108(9)	39(6)
H2	5280(30)	5820(20)	3271(10)	42(8)
H1	7911	7280	993	22
H2A	6130	6737	148	30
H2B	7594	6367	177	30
H3A	8262	8231	119	30
H3B	7292	7975	-379	30
H4A	6819	9712	33	40
H4B	5634	8878	49	40
H5A	5905	9686	892	33
H5B	7380	9357	926	33
H6A	5292	7849	992	22
H6B	6322	8121	1465	22
H7	7052	4810	462	17
H8A	7339	3258	1336	28
H8B	6061	3400	969	28
H9A	7264	1872	654	33
H9B	7141	2812	198	33
H10A	9262	2199	266	33
H10B	9338	2459	898	33
H11A	9115	4092	60	26
H11B	10335	3917	458	26
H12A	9101	5479	727	22

H12B	9215	4566	1195	22
H13	4984	4672	1444	17
H14A	4768	6181	2053	20
H14B	4258	6945	1562	20
H15A	2501	6196	2004	26
H15B	3021	4961	1916	26
H16A	1400	5317	1258	27
H16B	2105	6425	1073	27
H17A	2516	5018	451	24
H17B	3016	4203	923	24
H18A	4293	6187	597	22
H18B	4786	4945	500	22
H20A	11035	2975	2032	49
H20B	10964	3508	2619	49
H20C	10756	4275	2097	49
H22	8406	6294	3255	19
H23	9848	5136	2822	20
H25	6893	3396	2135	19
H26	5447	4569	2558	19
H4	3240(20)	5520(20)	3190(10)	30(7)
H27	2989	5586	4049	27
H28A	1566	4359	3608	56
H28B	2058	3812	4166	56
H28C	2629	3407	3612	56
H29A	4859	3868	3991	49
H29B	4264	4279	4539	49
H29C	5136	5101	4207	49

Table S20. Crystal data and structure refinement for 4c.

Identification code	Yi3h
Empirical formula	$C_{25}H_{39}BClF_4O_2PRu$
Formula weight	625.86
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.38368(11)
b/Å	11.82238(9)
c/Å	23.1436(2)
α/°	90.00
β/°	102.7232(10)
γ/°	90.00
Volume/Å^3	2771.34(4)
Z	4
ρ_{calc}g/cm^3	1.500
μ/mm^{-1}	6.428
F(000)	1288.0
Crystal size/mm^3	0.3138 × 0.2705 × 0.1982
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.84 to 148.04
Index ranges	$-12 \le h \le 11$, $-14 \le k \le 14$, $-27 \le l \le 28$
Reflections collected	27608
Independent reflections	10695 [R_{int} = 0.0213, R_{sigma} = 0.0240]
Data/restraints/parameters	10695/1/663
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0217, wR_2 = 0.0540
Final R indexes [all data]	R_1 = 0.0222, wR_2 = 0.0544
Largest diff. peak/hole / e Å^{-3}	0.47/-0.51
Flack parameter	0.000(5)

Table S21. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4c. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ru1	6396.56(17)	7923.19(13)	4028.92(7)	11.64(5)
Cl1	7110.1(6)	10696.1(5)	4771.5(3)	21.64(13)
P1	7638.3(6)	7910.9(6)	3305.7(2)	12.78(11)
O1	4084(2)	8758(2)	3114.3(9)	31.9(6)
O1X	4320(60)	6520(50)	3230(20)	31.9(6)
O2	6511(2)	5782.6(16)	5020.5(9)	21.2(4)
C1	6673(3)	6881(2)	4919.5(10)	15.7(5)
C2	7891(3)	7351(2)	4870.7(11)	15.0(5)
C3	8028(3)	8541(2)	4821.1(11)	14.4(5)
C4	6931(3)	9248(2)	4792.6(11)	14.9(5)

C5	5681(3)	8762(2)	4777.6(11)	16.4(5)
C6	5549(3)	7586(2)	4839.3(11)	15.0(5)
C7	4996(3)	8455(2)	3461.1(12)	20.6(6)
C8	9115(3)	7001(2)	3525.1(11)	17.5(5)
C9	10218(3)	7150(3)	3181.6(12)	26.2(6)
C10	11455(3)	6478(3)	3486.7(14)	32.2(7)
C11	11142(3)	5236(3)	3546.1(14)	32.6(7)
C12	10018(3)	5077(3)	3864.1(14)	28.2(7)
C13	8786(3)	5730(2)	3561.7(13)	23.3(6)
C14	6651(3)	7528(2)	2558.7(11)	17.0(5)
C15	7433(3)	7514(3)	2067.6(12)	27.1(6)
C16	6516(3)	7382(3)	1455.6(12)	31.9(7)
C17	5680(3)	6333(3)	1416.9(12)	26.9(6)
C18	4920(3)	6320(3)	1908.6(12)	27.7(6)
C19	5840(3)	6436(2)	2522.1(12)	24.8(6)
C20	8340(3)	9302(2)	3172.8(11)	16.6(5)
C21	7287(3)	10215(2)	2963.3(13)	23.8(6)
C22	7933(3)	11283(2)	2778.0(13)	28.8(6)
C23	9010(4)	11734(2)	3288.2(14)	32.7(7)
C24	10026(3)	10823(3)	3524.4(13)	30.3(7)
C25	9364(3)	9754(2)	3703.5(12)	21.9(6)
C26	5310(80)	7260(60)	3560(30)	20.6(6)
Ru1A	3654.29(17)	2086.11(14)	914.40(7)	12.83(5)
Cl1A	2695.7(7)	-321.2(6)	-85.1(4)	31.04(16)
P1A	2475.4(6)	2016.7(6)	1659.4(2)	13.72(12)
O1A	5675(3)	494(3)	1591.8(11)	40.4(7)
O1Y	5930(17)	3334(16)	1755(7)	40.4(7)
O2A	3643(2)	4568.1(17)	152.9(10)	25.2(4)
C1A	3396(3)	3461(2)	139.8(11)	15.7(5)
C2A	4473(3)	2720(2)	140.2(11)	16.9(6)
C3A	4261(3)	1554(2)	81.6(11)	16.9(5)
C4A	2973(3)	1106(2)	31.5(11)	16.8(5)
C5A	1937(3)	1820(2)	91.5(10)	13.8(5)
C6A	2153(2)	3000(2)	155.8(10)	14.7(5)
C7A	4884(3)	1114(3)	1347.1(14)	25.2(7)
C7Y	5070(20)	2960(20)	1458(9)	25.2(7)
C8A	3549(3)	2128(3)	2421.2(10)	19.5(5)
C9A	2972(3)	1633(3)	2925.4(11)	23.1(6)
C10A	3986(3)	1690(3)	3516.1(12)	28.2(6)
C11A	4481(3)	2888(3)	3665.6(12)	32.3(6)
C12A	5052(3)	3379(3)	3171.1(13)	33.6(8)
C13A	4042(3)	3329(3)	2577.8(13)	29.7(7)
C14A	1184(3)	3122(2)	1536.9(11)	15.6(5)
C15A	262(3)	3130(2)	1976.0(12)	20.1(5)
C16A	-926(3)	3896(2)	1742.0(13)	26.7(6)
C17A	-503(3)	5089(2)	1615.7(13)	26.1(6)

C18A	468(3)	5086(2)	1207.9(13)	22.0(6)
C19A	1657(3)	4335(2)	1459.1(12)	17.7(5)
C20A	1540(3)	688(2)	1691.2(11)	16.1(5)
C21A	331(3)	532(2)	1182.4(12)	19.6(6)
C22A	-457(3)	-502(2)	1305.6(13)	24.1(6)
C23A	390(3)	-1563(2)	1388.2(14)	27.5(6)
C24A	1638(3)	-1408(2)	1866.7(14)	26.9(6)
C25A	2417(3)	-365(2)	1745.7(12)	21.4(6)
F1	8641.7(16)	4598.3(13)	4988.0(7)	24.2(3)
F2	7585(2)	3347(2)	4299.5(10)	61.8(7)
F3	9212.9(16)	2733.9(14)	5054.7(9)	33.8(4)
F4	7264(2)	3300.1(17)	5230.2(13)	55.4(7)
B1	8166(3)	3471(3)	4884.3(17)	26.1(7)
F1A	1547.0(16)	5807.4(13)	91.7(7)	24.3(3)
F2A	2597.4(17)	7015.5(17)	-417.7(9)	37.7(4)
F3A	2757.7(19)	7278.8(16)	564.6(9)	43.2(5)
F4A	812.0(16)	7620.8(13)	-86.5(8)	25.0(4)
B1A	1934(3)	6959(3)	39.8(14)	21.6(6)

Table S22. Anisotropic Displacement Parameters ($Å^2×10^3$) for 4c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	11.33(9)	12.21(8)	12.02(8)	0.30(7)	3.98(7)	-0.22(7)
Cl1	22.7(3)	12.9(3)	30.2(3)	-3.8(2)	7.7(3)	-0.3(2)
P1	14.0(3)	13.0(3)	12.3(3)	-0.2(3)	5.1(2)	-0.8(3)
O1	21.0(11)	45.8(13)	25.1(11)	8(1)	-2.9(9)	9.8(10)
O1X	21.0(11)	45.8(13)	25.1(11)	8(1)	-2.9(9)	9.8(10)
O2	22.6(11)	15.0(9)	29(1)	3.8(8)	12.3(8)	1.5(8)
C1	26.1(14)	12.3(12)	10.7(10)	1.9(9)	8.4(9)	-0.8(10)
C2	14.3(12)	19.6(14)	10.9(11)	-0.3(9)	2.2(9)	2.4(10)
C3	15.2(12)	15.8(12)	11.8(11)	-2.7(9)	2.3(9)	-1.9(10)
C4	19.9(13)	11.2(11)	13.9(11)	-2.5(9)	4.2(10)	-0.9(10)
C5	17.6(13)	17.4(12)	16.5(12)	-6(1)	8.5(10)	0(1)
C6	14.2(13)	19.0(13)	14.7(12)	1.5(9)	9.1(10)	-1.2(10)
C7	22.7(15)	23.7(14)	18.1(14)	-1.4(11)	10.4(12)	-1.5(12)
C8	19.1(13)	17.4(12)	17.2(11)	-0.2(11)	6.2(9)	2.5(11)
C9	23.8(14)	32.1(14)	26.1(13)	-0.6(13)	12.7(11)	6.8(13)
C10	22.9(15)	45.0(18)	32.3(16)	4.9(14)	14.0(13)	11.5(14)
C11	28.2(16)	39.0(17)	31.0(16)	-1.0(13)	7.6(13)	18.1(14)
C12	28.6(16)	19.5(13)	34.7(16)	1.1(12)	3.1(13)	6.0(12)
C13	22.1(15)	18.8(13)	27.9(14)	-1.9(11)	3.5(11)	3.0(11)
C14	16.4(13)	20.0(12)	14.7(12)	-0.2(9)	3.9(10)	-1(1)
C15	27.2(15)	38.9(15)	17.3(13)	-6.8(11)	9.8(11)	-12.2(12)
C16	37.0(18)	43.8(18)	15.7(14)	-2.8(12)	7.3(12)	-9.8(14)
C17	24.5(15)	35.4(16)	20.2(13)	-9.0(12)	3.4(11)	-3.2(13)
C18	24.9(15)	34.4(16)	22.5(14)	-3.7(12)	2.2(12)	-8.1(13)

C19	32.3(16)	24.9(14)	15.1(13)	-1.9(10)	0.7(11)	-9.8(12)
C20	20.8(14)	15.6(12)	14.7(12)	-1.3(10)	6.4(10)	-4.4(11)
C21	28.3(15)	15.0(13)	30.3(15)	5.0(11)	11.3(12)	1.3(11)
C22	40.2(18)	19.1(13)	31.0(15)	4.9(12)	16.2(13)	-1.4(13)
C23	53(2)	20.6(14)	31.4(16)	-3.9(12)	23.1(15)	-14.2(14)
C24	38.9(18)	29.0(15)	25.4(15)	-4.6(12)	12.3(13)	-19.7(14)
C25	26.0(15)	20.5(13)	20.8(13)	-2.4(11)	8.6(11)	-8.0(11)
C26	22.7(15)	23.7(14)	18.1(14)	-1.4(11)	10.4(12)	-1.5(12)
Ru1A	10.50(9)	16.21(9)	11.99(8)	2.05(7)	2.92(7)	1.39(8)
Cl1A	24.4(3)	14.6(3)	51.7(4)	-7.4(3)	3.1(3)	-1.1(3)
P1A	13.6(3)	16.5(3)	11.5(3)	1.4(3)	3.5(2)	0.2(3)
O1A	31.2(14)	60.4(18)	28.2(13)	14.5(12)	3.5(11)	28.2(13)
O1Y	31.2(14)	60.4(18)	28.2(13)	14.5(12)	3.5(11)	28.2(13)
O2A	18.5(10)	13.2(9)	44.4(13)	5.5(8)	7.6(9)	0.3(8)
C1A	15.7(13)	13.3(12)	17.7(12)	3.8(10)	3.1(10)	1.1(10)
C2A	17.4(13)	19.8(14)	14.9(11)	4.5(10)	6.5(10)	0(1)
C3A	14.7(13)	20.4(13)	16.4(12)	-0.3(10)	5.1(10)	3.2(10)
C4A	20.2(13)	12.3(12)	17.8(12)	-2.2(9)	4(1)	0(1)
C5A	12.1(12)	16.8(13)	12.5(11)	0.7(9)	2.6(9)	-0.4(9)
C6A	12.7(11)	18.2(12)	12.8(10)	4.2(10)	1.6(9)	3.3(11)
C7A	24.0(17)	38.7(18)	14.9(14)	0.5(14)	8.7(13)	3.5(15)
C7Y	24.0(17)	38.7(18)	14.9(14)	0.5(14)	8.7(13)	3.5(15)
C8A	17.1(12)	27.9(13)	13.8(11)	3.5(11)	4.2(9)	-0.4(12)
C9A	22.7(14)	34.6(14)	13.1(12)	4.1(11)	5.9(10)	-0.7(11)
C10A	25.8(15)	44.5(17)	14.1(13)	4.5(11)	4.2(11)	3.9(13)
C11A	30.1(15)	50.2(18)	14.6(12)	-1.8(14)	0.6(11)	4.4(16)
C12A	32.1(17)	46.7(18)	17.6(14)	-4.1(13)	-4.2(12)	-12.5(15)
C13A	34.4(17)	33.4(16)	18.5(14)	1.8(11)	-0.8(12)	-9.6(13)
C14A	14.8(12)	15.9(14)	16.4(11)	-0.2(9)	4.3(9)	-0.3(10)
C15A	21.3(13)	18.5(14)	22.6(12)	1.4(10)	9.1(10)	2.3(10)
C16A	23.8(15)	29.3(15)	30.3(15)	0.0(12)	13.3(12)	6.5(12)
C17A	27.8(15)	25.6(14)	26.3(14)	-1.2(11)	8.7(12)	9.8(12)
C18A	24.1(15)	17.1(13)	25.3(14)	-0.4(10)	6.2(12)	1.2(11)
C19A	17.5(14)	15.7(12)	20.4(12)	-0.8(10)	5.5(10)	0(1)
C20A	17.6(13)	17.0(12)	14.4(12)	3.8(9)	4.8(10)	1.5(10)
C21A	20.4(14)	19.3(13)	18.4(13)	1(1)	2.9(10)	-4.0(11)
C22A	28.3(15)	19.4(13)	26.7(14)	0.0(11)	10.5(12)	-5.5(11)
C23A	35.4(17)	15.4(13)	36.0(16)	-3.2(12)	17.0(13)	-5.2(12)
C24A	29.6(16)	16.0(13)	37.6(16)	8.9(12)	12.5(13)	4.5(12)
C25A	22.2(14)	19.5(13)	25.5(14)	6.2(11)	11.8(11)	5.2(11)
F1	21.2(8)	17.1(7)	34.1(9)	2.0(6)	6.0(7)	-1.9(6)
F2	53.8(14)	51.7(13)	60.8(15)	-21.3(11)	-28.9(11)	4.9(11)
F3	14.9(8)	19.9(9)	64.6(12)	4.8(8)	4.5(8)	2.4(7)
F4	30.9(11)	29.9(10)	117(2)	15.6(11)	41.5(13)	0.9(8)
B1	12.8(15)	19.6(15)	43(2)	-1.9(14)	-0.5(13)	0.5(12)
F1A	21.7(8)	18.5(8)	32.9(9)	5.2(7)	6.6(7)	0.0(7)

