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Highly Cooperative Tetrametallic Ruthenium-μ-Oxo-μ-Hydroxo Catalyst for the Alcohol Oxidation Reaction

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Abstract: The tetrametallic ruthenium-oxo-hydroxo-hydride complex {[$(PCy_3)(CO)RuH]_4(\mu_4\text{-}O)(\mu_3\text{-}OH)(\mu_2\text{-}OH)$} (**1**) was synthesized in two steps from the monomeric complex $(PCy_3)(CO)RuHCl$ (**2**). The tetrameric complex **1** was found to be a highly effective catalyst for the transfer dehydrogenation of

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alcohols. Complex **1** showed a different catalytic activity pattern towards primary and secondary benzyl alcohols, as indicated by the Hammett correlation for the oxidation reaction of *p*-X-$C_6H_4CH_2OH$ ($\rho = -0.45$) and *p*-X-$C_6H_4CH(OH)CH_3$ ($\rho = +0.22$) (X = OMe, CH_3, H, Cl, CF_3). Both a sigmoidal curve from the plot of initial rate vs [$PhCH(OH)CH_3$] ($K_{0.5}$ = 0.34 *M*; Hill coefficient, $n = 4.2\pm0.1$) and the phosphine inhibition kinetics revealed the highly cooperative nature of the complex for the oxidation of secondary alcohols.

Introduction

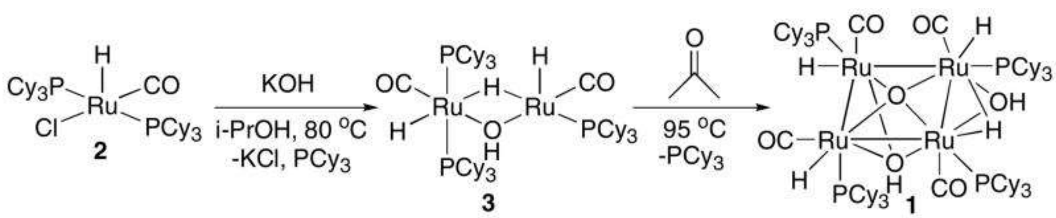
Considerable efforts have been devoted to the design of cooperative metal catalysts, for such catalysts may lead to increase in activity and serve as functional models for natural metalloenzymes.[1] For example, Jacobsen showed cooperative effects of chiral metal–salen complexes in catalytic asymmetric epoxide ring–opening and conjugate addition reactions.[2] Shibasaki also discovered cooperative effects of heterobimetallic catalysts for asymmetric conjugate addition and related reactions.[3] By employing a supramolecular approach, Mirkin and co-workers recently synthesized dimeric analogs of Jacobsen's epoxidation catalyst and demonstrated the allosteric nature in asymmetric epoxide ring-opening reactions.[4] Bimetallic Cu– and Zn–polypyridine[5] and tetrametallic Mn–oxo complexes[6] were found to exhibit cooperative catalytic activity for the hydrolysis of phosphate esters and the disproportionation of H_2O_2, respectively. Bimetallic cooperativity of cationic Rh complexes for cyclopropanation and hydroformylation reactions[7] and Ru complexes for alkyne coupling reactions[8] have also been well–documented. A number of different bimetallic supramolecular hosts have been found to bind guests allosterically.[9]

Despite such recent progress, however, only a few well–defined polymetallic catalysts have been shown to exhibit cooperative catalytic activity. Moreover, most synthetic metal catalysts contain only one or two substrate binding sites; multiple substrate binding sites are necessary for achieving high degrees of cooperativity. Inspired by recent reports on unusual reactivity of low–valent late metal complexes with "hard" oxygen and nitrogen ligands,[10] we have begun to utilize the ruthenium–hydroxo and –amido complexes for selective bond activation reactions.[11] Here we report the synthesis of a novel tetrametallic ruthenium–oxo–hydroxo complex {[$(PCy_3)(CO)RuH]_4$(μ_4-

O)(μ_3-OH)(μ_2-OH)} (**1**), and its cooperative catalytic activity for the alcohol oxidation reaction.

Results and Discussion

The tetrametallic complex **1** was synthesized in two steps from the ruthenium-hydride complex $(PCy_3)_2(CO)RuHCl$ (**2**) (Scheme 1). Thus, the reaction of **2** with KOH in 2-propanol produced the bimetallic complex **3**, which was isolated in 85% yield after recrystallization in hexanes.[12] The subsequent treatment of **3** with acetone at 95 °C yielded complex **1** in 84% yield as a brown–red solid. The ^1H NMR spectrum of **1** in CD_2Cl_2 exhibited four metal–hydride peaks at δ −18.64 (dt, J_{HP} = 13.2, 4.8 Hz), −15.28 (d, J_{HP} = 34.5 Hz), −15.01 (d, J_{HP} = 16.8 Hz) and −14.55 (d, J_{HP} = 20.1 Hz), of which the resonance at δ −18.64 was assigned to the bridging hydride on the basis of its coupling pattern. Two μ-hydroxo proton signals at δ −2.50 and −2.60 were found to readily undergo H/D exchange upon treatment with D_2O.



Scheme 1

The structure of **1** was further established by X–ray crystallography (Figure 1). The molecular structure of **1** showed a puckered butterfly geometry of the ruthenium core, which is supported by both μ_4–oxo and μ_3– and μ_2–hydroxo ligands. Two of the PCy_3 ligands on Ru(1) and Ru(4) occupy pseudo- axial positions, while the PCy_3 ligands on Ru(2) and Ru(3) can be viewed as pseudo-equatorial ones in relative to the metal core geometry. The anti geometry between two axial PCy_3 ligands (P(2) and P(3)) was also indicated by a relatively large coupling constant ($^3J_{PP}$ = 14.0 Hz) in the solution ^{31}P NMR.

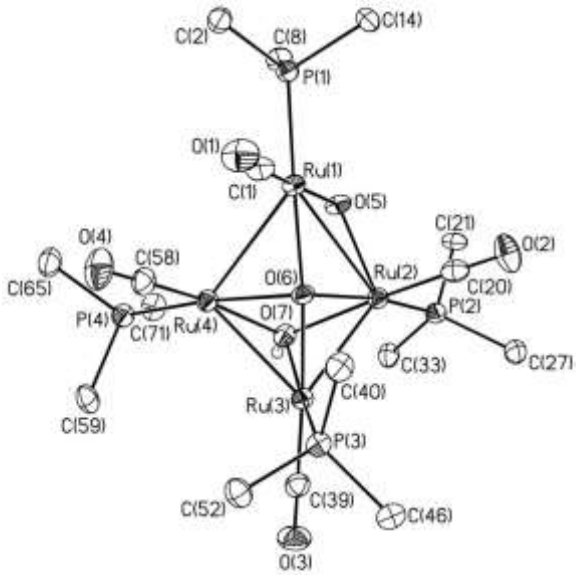
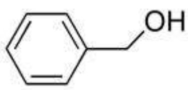
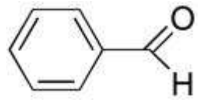
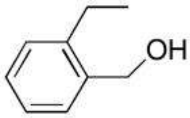
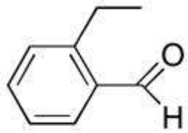
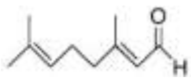
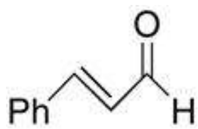
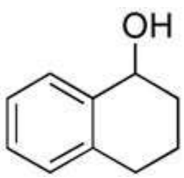
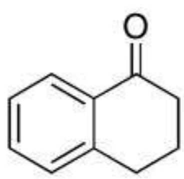
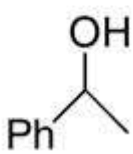
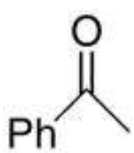
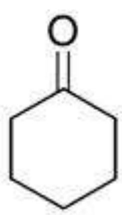
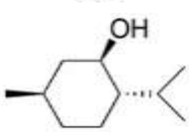
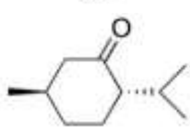
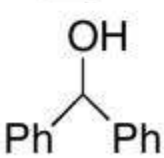
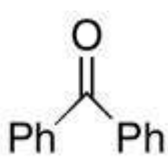
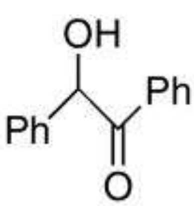
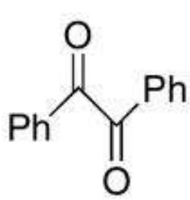


Figure 1. Molecular structure of **1** drawn with 50% thermal ellipsoids. Cyclohexyl groups are omitted for clarity.

Complex **1** was found to be a highly effective catalyst for the oxidation of both primary and secondary alcohols under transfer dehydrogenation conditions (Table 1). Considerably different reactivity pattern was noted between primary and secondary alcohol substrates. For example, the treatment of a primary alcohol $PhCH_2OH$ (1.0 mmol) in acetone (3 mL) in the presence of **1** (2.5 mol %) at 80 °C produced predominantly benzaldehyde (87% conversion after 22 h). For these *primary* alcohols, the red–brown color of reaction mixture (due to catalyst **1**) turned bright yellow after 15 min of heating at 80 °C, and the ruthenium catalyst could not be recovered from the reaction mixture because it was completely soluble in the solution (entry 1–4). In sharp contrast, the red-brown color of reaction mixture remained unchanged throughout the catalytic reaction for the *secondary* alcohols (entries 5–9) (Figure S1, Supporting Information). Furthermore, the catalyst **1** was readily recovered at the end of the catalysis by a simple filtration, as it became insoluble at room temperature. The ^{1}H NMR spectrum of the recovered catalyst was found to be identical to that of **1**, and its activity was found to be same after five repeated cycles. In general, the catalytic activity of **1** was found to be substantially higher than both mono- and bimetallic complexes **2** and **3**.[13]

Table 1. Catalytic oxidation of alcohols mediated by **1**.[a]

entry	alcohol	product	time (h)	convn (%)[b]	yield (%)[c]
1			22	87	84
2			18	100	62
3			3.5	95	85
4			19	100	85
5			18	100	94
6			20	100	97
7			4	100	86
8			6	100	98
9			6	100	97
10			16	83	79

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[a]Reaction conditions: alcohol (1.0 mmol), **1** (2.5 mol % Ru), acetone (3 mL), 80 °C.
[b]The conversion was determined by GC.
[c]Isolated yield.

Encouraged by these initial results, the Hammett study was performed for both primary and secondary benzyl alcohols, *p*-X-$C_6H_4CH_2OH$ and *p*-X-$C_6H_4CH(OH)CH_3$ (X = OMe, CH_3, H, Cl, CF_3), to compare the electronic effects of alcohol substrates on the oxidation reaction. As shown in Figure 2, an opposite trend was observed from the plots of $\log(k_X/k_H)$ vs σ_p between these primary and secondary alcohols ($\rho = -0.45$ for *p*-X-$C_6H_4CH_2OH$; $\rho = +0.22$ for *p*-X-$C_6H_4CHOHCH_3$). A negative Hammett ρ value, which is indicative of a developing positive charge on the α-carbon, has commonly been observed for the alcohol oxidation reactions. On the other hand, a positive ρ value has been much less commonly observed for alcohol oxidation reactions mediated by synthetic metal catalysts. Relatively large positive ρ values have been reported for enzymatic oxidation reactions of benzyl alcohols and amines, wherein carbanion character of carbonyl and imine carbon on the transition state has been implicated.[14] Very recently, Sigman observed a small, but positive ρ value of 0.03 from the palladium-catalyzed aerobic oxidation of benzyl alcohols.[15]

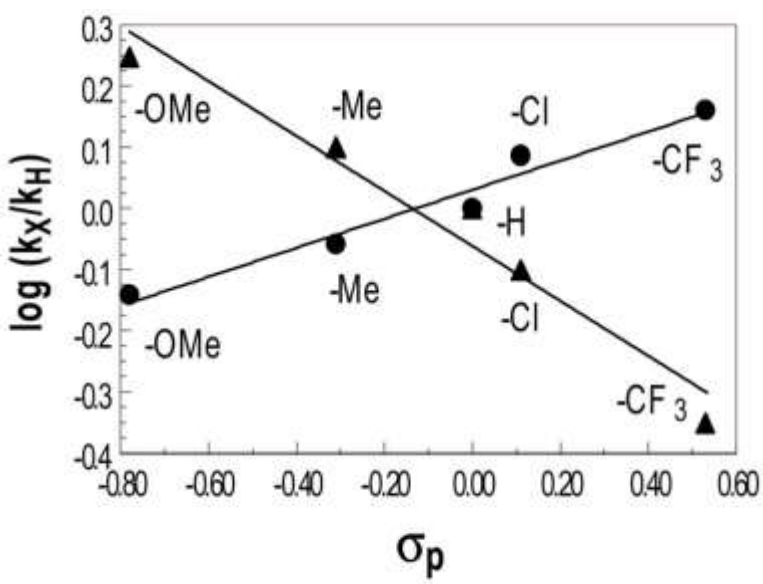

Figure 2 Hammett plots of *p*-X-$C_6H_4CH_2OH$ (▲) and *p*-X-$C_6H_4CH(OH)CH_3$ (●) (X = OMe, CH_3, H, Cl, CF_3).

We next examined the kinetics of the catalytic reaction to gain further insights on the reaction mechanism. The kinetic analysis for the oxidation reaction of secondary alcohols revealed the cooperative nature of complex **1**. Thus, the initial rate of the oxidation of 1-phenylethanol (0.05–0.4 mmol) in acetone–d_6 (0.5 mL) was monitored by NMR at 80 °C at different alcohol concentrations. The plot of initial rate (v_i) vs. [PhCH(OH)CH_3] showed a sigmoidal curve with saturation behavior typically seen for natural allosteric enzymes (Figure 3). The data was successfully fitted to the Hill equation, v_i/V_{max} = [PhCH(OH)CH_3]^4/($K_{0.5}^4$ + [PhCH(OH)CH_3]^4), from which $K_{0.5}$ = 0.34±0.01 *M* and the Hill coefficient, n = 4.2±0.1 were obtained. The similar value of n_{app} = 4.1 was also calculated from an Eadie–Scatchard plot (Figure S5, Supporting Information).

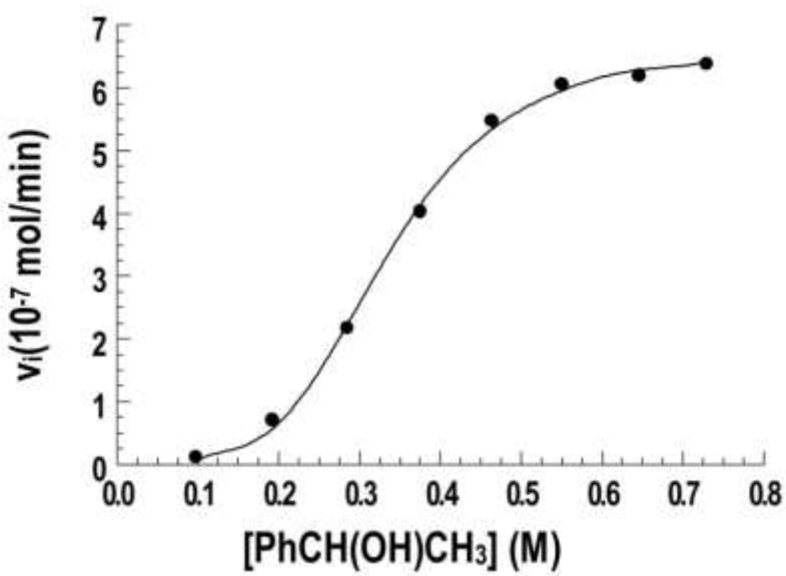

Figure 3 Plot of initial rate (v_i) vs [PhCH(OH)CH_3].