F2A	25.9(9)	37.3(10)	56.2(11)	9.7(10)	22.4(8)	-0.8(9)
F3A	35(1)	33.6(11)	47.8(11)	-2.0(9)	-19.1(9)	-1.6(8)
F4A	14.6(8)	20.3(8)	38.5(9)	1.9(7)	2.3(7)	3.2(6)
B1A	14.2(14)	17.3(15)	31.8(16)	3.3(13)	1.7(11)	-0.7(12)

Table S23. Bond Lengths for 4c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	P1	2.3271(6)	Ru1A	C4A	2.320(3)
Ru1	C1	2.364(2)	Ru1A	C5A	2.326(2)
Ru1	C2	2.308(3)	Ru1A	C6A	2.340(2)
Ru1	C3	2.323(3)	Ru1A	C7A	1.842(3)
Ru1	C4	2.335(2)	Ru1A	C7Y	2.00(2)
Ru1	C5	2.259(2)	Cl1A	C4A	1.723(3)
Ru1	C6	2.276(2)	P1A	C8A	1.871(3)
Ru1	C7	1.843(3)	P1A	C14A	1.849(3)
Ru1	C26	1.59(8)	P1A	C20A	1.856(3)
Cl1	C4	1.724(3)	O1A	C7A	1.152(4)
P1	C8	1.850(3)	O1Y	C7Y	1.10(3)
P1	C14	1.861(3)	O2A	C1A	1.333(3)
P1	C20	1.851(3)	C1A	C2A	1.421(4)
O1	C7	1.155(4)	C1A	C6A	1.408(4)
O1X	C26	1.43(10)	C2A	C3A	1.398(3)
O2	C1	1.336(3)	C3A	C4A	1.419(4)
C1	C2	1.408(4)	C4A	C5A	1.398(4)
C1	C6	1.414(4)	C5A	C6A	1.416(4)
C2	C3	1.421(3)	C8A	C9A	1.540(3)
C3	C4	1.403(4)	C8A	C13A	1.525(4)
C4	C5	1.413(4)	C9A	C10A	1.532(4)
C5	C6	1.407(4)	C10A	C11A	1.520(5)
C8	C9	1.542(3)	C11A	C12A	1.516(4)
C8	C13	1.547(4)	C12A	C13A	1.534(4)
C9	C10	1.542(4)	C14A	C15A	1.542(3)
C10	C11	1.517(5)	C14A	C19A	1.539(3)
C11	C12	1.522(4)	C15A	C16A	1.530(4)
C12	C13	1.527(4)	C16A	C17A	1.524(4)
C14	C15	1.535(4)	C17A	C18A	1.525(4)
C14	C19	1.534(4)	C18A	C19A	1.528(4)
C15	C16	1.531(4)	C20A	C21A	1.532(4)
C16	C17	1.505(4)	C20A	C25A	1.531(4)
C17	C18	1.520(4)	C21A	C22A	1.531(4)
C18	C19	1.533(4)	C22A	C23A	1.520(4)
C20	C21	1.537(4)	C23A	C24A	1.519(4)
C20	C25	1.533(4)	C24A	C25A	1.534(4)
C21	C22	1.535(4)	F1	B1	1.423(4)
C22	C23	1.532(4)	F2	B1	1.363(4)
C23	C24	1.522(5)	F3	B1	1.381(4)

C24	C25	1.539(4)	F4	B1	1.375(4)
Ru1A	P1A	2.3255(6)	F1A	B1A	1.432(3)
Ru1A	C1A	2.390(2)	F2A	B1A	1.386(4)
Ru1A	C2A	2.273(3)	F3A	B1A	1.376(4)
Ru1A	C3A	2.246(3)	F4A	B1A	1.380(3)

Table S24. Bond Angles for 4c.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Ru1	C1	130.06(7)	C2A	Ru1A	C5A	75.62(9)
P1	Ru1	C4	118.14(7)	C2A	Ru1A	C6A	63.86(9)
C2	Ru1	P1	103.26(7)	C3A	Ru1A	P1A	156.86(7)
C2	Ru1	C1	35.05(10)	C3A	Ru1A	C1A	63.46(9)
C2	Ru1	C3	35.74(8)	C3A	Ru1A	C2A	36.04(9)
C2	Ru1	C4	63.54(9)	C3A	Ru1A	C4A	36.17(10)
C3	Ru1	P1	98.41(7)	C3A	Ru1A	C5A	64.45(9)
C3	Ru1	C1	63.16(9)	C3A	Ru1A	C6A	75.64(9)
C3	Ru1	C4	35.06(9)	C4A	Ru1A	P1A	121.82(7)
C4	Ru1	C1	74.15(9)	C4A	Ru1A	C1A	73.54(9)
C5	Ru1	P1	151.92(7)	C4A	Ru1A	C5A	35.02(9)
C5	Ru1	C1	63.73(9)	C4A	Ru1A	C6A	63.01(9)
C5	Ru1	C2	75.79(10)	C5A	Ru1A	C1A	62.53(9)
C5	Ru1	C3	64.06(9)	C5A	Ru1A	C6A	35.33(9)
C5	Ru1	C4	35.76(9)	C6A	Ru1A	C1A	34.62(9)
C5	Ru1	C6	36.14(10)	C7A	Ru1A	P1A	89.43(10)
C6	Ru1	P1	165.45(7)	C7A	Ru1A	C1A	141.44(12)
C6	Ru1	C1	35.41(9)	C7A	Ru1A	C2A	107.41(12)
C6	Ru1	C2	64.10(10)	C7A	Ru1A	C3A	89.98(12)
C6	Ru1	C3	75.63(10)	C7A	Ru1A	C4A	101.99(12)
C6	Ru1	C4	64.16(9)	C7A	Ru1A	C5A	132.50(13)
C7	Ru1	P1	87.96(9)	C7A	Ru1A	C6A	164.55(12)
C7	Ru1	C1	136.47(11)	C7A	Ru1A	C7Y	69.8(7)
C7	Ru1	C2	168.53(10)	C7Y	Ru1A	P1A	89.2(6)
C7	Ru1	C3	141.19(11)	C7Y	Ru1A	C1A	93.8(7)
C7	Ru1	C4	109.23(11)	C7Y	Ru1A	C2A	88.6(6)
C7	Ru1	C5	93.21(11)	C7Y	Ru1A	C3A	112.2(6)
C7	Ru1	C6	105.05(11)	C7Y	Ru1A	C4A	148.4(6)
C26	Ru1	P1	86(2)	C7Y	Ru1A	C5A	155.6(7)
C26	Ru1	C1	106(3)	C7Y	Ru1A	C6A	120.7(7)
C26	Ru1	C2	133(3)	C8A	P1A	Ru1A	113.23(8)
C26	Ru1	C3	168(3)	C14A	P1A	Ru1A	110.11(8)
C26	Ru1	C4	150(3)	C14A	P1A	C8A	110.85(12)
C26	Ru1	C5	116(3)	C14A	P1A	C20A	103.64(12)
C26	Ru1	C6	98(2)	C20A	P1A	Ru1A	115.12(9)
C26	Ru1	C7	50(3)	C20A	P1A	C8A	103.33(12)
C8	P1	Ru1	111.30(8)	O2A	C1A	Ru1A	131.39(19)
C8	P1	C14	111.54(12)	O2A	C1A	C2A	117.2(2)

C8	P1	C20	103.26(13)	O2A	C1A	C6A	123.5(2)
C14	P1	Ru1	112.99(9)	C2A	C1A	Ru1A	67.80(14)
C20	P1	Ru1	114.49(9)	C6A	C1A	Ru1A	70.73(14)
C20	P1	C14	102.59(12)	C6A	C1A	C2A	119.2(2)
O2	C1	Ru1	131.54(18)	C1A	C2A	Ru1A	76.84(15)
O2	C1	C2	123.2(2)	C3A	C2A	Ru1A	70.91(16)
O2	C1	C6	117.6(2)	C3A	C2A	C1A	120.0(3)
C2	C1	Ru1	70.31(14)	C2A	C3A	Ru1A	73.05(17)
C2	C1	C6	119.1(2)	C2A	C3A	C4A	120.1(3)
C6	C1	Ru1	68.87(14)	C4A	C3A	Ru1A	74.76(15)
C1	C2	Ru1	74.64(15)	Cl1A	C4A	Ru1A	129.42(14)
C1	C2	C3	120.4(3)	C3A	C4A	Ru1A	69.07(14)
C3	C2	Ru1	72.70(16)	C3A	C4A	Cl1A	120.0(2)
C2	C3	Ru1	71.56(16)	C5A	C4A	Ru1A	72.74(14)
C4	C3	Ru1	72.94(15)	C5A	C4A	Cl1A	120.1(2)
C4	C3	C2	119.9(3)	C5A	C4A	C3A	119.9(2)
Cl1	C4	Ru1	130.83(13)	C4A	C5A	Ru1A	72.25(14)
C3	C4	Ru1	72.00(14)	C4A	C5A	C6A	119.9(2)
C3	C4	Cl1	120.1(2)	C6A	C5A	Ru1A	72.88(14)
C3	C4	C5	119.4(2)	C1A	C6A	Ru1A	74.64(14)
C5	C4	Ru1	69.17(14)	C1A	C6A	C5A	120.2(2)
C5	C4	Cl1	120.5(2)	C5A	C6A	Ru1A	71.79(15)
C4	C5	Ru1	75.06(15)	O1A	C7A	Ru1A	176.5(3)
C6	C5	Ru1	72.57(15)	O1Y	C7Y	Ru1A	172(2)
C6	C5	C4	120.6(3)	C9A	C8A	P1A	115.90(19)
C1	C6	Ru1	75.72(14)	C13A	C8A	P1A	112.87(19)
C5	C6	Ru1	71.29(15)	C13A	C8A	C9A	109.9(2)
C5	C6	C1	120.0(3)	C10A	C9A	C8A	110.7(2)
O1	C7	Ru1	177.1(3)	C11A	C10A	C9A	112.1(2)
C9	C8	P1	117.20(19)	C12A	C11A	C10A	110.7(3)
C9	C8	C13	109.7(2)	C11A	C12A	C13A	110.9(3)
C13	C8	P1	113.57(19)	C8A	C13A	C12A	112.1(3)
C8	C9	C10	110.1(2)	C15A	C14A	P1A	115.96(17)
C11	C10	C9	111.5(3)	C19A	C14A	P1A	115.88(18)
C10	C11	C12	111.5(2)	C19A	C14A	C15A	109.4(2)
C11	C12	C13	111.7(3)	C16A	C15A	C14A	109.8(2)
C12	C13	C8	110.1(2)	C17A	C16A	C15A	111.8(2)
C15	C14	P1	114.67(19)	C16A	C17A	C18A	112.0(2)
C19	C14	P1	116.06(18)	C17A	C18A	C19A	110.8(2)
C19	C14	C15	108.9(2)	C18A	C19A	C14A	109.5(2)
C16	C15	C14	111.3(2)	C21A	C20A	P1A	114.80(18)
C17	C16	C15	111.8(2)	C25A	C20A	P1A	112.62(18)
C16	C17	C18	110.6(2)	C25A	C20A	C21A	109.7(2)
C17	C18	C19	111.9(2)	C22A	C21A	C20A	109.5(2)
C18	C19	C14	110.4(2)	C23A	C22A	C21A	111.4(2)
C21	C20	P1	113.44(19)	C24A	C23A	C22A	111.6(2)

C25	C20	P1	113.92(18)	C23A	C24A	C25A	111.3(2)
C25	C20	C21	109.1(2)	C20A	C25A	C24A	110.0(2)
C22	C21	C20	110.0(2)	F2	B1	F1	109.2(3)
C23	C22	C21	111.1(2)	F2	B1	F3	111.4(3)
C24	C23	C22	111.2(2)	F2	B1	F4	110.7(3)
C23	C24	C25	111.2(3)	F3	B1	F1	108.7(2)
C20	C25	C24	110.1(2)	F4	B1	F1	107.2(3)
O1X	C26	Ru1	168(6)	F4	B1	F3	109.6(3)
P1A	Ru1A	C1A	126.12(7)	F2A	B1A	F1A	107.8(2)
P1A	Ru1A	C5A	99.70(6)	F3A	B1A	F1A	108.6(2)
P1A	Ru1A	C6A	101.54(6)	F3A	B1A	F2A	110.1(2)
C2A	Ru1A	P1A	161.01(7)	F3A	B1A	F4A	111.3(3)
C2A	Ru1A	C1A	35.36(9)	F4A	B1A	F1A	108.5(2)
C2A	Ru1A	C4A	64.19(10)	F4A	B1A	F2A	110.5(2)