The phosphine inhibition kinetics was conducted to further establish the cooperative nature of complex **1** (Figure 4). The Hill coefficient from the plot of initial rate vs [PhCH(OH)CH_3] was found to decrease to 2.4 upon addition of 1.0 equivalent of PCy_3, and the cooperativity was effectively lost with the addition of 2.0 equivalents of PCy_3, giving a Hill coefficient of 1.1. In contrast, the analogous inhibition kinetic plots for a primary benzyl alcohol, $PhCH_2OH$, gave hyperbolic curves which are commonly observed in Michaelis-Menton type of kinetics (Figure S6, Supporting Information).

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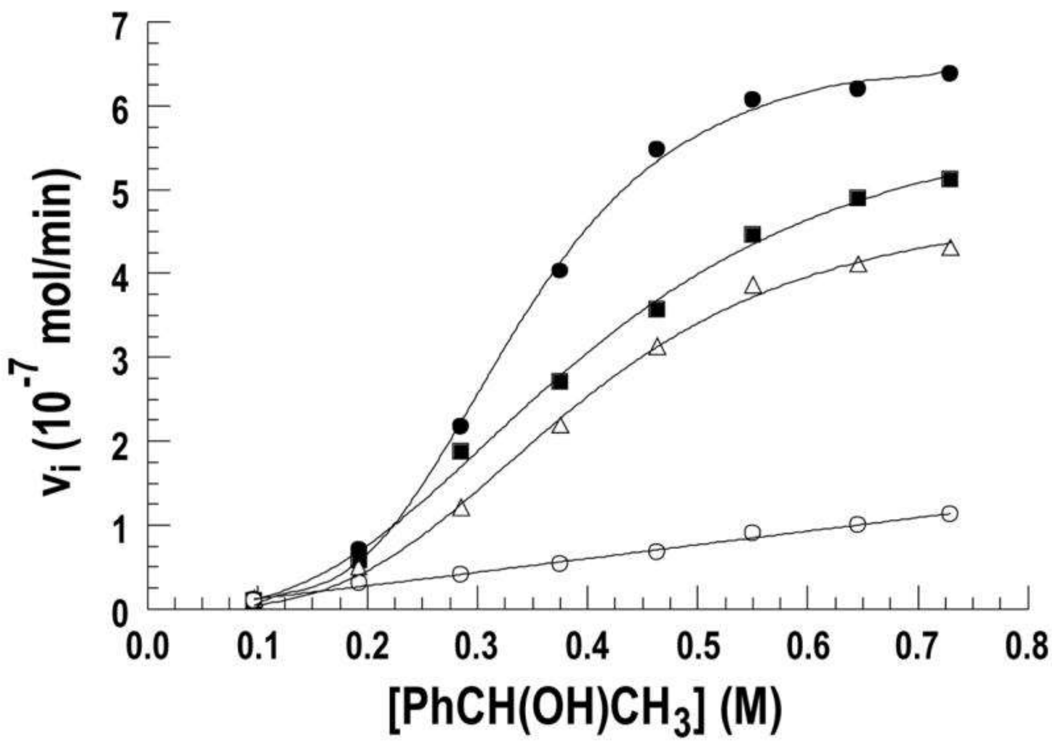
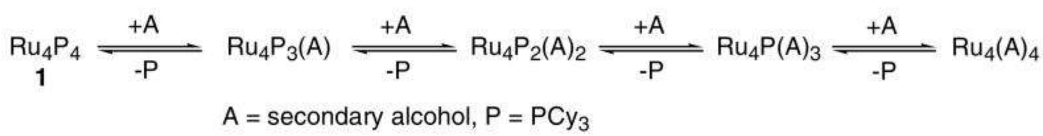


Figure 4 Plots of initial rate vs [PhCH(OH)CH$_3$] at various concentrations of added PCy_3. Without added PCy_3 (circ;); 1.0 equiv of PCy_3 (squf;); 1.5 equiv of PCy_3 (▵); 2.0 equiv of PCy_3 (○)

In an effort to detect possible intermediate species, the reaction of **1** with both primary and secondary benzyl alcohols (8 equiv) in benzene-d_6/acetone-d_6 (1:1) was monitored by VT NMR. For the PhCH(OH)CH$_3$case, the presence of complex **1** was clearly evident after 3 h at 40–60 °C as seen by ^{1}H NMR along with small amounts of secondary products, whose hydride signals are similar to that of **1** (Figure S7, Supporting Information). In contrast, a set of new peaks rapidly appeared at the expense of **1** upon warming to 40 °C for the reaction with PhCH$_2$OH. In this case, the new Ru-H peak at δ−14.79 (d, J_{PH} = 32.1 Hz) exhibited characteristic features of a monomeric ruthenium species similar to previously observed ruthenium-hydride complexes (PCy_3)(CO)(X)Ru(H)L_2 (X = OR; L = solvent).[11a] Both **1** and the new complex rapidly decomposed into a complex mixture of products within 10 min upon warming to 50 °C. These results further indicate the different reactivity pattern of **1** towards primary and secondary alcohols.

The exact cooperative mechanism of the catalytic reaction is not clear. We propose a plausible mechanistic model of the sequential cooperative binding of alcohol substrate as shown in Scheme 2 to explain the kinetic data. The Hill coefficient of n = 4 obtained from the secondary alcohol oxidation reaction clearly implicates characteristic features for a cooperative mechanism involving all four Ru centers.[16] Since PCy_3 is a much stronger σ–donor than an alcohol substrate, the initial dissociation of PCy_3 should lead to an electron–poor ruthenium center, which might promote the subsequent ligand dissociation by triggering the conformational change of the complex (e.g., by shortening bond lengths). Such strong cooperativity has been rarely observed in non–enzymatic catalysis; an allosteric substrate binding of dicarboxylic acids to a cerium–pyridylporphyrinate complex has been reported to give the Hill coefficient of n = 4.[17]



Scheme 2

Another important factor for cooperative activity appears to be the reversible nature of the catalytic reaction, and in this regard, both the alcohol dehydrogenation and reverse transfer hydrogenation reactions are well–known to proceed reversibly via a concerted "outer–sphere" mechanism.[18] In a preliminary result, we also demostrated the reversible nature of **1** by running the transfer hydrogenation of acetophenone.[19] Catalyst **1** did not exhibit any cooperative effects for the oxidation of primary alcohols because the sterically less demanding primary alcohols might have led to the rapid break-up of the tetrameric structure (as indicated by the formation of monomeric species). The resulting monomeric and/or dimeric complexes should favor the stepwise hydrogen transfer via an "inner–sphere" mechanism.[20]

Our kinetic and mechanistic results raise a number of intriguing questions. For instance, why does the Hammett study of secondary benzyl alcohols result in a positive ρ value of +0.22? The positive ρ value suggests a developing negative charge on the α-carbon of alcohol substrate, but normally the alcohol oxidation reactions proceed via a developing positive charge on the α-carbon. One possible explanation for this unusual observation is that sterically more demanding secondary alcohols would favor an "outer-sphere mechanism", which promotes hydrogen bonding interactions between Ru-OH and alcohol substrates. The hydrogen bonding interactions between late transition metal-hydride and -hydroxo complexes and protic substrates have been well documented,[21] and in our case, multiple number of hydrogen bonding interactions between the catalyst **1** and alcoholic substrates can be envisioned. Under such environments, the developing negative charge on the α-carbon can result from either a concerted hydrogen transfer via a 6-membered transition state similar to that of an Oppenhauer-type oxidation reaction or from an *anti*-1,2-hydrogen elimination promoted by an external base, such as free PCy_3 ligand.

Another unresolved issue is the homogeneous vs heterogeneous state of the catalytic reaction. Though the catalytic reaction appears to be "homogeneous", we still cannot rigorously rule out the possibility of the heterogeneous or colloidal nature of active species, especially for the catalytic reaction of secondary alcohols. In an effort to resolve this issue, Hg test was performed on the catalytic oxidation reaction of a secondary alcohol. Thus, the catalytic reaction of 1-phenylethanol was stirred vigorously in the presence of Hg(0) (2.0 g) in acetone at 80 °C, in which case, the ketone product was obtained in 92% yield after 20 h of reaction time. However, in light of recent reports by Süss-Fink and Finke on Ru_3-oxo complexes,[22] one must be very careful in distinguishing between homogeneous vs heterogeneous catalytic reactions and in establishing the nature of catalytically active species. Clearly, further research is warranted to determine both the nature of the reactive species and the steric and electronic influences on the cooperative activity of complex **1**.

In summary, the tetrametallic ruthenium–oxo–hydroxo complex **1** was found to exhibit strong cooperativity for the catalytic oxidation of secondary alcohols. Efforts are currently underway to establish the origin of cooperative activity as well as the nature of active species for the catalytic oxidation reaction.

Experimental Section

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. Benzene, hexanes, THF and Et_2O were distilled from purple solutions of sodium and benzophenone immediately prior to use. The NMR solvents were dried from activated molecular sieves (4 Å). All organic alcohols were received from commercial sources and used without further purification. The ^1H, ^{13}C and ^{31}P NMR spectra were recorded on a Varian Mercury 300 MHz FT-NMR spectrometer. Mass spectra were recorded from a Hewlett-Packard HP 5970 GC/MS spectrometer. High-resolution FAB mass spectra were performed at the Center of Mass Spectrometry, Washington University, St. Louis, MO. Elemental analyses were performed at the Midwest Microlab, Indianapolis, IN.

{[(PCy$_3$)$_2$(CO)RuH]$_4$(μ$_4$-O)(μ$_3$-OH)(μ$_2$-OH)} (1)

In a glove box, complex **3** (500 mg, 0.46 mmol) and acetone (5 mL) was added to 25 mL Schlenk tube equipped with a magnetic stirring bar and Teflon stopcock. The reaction tube was brought out of the glove box and stirred in an oil bath at 95 °C for 3 h. After the tube was cooled to room temperature, the resulting red solid was filtered, washed with 2-propanol (5 mL, 3 times), and recrystallized in CH_2Cl_2 to obtain product **1** in 84% yield.

Selected spectroscopic data for **1**: ^1H NMR (300 MHz, CD_2Cl_2) δ 2.25-1.15 (m, PCy_3), −2.50 and −2.60 (s, μ-OH), −14.56 (d, J_{PH} = 19.2 Hz, Ru-H), −15.02 (d, J_{PH} = 18.0 Hz, Ru-H), −15.28 (d, J_{PH} = 34.8 Hz, Ru-H), −18.64 (dt, J_{PH} = 13.2, 4.8 Hz, Ru-H-Ru); $^{31}P\{^1H\}$ NMR ($CDCl_3$, 121.6 MHz) δ 82.13 (s, PCy_3), 79.01 (d, J_{PP} = 14.0 Hz (PCy_3)), 71.96 (s, (PCy_3)), 68.89 (d, J_{PP} = 14.0 Hz, (PCy_3)); IR (CH_2Cl_2) ν_{OH} = 2926, 2849 cm^{-1}, ν_{CO} = 1925, 1912, 1894, 1868 cm^{-1}; Calcd for $C_{76}H_{138}O_7P_4Ru_4$: C 53.95, H 8.22. Found C 55.03, H 8.14.

(PCy₃)₂(CO)RuH(μ-OH)(μ-H)(PCy₃)(CO)RuH (3)

In a glove box, a 25 mL Schlenk tube equipped with a magnetic stirring bar and Teflon stopcock was charged with $(PCy_3)_2(CO)RuHCl$ (**1**) (726 mg, 1.0 mmol), KOH (6.5 mmol) and 2-propanol (5 mL). The reaction tube was brought out of the box and was stirred in an oil bath at 85 °C for 8 h. The solvent was removed under high vacuum, and the residue was washed with 2-propanol and benzene to obtain the product in 85% yield.

Selected spectroscopic data for **3**: ^{1}H NMR (300 MHz, CD_2Cl_2) δ 2.25–1.22 (m, PCy_3), −1.67 (s, Ru-OH), −8.05 (pseudo q, J_{PH} = 24.3, 18.0 Hz, Ru-H), −9.70 (dt, J_{PH} = 49.8, 5.7 Hz, Ru-H-Ru), −24.34 (dd, J_{PH} = 27.6, 5.7 Hz, Ru-H); ^{13}C{^{1}H} NMR (75 MHz, CD_2Cl_2) δ 208.7 (t, J_{PC} 14.6 Hz, CO), 207.0 (d, J_{PC} = 12.8 Hz, CO), 37.3, 36.8, 31.5, 30.7, 30.2, 28.4 and 27.2 (Pcy_3 carbons); ^{31}P{^{1}H} NMR (121.6 MHz, CD_2Cl_2) δ 80.7 (AB pattern, J_{AB} = 212 Hz, PCy_3), 74.1 (t, J = 37.5 Hz, PCy_3); IR (CH_2Cl_2) ν_{OH} = 3650, ν_{CO} = 1905, 1895 cm^{-1}.

General Procedure of the Catalytic Alcohol Oxidation Reaction

A 25 mL Schlenk tube equipped with a magnetic stirring bar and Teflon stopcock was charged with the alcohol (1.0 mmol) and acetone (3 mL). The reaction tube was cooled in a dry/ice acetone bath, degassed, and brought into a nitrogen filled glove box. Complex **1** (44 mg, 2.5 mol %) was added to the reaction tube. The reaction tube was sealed, brought out of the glove box, and stirred in an oil bath (preset to 80 °C) for 6–24 hrs. After the reaction was completed, the reaction tube was opened to air and the solution was filtered through a frit. The filtrate solution was analyzed by GC. Analytically pure oxidation product was obtained after column chromatography on silica gel (hexanes/EtOAc).

General Procedure for Kinetic Measurements

To a J-Young NMR tube equipped with a Teflon-coated screw cap, 1-phenylethanol (0.05–0.4 mmol) and aceteone-d_6 (0.5 mL) were added via a syringe. After degassing in a dry ice/acetone bath, the reaction tube was brought into the glove box, and **1** (4 mg) was added to the tube. The reaction tube was brought out of the glove box, and was stirred in an oil bath which was preset to 80 °C. The tube was removed from the oil bath at 15 min intervals, and immediately cooled in a dry ice/acetone bath. The rate of the product formation was determined by ^{1}H NMR by measuring the integration of the appearance of the product peak at δ 2.63 (PhC(O)CH_3) vs the disappearance of the alcohol peak at δ 1.92 (PhCH(OH)CH_3). The initial rate was obtained from a first order plot of [PhC(O)CH_3] vs. time. The data was fit to the Hill equation by using a nonlinear regression method (ProStat version 4.0). An analogous procedure was used to determine the product formation by measuring the disappearance of the benzyl alcohol peak at δ 4.43 ($C_6H_5CH_2OH$) against an internal standard (hexamethylbenzene).

General Procedure for Hammett Study

To each of five separate J-Young NMR tubes equipped with a Teflon-coated screw cap, *p*-X-$C_6H_4CH(OH)CH_3$ (X = OMe, Me, H, Cl, CF_3) (0.05–0.40 mmol) was added via syringe. Acetone-d_6 (400–450 μL) and benzene-d_6 (200–300 μL) were added to bring the total volume to 600 μL to each tube. The tubes were and brought into the glove box. The complex **1** (4 mg, 25 μmol) was added to each tube. The sealed tubes were brought out of the glove box, and the ^{1}H NMR spectrum of each sample was initially taken at room temperature. The tubes were placed in an oil bath preset to 85 °C. The tube was removed from the oil bath at 15 min intervals, and immediately cooled in a dry ice/acetone bath. The ^{1}H NMR spectrum of each sample was recorded at room temperature. The procedure was repeated for 4–5 times. The initial rate was determined by measuring the integration of the appearance of the product peak (ArC(O)CH_3) vs time. The plot of concentration vs rate was fit to the Hill equation by using a nonlinear regression method (ProStat version 4.0). An analogous procedure was used to determine the initial rates for *p*-X-$C_6H_4CH_2OH$ (X= OMe, Me, H, Cl, CF_3).