Table S25. Torsion Angles for 4c.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	P1	C8	C9	−163.99(18)	Ru1A	P1A	C8A	C9A	−156.69(18)
Ru1	P1	C8	C13	66.3(2)	Ru1A	P1A	C8A	C13A	75.4(2)
Ru1	P1	C14	C15	179.83(18)	Ru1A	P1A	C14A	C15A	176.28(16)
Ru1	P1	C14	C19	−51.8(2)	Ru1A	P1A	C14A	C19A	−53.4(2)
Ru1	P1	C20	C21	−60.5(2)	Ru1A	P1A	C20A	C21A	−71.0(2)
Ru1	P1	C20	C25	65.1(2)	Ru1A	P1A	C20A	C25A	55.5(2)
Ru1	C1	C2	C3	58.8(2)	Ru1A	C1A	C2A	C3A	58.5(2)
Ru1	C1	C6	C5	−58.1(2)	Ru1A	C1A	C6A	C5A	−57.7(2)
Ru1	C2	C3	C4	56.7(2)	Ru1A	C2A	C3A	C4A	60.4(2)
Ru1	C3	C4	Cl1	−127.32(18)	Ru1A	C3A	C4A	Cl1A	−124.34(19)
Ru1	C3	C4	C5	52.3(2)	Ru1A	C3A	C4A	C5A	54.1(2)
Ru1	C4	C5	C6	58.8(2)	Ru1A	C4A	C5A	C6A	57.3(2)
Ru1	C5	C6	C1	60.2(2)	Ru1A	C5A	C6A	C1A	59.1(2)
Cl1	C4	C5	Ru1	126.00(18)	Cl1A	C4A	C5A	Ru1A	126.04(19)
Cl1	C4	C5	C6	−175.2(2)	Cl1A	C4A	C5A	C6A	−176.65(19)
P1	Ru1	C1	O2	−70.0(3)	P1A	Ru1A	C1A	O2A	66.5(3)
P1	Ru1	C1	C2	47.40(17)	P1A	Ru1A	C1A	C2A	173.88(13)
P1	Ru1	C1	C6	−178.80(13)	P1A	Ru1A	C1A	C6A	−51.62(17)
P1	Ru1	C2	C1	−144.64(13)	P1A	Ru1A	C2A	C1A	−15.4(3)
P1	Ru1	C2	C3	85.98(16)	P1A	Ru1A	C2A	C3A	−144.01(18)
P1	Ru1	C3	C2	−101.04(16)	P1A	Ru1A	C3A	C2A	150.88(16)
P1	Ru1	C3	C4	128.27(14)	P1A	Ru1A	C3A	C4A	22.1(3)
P1	Ru1	C4	Cl1	52.8(2)	P1A	Ru1A	C4A	Cl1A	−57.7(2)
P1	Ru1	C4	C3	−61.73(16)	P1A	Ru1A	C4A	C3A	−

									169.97(13)
P1	Ru1	C4	C5	165.77(13)	P1A	Ru1A	C4A	C5A	57.31(16)
P1	Ru1	C5	C4	-27.4(2)	P1A	Ru1A	C5A	C4A	-133.49(14)
P1	Ru1	C5	C6	-156.94(13)	P1A	Ru1A	C5A	C6A	96.30(14)
P1	Ru1	C6	C1	3.7(4)	P1A	Ru1A	C6A	C1A	139.74(14)
P1	Ru1	C6	C5	132.8(2)	P1A	Ru1A	C6A	C5A	-90.54(14)
P1	Ru1	C7	O1	138(5)	P1A	Ru1A	C7A	O1A	161(6)
P1	Ru1	C26	O1X	134(31)	P1A	Ru1A	C7Y	O1Y	113(14)
P1	C8	C9	C10	170.6(2)	P1A	C8A	C9A	C10A	175.4(2)
P1	C8	C13	C12	-168.40(19)	P1A	C8A	C13A	C12A	-173.0(2)
P1	C14	C15	C16	-170.8(2)	P1A	C14A	C15A	C16A	-167.29(19)
P1	C14	C19	C18	171.3(2)	P1A	C14A	C19A	C18A	165.58(18)
P1	C20	C21	C22	-171.83(19)	P1A	C20A	C21A	C22A	-172.11(19)
P1	C20	C25	C24	172.2(2)	P1A	C20A	C25A	C24A	171.22(19)
O2	C1	C2	Ru1	127.4(2)	O2A	C1A	C2A	Ru1A	126.4(2)
O2	C1	C2	C3	-173.8(2)	O2A	C1A	C2A	C3A	-175.2(2)
O2	C1	C6	Ru1	-126.9(2)	O2A	C1A	C6A	Ru1A	-127.5(3)
O2	C1	C6	C5	175.1(2)	O2A	C1A	C6A	C5A	174.8(2)
C1	Ru1	P1	C8	-4.91(13)	C1A	Ru1A	P1A	C8A	-120.01(13)
C1	Ru1	P1	C14	121.50(12)	C1A	Ru1A	P1A	C14A	4.72(12)
C1	Ru1	P1	C20	-121.53(13)	C1A	Ru1A	P1A	C20A	121.41(12)
C1	Ru1	C2	C3	-129.4(2)	C1A	Ru1A	C2A	C3A	-128.7(3)
C1	Ru1	C3	C2	29.83(16)	C1A	Ru1A	C3A	C2A	30.34(16)
C1	Ru1	C3	C4	-100.85(18)	C1A	Ru1A	C3A	C4A	-98.42(17)
C1	Ru1	C4	Cl1	-179.8(2)	C1A	Ru1A	C4A	Cl1A	179.6(2)
C1	Ru1	C4	C3	65.63(16)	C1A	Ru1A	C4A	C3A	67.34(16)
C1	Ru1	C4	C5	-66.86(16)	C1A	Ru1A	C4A	C5A	-65.38(15)
C1	Ru1	C5	C4	99.44(17)	C1A	Ru1A	C5A	C4A	100.70(16)
C1	Ru1	C5	C6	-30.09(16)	C1A	Ru1A	C5A	C6A	-29.51(14)
C1	Ru1	C6	C5	129.1(2)	C1A	Ru1A	C6A	C5A	129.7(2)
C1	Ru1	C7	O1	-16(6)	C1A	Ru1A	C7A	O1A	-40(6)
C1	Ru1	C26	O1X	3(31)	C1A	Ru1A	C7Y	O1Y	-121(14)
C1	C2	C3	Ru1	-59.7(2)	C1A	C2A	C3A	Ru1A	-61.4(2)
C1	C2	C3	C4	-3.0(4)	C1A	C2A	C3A	C4A	-1.0(4)
C2	Ru1	P1	C8	20.83(12)	C2A	Ru1A	P1A	C8A	-109.1(2)
C2	Ru1	P1	C14	147.24(12)	C2A	Ru1A	P1A	C14A	15.7(2)
C2	Ru1	P1	C20	-95.79(12)	C2A	Ru1A	P1A	C20A	132.3(2)
C2	Ru1	C1	O2	-117.4(3)	C2A	Ru1A	C1A	O2A	-107.4(3)
C2	Ru1	C1	C6	133.8(2)	C2A	Ru1A	C1A	C6A	134.5(2)
C2	Ru1	C3	C4	-130.7(2)	C2A	Ru1A	C3A	C4A	-128.8(2)

C2	Ru1	C4	Cl1	144.2(2)	C2A	Ru1A	C4A	Cl1A	142.9(2)
C2	Ru1	C4	C3	29.66(15)	C2A	Ru1A	C4A	C3A	30.64(15)
C2	Ru1	C4	C5	−102.83(17)	C2A	Ru1A	C4A	C5A	−102.08(17)
C2	Ru1	C5	C4	64.21(16)	C2A	Ru1A	C5A	C4A	65.34(16)
C2	Ru1	C5	C6	−65.33(17)	C2A	Ru1A	C5A	C6A	−64.86(15)
C2	Ru1	C6	C1	−27.44(15)	C2A	Ru1A	C6A	C1A	−27.37(15)
C2	Ru1	C6	C5	101.68(18)	C2A	Ru1A	C6A	C5A	102.35(17)
C2	Ru1	C7	O1	−54(6)	C2A	Ru1A	C7A	O1A	−28(6)
C2	Ru1	C26	O1X	30(32)	C2A	Ru1A	C7Y	O1Y	−86(14)
C2	C1	C6	Ru1	51.1(2)	C2A	C1A	C6A	Ru1A	49.2(2)
C2	C1	C6	C5	−7.0(4)	C2A	C1A	C6A	C5A	−8.5(4)
C2	C3	C4	Ru1	−56.1(2)	C2A	C3A	C4A	Ru1A	−59.5(2)
C2	C3	C4	Cl1	176.6(2)	C2A	C3A	C4A	Cl1A	176.1(2)
C2	C3	C4	C5	−3.8(4)	C2A	C3A	C4A	C5A	−5.5(4)
C3	Ru1	P1	C8	56.92(12)	C3A	Ru1A	P1A	C8A	132.5(2)
C3	Ru1	P1	C14	−176.67(11)	C3A	Ru1A	P1A	C14A	−102.7(2)
C3	Ru1	P1	C20	−59.70(12)	C3A	Ru1A	P1A	C20A	13.9(2)
C3	Ru1	C1	O2	−147.8(3)	C3A	Ru1A	C1A	O2A	−138.3(3)
C3	Ru1	C1	C2	−30.40(14)	C3A	Ru1A	C1A	C2A	−30.90(16)
C3	Ru1	C1	C6	103.40(17)	C3A	Ru1A	C1A	C6A	103.61(17)
C3	Ru1	C2	C1	129.4(2)	C3A	Ru1A	C2A	C1A	128.7(3)
C3	Ru1	C4	Cl1	114.6(3)	C3A	Ru1A	C4A	Cl1A	112.2(3)
C3	Ru1	C4	C5	−132.5(2)	C3A	Ru1A	C4A	C5A	−132.7(2)
C3	Ru1	C5	C4	28.10(15)	C3A	Ru1A	C5A	C4A	28.73(15)
C3	Ru1	C5	C6	−101.44(18)	C3A	Ru1A	C5A	C6A	−101.48(16)
C3	Ru1	C6	C1	−63.63(15)	C3A	Ru1A	C6A	C1A	−63.84(16)
C3	Ru1	C6	C5	65.48(17)	C3A	Ru1A	C6A	C5A	65.88(15)
C3	Ru1	C7	O1	−121(5)	C3A	Ru1A	C7A	O1A	4(6)
C3	Ru1	C26	O1X	23(42)	C3A	Ru1A	C7Y	O1Y	−58(14)
C3	C4	C5	Ru1	−53.6(2)	C3A	C4A	C5A	Ru1A	−52.4(2)
C3	C4	C5	C6	5.2(4)	C3A	C4A	C5A	C6A	4.9(4)
C4	Ru1	P1	C8	87.67(12)	C4A	Ru1A	P1A	C8A	147.69(13)
C4	Ru1	P1	C14	−145.92(12)	C4A	Ru1A	P1A	C14A	−87.58(12)
C4	Ru1	P1	C20	−28.95(12)	C4A	Ru1A	P1A	C20A	29.11(12)
C4	Ru1	C1	O2	176.3(3)	C4A	Ru1A	C1A	O2A	−175.8(3)
C4	Ru1	C1	C2	−66.30(15)	C4A	Ru1A	C1A	C2A	−68.41(17)
C4	Ru1	C1	C6	67.50(15)	C4A	Ru1A	C1A	C6A	66.10(16)
C4	Ru1	C2	C1	100.27(17)	C4A	Ru1A	C2A	C1A	97.91(18)
C4	Ru1	C2	C3	−29.11(15)	C4A	Ru1A	C2A	C3A	−30.75(16)
C4	Ru1	C3	C2	130.7(2)	C4A	Ru1A	C3A	C2A	128.8(2)
C4	Ru1	C5	C6	−129.5(2)	C4A	Ru1A	C5A	C6A	−130.2(2)
C4	Ru1	C6	C1	−99.06(17)	C4A	Ru1A	C6A	C1A	−100.26(17)

C4	Ru1	C6	C5	30.05(16)	C4A	Ru1A	C6A	C5A	29.46(15)
C4	Ru1	C7	O1	-103(5)	C4A	Ru1A	C7A	O1A	39(6)
C4	Ru1	C26	O1X	-82(32)	C4A	Ru1A	C7Y	O1Y	-57(15)
C4	C5	C6	Ru1	-60.0(2)	C4A	C5A	C6A	Ru1A	-57.0(2)
C4	C5	C6	C1	0.2(4)	C4A	C5A	C6A	C1A	2.1(4)
C5	Ru1	P1	C8	105.44(18)	C5A	Ru1A	P1A	C8A	177.03(12)
C5	Ru1	P1	C14	−128.15(17)	C5A	Ru1A	P1A	C14A	-58.24(11)
C5	Ru1	P1	C20	-11.18(18)	C5A	Ru1A	P1A	C20A	58.45(11)
C5	Ru1	C1	O2	139.5(3)	C5A	Ru1A	C1A	O2A	148.2(3)
C5	Ru1	C1	C2	−103.12(16)	C5A	Ru1A	C1A	C2A	−104.42(17)
C5	Ru1	C1	C6	30.68(16)	C5A	Ru1A	C1A	C6A	30.09(15)
C5	Ru1	C2	C1	64.27(15)	C5A	Ru1A	C2A	C1A	62.51(16)
C5	Ru1	C2	C3	-65.11(17)	C5A	Ru1A	C2A	C3A	-66.15(17)
C5	Ru1	C3	C2	102.05(18)	C5A	Ru1A	C3A	C2A	100.90(18)
C5	Ru1	C3	C4	-28.64(15)	C5A	Ru1A	C3A	C4A	-27.86(14)
C5	Ru1	C4	Cl1	-112.9(3)	C5A	Ru1A	C4A	Cl1A	-115.1(3)
C5	Ru1	C4	C3	132.5(2)	C5A	Ru1A	C4A	C3A	132.7(2)
C5	Ru1	C6	C1	-129.1(2)	C5A	Ru1A	C6A	C1A	-129.7(2)
C5	Ru1	C7	O1	-70(5)	C5A	Ru1A	C7A	O1A	59(6)
C5	Ru1	C26	O1X	-65(31)	C5A	Ru1A	C7Y	O1Y	-135(13)
C6	Ru1	P1	C8	-7.7(3)	C6A	Ru1A	P1A	C8A	−147.05(13)
C6	Ru1	P1	C14	118.7(3)	C6A	Ru1A	P1A	C14A	-22.32(11)
C6	Ru1	P1	C20	-124.3(3)	C6A	Ru1A	P1A	C20A	94.37(12)
C6	Ru1	C1	O2	108.8(3)	C6A	Ru1A	C1A	O2A	118.1(3)
C6	Ru1	C1	C2	-133.8(2)	C6A	Ru1A	C1A	C2A	-134.5(2)
C6	Ru1	C2	C1	27.70(14)	C6A	Ru1A	C2A	C1A	26.83(15)
C6	Ru1	C2	C3	−101.68(18)	C6A	Ru1A	C2A	C3A	−101.82(19)
C6	Ru1	C3	C2	65.42(17)	C6A	Ru1A	C3A	C2A	65.10(17)
C6	Ru1	C3	C4	-65.27(16)	C6A	Ru1A	C3A	C4A	-63.67(15)
C6	Ru1	C4	Cl1	-143.3(2)	C6A	Ru1A	C4A	Cl1A	-144.8(2)
C6	Ru1	C4	C3	102.13(17)	C6A	Ru1A	C4A	C3A	103.00(17)
C6	Ru1	C4	C5	-30.36(16)	C6A	Ru1A	C4A	C5A	-29.72(14)
C6	Ru1	C5	C4	129.5(2)	C6A	Ru1A	C5A	C4A	130.2(2)
C6	Ru1	C7	O1	-36(5)	C6A	Ru1A	C7A	O1A	26(6)
C6	Ru1	C26	O1X	-32(31)	C6A	Ru1A	C7Y	O1Y	-144(14)
C6	C1	C2	Ru1	-50.4(2)	C6A	C1A	C2A	Ru1A	-50.5(2)
C6	C1	C2	C3	8.4(4)	C6A	C1A	C2A	C3A	8.0(4)
C7	Ru1	P1	C8	−161.55(13)	C7A	Ru1A	P1A	C8A	43.90(15)
C7	Ru1	P1	C14	-35.14(13)	C7A	Ru1A	P1A	C14A	168.63(14)
C7	Ru1	P1	C20	81.83(13)	C7A	Ru1A	P1A	C20A	-74.69(15)
C7	Ru1	C1	O2	74.9(3)	C7A	Ru1A	C1A	O2A	-87.1(3)
C7	Ru1	C1	C2	−167.73(17)	C7A	Ru1A	C1A	C2A	20.3(3)