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Acknowledgments

Financial support from the National Institute of Health, General Medical Sciences (Grant R15 GM55987) is gratefully acknowledged. We thank Prof. Daniel Sem for helpful suggestions on kinetic analysis.

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Supplementary Material

Supporting Information Available:

Experimental procedures and crystallographic data of **1** and **3**. This material is available free of charge via the Internet at http//:pubs.acs.org.

Supporting Information

Highly Cooperative Tetrametallic Ruthenium-μ-Oxo-μ-Hydroxo Catalyst for the Alcohol Oxidation Reaction

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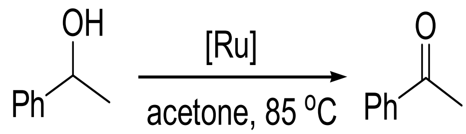
Table S1. Catalyst activity survey of selected Ruthenium Complexes.[a]



Entry	Catalyst	% yield[b]
1	**1**	98
2	**2**	30
3	**3**	trace
4	$[(COD)RuCl_2]_x$	0
5	$RuCl_3 3H_2O$	0
8	$(Pr_4N)^+RuO_4$	76

[a]Reaction conditions: 1-phenylethanol (1.0 mmol), acetone (3 mL), Ru catalyst (2.5 mol%), 85 °C, 6 h. [b]Determined by GC.

Figure S1. Plot of initial rate vs [*p*-Cl-$C_6H_4CH(OH)CH_3$].

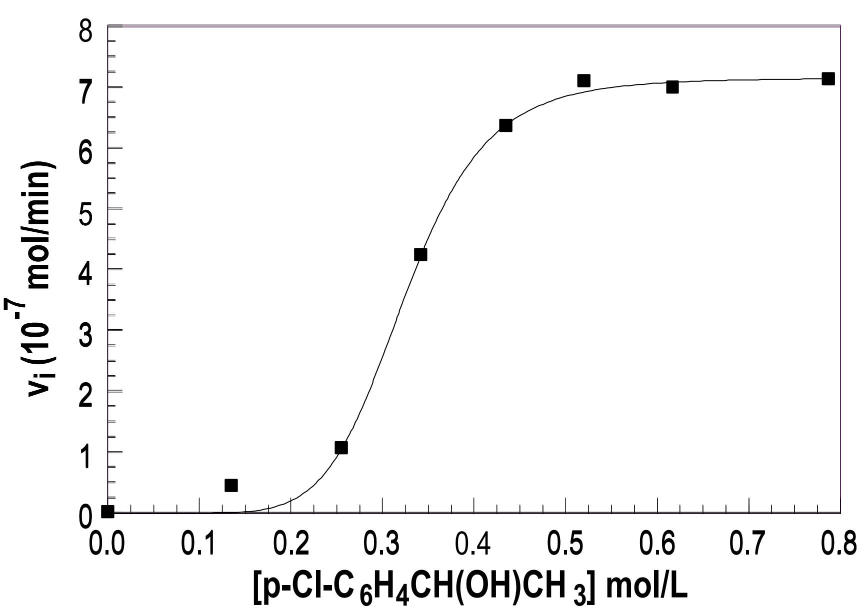


Figure S2. Plot of initial rate vs [p-CH_3-$C_6H_4CH(OH)CH_3$].

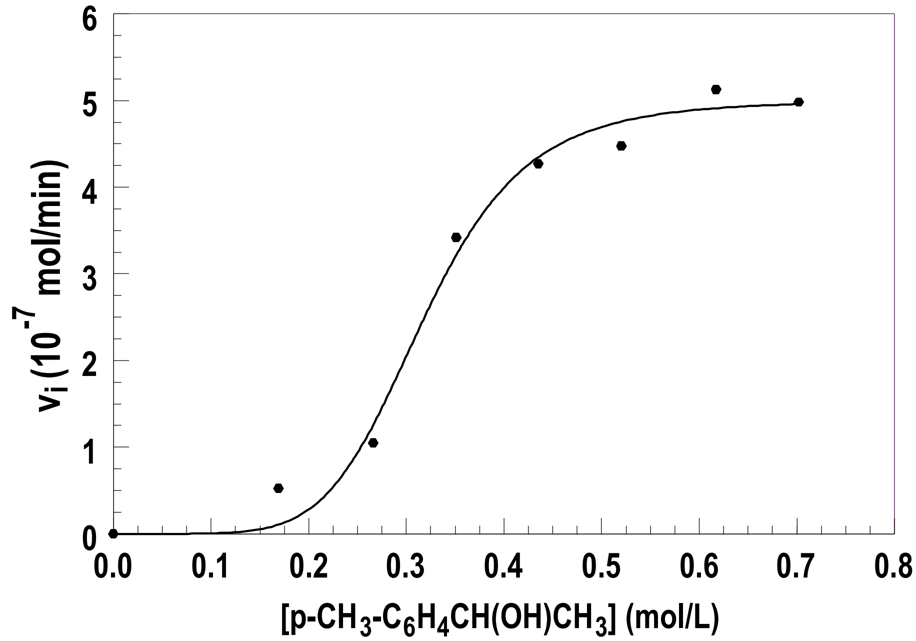


Figure S3. Plot of initial rate vs [p-CF_3-$C_6H_4CH_2OH$].

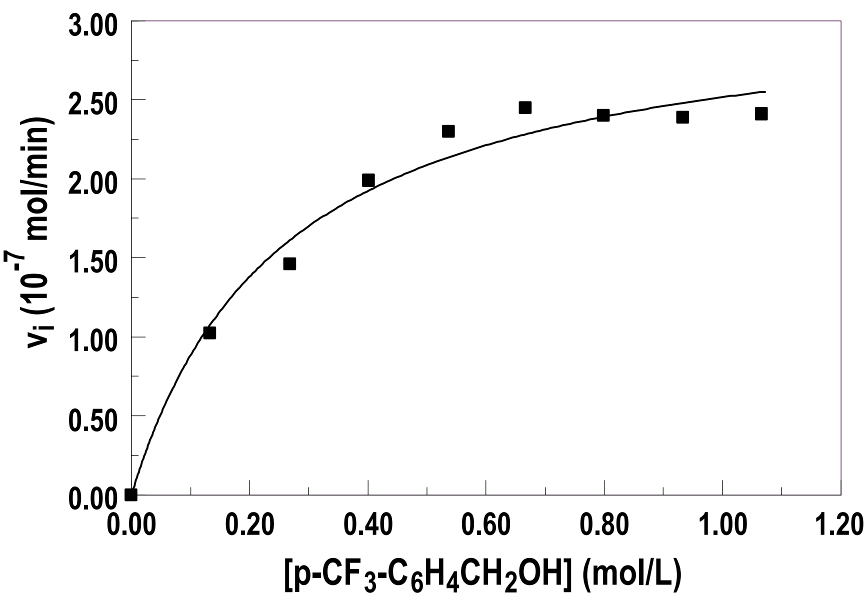


Figure S4. Plot of initial rate vs [p-CH_3-$C_6H_4CH_2OH$].

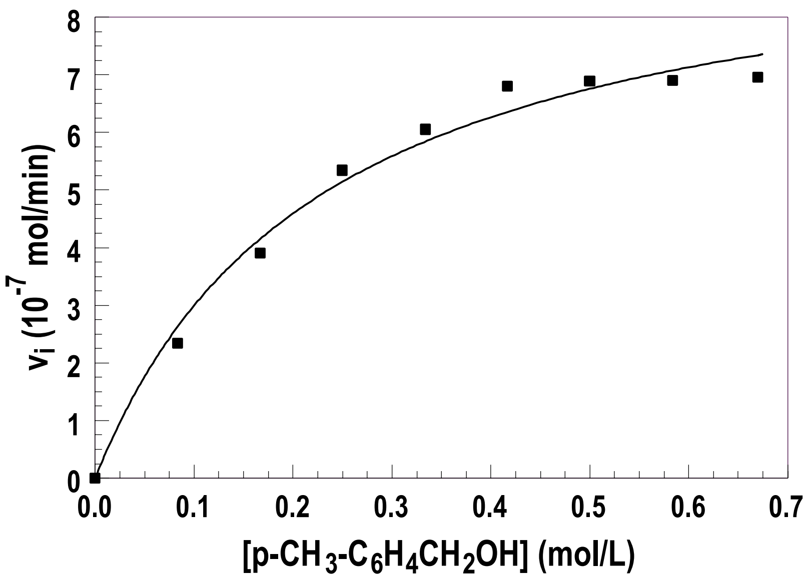
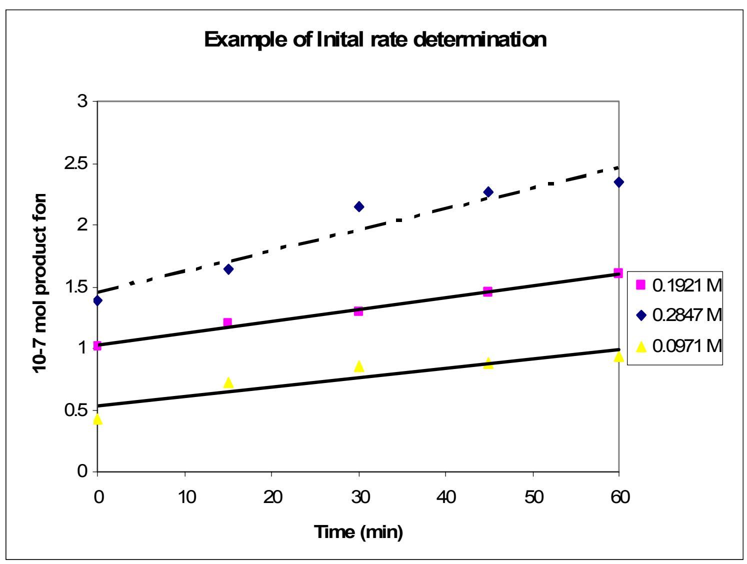


Table S2. Initital rate (v_i) vs [$PhCH(OH)CH_3$].

[$PhCH(OH)CH_3$] (M)	Rate (10^{-7} mol/min)
0.097	0.11 ± 0.06
0.192	0.70 ± 0.18
0.285	2.2 ± 0.64
0.375	4.0 ± 0.68
0.464	5.5 ± 0.32
0.550	6.1 ± 1.10
0.646	6.2 ± 0.05
0.729	6.4 ± 0.32



[a] Standard deviation determined from three separate trials.

Figure S5. The Eadie-Scatchard plot of v_i/[PhCH(OH)CH$_3$] vs v_i.

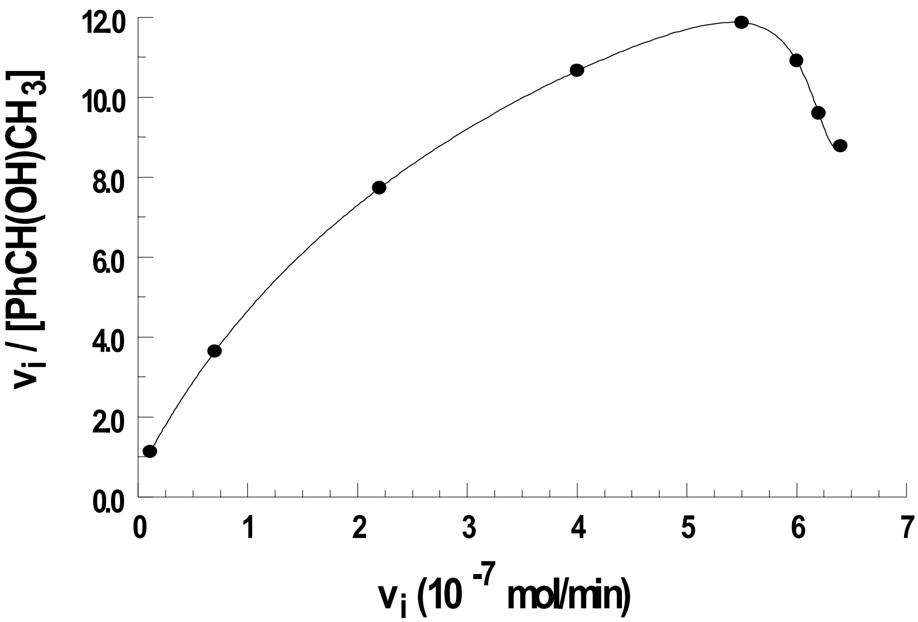


Table S3. Initital rate (v_i) vs [PhCH(OH)CH$_3$] with added PCy$_3$.

	Rate (10^{-7} mol/min)[a]			
[PhCH(OH)CH$_3$] (M)	No PCy$_3$	1.0 equiv	1.5 equiv	2.0 equiv
0.097	0.11 ± 0.06	0.11 ± 0.30	0.12 ±0.10	0.10 ± 0.1
0.192	0.70 ± 0.18	0.57 ± 0.63	0.51 ± 0.12	0.31 ± 0.12
0.285	2.2 ± 0.64	1.87 ± 0.15	1.21 ± 0.13	0.42 ± 0.12
0.375	4.0 ± 0.68	2.70 ± 0.25	2.19 ± 0.12	0.53 ± 0.11
0.464	5.5 ± 0.32	3.57 ± 1.50	3.13 ± 0.51	0.68 ± 0.51
0.550	6.1 ± 1.10	4.46 ± 0.38	3.86 ± 1.62	0.90 ± 1.62
0.646	6.2 ± 0.05	4.89 ± 0.36	4.11 ± 0.29	0.99 ± 0.29
0.729	6.4 ± 0.32	5.12 ± 0.36	4.31 ± 0.17	1.12 ± 0.17

[a]Standard deviation determined using data from three trials.

Table S4. Initital rate (v_i) vs [$PhCH_2OH$] with added PCy_3.

[$PhCH_2OH$] (mol/L)	Rate (10^{-7} mol/min) No PCy_3	1.0 Equiv PCy_3	1.5 Equiv PCy_3	2.0 Equiv PCy_3
0.0	0	0	0	0
0.080	1.85	1.74	1.04	1.00
0.177	2.99	2.10	1.99	1.23
0.274	3.49	3.14	2.10	1.98
0.371	3.83	3.25	2.34	1.99
0.451	4.40	3.20	2.46	2.04
0.548	4.23	3.29	2.50	2.09
0.644	4.36	3.26	2.57	2.07
0.725	4.34	3.25	2.54	2.11

Figure S6. Plot of the initial rate vs [$PhCH_2OH$] at different PCy_3. ■= No PCy_3; ▲= 1.0 equiv PCy_3; ●= 1.5 equiv PCy_3; ○= 2 equiv PCy_3.

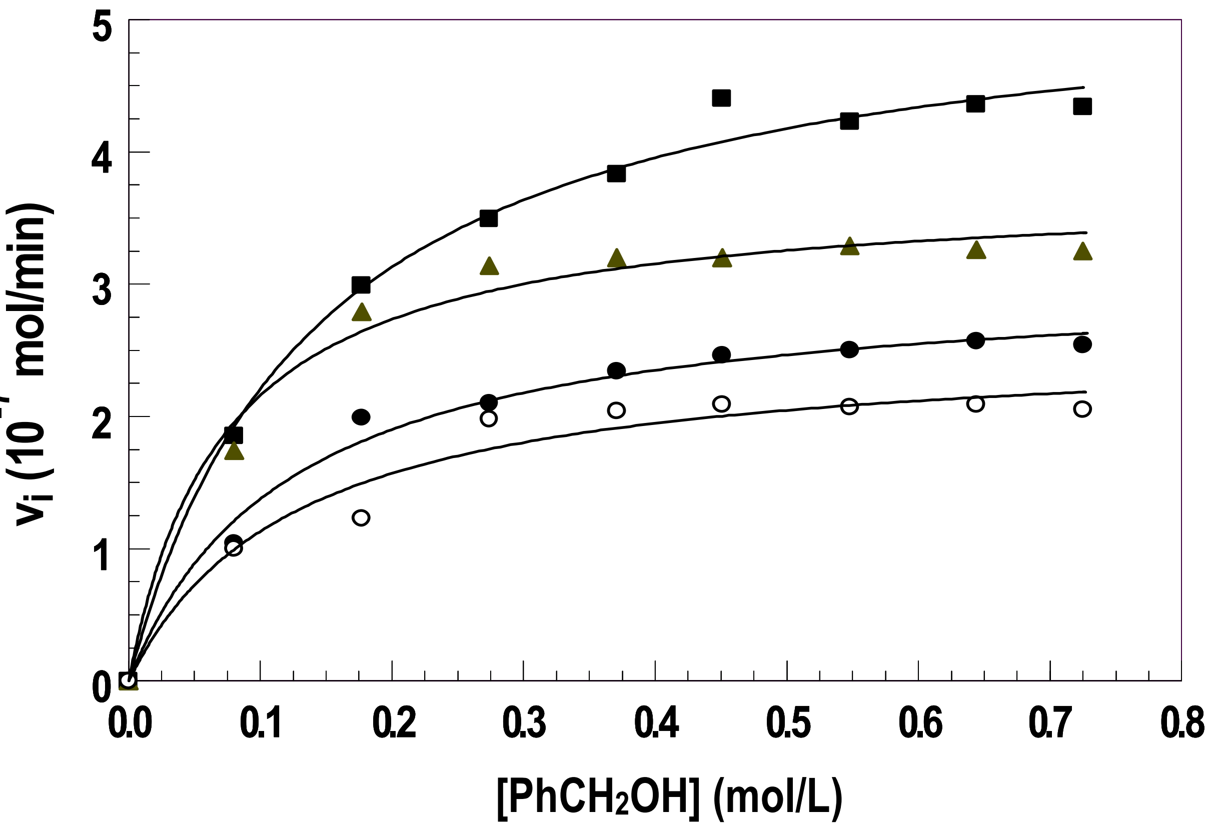
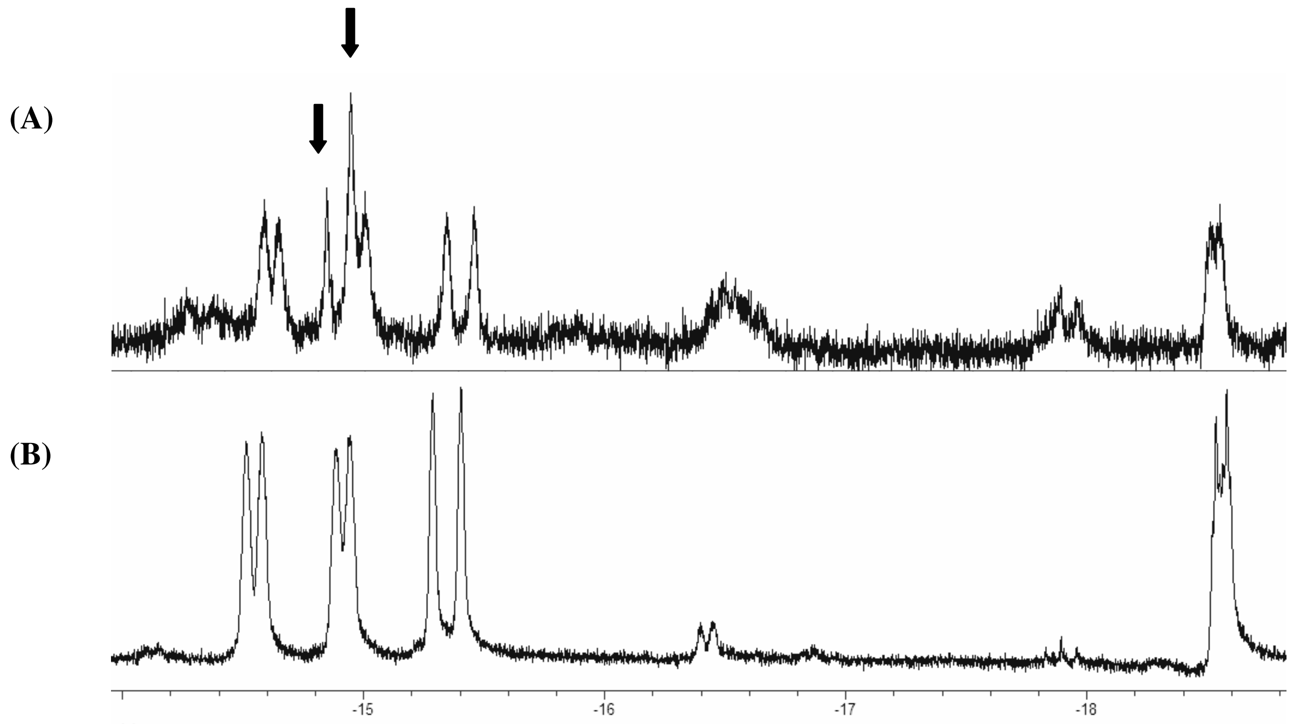


Figure S7. The ^{1}H NMR spectra of **1** and benzyl alcohols.



A. ^{1}H NMR spectrum of the reaction with **1** and $PhCH_2OH$ after 20 min at 40 °C. The appearance of a new peak at δ -14.79 (d, J_{PH} = 32.1 Hz) (black arrows) was observed in addition to the characteristic hydride peaks of **1**.

B. ^{1}H NMR spectrum of the reaction of **1** with $PhCH(OH)CH_3$ after 3 h at 40 °C.

Figure S8. Visual Comparison of the Reaction Flask for $PhCH_2OH$ and $PhCH(OH)CH_3$.

Reaction Flask of $PhCH_2OH$

(after 15 min at 80 °C)

Reaction Flask of $PhCH(OH)CH_3$

(after 3 h at 80 °C)

Crystallographic Experimental Section

Data Collection: A yellow air-sensitive crystal with approximate dimensions 0.43 x 0.38 x 0.31 mm^3 was selected under oil under ambient conditions and attached to the tip of a glass capillary. The crystal was mounted in a stream of cold nitrogen at 173(2) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α (ë = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.9 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3º in a 6º range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a large set of strong reflections from the actual data collection. The data was collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of a full sphere to a resolution of 0.80 Å. A data set was harvested by collecting three sets of frames with 0.3º scans in ω with an exposure time 30 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements.[1]

Structure Solution and Refinement of 1: The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement.[2] A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. There are also four hydride atoms in the vicinity of the Ru atoms as known from the results of other experimental techniques, but these hydrides were neither located nor refined. There are also three solvate molecules of benzene per molecule of complex in the lattice. The solvent molecules were refined with idealized geometries. The final least-squares refinement of 959 parameters against 17071 data resulted in residuals *R* (based on F^2 for *I*=2*ó*) and *wR* (based on F^2 for all data) of 0.0378 and 0.0954, respectively. The final difference Fourier map was featureless.

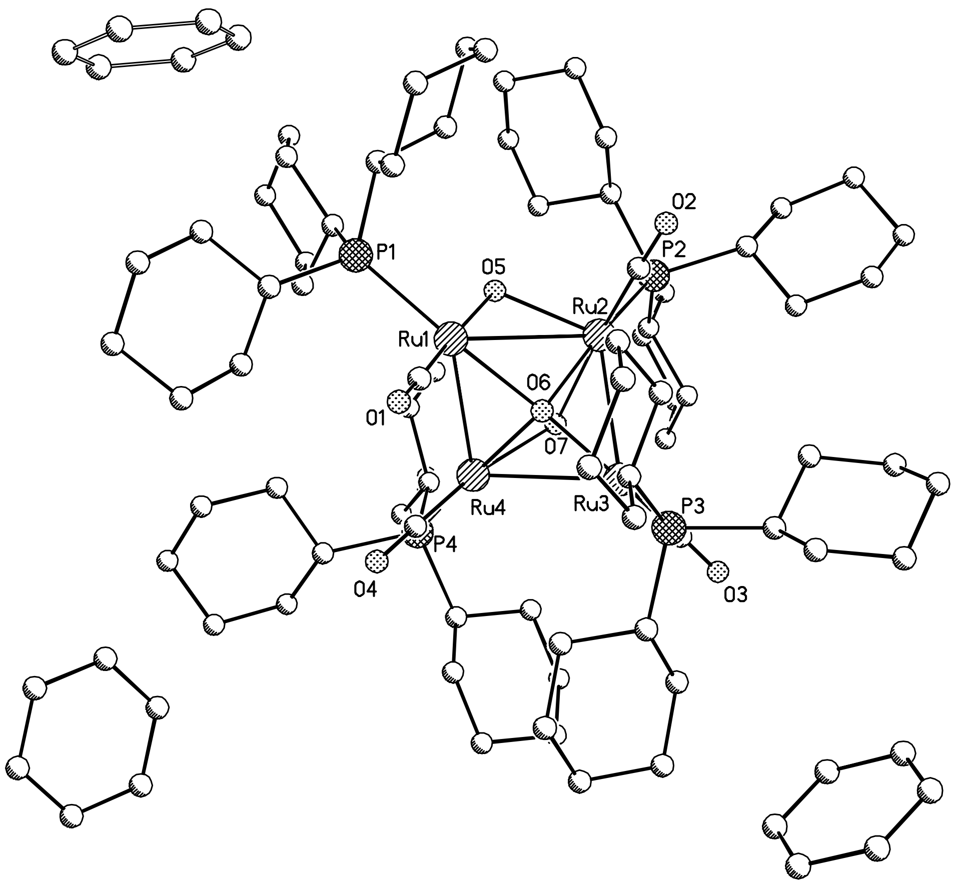
Structure Solution and Refinement of 3: The systematic absences in the diffraction data were uniquely consistent for the space groups $P2_1/n$ that yielded chemically reasonable and computationally stable results of refinement.[2] A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The three hydride H-atoms coordinated to Ru atoms were not located. The final least-squares refinement of 578 parameters against 11729 data resulted in residuals *R* (based on F^2 for I=2ó) and *wR* (based on F^2 for all data) of 0.0446 and 0.1086, respectively. The ORTEP diagrams are drawn with 30% probability ellipsoids.

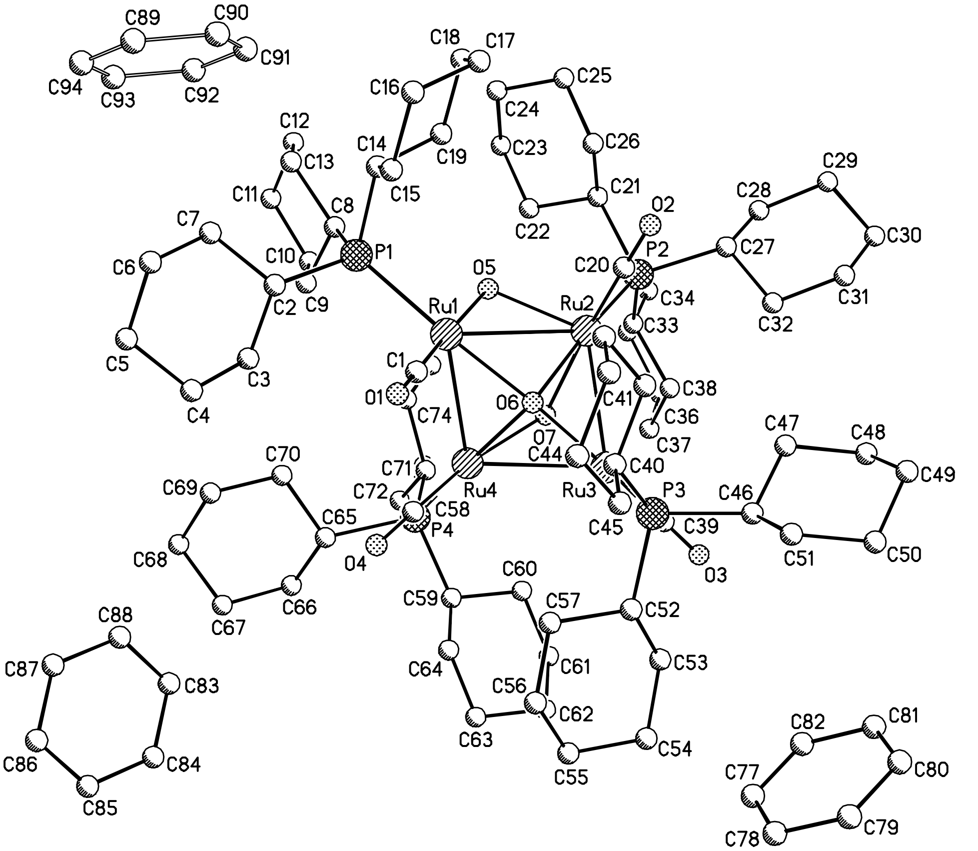
References

(1) Blessing, R. H. *Acta Cryst*. **1995**, *A51*, 33-38.

(2) All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).

Molecular structures of **1**.




C89
C90
C91
C94
C93
C92
C18
C17
C16
C25
C24
C12
C14
C23
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C13
C19
C11
C15
C21
C29
C8
C28
O2
C7
C22
C30
C27
C10
P1
C6
C20
P2
O5
C2
C9
C34
C31
Ru1
Ru2
C33
C32
C5
C1
C3
C38
O1
C41
O6
C36
C74
C4
O7
C37
C47
C48
C70
C44
C40
C49
C69
C71
C72
Ru4
Ru3
P3
C46
C58
C39
C65
P4
C45
C51
C50
C68
O4
O3
C60
C59
C57
C52
C66
C67
C88
C61
C53
C87
C83
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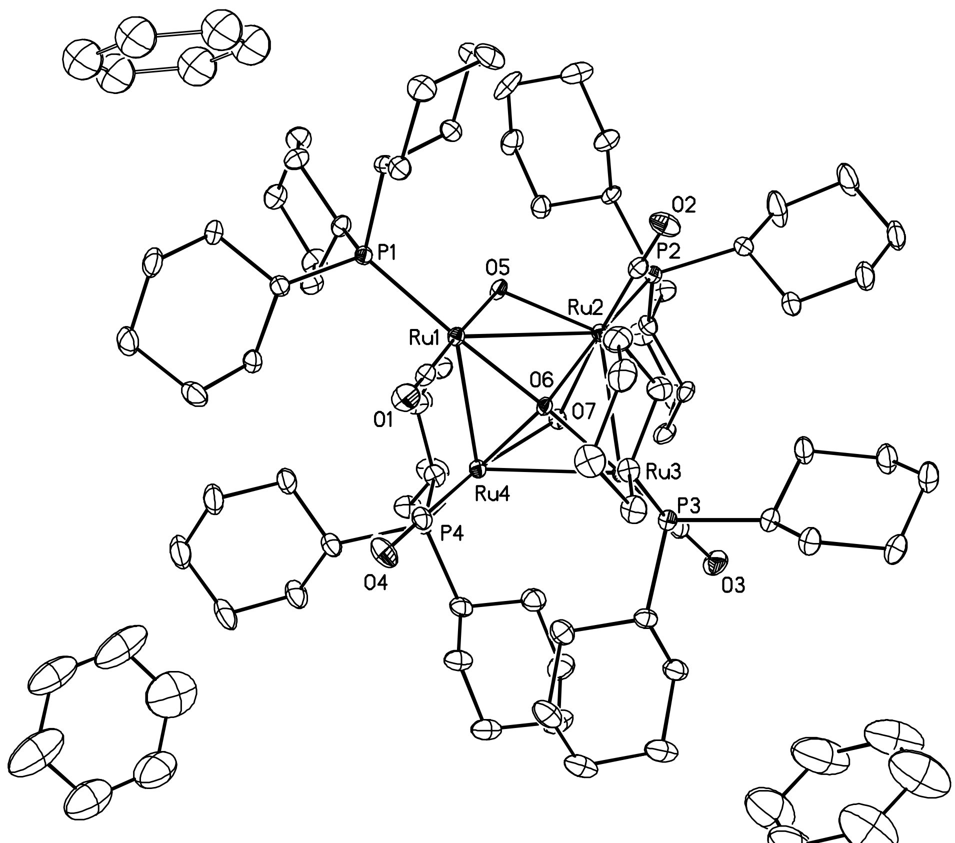
C77
C85
C78
C79