C7	Ru1	C1	C6	-33.9(2)	C7A	Ru1A	C1A	C6A	154.8(2)
C7	Ru1	C2	C1	47.4(6)	C7A	Ru1A	C2A	C1A	-166.91(18)
C7	Ru1	C2	C3	-82.0(6)	C7A	Ru1A	C2A	C3A	64.4(2)
C7	Ru1	C3	C2	161.69(18)	C7A	Ru1A	C3A	C2A	-120.6(2)
C7	Ru1	C3	C4	31.0(2)	C7A	Ru1A	C3A	C4A	110.64(18)
C7	Ru1	C4	Cl1	-45.4(2)	C7A	Ru1A	C4A	Cl1A	39.1(2)
C7	Ru1	C4	C3	-160.01(16)	C7A	Ru1A	C4A	C3A	-73.08(18)
C7	Ru1	C4	C5	67.50(18)	C7A	Ru1A	C4A	C5A	154.20(17)
C7	Ru1	C5	C4	-119.11(17)	C7A	Ru1A	C5A	C4A	-35.3(2)
C7	Ru1	C5	C6	111.36(18)	C7A	Ru1A	C5A	C6A	-165.47(18)
C7	Ru1	C6	C1	156.54(16)	C7A	Ru1A	C6A	C1A	-85.7(5)
C7	Ru1	C6	C5	-74.34(19)	C7A	Ru1A	C6A	C5A	44.0(5)
C7	Ru1	C26	O1X	-135(32)	C7A	Ru1A	C7Y	O1Y	23(14)
C8	P1	C14	C15	-53.9(2)	C7Y	Ru1A	P1A	C8A	-25.9(7)
C8	P1	C14	C19	74.5(2)	C7Y	Ru1A	P1A	C14A	98.9(7)
C8	P1	C20	C21	178.30(19)	C7Y	Ru1A	P1A	C20A	-144.4(7)
C8	P1	C20	C25	-56.1(2)	C7Y	Ru1A	C1A	O2A	-25.3(7)
C8	C9	C10	C11	56.5(3)	C7Y	Ru1A	C1A	C2A	82.1(6)
C9	C8	C13	C12	58.3(3)	C7Y	Ru1A	C1A	C6A	-143.4(6)
C9	C10	C11	C12	-54.8(3)	C7Y	Ru1A	C2A	C1A	-98.7(7)
C10	C11	C12	C13	55.3(3)	C7Y	Ru1A	C2A	C3A	132.7(7)
C11	C12	C13	C8	-56.9(3)	C7Y	Ru1A	C3A	C2A	-52.6(8)
C13	C8	C9	C10	-57.9(3)	C7Y	Ru1A	C3A	C4A	178.7(8)
C14	P1	C8	C9	68.8(2)	C7Y	Ru1A	C4A	Cl1A	109.9(14)
C14	P1	C8	C13	-60.9(2)	C7Y	Ru1A	C4A	C3A	-2.3(14)
C14	P1	C20	C21	62.2(2)	C7Y	Ru1A	C4A	C5A	-135.1(14)
C14	P1	C20	C25	-172.1(2)	C7Y	Ru1A	C5A	C4A	116.6(14)
C14	C15	C16	C17	-56.7(3)	C7Y	Ru1A	C5A	C6A	-13.6(14)
C15	C14	C19	C18	-57.5(3)	C7Y	Ru1A	C6A	C1A	43.8(7)
C15	C16	C17	C18	54.6(3)	C7Y	Ru1A	C6A	C5A	173.5(7)
C16	C17	C18	C19	-55.4(3)	C7Y	Ru1A	C7A	O1A	-109(6)
C17	C18	C19	C14	57.6(3)	C8A	P1A	C14A	C15A	-57.6(2)
C19	C14	C15	C16	57.3(3)	C8A	P1A	C14A	C19A	72.7(2)
C20	P1	C8	C9	-40.7(2)	C8A	P1A	C20A	C21A	165.0(2)
C20	P1	C8	C13	-170.36(19)	C8A	P1A	C20A	C25A	-68.5(2)
C20	P1	C14	C15	56.0(2)	C8A	C9A	C10A	C11A	56.1(3)
C20	P1	C14	C19	-175.6(2)	C9A	C8A	C13A	C12A	55.9(3)
C20	C21	C22	C23	-57.6(3)	C9A	C10A	C11A	C12A	-56.1(3)
C21	C20	C25	C24	-59.9(3)	C10A	C11A	C12A	C13A	55.4(4)
C21	C22	C23	C24	54.8(3)	C11A	C12A	C13A	C8A	-56.4(4)
C22	C23	C24	C25	-54.7(3)	C13A	C8A	C9A	C10A	-55.2(3)
C23	C24	C25	C20	57.6(3)	C14A	P1A	C8A	C9A	79.0(2)

C25	C20	C21	C22	60.0(3)	C14A	P1A	C8A	C13A	-49.0(2)
C26	Ru1	P1	C8	-112(3)	C14A	P1A	C20A	C21A	49.3(2)
C26	Ru1	P1	C14	14(3)	C14A	P1A	C20A	C25A	175.76(18)
C26	Ru1	P1	C20	131(3)	C14A	C15A	C16A	C17A	-55.6(3)
C26	Ru1	C1	O2	28(3)	C15A	C14A	C19A	C18A	-61.0(3)
C26	Ru1	C1	C2	145(3)	C15A	C16A	C17A	C18A	53.5(3)
C26	Ru1	C1	C6	-81(3)	C16A	C17A	C18A	C19A	-54.8(3)
C26	Ru1	C2	C1	-48(3)	C17A	C18A	C19A	C14A	58.5(3)
C26	Ru1	C2	C3	-178(3)	C19A	C14A	C15A	C16A	59.4(3)
C26	Ru1	C3	C2	9(13)	C20A	P1A	C8A	C9A	-31.5(2)
C26	Ru1	C3	C4	-122(13)	C20A	P1A	C8A	C13A	-159.4(2)
C26	Ru1	C4	Cl1	-86(5)	C20A	P1A	C14A	C15A	52.6(2)
C26	Ru1	C4	C3	160(5)	C20A	P1A	C14A	C19A	-177.05(19)
C26	Ru1	C4	C5	27(5)	C20A	C21A	C22A	C23A	-57.5(3)
C26	Ru1	C5	C4	-165(3)	C21A	C20A	C25A	C24A	-59.6(3)
C26	Ru1	C5	C6	65(3)	C21A	C22A	C23A	C24A	54.7(3)
C26	Ru1	C6	C1	106(3)	C22A	C23A	C24A	C25A	-54.1(3)
C26	Ru1	C6	C5	-124(3)	C23A	C24A	C25A	C20A	56.6(3)
C26	Ru1	C7	O1	52(6)	C25A	C20A	C21A	C22A	59.9(3)

Table S26. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4c.

Atom	*x*	*y*	*z*	U(eq)
H	6080(30)	6770(30)	3755(15)	32(9)
H2	7150(30)	5410(30)	5034(13)	12(7)
H2A	8624	6870	4871	18
H3	8862	8857	4807	17
H5	4923	9233	4725	20
H6	4704	7267	4827	18
H8	9524	7227	3941	21
H9A	10443	7962	3167	31
H9B	9907	6878	2770	31
H10A	12142	6553	3253	39
H10B	11811	6800	3885	39
H11A	11939	4843	3769	39
H11B	10895	4891	3147	39
H12A	10307	5339	4279	34
H12B	9802	4262	3872	34
H13A	8089	5634	3789	28
H13B	8448	5427	3158	28
H14	5989	8149	2448	20
H15A	7938	8227	2080	32
H15B	8071	6879	2138	32
H16A	5935	8053	1371	38
H16B	7053	7345	1152	38
H17A	6251	5655	1450	32

H17B	5051	6309	1028	32
H18A	4421	5603	1890	33
H18B	4277	6951	1847	33
H19A	6442	5777	2598	30
H19B	5310	6446	2829	30
H20	8812	9190	2844	20
H21A	6615	9926	2623	29
H21B	6840	10400	3287	29
H22A	8325	11107	2435	35
H22B	7252	11873	2654	35
H23A	9455	12386	3148	39
H23B	8601	12000	3612	39
H24A	10669	11118	3873	36
H24B	10515	10626	3216	36
H25A	10041	9167	3844	26
H25B	8927	9935	4032	26
HA	4350(40)	3010(30)	1334(14)	30(9)
H2AA	3040(40)	4940(30)	188(16)	32(10)
H2AB	5339	3017	180	20
H3A	4980	1060	75	20
H5A	1090	1514	89	17
H6A	1457	3483	210	18
H8A	4353	1668	2414	23
H9AA	2172	2063	2957	28
H9AB	2712	836	2834	28
H10C	3578	1403	3836	34
H10D	4744	1195	3496	34
H11C	3742	3368	3728	39
H11D	5167	2882	4038	39
H12C	5852	2950	3140	40
H12D	5313	4175	3265	40
H13C	3282	3821	2599	36
H13D	4453	3624	2261	36
H14A	596	2929	1146	19
H15C	-45	2351	2028	24
H15D	749	3408	2367	24
H16C	-1463	3567	1373	32
H16D	-1484	3932	2038	32
H17C	-86	5460	1994	31
H17D	-1293	5534	1429	31
H18C	772	5868	1162	26
H18D	19	4805	812	26
H19C	2136	4635	1846	21
H19D	2270	4332	1186	21
H20A	1201	727	2063	19
H21C	-233	1215	1144	23

H21D	617	424	805	23
H22C	-795	-365	1667	29
H22D	-1224	-613	971	29
H23C	-127	-2202	1497	33
H23D	632	-1755	1009	33
H24C	2200	-2089	1884	32
H24D	1401	-1323	2256	32
H25C	3201	-261	2073	26
H25D	2726	-475	1374	26

Table S27. Atomic Occupancy for 4c.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
O1	0.963(4)	O1X	0.037(4)	C7	0.963(4)
C26	0.037(4)	O1A	0.862(4)	O1Y	0.138(4)
C7A	0.862(4)	C7Y	0.138(4)		

Table S28. Crystal Data and Structure Refinement for 5.

Identification code	yi2r
Empirical formula	$C_{54.78}H_{82.56}BCl_{1.56}F_4O_6P_2Ru_2$
Formula weight	1243.55
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	19.8500(4)
b/Å	17.9759(3)
c/Å	16.6953(3)
α/°	90.00
β/°	107.1132(19)
γ/°	90.00
Volume/Å^3	5693.49(17)
Z	4
ρ_{calc}mg/mm^3	1.451
m/mm^{-1}	0.720
F(000)	2579.0
Crystal size/mm^3	0.6545 × 0.082 × 0.0667
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.62 to 58.94°
Index ranges	-26 ≤ h ≤ 25, -23 ≤ k ≤ 23, -23 ≤ l ≤ 21
Reflections collected	32469
Independent reflections	7101 [R_{int} = 0.0353, R_{sigma} = 0.0322]
Data/restraints/parameters	7101/24/389
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0324, wR_2 = 0.0730
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.0766
Largest diff. peak/hole/e Å^{-3}	0.85/-0.60

Table S29. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ru1	4677.43(9)	6496.55(9)	3101.28(10)	15.62(6)
P1	3657.5(3)	5834.1(3)	3018.6(3)	15.72(11)
O1	4362.0(8)	7081.8(8)	1979.5(9)	18.9(3)
O2	4305.8(8)	7377.3(9)	3647.2(10)	22.5(3)
O3	5400.1(9)	5621.9(10)	4634.7(10)	27.8(4)
C1	4235.3(11)	7813.5(12)	1887.3(14)	22.0(5)
C2	4110.7(12)	8273.8(13)	2521.9(16)	25.0(5)
C3	3984.5(13)	9041.4(14)	2340.1(18)	32.8(6)
C4	3984.6(14)	9342.6(14)	1588.2(19)	37.5(7)
C5	4105.0(13)	8885.6(15)	974.5(17)	34.5(6)
C6	4214.8(12)	8131.3(14)	1111.7(15)	26.6(5)
C7	4133.6(12)	8017.0(13)	3360.1(16)	26.1(5)

C8	3949.6(16)	8546.2(15)	3963(2)	39.3(7)
C9	2983.0(11)	5921.8(12)	1990.8(12)	16.8(4)
C10	2686.9(11)	6717.5(12)	1832.1(13)	18.8(4)
C11	2200.0(12)	6802.6(13)	939.0(13)	21.7(5)
C12	2573.6(12)	6580.7(12)	296.7(13)	21.6(5)
C13	2801.4(12)	5770.3(12)	422.9(13)	21.0(4)
C14	3302.7(11)	5657.9(12)	1303.5(12)	18.2(4)
C15	3738.5(11)	4818.0(12)	3245.6(13)	18.9(4)
C16	4352.2(12)	4429.6(12)	3023.4(14)	22.0(5)
C17	4423.0(13)	3619.1(13)	3316.1(15)	25.6(5)
C18	3741.5(13)	3180.1(13)	2964.1(15)	27.2(5)
C19	3130.6(13)	3573.2(13)	3166.7(16)	26.1(5)
C20	3053.2(12)	4377.2(12)	2852.7(14)	22.0(5)
C21	3241.3(11)	6222.1(12)	3788.9(13)	18.8(4)
C22	3733.6(12)	6203.6(13)	4692.7(13)	22.9(5)
C23	3418.4(13)	6649.3(14)	5273.6(14)	25.1(5)
C24	2683.3(14)	6384.6(14)	5240.1(15)	28.0(5)
C25	2197.5(13)	6364.3(14)	4340.6(15)	27.2(5)
C26	2516.8(12)	5906.2(13)	3765.6(14)	22.3(5)
C27	5106.2(12)	5961.6(13)	4046.3(13)	20.6(4)
F1	787(8)	5637(7)	1629(10)	163(5)
F2	440(2)	6475(2)	694(3)	65.6(12)
F3	-309(5)	5902(4)	1201(8)	177(4)
F4	257(4)	5259(3)	504(6)	148(3)
B1	327(6)	5818(6)	1058(7)	66(3)
Cl3	-190(5)	6855(4)	1085(10)	105(6)
Cl4	885(6)	6162(12)	2300(17)	191(12)
C2S	253(16)	5973(15)	1330(20)	103(6)
Cl1	-355(4)	6825(4)	1743(9)	124(4)
Cl2	882(4)	5868(4)	1708(5)	65.8(19)
C1S	190(9)	6063(11)	2057(17)	103(6)