O2
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P2
O5
Ru2
Ru1
O6
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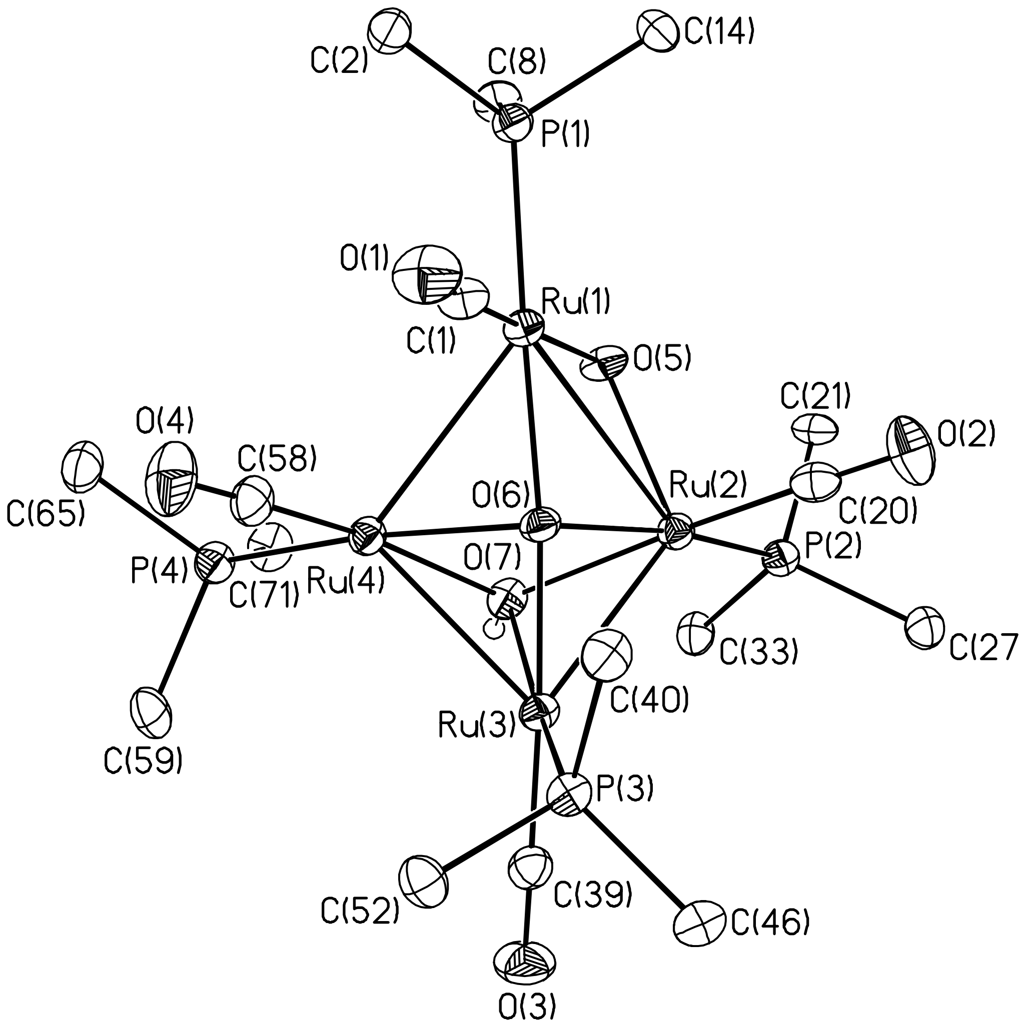
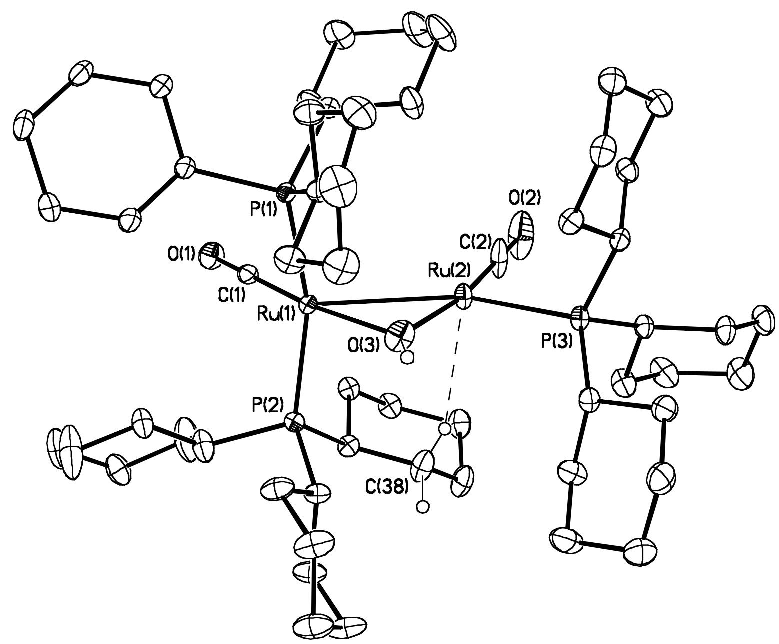
Ru3
Ru4
P3
P4
O4
O3


C(2)
C(8)
C(14)
P(1)
O(1)
Ru(1)
C(1)
O(5)
C(21)
O(4)
O(2)
C(58)
Ru(2)
O(6)
C(65)
C(20)
P(2)
O(7)
P(4)
C(71)
Ru(4)
C(33)
C(27)
C(40)
Ru(3)
C(59)
P(3)
C(52)
C(39)
C(46)
O(3)

Molecular structure of **3** drawn with 30% thermal ellipsoids.



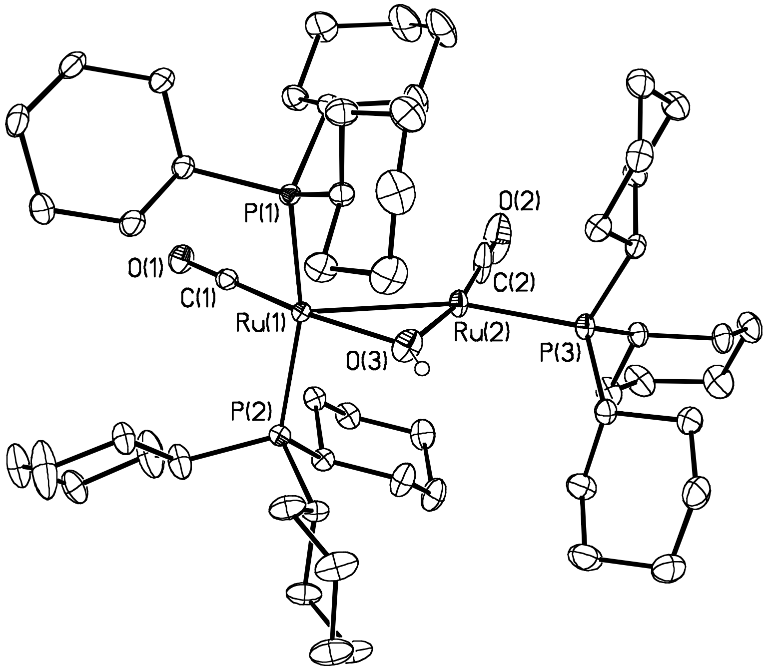

O(2)
P(1)
O(1)
C(1)
C(2)
Ru(1)
Ru(2)
P(3)
O(3)
P(2)

Table S2. Crystal data and structure refinement for **1**.

Identification code	yi03	
Empirical formula	$C_{91} H_{153} O_7 P_4 Ru_4$	
Formula weight	1887.29	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 25.2996(17) Å	α= 90°.
	b = 15.0050(11) Å	β= 98.190(2)°.
	c = 24.7448(17) Å	γ = 90°.
Volume	9297.8(11) $Å^3$	
Z	4	
Density (calculated)	1.348 Mg/m^3	
Absorption coefficient	0.756 mm^{-1}	
F(000)	3964	
Crystal size	0.43 x 0.38 x 0.31 mm^3	
Theta range for data collection	1.58 to 26.36°.	
Index ranges	-31<=h<=31, 0<=k<=18, 0<=l<=30	
Reflections collected	17071	
Independent reflections	17071 [R(int) = 0.0000]	
Completeness to theta = 26.36°	89.8 %	
Absorption correction	Multi-scan with SADABS	
Max. and min. transmission	0.7995 and 0.7370	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17071 / 36 / 947	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0973	
R indices (all data)	R1 = 0.0536, wR2 = 0.1061	
Largest diff. peak and hole	0.905 and -0.703 e.$Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	1984(1)	1552(1)	3133(1)	18(1)
Ru(2)	2648(1)	660(1)	4165(1)	18(1)
Ru(3)	3467(1)	1808(1)	4103(1)	18(1)
Ru(4)	2615(1)	2906(1)	3810(1)	18(1)
P(1)	1102(1)	1450(1)	2802(1)	20(1)
P(2)	2555(1)	-131(1)	4938(1)	20(1)
P(3)	4051(1)	1610(1)	3494(1)	21(1)
P(4)	2455(1)	4172(1)	4290(1)	23(1)
O(1)	2215(1)	2066(2)	2032(1)	37(1)
O(2)	2634(1)	-1080(2)	3589(1)	41(1)
O(3)	4380(1)	2185(2)	4986(1)	39(1)
O(4)	2630(1)	4054(2)	2835(1)	42(1)
O(5)	1847(1)	1033(2)	3916(1)	22(1)
O(6)	2775(1)	1616(2)	3551(1)	19(1)
O(7)	2748(1)	1998(2)	4505(1)	20(1)
C(1)	2129(2)	1892(3)	2471(2)	25(1)
C(2)	888(2)	2200(3)	2215(2)	24(1)
C(3)	1037(2)	3184(3)	2329(2)	30(1)
C(4)	984(2)	3708(3)	1794(2)	40(1)
C(5)	424(2)	3639(3)	1478(2)	42(1)
C(6)	251(2)	2674(3)	1386(2)	39(1)
C(7)	315(2)	2139(3)	1924(2)	31(1)
C(8)	661(2)	1581(3)	3342(2)	25(1)
C(9)	678(2)	2506(3)	3599(2)	31(1)
C(10)	433(2)	2491(3)	4134(2)	39(1)
C(11)	-140(2)	2157(3)	4029(2)	34(1)
C(12)	-180(2)	1257(3)	3741(2)	37(1)
C(13)	76(2)	1277(3)	3218(2)	31(1)
C(14)	886(2)	328(2)	2526(2)	22(1)
C(15)	1139(2)	70(3)	2023(2)	27(1)
C(16)	972(2)	-871(3)	1832(2)	36(1)
C(17)	1106(2)	-1560(3)	2282(2)	43(1)
C(18)	844(2)	-1312(3)	2775(2)	36(1)
C(19)	1012(2)	-380(3)	2981(2)	27(1)
C(20)	2637(2)	-393(3)	3808(2)	24(1)
C(21)	1872(1)	-554(3)	4980(2)	23(1)
C(22)	1459(2)	194(3)	5008(2)	31(1)
C(23)	909(2)	-189(3)	5074(2)	39(1)
C(24)	712(2)	-845(4)	4613(2)	48(1)
C(25)	1124(2)	-1575(3)	4568(2)	47(1)
C(26)	1674(2)	-1177(3)	4503(2)	36(1)
C(27)	2970(2)	-1161(3)	5053(2)	25(1)
C(28)	2913(2)	-1707(4)	5557(2)	62(2)
C(29)	3215(2)	-2601(3)	5545(3)	64(2)
C(30)	3799(2)	-2450(3)	5513(2)	45(1)
C(31)	3870(2)	-1886(3)	5030(2)	52(1)
C(32)	3558(2)	-1005(3)	5016(2)	42(1)
C(33)	2674(2)	605(3)	5548(2)	25(1)
C(34)	2503(2)	272(3)	6086(2)	35(1)
C(35)	2515(2)	1035(3)	6491(2)	42(1)
C(36)	3071(2)	1444(3)	6604(2)	38(1)

C(37)	3266(2)	1744(3)	6079(2)	34(1)
C(38)	3243(2)	980(3)	5665(2)	26(1)
C(39)	4028(2)	2038(3)	4646(2)	24(1)
C(40)	3686(2)	1218(3)	2826(2)	26(1)
C(41)	3486(2)	255(3)	2868(2)	30(1)
C(42)	3114(2)	-25(3)	2349(2)	39(1)
C(43)	3386(2)	78(3)	1842(2)	42(1)
C(44)	3585(2)	1043(3)	1799(2)	40(1)
C(45)	3960(2)	1322(3)	2312(2)	33(1)
C(46)	4613(2)	844(3)	3730(2)	26(1)
C(47)	4452(2)	23(3)	4042(2)	35(1)
C(48)	4944(2)	-504(3)	4289(2)	42(1)
C(49)	5289(2)	-781(3)	3863(2)	41(1)
C(50)	5453(2)	41(3)	3569(2)	35(1)
C(51)	4967(2)	566(3)	3303(2)	32(1)
C(52)	4405(2)	2616(3)	3300(2)	25(1)
C(53)	4770(2)	3052(3)	3777(2)	34(1)
C(54)	5084(2)	3829(3)	3576(2)	49(1)
C(55)	4725(2)	4518(3)	3273(2)	48(1)
C(56)	4338(2)	4090(3)	2810(2)	44(1)
C(57)	4023(2)	3324(3)	3020(2)	33(1)
C(58)	2622(2)	3595(3)	3213(2)	26(1)
C(59)	3063(2)	4796(3)	4590(2)	30(1)
C(60)	3427(2)	4252(3)	5021(2)	39(1)
C(61)	3918(2)	4785(4)	5259(2)	48(1)
C(62)	4226(2)	5133(4)	4809(2)	53(1)
C(63)	3869(2)	5659(3)	4381(2)	44(1)
C(64)	3383(2)	5109(3)	4141(2)	38(1)
C(65)	2047(2)	5032(3)	3879(2)	31(1)
C(66)	2021(2)	5984(3)	4094(2)	44(1)
C(67)	1759(2)	6597(3)	3633(2)	51(1)
C(68)	1204(2)	6273(3)	3396(2)	62(2)
C(69)	1209(2)	5323(3)	3208(3)	62(2)
C(70)	1486(2)	4705(3)	3660(2)	42(1)
C(71)	2158(2)	3884(3)	4911(2)	28(1)
C(72)	2064(2)	4652(3)	5296(2)	38(1)
C(73)	1929(2)	4284(3)	5839(2)	50(1)
C(74)	1458(2)	3653(3)	5756(2)	47(1)
C(75)	1534(2)	2912(3)	5360(2)	36(1)
C(76)	1667(2)	3282(3)	4819(2)	37(1)
C(77)	5983(2)	2835(3)	2350(2)	108(3)
C(78)	6263(2)	2762(3)	1908(2)	98(3)
C(79)	6562(2)	2003(4)	1844(2)	118(3)
C(80)	6582(2)	1316(3)	2223(3)	127(3)
C(81)	6303(3)	1388(3)	2666(2)	115(3)
C(82)	6004(2)	2148(4)	2730(2)	128(4)
C(83)	2185(2)	6771(4)	1987(2)	120(3)
C(84)	2451(2)	7568(4)	1932(2)	97(3)
C(85)	2286(2)	8128(3)	1492(3)	102(3)
C(86)	1853(2)	7890(4)	1108(2)	119(3)
C(87)	1586(2)	7093(4)	1164(2)	90(3)
C(88)	1752(2)	6533(3)	1603(3)	115(4)
C(89)	-111(6)	-79(18)	-530(7)	94(8)
C(90)	208(6)	-629(18)	-167(8)	108(9)
C(91)	221(6)	-520(20)	392(7)	113(11)
C(92)	-85(7)	150(20)	589(8)	153(15)

C(93)	-404(6)	700(20)	226(10)	117(10)
C(94)	-417(6)	584(18)	-334(9)	100(9)

Table S4. Bond lengths [Å] and angles [°] for **1**.

Ru(1)-C(1)	1.802(4)
Ru(1)-O(6)	2.120(2)
Ru(1)-O(5)	2.161(2)
Ru(1)-P(1)	2.2704(10)
Ru(1)-Ru(4)	2.9543(4)
Ru(1)-Ru(2)	3.1489(4)
Ru(2)-C(20)	1.808(4)
Ru(2)-O(5)	2.109(2)
Ru(2)-O(6)	2.146(2)
Ru(2)-O(7)	2.177(2)
Ru(2)-P(2)	2.2914(10)
Ru(2)-Ru(3)	2.7145(4)
Ru(3)-C(39)	1.843(4)
Ru(3)-O(6)	2.082(2)
Ru(3)-O(7)	2.211(2)
Ru(3)-P(3)	2.2769(10)
Ru(3)-Ru(4)	2.7273(4)
Ru(4)-C(58)	1.806(4)
Ru(4)-O(6)	2.097(2)
Ru(4)-O(7)	2.183(2)
Ru(4)-P(4)	2.3054(10)
P(1)-C(2)	1.855(4)
P(1)-C(14)	1.868(4)
P(1)-C(8)	1.870(4)
P(2)-C(21)	1.859(4)
P(2)-C(33)	1.859(4)
P(2)-C(27)	1.866(4)
P(3)-C(52)	1.853(4)
P(3)-C(46)	1.855(4)
P(3)-C(40)	1.870(4)
P(4)-C(71)	1.856(4)
P(4)-C(65)	1.861(4)
P(4)-C(59)	1.864(4)
O(1)-C(1)	1.168(5)
O(2)-C(20)	1.165(5)
O(3)-C(39)	1.156(5)
O(4)-C(58)	1.164(5)
C(2)-C(7)	1.528(5)
C(2)-C(3)	1.540(5)
C(3)-C(4)	1.530(6)
C(4)-C(5)	1.521(6)
C(5)-C(6)	1.519(7)
C(6)-C(7)	1.542(6)
C(8)-C(9)	1.524(5)
C(8)-C(13)	1.538(5)
C(9)-C(10)	1.541(6)
C(10)-C(11)	1.520(6)
C(11)-C(12)	1.523(6)
C(12)-C(13)	1.527(6)
C(14)-C(15)	1.529(5)
C(14)-C(19)	1.548(5)
C(15)-C(16)	1.529(5)
C(16)-C(17)	1.522(6)
C(17)-C(18)	1.514(6)

C(18)-C(19)	1.528(6)
C(21)-C(26)	1.532(5)
C(21)-C(22)	1.541(5)
C(22)-C(23)	1.537(5)
C(23)-C(24)	1.534(7)
C(24)-C(25)	1.528(7)
C(25)-C(26)	1.543(6)
C(27)-C(28)	1.515(6)
C(27)-C(32)	1.522(6)
C(28)-C(29)	1.545(7)
C(29)-C(30)	1.509(7)
C(30)-C(31)	1.495(7)
C(31)-C(32)	1.538(6)
C(33)-C(38)	1.534(5)
C(33)-C(34)	1.540(5)
C(34)-C(35)	1.519(6)
C(35)-C(36)	1.524(6)
C(36)-C(37)	1.523(6)
C(37)-C(38)	1.532(5)
C(40)-C(41)	1.539(5)
C(40)-C(45)	1.540(5)
C(41)-C(42)	1.539(6)
C(42)-C(43)	1.523(6)
C(43)-C(44)	1.542(6)
C(44)-C(45)	1.532(6)
C(46)-C(51)	1.536(5)
C(46)-C(47)	1.538(6)
C(47)-C(48)	1.527(6)
C(48)-C(49)	1.518(6)
C(49)-C(50)	1.520(6)
C(50)-C(51)	1.528(6)
C(52)-C(57)	1.533(6)
C(52)-C(53)	1.538(6)
C(53)-C(54)	1.533(6)
C(54)-C(55)	1.505(7)
C(55)-C(56)	1.537(7)
C(56)-C(57)	1.530(6)
C(59)-C(64)	1.536(6)
C(59)-C(60)	1.540(6)
C(60)-C(61)	1.524(6)
C(61)-C(62)	1.538(7)
C(62)-C(63)	1.512(7)
C(63)-C(64)	1.529(6)
C(65)-C(70)	1.527(6)
C(65)-C(66)	1.530(6)
C(66)-C(67)	1.540(6)
C(67)-C(68)	1.521(7)
C(68)-C(69)	1.499(7)
C(69)-C(70)	1.541(6)
C(71)-C(76)	1.527(6)
C(71)-C(72)	1.535(5)
C(72)-C(73)	1.535(6)
C(73)-C(74)	1.511(7)
C(74)-C(75)	1.514(6)
C(75)-C(76)	1.532(6)
C(77)-C(78)	1.3900

C(77)-C(82)	1.3900
C(78)-C(79)	1.3900
C(79)-C(80)	1.3900
C(80)-C(81)	1.3900
C(81)-C(82)	1.3900
C(83)-C(84)	1.3900
C(83)-C(88)	1.3900
C(84)-C(85)	1.3900
C(85)-C(86)	1.3900
C(86)-C(87)	1.3900
C(87)-C(88)	1.3900
C(89)-C(90)	1.3900
C(89)-C(94)	1.3900
C(90)-C(91)	1.3900
C(91)-C(92)	1.3900
C(92)-C(93)	1.3900
C(93)-C(94)	1.3900
C(1)-Ru(1)-O(6)	97.54(14)
C(1)-Ru(1)-O(5)	174.91(14)
O(6)-Ru(1)-O(5)	80.77(9)
C(1)-Ru(1)-P(1)	90.42(12)
O(6)-Ru(1)-P(1)	171.97(7)
O(5)-Ru(1)-P(1)	91.40(7)
C(1)-Ru(1)-Ru(4)	99.03(12)
O(6)-Ru(1)-Ru(4)	45.20(6)
O(5)-Ru(1)-Ru(4)	83.22(7)
P(1)-Ru(1)-Ru(4)	132.48(3)
C(1)-Ru(1)-Ru(2)	134.73(12)
O(6)-Ru(1)-Ru(2)	42.75(7)
O(5)-Ru(1)-Ru(2)	41.85(6)
P(1)-Ru(1)-Ru(2)	130.38(3)
Ru(4)-Ru(1)-Ru(2)	69.453(11)
C(20)-Ru(2)-O(5)	98.14(14)
C(20)-Ru(2)-O(6)	103.39(13)
O(5)-Ru(2)-O(6)	81.35(9)
C(20)-Ru(2)-O(7)	170.79(14)
O(5)-Ru(2)-O(7)	85.56(10)
O(6)-Ru(2)-O(7)	68.70(9)
C(20)-Ru(2)-P(2)	87.63(12)
O(5)-Ru(2)-P(2)	99.98(7)
O(6)-Ru(2)-P(2)	168.65(7)
O(7)-Ru(2)-P(2)	100.08(7)
C(20)-Ru(2)-Ru(3)	119.05(12)
O(5)-Ru(2)-Ru(3)	121.63(7)
O(6)-Ru(2)-Ru(3)	49.02(6)
O(7)-Ru(2)-Ru(3)	52.36(7)
P(2)-Ru(2)-Ru(3)	123.07(3)
C(20)-Ru(2)-Ru(1)	90.32(12)
O(5)-Ru(2)-Ru(1)	43.12(7)
O(6)-Ru(2)-Ru(1)	42.11(6)
O(7)-Ru(2)-Ru(1)	86.63(6)
P(2)-Ru(2)-Ru(1)	142.26(3)
Ru(3)-Ru(2)-Ru(1)	90.462(12)
C(39)-Ru(3)-O(6)	173.21(14)
C(39)-Ru(3)-O(7)	104.22(14)

O(6)-Ru(3)-O(7)	69.18(9)
C(39)-Ru(3)-P(3)	90.06(12)
O(6)-Ru(3)-P(3)	96.45(7)
O(7)-Ru(3)-P(3)	165.42(7)
C(39)-Ru(3)-Ru(2)	126.34(12)
O(6)-Ru(3)-Ru(2)	51.11(7)
O(7)-Ru(3)-Ru(2)	51.21(6)
P(3)-Ru(3)-Ru(2)	121.84(3)
C(39)-Ru(3)-Ru(4)	125.33(12)
O(6)-Ru(3)-Ru(4)	49.49(7)
O(7)-Ru(3)-Ru(4)	51.16(6)
P(3)-Ru(3)-Ru(4)	117.76(3)
Ru(2)-Ru(3)-Ru(4)	79.521(13)
C(58)-Ru(4)-O(6)	104.68(13)
C(58)-Ru(4)-O(7)	169.74(14)
O(6)-Ru(4)-O(7)	69.47(9)
C(58)-Ru(4)-P(4)	88.43(12)
O(6)-Ru(4)-P(4)	166.81(7)
O(7)-Ru(4)-P(4)	97.35(7)
C(58)-Ru(4)-Ru(3)	117.66(13)
O(6)-Ru(4)-Ru(3)	49.01(6)
O(7)-Ru(4)-Ru(3)	52.10(6)
P(4)-Ru(4)-Ru(3)	123.45(3)
C(58)-Ru(4)-Ru(1)	89.81(12)
O(6)-Ru(4)-Ru(1)	45.85(6)
O(7)-Ru(4)-Ru(1)	91.58(7)
P(4)-Ru(4)-Ru(1)	137.56(3)
Ru(3)-Ru(4)-Ru(1)	94.469(13)
C(2)-P(1)-C(14)	102.92(17)
C(2)-P(1)-C(8)	110.99(18)
C(14)-P(1)-C(8)	100.52(17)
C(2)-P(1)-Ru(1)	113.83(13)
C(14)-P(1)-Ru(1)	114.47(13)
C(8)-P(1)-Ru(1)	112.95(13)
C(21)-P(2)-C(33)	101.70(17)
C(21)-P(2)-C(27)	102.43(18)
C(33)-P(2)-C(27)	110.19(18)
C(21)-P(2)-Ru(2)	115.50(13)
C(33)-P(2)-Ru(2)	110.22(13)
C(27)-P(2)-Ru(2)	115.71(13)
C(52)-P(3)-C(46)	102.16(18)
C(52)-P(3)-C(40)	102.85(18)
C(46)-P(3)-C(40)	110.06(18)
C(52)-P(3)-Ru(3)	116.65(13)
C(46)-P(3)-Ru(3)	114.39(13)
C(40)-P(3)-Ru(3)	109.92(13)
C(71)-P(4)-C(65)	110.83(19)
C(71)-P(4)-C(59)	101.26(19)
C(65)-P(4)-C(59)	103.36(19)
C(71)-P(4)-Ru(4)	110.89(13)
C(65)-P(4)-Ru(4)	114.51(14)
C(59)-P(4)-Ru(4)	115.03(13)
Ru(2)-O(5)-Ru(1)	95.03(10)
Ru(3)-O(6)-Ru(4)	81.50(9)
Ru(3)-O(6)-Ru(1)	166.86(13)
Ru(4)-O(6)-Ru(1)	88.96(9)

Ru(3)-O(6)-Ru(2)	79.88(8)
Ru(4)-O(6)-Ru(2)	110.23(11)
Ru(1)-O(6)-Ru(2)	95.14(10)
Ru(2)-O(7)-Ru(4)	105.95(10)
Ru(2)-O(7)-Ru(3)	76.43(8)
Ru(4)-O(7)-Ru(3)	76.74(8)
O(1)-C(1)-Ru(1)	176.2(4)
C(7)-C(2)-C(3)	109.5(3)
C(7)-C(2)-P(1)	119.0(3)
C(3)-C(2)-P(1)	113.7(3)
C(4)-C(3)-C(2)	110.2(3)
C(5)-C(4)-C(3)	111.7(4)
C(6)-C(5)-C(4)	111.7(4)
C(5)-C(6)-C(7)	112.0(4)
C(2)-C(7)-C(6)	110.6(3)
C(9)-C(8)-C(13)	108.9(3)
C(9)-C(8)-P(1)	114.2(3)
C(13)-C(8)-P(1)	118.7(3)
C(8)-C(9)-C(10)	110.7(3)
C(11)-C(10)-C(9)	110.4(4)
C(10)-C(11)-C(12)	111.8(3)
C(11)-C(12)-C(13)	111.8(4)
C(12)-C(13)-C(8)	110.4(3)
C(15)-C(14)-C(19)	110.5(3)
C(15)-C(14)-P(1)	113.0(3)
C(19)-C(14)-P(1)	109.5(3)
C(16)-C(15)-C(14)	110.9(3)
C(17)-C(16)-C(15)	112.2(4)
C(18)-C(17)-C(16)	110.3(4)
C(17)-C(18)-C(19)	111.2(4)
C(18)-C(19)-C(14)	111.6(3)
O(2)-C(20)-Ru(2)	178.5(4)
C(26)-C(21)-C(22)	109.2(3)
C(26)-C(21)-P(2)	111.7(3)
C(22)-C(21)-P(2)	113.2(3)
C(23)-C(22)-C(21)	111.2(3)
C(24)-C(23)-C(22)	111.4(4)
C(25)-C(24)-C(23)	111.2(4)
C(24)-C(25)-C(26)	111.3(4)
C(21)-C(26)-C(25)	110.9(4)
C(28)-C(27)-C(32)	109.9(4)
C(28)-C(27)-P(2)	117.2(3)
C(32)-C(27)-P(2)	113.3(3)
C(27)-C(28)-C(29)	110.5(4)
C(30)-C(29)-C(28)	111.1(4)
C(31)-C(30)-C(29)	110.9(4)
C(30)-C(31)-C(32)	112.7(4)
C(27)-C(32)-C(31)	111.7(4)
C(38)-C(33)-C(34)	109.1(3)
C(38)-C(33)-P(2)	114.3(3)
C(34)-C(33)-P(2)	118.4(3)
C(35)-C(34)-C(33)	110.1(4)
C(34)-C(35)-C(36)	110.9(4)
C(37)-C(36)-C(35)	111.4(4)
C(36)-C(37)-C(38)	111.3(4)
C(37)-C(38)-C(33)	110.3(3)