Table S30. Anisotropic Displacement Parameters ($Å^2×10^3$) for 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	13.98(10)	18.53(9)	14.37(9)	-0.68(6)	4.20(6)	0.31(6)
P1	14.6(3)	18.5(3)	14.3(2)	1.40(19)	4.6(2)	1.2(2)
O1	15.5(7)	20.2(7)	21.0(7)	2.9(6)	5.5(6)	1.2(6)
O2	19.0(8)	22.6(8)	28.3(8)	-5.0(6)	10.5(6)	-1.0(6)
O3	23.0(9)	41.6(10)	18.3(8)	6.4(7)	4.9(7)	6.4(7)
C1	10.4(10)	22.4(11)	29.8(12)	3.3(9)	0.5(8)	1.0(8)
C2	13.9(11)	22.2(11)	36.8(13)	-1.1(10)	4.2(9)	-0.4(9)
C3	22.7(13)	23.7(12)	47.6(16)	-2.3(11)	3.6(11)	2.1(10)
C4	29.0(14)	21.5(12)	51.9(17)	6.4(11)	-4.0(12)	1.3(10)
C5	24.9(13)	31.1(13)	39.0(14)	12.7(11)	-3.8(11)	-2.2(11)
C6	18.0(12)	28.7(12)	28.6(12)	6.4(10)	-0.3(9)	-1.2(9)

C7	16.2(11)	23.3(11)	40.5(14)	-5.6(10)	10.8(10)	-2.2(9)
C8	43.4(17)	29.5(14)	55.0(18)	-7.6(12)	30.1(14)	1.4(12)
C9	14.7(10)	20.2(10)	15.3(9)	0.8(8)	3.9(8)	0.0(8)
C10	17.3(11)	20(1)	19(1)	1.0(8)	5.3(8)	1.1(8)
C11	20.2(11)	22.4(11)	20.2(11)	2.3(8)	2.4(9)	4.0(9)
C12	22.5(12)	24.1(11)	16.9(10)	1.8(8)	3.7(9)	2.6(9)
C13	22.4(12)	23.3(11)	16.1(10)	-2.0(8)	3.6(8)	0.8(9)
C14	17.9(11)	19.9(10)	15.5(10)	-0.3(8)	3.1(8)	2.1(8)
C15	20.5(11)	19.4(10)	17.7(10)	3.3(8)	7.0(8)	1.5(8)
C16	20.8(12)	22.7(11)	24.1(11)	2.0(9)	8.8(9)	1.8(9)
C17	29.4(13)	24.6(12)	24.5(11)	3.8(9)	10.5(10)	7.9(10)
C18	35.7(14)	20.6(11)	28.2(12)	2.4(9)	14(1)	1.4(10)
C19	29.4(13)	21.9(11)	30.1(12)	3.3(9)	13.9(10)	-1.1(9)
C20	21.7(12)	21.3(11)	24.5(11)	2.0(9)	9.2(9)	-0.6(9)
C21	19.0(11)	21.5(10)	17.5(10)	1.6(8)	7.7(8)	2.3(9)
C22	24.1(12)	29.1(12)	16.5(10)	0.9(9)	7.3(9)	3.6(10)
C23	27.8(13)	29.9(12)	20.0(11)	-1.7(9)	10.8(9)	3.3(10)
C24	34.1(14)	27.6(12)	29.5(12)	-2(1)	20.6(11)	2.1(10)
C25	23.0(13)	30.2(12)	33.0(13)	-3.3(10)	15.1(10)	1(1)
C26	20.4(12)	23.7(11)	25.1(11)	1.1(9)	10.4(9)	0.4(9)
C27	17.0(11)	28.0(11)	19(1)	-3.0(9)	8.9(8)	-2.2(9)
F1	168(9)	109(9)	195(9)	79(7)	28(7)	7(7)
F2	45(2)	67(3)	85(3)	28(2)	19(2)	-8.3(19)
F3	149(6)	126(6)	318(12)	103(7)	166(8)	20(5)
F4	182(8)	56(3)	219(8)	38(4)	79(6)	4(4)
B1	70(7)	55(5)	99(7)	33(5)	63(6)	13(5)
Cl3	62(5)	35(3)	165(11)	-5(5)	-50(6)	-2(3)
Cl4	56(6)	181(17)	280(20)	135(16)	-32(11)	-24(9)
C2S	35(8)	93(11)	181(17)	95(13)	33(8)	18(7)
Cl1	71(4)	79(4)	192(10)	-26(5)	-9(5)	3(3)
Cl2	60(3)	49(3)	90(4)	20(3)	25(3)	-9(2)
C1S	35(8)	93(11)	181(17)	95(13)	33(8)	18(7)

Table S31 Bond Lengths for 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Ru1[1]	2.6802(3)	C11	C12	1.526(3)
Ru1	P1	2.3177(6)	C12	C13	1.521(3)
Ru1	O1	2.0775(14)	C13	C14	1.527(3)
Ru1	O1[1]	2.2163(15)	C15	C16	1.541(3)
Ru1	O2	2.0682(15)	C15	C20	1.544(3)
Ru1	C27	1.830(2)	C16	C17	1.530(3)
P1	C9	1.847(2)	C17	C18	1.527(4)
P1	C15	1.863(2)	C18	C19	1.525(3)
P1	C21	1.857(2)	C19	C20	1.530(3)
O1	Ru1[1]	2.2163(15)	C21	C22	1.538(3)
O1	C1	1.340(3)	C21	C26	1.536(3)

O2	C7	1.254(3)	C22	C23	1.527(3)
O3	C27	1.158(3)	C23	C24	1.520(3)
C1	C2	1.422(3)	C24	C25	1.528(3)
C1	C6	1.405(3)	C25	C26	1.536(3)
C2	C3	1.419(3)	F1	B1	1.156(14)
C2	C7	1.461(4)	F2	B1	1.377(10)
C3	C4	1.367(4)	F3	B1	1.359(10)
C4	C5	1.388(4)	F4	B1	1.344(12)
C5	C6	1.382(3)	Cl3	C2S	1.80(2)
C7	C8	1.506(3)	Cl4	C2S	1.76(2)
C9	C10	1.539(3)	Cl1	C1S	1.728(14)
C9	C14	1.540(3)	Cl2	C1S	1.679(16)
C10	C11	1.527(3)			

Table S32 Bond Angles for 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Ru1	Ru1[1]	123.844(15)	O2	C7	C8	114.6(2)
O1[1]	Ru1	Ru1[1]	49.09(4)	C2	C7	C8	119.7(2)
O1	Ru1	Ru1[1]	53.73(4)	C10	C9	P1	112.02(14)
O1	Ru1	P1	100.38(4)	C10	C9	C14	112.21(17)
O1[1]	Ru1	P1	172.91(4)	C14	C9	P1	108.72(14)
O1	Ru1	O1[1]	75.00(7)	C11	C10	C9	111.16(17)
O2	Ru1	Ru1[1]	129.87(4)	C12	C11	C10	111.18(18)
O2	Ru1	P1	90.06(5)	C13	C12	C11	109.82(18)
O2	Ru1	O1[1]	95.06(6)	C12	C13	C14	110.05(17)
O2	Ru1	O1	87.57(6)	C13	C14	C9	112.45(17)
C27	Ru1	Ru1[1]	116.26(7)	C16	C15	P1	114.97(15)
C27	Ru1	P1	87.59(7)	C16	C15	C20	108.99(18)
C27	Ru1	O1[1]	96.42(8)	C20	C15	P1	113.84(15)
C27	Ru1	O1	169.66(8)	C17	C16	C15	111.06(18)
C27	Ru1	O2	99.09(8)	C18	C17	C16	112.43(19)
C9	P1	Ru1	113.16(7)	C19	C18	C17	110.3(2)
C9	P1	C15	105.57(10)	C18	C19	C20	111.60(19)
C9	P1	C21	105.24(10)	C19	C20	C15	110.62(19)
C15	P1	Ru1	118.04(7)	C22	C21	P1	112.81(15)
C21	P1	Ru1	108.94(7)	C26	C21	P1	116.60(15)
C21	P1	C15	104.88(10)	C26	C21	C22	109.67(18)
Ru1	O1	Ru1[1]	77.17(5)	C23	C22	C21	110.55(19)
C1	O1	Ru1[1]	126.50(13)	C24	C23	C22	112.4(2)
C1	O1	Ru1	126.69(14)	C23	C24	C25	111.40(19)
C7	O2	Ru1	128.75(16)	C24	C25	C26	111.7(2)
O1	C1	C2	123.6(2)	C21	C26	C25	109.97(19)
O1	C1	C6	117.3(2)	O3	C27	Ru1	177.43(19)
C6	C1	C2	119.1(2)	F1	B1	F2	114.4(11)
C1	C2	C7	124.5(2)	F1	B1	F3	115.9(12)
C3	C2	C1	117.7(2)	F1	B1	F4	104.6(11)

C3	C2	C7	117.8(2)	F3	B1	F2	105.2(7)
C4	C3	C2	122.3(3)	F4	B1	F2	109.5(8)
C3	C4	C5	119.3(2)	F4	B1	F3	106.9(10)
C6	C5	C4	120.8(3)	Cl4	C2S	Cl3	102.1(16)
C5	C6	C1	120.8(2)	Cl2	C1S	Cl1	124.2(11)
O2	C7	C2	125.7(2)				

Table S33 Torsion Angles for 5.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1[1]	Ru1	P1	C9	-45.05(8)	C1	C2	C3	C4	-0.4(4)
Ru1[1]	Ru1	P1	C15	78.91(8)	C1	C2	C7	O2	4.6(4)
Ru1[1]	Ru1	P1	C21	-161.73(7)	C1	C2	C7	C8	-176.3(2)
Ru1[1]	Ru1	O1	C1	−126.24(18)	C2	C1	C6	C5	2.7(3)
Ru1[1]	Ru1	O2	C7	23.0(2)	C2	C3	C4	C5	0.6(4)
Ru1[1]	Ru1	C27	O3	14(5)	C3	C2	C7	O2	-172.6(2)
Ru1	P1	C9	C10	-67.08(16)	C3	C2	C7	C8	6.4(3)
Ru1	P1	C9	C14	57.51(15)	C3	C4	C5	C6	0.9(4)
Ru1	P1	C15	C16	-30.42(18)	C4	C5	C6	C1	-2.5(4)
Ru1	P1	C15	C20	−157.16(13)	C6	C1	C2	C3	-1.2(3)
Ru1	P1	C21	C22	-57.78(17)	C6	C1	C2	C7	-178.5(2)
Ru1	P1	C21	C26	173.98(14)	C7	C2	C3	C4	177.0(2)
Ru1[1]	O1	C1	C2	-119.9(2)	C9	P1	C15	C16	97.24(17)
Ru1	O1	C1	C2	-17.9(3)	C9	P1	C15	C20	-29.51(18)
Ru1[1]	O1	C1	C6	61.2(2)	C9	P1	C21	C22	-179.41(16)
Ru1	O1	C1	C6	163.15(15)	C9	P1	C21	C26	52.35(18)
Ru1	O2	C7	C2	4.7(3)	C9	C10	C11	C12	-55.5(2)
Ru1	O2	C7	C8	−174.42(17)	C10	C9	C14	C13	-50.8(2)
P1	Ru1	O1	Ru1[1]	-124.60(3)	C10	C11	C12	C13	60.6(2)
P1	Ru1	O1	C1	109.16(16)	C11	C12	C13	C14	-59.8(2)
P1	Ru1	O2	C7	−113.63(19)	C12	C13	C14	C9	55.4(2)
P1	Ru1	C27	O3	141(5)	C14	C9	C10	C11	50.3(2)
P1	C9	C10	C11	172.90(15)	C15	P1	C9	C10	162.39(15)
P1	C9	C14	C13	−175.28(15)	C15	P1	C9	C14	-73.03(16)
P1	C15	C16	C17	174.02(15)	C15	P1	C21	C22	69.48(18)
P1	C15	C20	C19	−172.03(15)	C15	P1	C21	C26	-58.76(18)
P1	C21	C22	C23	169.97(16)	C15	C16	C17	C18	55.9(3)
P1	C21	C26	C25	−171.31(16)	C16	C15	C20	C19	58.2(2)
O1[1]	Ru1	P1	C9	-40.8(3)	C16	C17	C18	C19	-54.2(3)
O1	Ru1	P1	C9	7.99(9)	C17	C18	C19	C20	55.3(3)

O1[1]	Ru1	P1	C15	83.2(3)	C18	C19	C20	C15	-58.4(3)
O1	Ru1	P1	C15	131.95(9)	C20	C15	C16	C17	-56.8(2)
O1[1]	Ru1	P1	C21	-157.5(3)	C21	P1	C9	C10	51.77(17)
O1	Ru1	P1	C21	-108.69(8)	C21	P1	C9	C14	176.36(14)
O1[1]	Ru1	O1	Ru1[1]	49.89(6)	C21	P1	C15	C16	-151.89(16)
O1[1]	Ru1	O1	C1	-76.35(15)	C21	P1	C15	C20	81.36(17)
O1[1]	Ru1	O2	C7	61.46(19)	C21	C22	C23	C24	55.6(3)
O1	Ru1	O2	C7	-13.24(19)	C22	C21	C26	C25	58.9(2)
O1[1]	Ru1	C27	O3	-33(5)	C22	C23	C24	C25	-53.0(3)
O1	Ru1	C27	O3	0(5)	C23	C24	C25	C26	53.7(3)
O1	C1	C2	C3	179.9(2)	C24	C25	C26	C21	-57.0(3)
O1	C1	C2	C7	2.7(4)	C26	C21	C22	C23	-58.3(2)
O1	C1	C6	C5	-178.3(2)	C27	Ru1	P1	C9	-165.37(10)
O2	Ru1	P1	C9	95.54(9)	C27	Ru1	P1	C15	-41.41(10)
O2	Ru1	P1	C15	-140.51(9)	C27	Ru1	P1	C21	77.95(10)
O2	Ru1	P1	C21	-21.15(8)	C27	Ru1	O1	Ru1[1]	15.3(5)
O2	Ru1	O1	Ru1[1]	145.79(5)	C27	Ru1	O1	C1	-110.9(5)
O2	Ru1	O1	C1	19.55(17)	C27	Ru1	O2	C7	158.80(19)
O2	Ru1	C27	O3	-129(5)					

Table S34. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.

Atom	*x*	*y*	*z*	U(eq)
H	5000	5850(19)	2500	20(9)
H3	3897	9357	2755	39
H4	3903	9860	1487	45
H5	4112	9094	454	41
H6	4277	7824	676	32
H8A	3946	8277	4472	59
H8B	3483	8760	3701	59
H8C	4301	8945	4109	59
H9	2584	5581	1989	20
H10A	2422	6834	2235	23
H10B	3082	7075	1925	23
H11A	1778	6486	866	26
H11B	2042	7326	844	26
H12A	2252	6651	-276	26
H12B	2992	6901	361	26
H13A	3040	5627	2	25
H13B	2382	5449	343	25
H14A	3744	5936	1356	22
H14B	3423	5124	1388	22
H15	3840	4768	3866	23
H16A	4269	4447	2409	26

H16B	4797	4698	3293	26
H17A	4804	3378	3138	31
H17B	4558	3606	3936	31
H18A	3638	3131	2349	33
H18B	3798	2674	3209	33
H19A	3211	3569	3781	31
H19B	2688	3300	2903	31
H20A	2657	4618	3001	26
H20B	2944	4382	2235	26
H21	3160	6761	3644	23
H22A	3807	5682	4889	28
H22B	4198	6415	4708	28
H23A	3730	6606	5856	30
H23B	3397	7181	5113	30
H24A	2482	6722	5578	34
H24B	2714	5881	5487	34
H25A	2111	6879	4123	33
H25B	1739	6146	4336	33
H26A	2568	5381	3953	27
H26B	2199	5921	3184	27
H2SA	-77	5577	1390	123
H2SB	479	5825	903	123
H1SA	377	6095	2675	123
H1SB	-120	5620	1934	123

Table S35. Atomic Occupancy for 5.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
F1	0.50	F2	0.50	F3	0.50
F4	0.50	B1	0.50	Cl3	0.157(6)
Cl4	0.157(6)	C2S	0.157(6)	H2SA	0.157(6)
H2SB	0.157(6)	Cl1	0.235(6)	Cl2	0.235(6)
C1S	0.235(6)	H1SA	0.235(6)	H1SB	0.235(6)

Table S36. Crystal Data and Structure Refinement for 6.

Identification code	Yi2x
Empirical formula	$C_{58}H_{88}BO_9F_4P_2Ru_2$
Formula weight	1280.17
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.44999(18)
b/Å	11.75213(19)
c/Å	23.6747(2)
α/°	96.5819(10)
β/°	100.9333(10)
γ/°	111.4618(15)
Volume/Å^3	2851.36(7)
Z	2
ρ_{calc}mg/mm^3	1.491
m/mm^{-1}	5.387
F(000)	1334.0
Crystal size/mm^3	0.2265 × 0.1198 × 0.0692
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection	7.76 to 147.42°
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -29 ≤ l ≤ 29
Reflections collected	22228
Independent reflections	22228 [R_{int} = 0.0000, R_{sigma} = 0.0144]
Data/restraints/parameters	22228/0/688
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0433, wR_2 = 0.1299
Final R indexes [all data]	R_1 = 0.0470, wR_2 = 0.1342
Largest diff. peak/hole / e Å^{-3}	1.04/-0.92

Table S37. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ru1	2665.24(16)	6693.10(16)	2709.09(7)	23.34(6)
Ru2	3889.52(16)	5054.57(16)	2295.95(7)	22.72(6)
P1	3490.6(6)	8204.0(6)	3552.0(3)	25.56(12)
P2	4623.5(6)	5022.9(5)	1457.7(2)	24.10(12)
O1	2087(2)	8378.5(18)	1954.7(8)	37.2(4)
O2	6318.6(18)	5032.4(19)	3005.2(8)	37.7(4)
O3	841.6(16)	5936.2(16)	2840.6(7)	28.7(3)
O4	3045.6(16)	5279.8(16)	3064.0(7)	25.8(3)
O5	2902.8(16)	3155.9(16)	2136.5(7)	27.5(3)
O6	2143.7(15)	5176.3(15)	1937.4(7)	25.3(3)

O7	4446.7(16)	6958.1(15)	2553.6(7)	26.7(3)
C1	4565(2)	9752(2)	3446.8(11)	29.9(5)
C2	5679(3)	10580(3)	3980.2(12)	37.8(6)
C3	6592(3)	11717(3)	3804.7(15)	46.4(7)
C4	5881(3)	12472(3)	3538.2(14)	43.6(7)
C5	4738(3)	11662(3)	3028.3(13)	37.8(6)
C6	3832(3)	10517(3)	3211.7(12)	34.3(5)
C7	2198(2)	8324(2)	3891.3(10)	28.2(5)
C8	1107(2)	8545(3)	3484.7(11)	31.5(5)
C9	-39(3)	8320(3)	3768.8(12)	36.8(6)
C10	383(3)	9146(3)	4377.9(12)	39.3(6)
C11	1504(3)	8982(3)	4771.3(12)	38.9(6)
C12	2639(3)	9214(3)	4486.4(11)	33.5(5)
C13	4561(3)	7866(2)	4140.8(11)	30.8(5)
C14	3865(3)	6834(3)	4442.6(12)	36.5(6)
C15	4843(3)	6684(3)	4934.8(13)	45.0(7)
C16	5889(3)	6422(3)	4708.6(14)	48.3(8)
C17	6595(3)	7442(3)	4410.3(13)	44.0(7)
C18	5640(3)	7615(3)	3914.1(12)	34.1(5)
C19	3809(2)	5614(2)	877.4(10)	27.7(5)
C20	2399(2)	4721(3)	576.1(11)	30.9(5)
C21	1806(3)	5284(3)	107.6(12)	35.3(6)
C22	1872(3)	6565(3)	358.7(12)	38.8(6)
C23	3261(3)	7451(3)	649.7(12)	36.7(6)
C24	3888(3)	6918(2)	1118.1(11)	32.1(5)
C25	4294(2)	3405(2)	1109.1(10)	27.2(5)
C26	4945(2)	2735(2)	1507.2(11)	29.0(5)
C27	4399(3)	1341(2)	1232.4(12)	35.6(6)
C28	4526(3)	1105(3)	600.4(12)	38.7(6)
C29	3951(3)	1829(3)	221.5(11)	35.3(6)
C30	4538(3)	3212(2)	496.1(11)	31.2(5)
C31	6393(2)	5930(2)	1564.2(11)	29.6(5)
C32	6995(3)	7100(3)	2045.8(12)	33.5(5)
C33	8473(3)	7697(3)	2140.4(13)	38.2(6)
C34	8842(3)	8008(3)	1576.3(13)	39.0(6)
C35	8239(3)	6862(3)	1091.7(13)	39.1(6)
C36	6769(3)	6279(3)	995.0(12)	33.6(5)
C37	2329(2)	7773(2)	2275.1(11)	29.8(5)
C38	5387(2)	5032(2)	2713.2(11)	28.6(5)
C39	266(2)	4909(2)	2971.9(11)	30.4(5)
C40	874(3)	4066(2)	3160.5(11)	31.2(5)
C41	2214(2)	4318(2)	3221.3(10)	27.6(5)
C42	2699(3)	3489(2)	3463.7(11)	30.9(5)
C43	1903(3)	2437(3)	3611.6(13)	38.7(6)
C44	572(3)	2133(3)	3509.2(15)	44.3(7)
C45	77(3)	2938(3)	3289.1(14)	40.7(6)

C46	-1148(3)	4566(3)	2931.3(14)	40.9(6)
C47	1709(2)	2511(2)	1971.4(10)	28.1(5)
C48	724(2)	2973(2)	1760.2(11)	29.1(5)
C49	976(2)	4247(2)	1748(1)	26.3(5)
C50	-65(2)	4565(3)	1517.0(11)	30.6(5)
C51	-1310(3)	3686(3)	1324.6(12)	36.4(6)
C52	-1586(3)	2450(3)	1352.4(13)	40.6(6)
C53	-586(3)	2102(3)	1566.7(12)	36.1(6)
C54	1323(3)	1160(2)	2003.2(12)	36.4(6)
O8	271(3)	5433(2)	4489.1(11)	56.8(6)
C55	-888(4)	5354(4)	4668.6(18)	60.4(9)
C56	666(4)	4511(4)	4694.6(18)	61.4(9)
O9	824(2)	802(2)	533.7(10)	49.0(5)
C57	-228(4)	1024(3)	206.2(16)	54.1(8)
C58	521(4)	-503(3)	420.6(16)	58.3(9)
F1	5603(2)	9320.1(18)	2237.4(9)	58.2(5)
F2	6930(2)	11363.2(17)	2336.1(10)	56.0(5)
F3	7042(3)	9835(2)	1694.2(14)	91.6(10)
F4	7710(3)	10001(3)	2682.7(19)	134.5(17)
B1	6853(4)	10144(4)	2240(2)	52.2(9)

Table S38. Anisotropic Displacement Parameters ($Å^2×10^3$) for 6. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	20.88(10)	23.94(10)	22.55(10)	5.35(7)	5.10(7)	5.89(7)
Ru2	19.64(10)	23.52(10)	22.03(10)	5.56(7)	5.12(7)	5.01(7)
P1	24.6(3)	26.5(3)	22.6(3)	5.0(2)	4.3(2)	7.6(2)
P2	21.9(3)	25.5(3)	21.7(3)	6.0(2)	5.4(2)	5.3(2)
O1	42.6(11)	37.1(10)	33.4(9)	14.4(8)	4.8(8)	17.7(9)
O2	25.9(9)	47.0(11)	38.2(10)	14.3(9)	2.7(8)	13.1(8)
O3	25.4(8)	29.5(9)	29.3(8)	5.7(7)	8.1(7)	8.1(7)
O4	24.6(8)	27.4(8)	25.4(8)	7.8(6)	9.1(6)	8.3(7)
O5	25.4(8)	27.5(8)	26.7(8)	7.3(7)	6.4(7)	6.7(7)
O6	20.1(8)	24.7(8)	26.1(8)	2.7(6)	3.8(6)	4.9(7)
O7	25.0(8)	27.1(8)	27.0(8)	3.9(7)	7.1(7)	9.6(7)
C1	30.4(12)	28.1(12)	25.7(11)	5.6(9)	5.6(10)	6.1(10)
C2	35.9(14)	33.6(13)	31.5(13)	5.2(11)	3.0(11)	2.9(12)
C3	35.3(15)	39.7(16)	52.2(18)	12.4(14)	3.8(13)	3.9(13)
C4	42.3(16)	33.6(14)	44.6(16)	12.1(12)	9.7(13)	2.7(13)
C5	41.8(15)	35.5(14)	40.0(15)	14.6(12)	14.0(12)	15.9(13)
C6	33.0(13)	32.8(13)	34.0(13)	6.3(11)	7.3(11)	10.4(11)
C7	27.9(12)	30.0(12)	23.8(11)	5.2(9)	5.9(9)	8.6(10)
C8	29.6(13)	36.7(13)	27.8(12)	5.2(10)	7.2(10)	13.2(11)
C9	29.8(13)	43.2(15)	35.0(13)	3.5(11)	10.8(11)	11.8(12)
C10	37.6(15)	47.8(16)	35.0(14)	5.0(12)	14.8(12)	17.9(13)
C11	44.3(16)	42.6(15)	26.8(12)	3.5(11)	11.3(12)	13.7(13)

C12	35.4(14)	36.8(14)	25.4(12)	3.9(10)	6.3(10)	12.6(12)
C13	29.8(12)	32.7(13)	25.2(11)	6.1(10)	2.3(10)	9.3(11)
C14	41.8(15)	36.8(14)	27.3(12)	9.9(11)	6.8(11)	11.4(12)
C15	62(2)	42.9(16)	28.9(13)	12.2(12)	3.1(13)	21.6(15)
C16	56.4(19)	45.9(17)	36.9(15)	8.1(13)	-7.9(14)	23.8(16)
C17	41.2(16)	45.3(16)	41.7(15)	2.8(13)	-4.0(13)	21.9(14)
C18	29.3(13)	36.8(14)	32.3(13)	4.8(11)	1.1(10)	12.8(11)
C19	23.6(11)	29.6(12)	25.7(11)	7.4(9)	3.9(9)	6.3(10)
C20	25.2(12)	34.5(13)	27.9(12)	7.2(10)	4.3(10)	7.1(11)
C21	31.4(13)	45.2(15)	28.2(12)	8.8(11)	4.1(10)	15.3(12)
C22	38.4(15)	48.5(16)	32.9(13)	11.3(12)	4.7(11)	22.3(13)
C23	39.7(15)	36.2(14)	36.6(14)	13.5(11)	10.4(12)	15.9(12)
C24	33.1(13)	29.7(12)	32.3(12)	8.5(10)	7.5(10)	10.8(11)
C25	25.3(11)	26.5(12)	25.3(11)	5.5(9)	5.6(9)	5.5(10)
C26	28.0(12)	30.0(12)	28.5(12)	7.8(10)	7.6(10)	10.1(10)
C27	38.8(14)	29.7(13)	37.2(14)	8.2(11)	10.7(11)	11.3(12)
C28	44.0(16)	31.5(13)	37.0(14)	0.5(11)	10.3(12)	12.9(12)
C29	35.8(14)	36.9(14)	28.6(12)	2.8(10)	8.0(11)	10.4(12)
C30	32.1(13)	34.8(13)	26.6(12)	7.4(10)	9.5(10)	11.4(11)
C31	24.0(11)	33.8(13)	27.8(12)	9.3(10)	7.0(9)	6.8(10)
C32	28.5(13)	33.2(13)	32.3(13)	5.7(10)	8.3(10)	4.9(11)
C33	29.9(13)	35.7(14)	38.3(14)	6.0(11)	2.4(11)	4.4(12)
C34	24.3(12)	38.0(15)	47.4(16)	11.6(12)	10.7(11)	2.3(11)
C35	35.2(14)	38.4(14)	44.2(15)	10.6(12)	18.5(12)	10.2(12)
C36	29.4(13)	34.9(13)	31.7(13)	7(1)	10.7(10)	5.9(11)
C37	24.6(11)	29.0(12)	31.5(12)	1.6(10)	7.5(10)	6.9(10)
C38	28.2(12)	27.7(12)	30.0(12)	10.0(9)	12.8(10)	7.4(10)
C39	27.1(12)	30.7(12)	29.8(12)	4.2(10)	10.3(10)	6.6(10)
C40	29.4(13)	31.2(13)	32.1(12)	7.9(10)	12.9(10)	8.1(11)
C41	29.9(12)	27.1(12)	24.2(11)	6.1(9)	10.1(9)	7.8(10)
C42	34.6(13)	32.8(13)	28.4(12)	9(1)	10.5(10)	14.7(11)
C43	49.8(17)	36.2(14)	39.2(14)	17.2(12)	19.1(13)	20.6(13)
C44	46.1(17)	36.9(15)	57.2(18)	23.1(14)	28.1(15)	13.2(13)
C45	35.9(14)	38.1(15)	52.8(17)	17.4(13)	20.9(13)	12.8(13)
C46	28.9(14)	43.8(16)	51.3(17)	13.4(13)	15.9(12)	12.0(12)
C47	26.7(12)	26.7(12)	25.1(11)	4.5(9)	7.1(9)	4.1(10)
C48	27.8(12)	29.7(12)	25.3(11)	5.4(9)	8.3(10)	5.8(10)
C49	22.6(11)	29.1(12)	21.7(10)	4.1(9)	4.8(9)	4.7(10)
C50	26.2(12)	33.3(13)	28.5(12)	6.8(10)	4.7(10)	8.3(11)
C51	25.1(12)	45.3(15)	35.4(13)	6.6(11)	3.4(10)	12.7(12)
C52	23.7(12)	41.0(15)	45.4(16)	5.3(12)	3.9(11)	2.8(12)
C53	29.9(13)	31.1(13)	39.9(14)	7.1(11)	7.9(11)	4.3(11)
C54	36.0(14)	26.6(12)	36.6(14)	7(1)	2.6(11)	4.2(11)
O8	69.0(16)	64.8(15)	53.5(13)	30.6(12)	33.3(12)	31.4(14)
C55	58(2)	64(2)	63(2)	22.8(19)	19.6(18)	22.5(19)
C56	67(2)	67(2)	64(2)	24.4(19)	31.9(19)	31(2)