O(3)-C(39)-Ru(3)	179.8(4)
C(41)-C(40)-C(45)	110.0(3)
C(41)-C(40)-P(3)	111.2(3)
C(45)-C(40)-P(3)	118.3(3)
C(42)-C(41)-C(40)	111.6(4)
C(43)-C(42)-C(41)	111.4(4)
C(42)-C(43)-C(44)	110.0(4)
C(45)-C(44)-C(43)	111.7(4)
C(44)-C(45)-C(40)	111.0(4)
C(51)-C(46)-C(47)	110.4(3)
C(51)-C(46)-P(3)	116.6(3)
C(47)-C(46)-P(3)	114.2(3)
C(48)-C(47)-C(46)	111.0(3)
C(49)-C(48)-C(47)	112.3(4)
C(48)-C(49)-C(50)	109.5(4)
C(49)-C(50)-C(51)	111.5(4)
C(50)-C(51)-C(46)	110.9(3)
C(57)-C(52)-C(53)	108.8(3)
C(57)-C(52)-P(3)	112.7(3)
C(53)-C(52)-P(3)	114.0(3)
C(54)-C(53)-C(52)	111.0(4)
C(55)-C(54)-C(53)	112.3(4)
C(54)-C(55)-C(56)	111.1(4)
C(57)-C(56)-C(55)	111.6(4)
C(56)-C(57)-C(52)	110.4(4)
O(4)-C(58)-Ru(4)	178.5(4)
C(64)-C(59)-C(60)	109.8(4)
C(64)-C(59)-P(4)	110.9(3)
C(60)-C(59)-P(4)	112.8(3)
C(61)-C(60)-C(59)	111.3(4)
C(60)-C(61)-C(62)	111.6(4)
C(63)-C(62)-C(61)	111.8(4)
C(62)-C(63)-C(64)	111.0(4)
C(63)-C(64)-C(59)	111.2(4)
C(70)-C(65)-C(66)	109.8(4)
C(70)-C(65)-P(4)	112.7(3)
C(66)-C(65)-P(4)	120.4(3)
C(65)-C(66)-C(67)	109.7(4)
C(68)-C(67)-C(66)	111.7(4)
C(69)-C(68)-C(67)	112.1(4)
C(68)-C(69)-C(70)	111.7(4)
C(65)-C(70)-C(69)	111.6(4)
C(76)-C(71)-C(72)	110.0(3)
C(76)-C(71)-P(4)	115.4(3)
C(72)-C(71)-P(4)	117.2(3)
C(71)-C(72)-C(73)	110.3(4)
C(74)-C(73)-C(72)	112.2(4)
C(73)-C(74)-C(75)	112.2(4)
C(74)-C(75)-C(76)	111.3(4)
C(71)-C(76)-C(75)	111.0(4)
C(78)-C(77)-C(82)	120.0
C(79)-C(78)-C(77)	120.0
C(78)-C(79)-C(80)	120.0
C(79)-C(80)-C(81)	120.0
C(82)-C(81)-C(80)	120.0
C(81)-C(82)-C(77)	120.0

C(84)-C(83)-C(88)	120.0
C(83)-C(84)-C(85)	120.0
C(84)-C(85)-C(86)	120.0
C(87)-C(86)-C(85)	120.0
C(86)-C(87)-C(88)	120.0
C(87)-C(88)-C(83)	120.0
C(90)-C(89)-C(94)	120.0
C(89)-C(90)-C(91)	120.0
C(92)-C(91)-C(90)	120.0
C(91)-C(92)-C(93)	120.0
C(94)-C(93)-C(92)	120.0
C(93)-C(94)-C(89)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2$x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	18(1)	21(1)	17(1)	1(1)	1(1)	1(1)
Ru(2)	18(1)	18(1)	17(1)	0(1)	1(1)	1(1)
Ru(3)	17(1)	20(1)	18(1)	0(1)	1(1)	1(1)
Ru(4)	20(1)	18(1)	17(1)	0(1)	1(1)	2(1)
P(1)	19(1)	21(1)	19(1)	1(1)	2(1)	1(1)
P(2)	20(1)	20(1)	19(1)	0(1)	2(1)	0(1)
P(3)	20(1)	23(1)	21(1)	1(1)	3(1)	2(1)
P(4)	25(1)	22(1)	21(1)	-1(1)	2(1)	2(1)
O(1)	37(2)	51(2)	23(2)	9(1)	5(1)	-5(2)
O(2)	58(2)	26(2)	40(2)	-10(1)	15(2)	-5(2)
O(3)	31(2)	49(2)	33(2)	1(2)	-10(2)	-5(2)
O(4)	68(2)	34(2)	24(2)	9(1)	8(2)	5(2)
O(5)	14(1)	32(2)	19(1)	6(1)	2(1)	2(1)
O(6)	17(1)	21(1)	18(1)	-1(1)	-2(1)	2(1)
O(7)	24(1)	22(1)	14(1)	-1(1)	2(1)	3(1)
C(1)	18(2)	30(2)	26(2)	0(2)	1(2)	1(2)
C(2)	23(2)	22(2)	25(2)	2(2)	3(2)	2(2)
C(3)	28(2)	27(2)	31(2)	4(2)	-6(2)	2(2)
C(4)	45(3)	31(2)	43(3)	13(2)	9(2)	-1(2)
C(5)	35(3)	47(3)	44(3)	24(2)	5(2)	6(2)
C(6)	30(2)	49(3)	35(3)	11(2)	-9(2)	5(2)
C(7)	25(2)	32(2)	33(2)	6(2)	-5(2)	4(2)
C(8)	22(2)	31(2)	23(2)	1(2)	5(2)	1(2)
C(9)	26(2)	32(2)	34(2)	-6(2)	7(2)	0(2)
C(10)	35(3)	45(3)	39(3)	-10(2)	12(2)	2(2)
C(11)	29(2)	45(3)	31(2)	-3(2)	9(2)	4(2)
C(12)	33(3)	41(3)	39(3)	2(2)	16(2)	-1(2)
C(13)	25(2)	36(2)	33(2)	-6(2)	7(2)	-4(2)
C(14)	24(2)	20(2)	23(2)	-2(2)	2(2)	-4(2)
C(15)	31(2)	29(2)	19(2)	-1(2)	0(2)	0(2)
C(16)	44(3)	35(2)	29(2)	-9(2)	4(2)	-2(2)
C(17)	56(3)	21(2)	53(3)	-9(2)	14(3)	0(2)
C(18)	45(3)	24(2)	40(3)	3(2)	8(2)	-2(2)
C(19)	29(2)	25(2)	28(2)	2(2)	5(2)	-1(2)
C(20)	20(2)	32(2)	18(2)	4(2)	2(2)	-1(2)
C(21)	18(2)	31(2)	20(2)	1(2)	-2(2)	-5(2)
C(22)	26(2)	35(2)	32(2)	6(2)	8(2)	3(2)
C(23)	25(2)	53(3)	41(3)	9(2)	13(2)	3(2)
C(24)	18(2)	86(4)	37(3)	-3(3)	-4(2)	-9(2)
C(25)	40(3)	53(3)	50(3)	-17(2)	11(2)	-19(2)
C(26)	30(2)	44(3)	33(2)	-8(2)	-2(2)	-8(2)
C(27)	25(2)	22(2)	29(2)	1(2)	4(2)	0(2)
C(28)	60(4)	57(3)	76(4)	42(3)	34(3)	32(3)
C(29)	57(3)	43(3)	100(5)	40(3)	35(3)	22(3)
C(30)	44(3)	35(3)	53(3)	3(2)	-4(2)	19(2)
C(31)	36(3)	39(3)	84(4)	20(3)	20(3)	17(2)
C(32)	30(2)	27(2)	70(4)	8(2)	8(2)	8(2)
C(33)	30(2)	22(2)	22(2)	0(2)	3(2)	2(2)
C(34)	40(3)	44(3)	19(2)	-1(2)	0(2)	-10(2)
C(35)	49(3)	54(3)	25(2)	-7(2)	10(2)	-9(2)
C(36)	40(3)	41(3)	31(2)	-11(2)	-2(2)	7(2)

C(37)	25(2)	37(2)	39(3)	-15(2)	-1(2)	-3(2)
C(38)	20(2)	32(2)	26(2)	-4(2)	-4(2)	2(2)
C(39)	23(2)	25(2)	25(2)	3(2)	4(2)	1(2)
C(40)	28(2)	27(2)	22(2)	-2(2)	4(2)	3(2)
C(41)	31(2)	29(2)	29(2)	-7(2)	6(2)	-1(2)
C(42)	38(3)	37(3)	42(3)	-14(2)	2(2)	-3(2)
C(43)	44(3)	49(3)	29(2)	-12(2)	-8(2)	4(2)
C(44)	50(3)	48(3)	23(2)	-3(2)	5(2)	2(2)
C(45)	38(3)	39(3)	21(2)	2(2)	3(2)	0(2)
C(46)	22(2)	31(2)	25(2)	1(2)	2(2)	3(2)
C(47)	30(2)	35(2)	40(3)	13(2)	11(2)	13(2)
C(48)	38(3)	43(3)	46(3)	16(2)	9(2)	14(2)
C(49)	32(3)	43(3)	48(3)	4(2)	6(2)	16(2)
C(50)	24(2)	48(3)	32(2)	-4(2)	6(2)	9(2)
C(51)	29(2)	38(2)	31(2)	0(2)	5(2)	7(2)
C(52)	27(2)	24(2)	26(2)	-1(2)	9(2)	-3(2)
C(53)	37(3)	27(2)	38(3)	2(2)	3(2)	-6(2)
C(54)	55(3)	35(3)	60(3)	2(2)	15(3)	-15(2)
C(55)	63(3)	31(3)	55(3)	2(2)	21(3)	-13(2)
C(56)	61(3)	34(3)	40(3)	11(2)	16(2)	0(2)
C(57)	39(3)	31(2)	29(2)	4(2)	7(2)	1(2)
C(58)	31(2)	21(2)	25(2)	-4(2)	3(2)	5(2)
C(59)	36(2)	20(2)	35(2)	-7(2)	8(2)	-3(2)
C(60)	43(3)	35(3)	38(3)	-3(2)	1(2)	-4(2)
C(61)	41(3)	53(3)	46(3)	-10(2)	-4(2)	-6(2)
C(62)	36(3)	51(3)	71(4)	-19(3)	10(3)	-12(2)
C(63)	44(3)	35(3)	56(3)	-11(2)	21(2)	-12(2)
C(64)	42(3)	31(2)	43(3)	-7(2)	15(2)	-9(2)
C(65)	38(3)	22(2)	32(2)	1(2)	2(2)	5(2)
C(66)	57(3)	27(2)	45(3)	-5(2)	-2(3)	11(2)
C(67)	75(4)	23(2)	51(3)	2(2)	-5(3)	15(2)
C(68)	68(4)	38(3)	71(4)	3(3)	-25(3)	17(3)
C(69)	60(4)	35(3)	78(4)	3(3)	-34(3)	10(3)
C(70)	42(3)	26(2)	53(3)	1(2)	-7(2)	9(2)
C(71)	32(2)	31(2)	22(2)	-1(2)	10(2)	3(2)
C(72)	46(3)	37(3)	35(3)	-12(2)	15(2)	-5(2)
C(73)	71(4)	50(3)	35(3)	-12(2)	23(3)	-13(3)
C(74)	58(3)	50(3)	39(3)	-6(2)	26(3)	-5(3)
C(75)	35(3)	42(3)	29(2)	0(2)	3(2)	-7(2)
C(76)	40(3)	39(3)	33(2)	-5(2)	14(2)	-4(2)
C(77)	142(8)	69(5)	125(7)	2(5)	57(6)	4(5)
C(78)	140(7)	46(4)	117(7)	-9(4)	51(6)	1(4)
C(79)	195(10)	82(6)	82(6)	-11(5)	39(6)	-7(6)
C(80)	201(11)	77(6)	112(7)	-6(5)	54(7)	-16(6)
C(81)	157(9)	82(6)	114(7)	-4(5)	42(6)	-46(6)
C(82)	157(9)	64(5)	185(10)	-21(6)	98(8)	-25(6)
C(83)	106(7)	112(7)	153(9)	-45(6)	48(7)	11(6)
C(84)	71(5)	79(5)	139(8)	-38(5)	1(5)	-12(4)
C(85)	63(5)	100(6)	145(8)	-52(6)	29(5)	-4(4)
C(86)	56(5)	152(8)	154(8)	-89(7)	32(5)	-3(5)
C(87)	43(4)	108(6)	122(7)	-70(5)	25(4)	-10(4)
C(88)	43(4)	125(7)	181(10)	-98(7)	29(5)	-4(4)
C(89)	95(15)	130(20)	42(10)	53(11)	-27(10)	-50(14)
C(90)	57(11)	180(20)	79(16)	59(14)	-35(12)	-68(12)
C(91)	67(17)	140(20)	120(20)	78(17)	-34(15)	-75(17)
C(92)	150(30)	190(30)	130(20)	10(20)	50(20)	-90(20)

C(93)	101(19)	150(20)	110(20)	16(15)	26(15)	-86(16)
C(94)	52(13)	150(20)	82(15)	66(14)	-39(10)	-59(13)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(5)	1535	989	4087	26
H(7)	2746	2163	4896	24
H(2A)	1111	2014	1933	28
H(3B)	798	3445	2572	36
H(3A)	1408	3224	2517	36
H(4A)	1069	4343	1874	48
H(4B)	1244	3477	1566	48
H(5A)	169	3949	1682	50
H(5B)	414	3939	1120	50
H(6A)	467	2392	1130	47
H(6B)	-128	2657	1216	47
H(7A)	67	2376	2164	37
H(7B)	221	1507	1844	37
H(8)	823	1181	3645	30
H(9A)	477	2930	3340	37
H(9B)	1053	2713	3674	37
H(10A)	647	2097	4402	47
H(10B)	440	3099	4290	47
H(11A)	-363	2597	3802	41
H(11B)	-280	2102	4381	41
H(12A)	-561	1089	3650	44
H(12B)	-1	799	3990	44
H(13A)	-125	1690	2952	37
H(13B)	60	675	3053	37
H(14)	490	344	2417	27
H(15A)	1027	499	1725	32
H(15B)	1533	98	2112	32
H(16A)	583	-880	1706	43
H(16B)	1156	-1032	1518	43
H(17A)	978	-2154	2146	51
H(17B)	1498	-1592	2387	51
H(18A)	947	-1751	3070	43
H(18B)	451	-1333	2676	43
H(19A)	1400	-377	3114	33
H(19B)	822	-226	3291	33
H(21)	1889	-910	5324	28
H(22A)	1583	591	5320	37
H(22B)	1429	555	4669	37
H(23A)	932	-499	5430	47
H(23B)	649	304	5073	47
H(24A)	373	-1119	4685	58
H(24B)	641	-518	4263	58
H(25A)	999	-1958	4249	56
H(25B)	1159	-1953	4899	56
H(26A)	1934	-1665	4488	43
H(26B)	1645	-841	4156	43
H(27)	2839	-1558	4738	30
H(28A)	2531	-1824	5572	74
H(28B)	3059	-1368	5888	74
H(29A)	3178	-2946	5879	77

H(29B)	3054	-2954	5225	77
H(30A)	3969	-2153	5851	54
H(30B)	3978	-3031	5484	54
H(31A)	3749	-2225	4692	62
H(31B)	4254	-1753	5039	62
H(32A)	3715	-624	5324	51
H(32B)	3591	-685	4672	51
H(33)	2444	1138	5447	30
H(34A)	2138	22	6013	42
H(34B)	2748	-207	6242	42
H(35A)	2409	813	6836	51
H(35B)	2255	1498	6342	51
H(36A)	3064	1962	6851	46
H(36B)	3323	1000	6791	46
H(37A)	3639	1961	6163	41
H(37B)	3042	2244	5917	41
H(38A)	3493	502	5812	32
H(38B)	3355	1200	5322	32
H(40)	3357	1594	2758	31
H(41A)	3796	-154	2926	36
H(41B)	3292	205	3187	36
H(42A)	3006	-655	2384	47
H(42B)	2787	346	2309	47
H(43A)	3131	-71	1512	50
H(43B)	3692	-339	1862	50
H(44A)	3776	1095	1477	48
H(44B)	3275	1451	1744	48
H(45A)	4069	1951	2276	39
H(45B)	4286	949	2350	39
H(46)	4854	1194	4007	31
H(47A)	4252	218	4336	42
H(47B)	4216	-365	3790	42
H(48A)	5160	-136	4570	51
H(48B)	4828	-1043	4470	51
H(49A)	5086	-1193	3597	49
H(49B)	5610	-1097	4041	49
H(50A)	5669	-143	3284	42
H(50B)	5677	428	3832	42
H(51A)	4756	195	3019	39
H(51B)	5087	1104	3124	39
H(52)	4638	2423	3028	30
H(53A)	4551	3273	4050	41
H(53B)	5023	2602	3956	41
H(54A)	5302	4114	3894	59
H(54B)	5330	3596	3333	59
H(55A)	4944	4972	3119	58
H(55B)	4518	4821	3530	58
H(56A)	4086	4548	2639	53
H(56B)	4543	3862	2527	53
H(57A)	3787	3052	2711	39
H(57B)	3797	3558	3283	39
H(59)	2944	5339	4774	36
H(60A)	3223	4080	5318	47
H(60B)	3541	3700	4852	47
H(61A)	4157	4402	5513	57
H(61B)	3806	5295	5470	57