O9	41.6(12)	49.5(12)	41.8(11)	2.7(9)	0.8(9)	9.1(10)
C57	45.0(18)	50.4(18)	57(2)	0.6(16)	2.9(15)	15.3(15)
C58	62(2)	50.6(19)	50.4(19)	12.4(15)	0.4(17)	14.9(18)
F1	62.6(12)	41.9(10)	64.8(12)	9.2(9)	32.8(10)	6.9(9)
F2	52.8(11)	37.6(9)	76.3(13)	6.9(9)	27.1(10)	12.5(9)
F3	120(2)	41.7(11)	133(2)	19.9(13)	99(2)	21.4(13)
F4	97(2)	65.7(17)	187(4)	-30(2)	-70(2)	39.5(17)
B1	43(2)	37.0(18)	72(3)	8.1(17)	19.5(19)	9.6(16)

Table S39. Bond Lengths for 6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Ru2	2.9484(2)	C20	C21	1.529(3)
Ru1	P1	2.2962(6)	C21	C22	1.523(4)
Ru1	O3	2.0492(17)	C22	C23	1.516(4)
Ru1	O4	2.0893(16)	C23	C24	1.524(3)
Ru1	O6	2.2210(16)	C25	C26	1.548(3)
Ru1	O7	2.0590(16)	C25	C30	1.536(3)
Ru1	C37	1.822(3)	C26	C27	1.534(4)
Ru2	P2	2.2989(6)	C27	C28	1.534(4)
Ru2	O4	2.2481(16)	C28	C29	1.524(4)
Ru2	O5	2.0490(17)	C29	C30	1.520(4)
Ru2	O6	2.0810(16)	C31	C32	1.521(4)
Ru2	O7	2.0685(16)	C31	C36	1.545(3)
Ru2	C38	1.820(3)	C32	C33	1.535(4)
P1	C1	1.863(3)	C33	C34	1.519(4)
P1	C7	1.853(3)	C34	C35	1.507(4)
P1	C13	1.854(2)	C35	C36	1.526(4)
P2	C19	1.857(2)	C39	C40	1.468(4)
P2	C25	1.853(2)	C39	C46	1.499(4)
P2	C31	1.862(3)	C40	C41	1.427(4)
O1	C37	1.161(3)	C40	C45	1.413(4)
O2	C38	1.156(3)	C41	C42	1.410(3)
O3	C39	1.253(3)	C42	C43	1.370(4)
O4	C41	1.329(3)	C43	C44	1.397(4)
O5	C47	1.252(3)	C44	C45	1.371(4)
O6	C49	1.331(3)	C47	C48	1.454(4)
C1	C2	1.538(4)	C47	C54	1.499(3)
C1	C6	1.521(4)	C48	C49	1.423(4)
C2	C3	1.524(4)	C48	C53	1.420(4)
C3	C4	1.519(4)	C49	C50	1.409(3)
C4	C5	1.517(4)	C50	C51	1.369(4)
C5	C6	1.535(4)	C51	C52	1.381(4)
C7	C8	1.547(3)	C52	C53	1.381(4)
C7	C12	1.530(3)	O8	C55	1.444(4)
C8	C9	1.538(3)	O8	C56	1.418(5)
C9	C10	1.525(4)	C55	C56[1]	1.460(5)

C10	C11	1.523(4)	C56	C55[1]	1.460(5)
C11	C12	1.528(4)	O9	C57	1.429(4)
C13	C14	1.524(4)	O9	C58	1.423(4)
C13	C18	1.544(4)	C57	C58[2]	1.464(5)
C14	C15	1.530(4)	C58	C57[2]	1.464(5)
C15	C16	1.514(5)	F1	B1	1.402(4)
C16	C17	1.514(5)	F2	B1	1.392(4)
C17	C18	1.531(4)	F3	B1	1.379(5)
C19	C20	1.539(3)	F4	B1	1.364(5)
C19	C24	1.537(3)			

[1]-X,1-Y,1-Z; [2]-X,-Y,-Z

Table S40. Bond Angles for 6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Ru1	Ru2	126.289(16)	C11	C10	C9	111.3(2)
O3	Ru1	Ru2	120.15(5)	C10	C11	C12	111.2(2)
O3	Ru1	P1	94.79(5)	C11	C12	C7	110.0(2)
O3	Ru1	O4	87.93(7)	C14	C13	P1	115.10(19)
O3	Ru1	O6	91.30(6)	C14	C13	C18	111.1(2)
O3	Ru1	O7	164.40(7)	C18	C13	P1	110.80(17)
O4	Ru1	Ru2	49.48(4)	C13	C14	C15	110.1(2)
O4	Ru1	P1	98.10(5)	C16	C15	C14	111.6(2)
O4	Ru1	O6	75.57(6)	C17	C16	C15	111.4(3)
O6	Ru1	Ru2	44.78(4)	C16	C17	C18	110.7(3)
O6	Ru1	P1	171.07(4)	C17	C18	C13	111.1(2)
O7	Ru1	Ru2	44.54(5)	C20	C19	P2	113.83(17)
O7	Ru1	P1	94.72(5)	C24	C19	P2	110.91(17)
O7	Ru1	O4	78.51(6)	C24	C19	C20	110.8(2)
O7	Ru1	O6	77.97(6)	C21	C20	C19	110.2(2)
C37	Ru1	Ru2	121.21(8)	C22	C21	C20	112.2(2)
C37	Ru1	P1	91.38(8)	C23	C22	C21	110.6(2)
C37	Ru1	O3	95.13(9)	C22	C23	C24	111.1(2)
C37	Ru1	O4	169.77(9)	C23	C24	C19	112.5(2)
C37	Ru1	O6	94.57(9)	C26	C25	P2	113.90(16)
C37	Ru1	O7	96.97(9)	C30	C25	P2	116.91(17)
P2	Ru2	Ru1	126.622(16)	C30	C25	C26	109.4(2)
O4	Ru2	Ru1	44.95(4)	C27	C26	C25	109.7(2)
O4	Ru2	P2	171.47(4)	C26	C27	C28	112.5(2)
O5	Ru2	Ru1	119.64(5)	C29	C28	C27	111.4(2)
O5	Ru2	P2	93.90(5)	C30	C29	C28	111.2(2)
O5	Ru2	O4	90.85(6)	C29	C30	C25	110.0(2)
O5	Ru2	O6	87.97(7)	C32	C31	P2	115.37(17)
O5	Ru2	O7	163.70(7)	C32	C31	C36	108.7(2)
O6	Ru2	Ru1	48.75(4)	C36	C31	P2	113.52(17)
O6	Ru2	P2	97.93(5)	C31	C32	C33	111.0(2)
O6	Ru2	O4	75.14(6)	C34	C33	C32	111.3(2)

O7	Ru2	Ru1	44.28(4)	C35	C34	C33	110.7(2)
O7	Ru2	P2	99.47(5)	C34	C35	C36	111.0(2)
O7	Ru2	O4	74.77(6)	C35	C36	C31	111.0(2)
O7	Ru2	O6	81.03(6)	O1	C37	Ru1	173.9(2)
C38	Ru2	Ru1	123.73(8)	O2	C38	Ru2	176.3(2)
C38	Ru2	P2	90.00(8)	O3	C39	C40	125.1(2)
C38	Ru2	O4	96.71(8)	O3	C39	C46	115.0(2)
C38	Ru2	O5	94.26(9)	C40	C39	C46	119.9(2)
C38	Ru2	O6	171.60(9)	C41	C40	C39	124.0(2)
C38	Ru2	O7	95.01(9)	C45	C40	C39	117.6(2)
C1	P1	Ru1	113.16(8)	C45	C40	C41	118.4(2)
C7	P1	Ru1	111.91(8)	O4	C41	C40	124.7(2)
C7	P1	C1	111.48(12)	O4	C41	C42	117.2(2)
C7	P1	C13	103.63(11)	C42	C41	C40	118.0(2)
C13	P1	Ru1	113.08(8)	C43	C42	C41	121.5(3)
C13	P1	C1	102.85(12)	C42	C43	C44	120.7(3)
C19	P2	Ru2	113.62(8)	C45	C44	C43	119.2(3)
C19	P2	C31	105.53(11)	C44	C45	C40	121.9(3)
C25	P2	Ru2	110.97(8)	O5	C47	C48	125.3(2)
C25	P2	C19	104.58(11)	O5	C47	C54	114.7(2)
C25	P2	C31	106.02(11)	C48	C47	C54	120.0(2)
C31	P2	Ru2	115.27(8)	C49	C48	C47	124.5(2)
C39	O3	Ru1	129.89(16)	C53	C48	C47	118.1(2)
Ru1	O4	Ru2	85.57(6)	C53	C48	C49	117.4(2)
C41	O4	Ru1	127.19(15)	O6	C49	C48	124.4(2)
C41	O4	Ru2	122.63(14)	O6	C49	C50	116.9(2)
C47	O5	Ru2	129.75(16)	C50	C49	C48	118.7(2)
Ru2	O6	Ru1	86.47(6)	C51	C50	C49	121.6(3)
C49	O6	Ru1	123.19(14)	C50	C51	C52	120.7(3)
C49	O6	Ru2	127.44(15)	C53	C52	C51	119.2(3)
Ru1	O7	Ru2	91.18(7)	C52	C53	C48	122.3(3)
C2	C1	P1	116.24(18)	C56	O8	C55	108.8(3)
C6	C1	P1	113.46(18)	O8	C55	C56[1]	110.6(3)
C6	C1	C2	108.8(2)	O8	C56	C55[1]	112.0(3)
C3	C2	C1	110.3(2)	C58	O9	C57	108.9(3)
C4	C3	C2	111.7(3)	O9	C57	C58[2]	111.2(3)
C5	C4	C3	111.2(3)	O9	C58	C57[2]	112.4(3)
C4	C5	C6	111.1(2)	F2	B1	F1	109.3(3)
C1	C6	C5	110.6(2)	F3	B1	F1	106.8(3)
C8	C7	P1	115.37(17)	F3	B1	F2	110.2(3)
C12	C7	P1	116.64(18)	F4	B1	F1	107.9(4)
C12	C7	C8	109.4(2)	F4	B1	F2	110.0(3)
C9	C8	C7	109.6(2)	F4	B1	F3	112.6(4)
C10	C9	C8	111.5(2)				

[1]-X,1-Y,1-Z; [2]-X,-Y,-Z

Table S41. Torsion Angles for 6.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	Ru2	P2	C19	-24.71(9)	O6	Ru2	O7	Ru1	37.42(6)
Ru1	Ru2	P2	C25	-142.21(8)	O6	Ru2	C38	O2	8(4)
Ru1	Ru2	P2	C31	97.28(9)	O6	C49	C50	C51	-178.2(2)
Ru1	Ru2	O4	C41	132.09(19)	O7	Ru1	Ru2	P2	-62.07(7)
Ru1	Ru2	O5	C47	30.0(2)	O7	Ru1	Ru2	O4	119.66(9)
Ru1	Ru2	O6	C49	-130.1(2)	O7	Ru1	Ru2	O5	176.56(8)
Ru1	Ru2	C38	O2	33(4)	O7	Ru1	Ru2	O6	-127.03(9)
Ru1	P1	C1	C2	148.50(18)	O7	Ru1	Ru2	C38	57.70(11)
Ru1	P1	C1	C6	84.25(18)	O7	Ru1	P1	C1	54.07(10)
Ru1	P1	C7	C8	-55.1(2)	O7	Ru1	P1	C7	-178.96(10)
Ru1	P1	C7	C12	174.44(16)	O7	Ru1	P1	C13	-62.37(11)
Ru1	P1	C13	C14	-73.7(2)	O7	Ru1	O3	C39	17.7(4)
Ru1	P1	C13	C18	53.4(2)	O7	Ru1	O4	Ru2	-38.46(6)
Ru1	O3	C39	C40	10.8(4)	O7	Ru1	O4	C41	-166.78(19)
Ru1	O3	C39	C46	-169.87(18)	O7	Ru1	O6	Ru2	34.93(6)
Ru1	O4	C41	C40	1.5(3)	O7	Ru1	O6	C49	168.36(18)
Ru1	O4	C41	C42	-178.71(16)	O7	Ru1	C37	O1	77(2)
Ru1	O6	C49	C48	-114.1(2)	O7	Ru2	P2	C19	-63.41(10)
Ru1	O6	C49	C50	66.4(3)	O7	Ru2	P2	C25	179.08(9)
Ru2	Ru1	P1	C1	88.31(9)	O7	Ru2	P2	C31	58.57(10)
Ru2	Ru1	P1	C7	-144.72(9)	O7	Ru2	O4	Ru1	38.96(6)
Ru2	Ru1	P1	C13	-28.13(10)	O7	Ru2	O4	C41	171.05(18)
Ru2	Ru1	O3	C39	27.7(2)	O7	Ru2	O5	C47	38.6(4)
Ru2	Ru1	O4	C41	-128.3(2)	O7	Ru2	O6	Ru1	-34.35(6)
Ru2	Ru1	O6	C49	133.43(19)	O7	Ru2	O6	C49	-164.41(19)
Ru2	Ru1	C37	O1	37(2)	O7	Ru2	C38	O2	70(4)
Ru2	P2	C19	C20	-72.14(18)	C1	P1	C7	C8	72.8(2)
Ru2	P2	C19	C24	53.66(19)	C1	P1	C7	C12	-57.7(2)
Ru2	P2	C25	C26	-59.89(18)	C1	P1	C13	C14	163.94(19)
Ru2	P2	C25	C30	170.85(16)	C1	P1	C13	C18	-69.0(2)
Ru2	P2	C31	C32	-33.2(2)	C1	C2	C3	C4	57.0(3)
Ru2	P2	C31	C36	159.63(16)	C2	C1	C6	C5	59.5(3)
Ru2	O4	C41	C40	-110.3(2)	C2	C3	C4	C5	-54.3(4)
Ru2	O4	C41	C42	69.5(3)	C3	C4	C5	C6	54.1(3)
Ru2	O5	C47	C48	10.5(4)	C4	C5	C6	C1	-57.6(3)
Ru2	O5	C47	C54	169.58(17)	C6	C1	C2	C3	-59.2(3)
Ru2	O6	C49	C48	-0.1(3)	C7	P1	C1	C2	84.3(2)

Ru2	O6	C49	C50	−179.49(16)	C7	P1	C1	C6	−42.9(2)
P1	Ru1	Ru2	P2	−115.15(3)	C7	P1	C13	C14	47.7(2)
P1	Ru1	Ru2	O4	66.57(6)	C7	P1	C13	C18	174.82(19)
P1	Ru1	Ru2	O5	123.48(6)	C7	C8	C9	C10	56.7(3)
P1	Ru1	Ru2	O6	179.89(6)	C8	C7	C12	C11	60.1(3)
P1	Ru1	Ru2	O7	−53.09(7)	C8	C9	C10	C11	−54.6(3)
P1	Ru1	Ru2	C38	4.61(9)	C9	C10	C11	C12	55.0(3)
P1	Ru1	O3	C39	−109.7(2)	C10	C11	C12	C7	−58.1(3)
P1	Ru1	O4	Ru2	−131.66(4)	C12	C7	C8	C9	−59.3(3)
P1	Ru1	O4	C41	100.01(18)	C13	P1	C1	C2	−26.2(2)
P1	Ru1	O6	Ru2	−0.6(3)	C13	P1	C1	C6	−153.41(18)
P1	Ru1	O6	C49	132.8(3)	C13	P1	C7	C8	−177.23(19)
P1	Ru1	O7	Ru2	139.71(5)	C13	P1	C7	C12	52.3(2)
P1	Ru1	C37	O1	172(2)	C13	C14	C15	C16	−56.7(3)
P1	C1	C2	C3	171.3(2)	C14	C13	C18	C17	−55.5(3)
P1	C1	C6	C5	−169.49(18)	C14	C15	C16	C17	57.3(3)
P1	C7	C8	C9	166.84(18)	C15	C16	C17	C18	−56.1(3)
P1	C7	C12	C11	−166.64(19)	C16	C17	C18	C13	55.1(3)
P1	C13	C14	C15	−177.54(19)	C18	C13	C14	C15	55.5(3)
P1	C13	C18	C17	175.3(2)	C19	P2	C25	C26	177.22(17)
P2	Ru2	O4	Ru1	−9.4(3)	C19	P2	C25	C30	48.0(2)
P2	Ru2	O4	C41	122.7(3)	C19	P2	C31	C32	93.0(2)
P2	Ru2	O5	C47	−106.6(2)	C19	P2	C31	C36	−33.4(2)
P2	Ru2	O6	Ru1	−132.76(4)	C19	C20	C21	C22	−56.5(3)
P2	Ru2	O6	C49	97.18(18)	C20	C19	C24	C23	−54.1(3)
P2	Ru2	O7	Ru1	134.04(5)	C20	C21	C22	C23	57.3(3)
P2	Ru2	C38	O2	169(4)	C21	C22	C23	C24	−55.5(3)
P2	C19	C20	C21	179.85(17)	C22	C23	C24	C19	54.8(3)
P2	C19	C24	C23	178.43(18)	C24	C19	C20	C21	54.0(3)
P2	C25	C26	C27	168.61(17)	C25	P2	C19	C20	49.0(2)
P2	C25	C30	C29	−167.66(18)	C25	P2	C19	C24	174.81(18)
P2	C31	C32	C33	173.95(18)	C25	P2	C31	C32	−156.39(18)
P2	C31	C36	C35	−172.30(18)	C25	P2	C31	C36	77.2(2)
O3	Ru1	Ru2	P2	121.74(6)	C25	C26	C27	C28	54.7(3)
O3	Ru1	Ru2	O4	−56.54(8)	C26	C25	C30	C29	61.0(3)
O3	Ru1	Ru2	O5	0.37(7)	C26	C27	C28	C29	−52.7(3)
O3	Ru1	Ru2	O6	56.78(8)	C27	C28	C29	C30	54.3(3)
O3	Ru1	Ru2	O7	−176.20(9)	C28	C29	C30	C25	−59.0(3)

O3	Ru1	Ru2	C38	−118.50(11)	C30	C25	C26	C27	−58.5(3)
O3	Ru1	P1	C1	−138.31(10)	C31	P2	C19	C20	160.62(18)
O3	Ru1	P1	C7	−11.34(10)	C31	P2	C19	C24	−73.6(2)
O3	Ru1	P1	C13	105.25(11)	C31	P2	C25	C26	65.96(19)
O3	Ru1	O4	Ru2	133.79(6)	C31	P2	C25	C30	−63.3(2)
O3	Ru1	O4	C41	5.47(18)	C31	C32	C33	C34	57.2(3)
O3	Ru1	O6	Ru2	−133.65(6)	C32	C31	C36	C35	57.8(3)
O3	Ru1	O6	C49	−0.22(18)	C32	C33	C34	C35	−55.9(3)
O3	Ru1	O7	Ru2	12.3(3)	C33	C34	C35	C36	56.4(3)
O3	Ru1	C37	O1	−93(2)	C34	C35	C36	C31	−58.0(3)
O3	C39	C40	C41	0.3(4)	C36	C31	C32	C33	−57.2(3)
O3	C39	C40	C45	−179.7(3)	C37	Ru1	Ru2	P2	3.52(9)
O4	Ru1	Ru2	P2	178.27(6)	C37	Ru1	Ru2	O4	−174.75(11)
O4	Ru1	Ru2	O5	56.90(8)	C37	Ru1	Ru2	O5	−117.85(11)
O4	Ru1	Ru2	O6	113.31(8)	C37	Ru1	Ru2	O6	−61.44(11)
O4	Ru1	Ru2	O7	−119.66(9)	C37	Ru1	Ru2	O7	65.59(11)
O4	Ru1	Ru2	C38	−61.96(11)	C37	Ru1	Ru2	C38	123.29(12)
O4	Ru1	P1	C1	133.11(10)	C37	Ru1	P1	C1	−43.04(12)
O4	Ru1	P1	C7	−99.92(10)	C37	Ru1	P1	C7	83.93(12)
O4	Ru1	P1	C13	16.66(11)	C37	Ru1	P1	C13	−159.49(12)
O4	Ru1	O3	C39	−11.7(2)	C37	Ru1	O3	C39	158.5(2)
O4	Ru1	O6	Ru2	−46.12(6)	C37	Ru1	O4	Ru2	26.1(5)
O4	Ru1	O6	C49	87.30(18)	C37	Ru1	O4	C41	−102.2(5)
O4	Ru1	O7	Ru2	42.38(6)	C37	Ru1	O6	Ru2	131.10(9)
O4	Ru1	C37	O1	14(3)	C37	Ru1	O6	C49	−95.47(18)
O4	Ru2	P2	C19	−16.5(3)	C37	Ru1	O7	Ru2	−128.31(9)
O4	Ru2	P2	C25	−134.0(3)	C38	Ru2	P2	C19	−158.49(12)
O4	Ru2	P2	C31	105.5(3)	C38	Ru2	P2	C25	84.00(11)
O4	Ru2	O5	C47	66.3(2)	C38	Ru2	P2	C31	−36.51(12)
O4	Ru2	O6	Ru1	42.16(5)	C38	Ru2	O4	Ru1	132.34(9)
O4	Ru2	O6	C49	−87.89(18)	C38	Ru2	O4	C41	−95.57(19)
O4	Ru2	O7	Ru1	−39.51(6)	C38	Ru2	O5	C47	163.1(2)
O4	Ru2	C38	O2	−6(4)	C38	Ru2	O6	Ru1	28.0(6)
O4	C41	C42	C43	−176.7(2)	C38	Ru2	O6	C49	−102.1(6)
O5	Ru2	P2	C19	107.24(10)	C38	Ru2	O7	Ru1	−135.12(9)
O5	Ru2	P2	C25	−10.27(10)	C39	C40	C41	O4	−6.6(4)
O5	Ru2	P2	C31	−130.78(10)	C39	C40	C41	C42	173.6(2)
O5	Ru2	O4	Ru1	−133.27(6)	C39	C40	C45	C44	−175.2(3)
O5	Ru2	O4	C41	−1.18(18)	C40	C41	C42	C43	3.2(4)
O5	Ru2	O6	Ru1	133.58(6)	C41	C40	C45	C44	4.8(4)

O5	Ru2	O6	C49	3.52(18)	C41	C42	C43	C44	1.9(4)
O5	Ru2	O7	Ru1	-10.7(3)	C42	C43	C44	C45	-3.7(5)
O5	Ru2	C38	O2	-97(4)	C43	C44	C45	C40	0.2(5)
O5	C47	C48	C49	-4.3(4)	C45	C40	C41	O4	173.4(2)
O5	C47	C48	C53	177.4(2)	C45	C40	C41	C42	-6.4(4)
O6	Ru1	Ru2	P2	64.96(6)	C46	C39	C40	C41	-179.0(2)
O6	Ru1	Ru2	O4	-113.31(8)	C46	C39	C40	C45	1.0(4)
O6	Ru1	Ru2	O5	-56.41(8)	C47	C48	C49	O6	-1.1(4)
O6	Ru1	Ru2	O7	127.03(9)	C47	C48	C49	C50	178.3(2)
O6	Ru1	Ru2	C38	-175.28(11)	C47	C48	C53	C52	-179.2(3)
O6	Ru1	P1	C1	88.8(3)	C48	C49	C50	C51	2.3(4)
O6	Ru1	P1	C7	-144.2(3)	C49	C48	C53	C52	2.4(4)
O6	Ru1	P1	C13	-27.6(3)	C49	C50	C51	C52	0.1(4)
O6	Ru1	O3	C39	63.8(2)	C50	C51	C52	C53	-1.2(4)
O6	Ru1	O4	Ru2	41.91(5)	C51	C52	C53	C48	-0.1(4)
O6	Ru1	O4	C41	-86.41(18)	C53	C48	C49	O6	177.1(2)
O6	Ru1	O7	Ru2	-35.10(6)	C53	C48	C49	C50	-3.4(3)
O6	Ru1	C37	O1	-1(2)	C54	C47	C48	C49	175.8(2)
O6	Ru2	P2	C19	18.75(10)	C54	C47	C48	C53	-2.5(4)
O6	Ru2	P2	C25	-98.76(10)	C55	O8	C56	C55[1]	-57.4(5)
O6	Ru2	P2	C31	140.73(10)	C56	O8	C55	C56[1]	56.5(5)
O6	Ru2	O4	Ru1	-45.59(6)	C57	O9	C58	C57[2]	56.3(4)
O6	Ru2	O4	C41	86.50(18)	C58	O9	C57	C58[2]	-55.6(4)
O6	Ru2	O5	C47	-8.8(2)					

[1]-X,1-Y,1-Z; [2]-X,-Y,-Z

Table S42. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6.

Atom	*x*	*y*	*z*	U(eq)
H1	4988	9571	3135	36
H2A	5320	10854	4293	45
H2B	6166	10092	4137	45
H3A	7285	12253	4155	56
H3B	7006	11440	3517	56
H4A	5569	12846	3843	52
H4B	6487	13159	3399	52
H5A	5059	11382	2701	45
H5B	4250	12159	2886	45
H6A	3460	10794	3518	41
H6B	3109	9993	2869	41
H7	1760	7477	3975	34
H8A	1439	9412	3420	38
H8B	816	7969	3099	38
H9A	-720	8496	3515	44
H9B	-414	7432	3801	44
H10A	651	10030	4341	47

H10B	-359	8931	4560	47
H11A	1204	8123	4848	47
H11B	1796	9572	5153	47
H12A	3347	9084	4746	40
H12B	2978	10089	4432	40
H13	5004	8646	4450	37
H14A	3400	6038	4152	44
H14B	3219	7043	4607	44
H15A	5248	7457	5242	54
H15B	4384	5989	5116	54
H16A	6517	6357	5040	58
H16B	5493	5614	4426	58
H17A	7239	7223	4248	53
H17B	7066	8236	4702	53
H18A	5246	6854	3600	41
H18B	6112	8324	3743	41
H19	4302	5706	568	33
H20A	2376	3911	392	37
H20B	1884	4569	872	37
H21A	2273	5358	-207	42
H21B	889	4715	-70	42
H22A	1506	6906	39	47
H22B	1345	6485	650	47
H23A	3278	8261	832	44
H23B	3764	7604	349	44
H24A	3453	6871	1443	39
H24B	4810	7490	1279	39
H25	3341	2932	1051	33
H26A	5894	3106	1553	35
H26B	4778	2846	1901	35
H27A	3473	957	1234	43
H27B	4866	932	1475	43
H28A	5453	1359	604	46
H28B	4074	202	428	46
H29A	4114	1714	-173	42
H29B	3001	1496	173	42
H30A	4145	3660	244	37
H30B	5482	3558	528	37
H31	6827	5367	1687	36
H32A	6785	6883	2417	40
H32B	6624	7708	1937	40
H33A	8838	8470	2446	46
H33B	8850	7114	2281	46
H34A	8544	8657	1458	47
H34B	9797	8345	1644	47
H35A	8601	6244	1195	47

H35B	8455	7092	724	47
H36A	6398	5520	681	40
H36B	6401	6876	866	40
H42	3597	3665	3526	37
H43	2261	1909	3785	46
H44	17	1378	3591	53
H45	-828	2731	3221	49
H46A	-1311	4486	3319	61
H46B	-1656	3771	2654	61
H46C	-1399	5219	2794	61
H50	100	5409	1494	37
H51	-1992	3929	1170	44
H52	-2454	1847	1226	49
H53	-781	1251	1585	43
H54A	2102	994	2127	55
H54B	817	641	1616	55
H54C	796	961	2288	55
H55A	-1601	4539	4475	72
H55B	-1150	6020	4544	72
H56A	1474	4575	4582	74
H56B	-10	3673	4504	74
H57A	-3	1934	263	65
H57B	-1006	641	354	65
H58A	-236	-936	574	70
H58B	1264	-657	633	70

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