H(62A)	4523	5518	4975	63
H(62B)	4381	4623	4633	63
H(63A)	4074	5834	4086	52
H(63B)	3748	6209	4547	52
H(64A)	3503	4584	3949	45
H(64B)	3150	5474	3871	45
H(65)	2224	5098	3545	38
H(66A)	2385	6200	4229	53
H(66B)	1810	5995	4401	53
H(67A)	1732	7209	3777	62
H(67B)	1986	6621	3339	62
H(68A)	964	6327	3676	75
H(68B)	1062	6656	3083	75
H(69A)	1397	5286	2885	75
H(69B)	837	5119	3098	75
H(70A)	1269	4678	3963	50
H(70B)	1507	4096	3511	50
H(71)	2437	3510	5131	33
H(72A)	1766	5030	5122	46
H(72B)	2389	5027	5365	46
H(73A)	2244	3967	6031	60
H(73B)	1846	4787	6072	60
H(74A)	1131	3992	5617	57
H(74B)	1408	3391	6113	57
H(75A)	1203	2552	5290	43
H(75B)	1827	2516	5524	43
H(76A)	1734	2782	4576	44
H(76B)	1358	3626	4635	44
H(77)	5779	3354	2394	130
H(78)	6249	3232	1648	117
H(79)	6753	1953	1541	141
H(80)	6787	797	2180	152
H(81)	6317	919	2925	139
H(82)	5813	2198	3032	154
H(83)	2298	6388	2287	145
H(84)	2747	7731	2194	117
H(85)	2468	8673	1455	122
H(86)	1740	8273	808	143
H(87)	1290	6930	901	108
H(88)	1570	5988	1640	138
H(89)	-120	-156	-912	113
H(90)	417	-1082	-301	130
H(91)	439	-892	640	136
H(92)	-76	224	971	183
H(93)	-613	1150	360	140
H(94)	-635	960	-582	120

Table S7. Torsion angles [°] for **1**.

C(1)-Ru(1)-Ru(2)-C(20)	-72.9(2)
O(6)-Ru(1)-Ru(2)-C(20)	-109.82(15)
O(5)-Ru(1)-Ru(2)-C(20)	101.60(16)
P(1)-Ru(1)-Ru(2)-C(20)	75.95(12)
Ru(4)-Ru(1)-Ru(2)-C(20)	-155.14(12)
C(1)-Ru(1)-Ru(2)-O(5)	-174.5(2)
O(6)-Ru(1)-Ru(2)-O(5)	148.58(14)
P(1)-Ru(1)-Ru(2)-O(5)	-25.65(11)
Ru(4)-Ru(1)-Ru(2)-O(5)	103.26(10)
C(1)-Ru(1)-Ru(2)-O(6)	36.9(2)
O(5)-Ru(1)-Ru(2)-O(6)	-148.58(14)
P(1)-Ru(1)-Ru(2)-O(6)	-174.23(10)
Ru(4)-Ru(1)-Ru(2)-O(6)	-45.32(9)
C(1)-Ru(1)-Ru(2)-O(7)	98.38(19)
O(6)-Ru(1)-Ru(2)-O(7)	61.48(11)
O(5)-Ru(1)-Ru(2)-O(7)	-87.10(12)
P(1)-Ru(1)-Ru(2)-O(7)	-112.75(7)
Ru(4)-Ru(1)-Ru(2)-O(7)	16.16(7)
C(1)-Ru(1)-Ru(2)-P(2)	-159.47(18)
O(6)-Ru(1)-Ru(2)-P(2)	163.63(10)
O(5)-Ru(1)-Ru(2)-P(2)	15.05(11)
P(1)-Ru(1)-Ru(2)-P(2)	-10.60(6)
Ru(4)-Ru(1)-Ru(2)-P(2)	118.31(4)
C(1)-Ru(1)-Ru(2)-Ru(3)	46.13(18)
O(6)-Ru(1)-Ru(2)-Ru(3)	9.23(9)
O(5)-Ru(1)-Ru(2)-Ru(3)	-139.35(10)
P(1)-Ru(1)-Ru(2)-Ru(3)	-165.00(4)
Ru(4)-Ru(1)-Ru(2)-Ru(3)	-36.089(11)
C(20)-Ru(2)-Ru(3)-C(39)	-105.5(2)
O(5)-Ru(2)-Ru(3)-C(39)	132.33(17)
O(6)-Ru(2)-Ru(3)-C(39)	172.05(17)
O(7)-Ru(2)-Ru(3)-C(39)	78.47(17)
P(2)-Ru(2)-Ru(3)-C(39)	2.26(15)
Ru(1)-Ru(2)-Ru(3)-C(39)	163.86(15)
C(20)-Ru(2)-Ru(3)-O(6)	82.43(16)
O(5)-Ru(2)-Ru(3)-O(6)	-39.72(12)
O(7)-Ru(2)-Ru(3)-O(6)	-93.58(12)
P(2)-Ru(2)-Ru(3)-O(6)	-169.79(9)
Ru(1)-Ru(2)-Ru(3)-O(6)	-8.19(8)
C(20)-Ru(2)-Ru(3)-O(7)	176.01(16)
O(5)-Ru(2)-Ru(3)-O(7)	53.86(11)
O(6)-Ru(2)-Ru(3)-O(7)	93.58(12)
P(2)-Ru(2)-Ru(3)-O(7)	-76.21(9)
Ru(1)-Ru(2)-Ru(3)-O(7)	85.39(8)
C(20)-Ru(2)-Ru(3)-P(3)	11.76(14)
O(5)-Ru(2)-Ru(3)-P(3)	-110.39(9)
O(6)-Ru(2)-Ru(3)-P(3)	-70.67(9)
O(7)-Ru(2)-Ru(3)-P(3)	-164.25(9)
P(2)-Ru(2)-Ru(3)-P(3)	119.54(4)
Ru(1)-Ru(2)-Ru(3)-P(3)	-78.86(3)
C(20)-Ru(2)-Ru(3)-Ru(4)	128.04(14)
O(5)-Ru(2)-Ru(3)-Ru(4)	5.89(8)
O(6)-Ru(2)-Ru(3)-Ru(4)	45.61(8)
O(7)-Ru(2)-Ru(3)-Ru(4)	-47.97(8)

P(2)-Ru(2)-Ru(3)-Ru(4)	-124.18(3)
Ru(1)-Ru(2)-Ru(3)-Ru(4)	37.417(11)
C(39)-Ru(3)-Ru(4)-C(58)	99.9(2)
O(6)-Ru(3)-Ru(4)-C(58)	-85.63(16)
O(7)-Ru(3)-Ru(4)-C(58)	179.34(16)
P(3)-Ru(3)-Ru(4)-C(58)	-12.06(14)
Ru(2)-Ru(3)-Ru(4)-C(58)	-132.64(14)
C(39)-Ru(3)-Ru(4)-O(6)	-174.43(17)
O(7)-Ru(3)-Ru(4)-O(6)	-95.03(12)
P(3)-Ru(3)-Ru(4)-O(6)	73.57(9)
Ru(2)-Ru(3)-Ru(4)-O(6)	-47.02(9)
C(39)-Ru(3)-Ru(4)-O(7)	-79.40(17)
O(6)-Ru(3)-Ru(4)-O(7)	95.03(12)
P(3)-Ru(3)-Ru(4)-O(7)	168.60(9)
Ru(2)-Ru(3)-Ru(4)-O(7)	48.02(8)
C(39)-Ru(3)-Ru(4)-P(4)	-8.06(15)
O(6)-Ru(3)-Ru(4)-P(4)	166.37(9)
O(7)-Ru(3)-Ru(4)-P(4)	71.34(9)
P(3)-Ru(3)-Ru(4)-P(4)	-120.06(4)
Ru(2)-Ru(3)-Ru(4)-P(4)	119.35(3)
C(39)-Ru(3)-Ru(4)-Ru(1)	-167.92(15)
O(6)-Ru(3)-Ru(4)-Ru(1)	6.51(9)
O(7)-Ru(3)-Ru(4)-Ru(1)	-88.53(8)
P(3)-Ru(3)-Ru(4)-Ru(1)	80.08(3)
Ru(2)-Ru(3)-Ru(4)-Ru(1)	-40.511(12)
C(1)-Ru(1)-Ru(4)-C(58)	19.20(17)
O(6)-Ru(1)-Ru(4)-C(58)	110.89(15)
O(5)-Ru(1)-Ru(4)-C(58)	-165.41(14)
P(1)-Ru(1)-Ru(4)-C(58)	-79.74(13)
Ru(2)-Ru(1)-Ru(4)-C(58)	153.75(12)
C(1)-Ru(1)-Ru(4)-O(6)	-91.68(15)
O(5)-Ru(1)-Ru(4)-O(6)	83.71(11)
P(1)-Ru(1)-Ru(4)-O(6)	169.37(10)
Ru(2)-Ru(1)-Ru(4)-O(6)	42.86(9)
C(1)-Ru(1)-Ru(4)-O(7)	-150.63(14)
O(6)-Ru(1)-Ru(4)-O(7)	-58.95(11)
O(5)-Ru(1)-Ru(4)-O(7)	24.76(9)
P(1)-Ru(1)-Ru(4)-O(7)	110.42(7)
Ru(2)-Ru(1)-Ru(4)-O(7)	-16.09(6)
C(1)-Ru(1)-Ru(4)-P(4)	106.66(13)
O(6)-Ru(1)-Ru(4)-P(4)	-161.66(10)
O(5)-Ru(1)-Ru(4)-P(4)	-77.95(8)
P(1)-Ru(1)-Ru(4)-P(4)	7.71(6)
Ru(2)-Ru(1)-Ru(4)-P(4)	-118.79(4)
C(1)-Ru(1)-Ru(4)-Ru(3)	-98.53(12)
O(6)-Ru(1)-Ru(4)-Ru(3)	-6.85(9)
O(5)-Ru(1)-Ru(4)-Ru(3)	76.86(7)
P(1)-Ru(1)-Ru(4)-Ru(3)	162.52(4)
Ru(2)-Ru(1)-Ru(4)-Ru(3)	36.018(11)
C(1)-Ru(1)-P(1)-C(2)	-27.50(19)
O(6)-Ru(1)-P(1)-C(2)	144.8(5)
O(5)-Ru(1)-P(1)-C(2)	157.25(15)
Ru(4)-Ru(1)-P(1)-C(2)	75.18(14)
Ru(2)-Ru(1)-P(1)-C(2)	174.05(13)
C(1)-Ru(1)-P(1)-C(14)	90.50(18)
O(6)-Ru(1)-P(1)-C(14)	-97.2(5)

O(5)-Ru(1)-P(1)-C(14)	-84.74(15)
Ru(4)-Ru(1)-P(1)-C(14)	-166.82(13)
Ru(2)-Ru(1)-P(1)-C(14)	-67.95(14)
C(1)-Ru(1)-P(1)-C(8)	-155.25(19)
O(6)-Ru(1)-P(1)-C(8)	17.0(5)
O(5)-Ru(1)-P(1)-C(8)	29.50(15)
Ru(4)-Ru(1)-P(1)-C(8)	-52.57(15)
Ru(2)-Ru(1)-P(1)-C(8)	46.29(15)
C(20)-Ru(2)-P(2)-C(21)	-76.95(18)
O(5)-Ru(2)-P(2)-C(21)	20.90(16)
O(6)-Ru(2)-P(2)-C(21)	116.6(4)
O(7)-Ru(2)-P(2)-C(21)	108.12(15)
Ru(3)-Ru(2)-P(2)-C(21)	159.48(14)
Ru(1)-Ru(2)-P(2)-C(21)	10.52(15)
C(20)-Ru(2)-P(2)-C(33)	168.53(18)
O(5)-Ru(2)-P(2)-C(33)	-93.62(15)
O(6)-Ru(2)-P(2)-C(33)	2.1(4)
O(7)-Ru(2)-P(2)-C(33)	-6.40(15)
Ru(3)-Ru(2)-P(2)-C(33)	44.96(14)
Ru(1)-Ru(2)-P(2)-C(33)	-104.00(14)
C(20)-Ru(2)-P(2)-C(27)	42.68(19)
O(5)-Ru(2)-P(2)-C(27)	140.53(16)
O(6)-Ru(2)-P(2)-C(27)	-123.7(4)
O(7)-Ru(2)-P(2)-C(27)	-132.25(16)
Ru(3)-Ru(2)-P(2)-C(27)	-80.89(15)
Ru(1)-Ru(2)-P(2)-C(27)	130.15(14)
C(39)-Ru(3)-P(3)-C(52)	-69.43(19)
O(6)-Ru(3)-P(3)-C(52)	108.63(16)
O(7)-Ru(3)-P(3)-C(52)	99.1(3)
Ru(2)-Ru(3)-P(3)-C(52)	156.29(14)
Ru(4)-Ru(3)-P(3)-C(52)	61.42(15)
C(39)-Ru(3)-P(3)-C(46)	49.67(19)
O(6)-Ru(3)-P(3)-C(46)	-132.27(16)
O(7)-Ru(3)-P(3)-C(46)	-141.8(3)
Ru(2)-Ru(3)-P(3)-C(46)	-84.61(15)
Ru(4)-Ru(3)-P(3)-C(46)	-179.49(14)
C(39)-Ru(3)-P(3)-C(40)	174.05(18)
O(6)-Ru(3)-P(3)-C(40)	-7.89(15)
O(7)-Ru(3)-P(3)-C(40)	-17.4(3)
Ru(2)-Ru(3)-P(3)-C(40)	39.77(14)
Ru(4)-Ru(3)-P(3)-C(40)	-55.10(14)
C(58)-Ru(4)-P(4)-C(71)	159.3(2)
O(6)-Ru(4)-P(4)-C(71)	-26.9(4)
O(7)-Ru(4)-P(4)-C(71)	-29.23(16)
Ru(3)-Ru(4)-P(4)-C(71)	-78.15(15)
Ru(1)-Ru(4)-P(4)-C(71)	71.28(15)
C(58)-Ru(4)-P(4)-C(65)	33.0(2)
O(6)-Ru(4)-P(4)-C(65)	-153.2(3)
O(7)-Ru(4)-P(4)-C(65)	-155.55(17)
Ru(3)-Ru(4)-P(4)-C(65)	155.53(15)
Ru(1)-Ru(4)-P(4)-C(65)	-55.04(16)
C(58)-Ru(4)-P(4)-C(59)	-86.6(2)
O(6)-Ru(4)-P(4)-C(59)	87.2(3)
O(7)-Ru(4)-P(4)-C(59)	84.90(16)
Ru(3)-Ru(4)-P(4)-C(59)	35.98(16)
Ru(1)-Ru(4)-P(4)-C(59)	-174.59(14)

C(20)-Ru(2)-O(5)-Ru(1)	-81.70(14)
O(6)-Ru(2)-O(5)-Ru(1)	20.71(9)
O(7)-Ru(2)-O(5)-Ru(1)	89.81(10)
P(2)-Ru(2)-O(5)-Ru(1)	-170.71(7)
Ru(3)-Ru(2)-O(5)-Ru(1)	49.91(11)
C(1)-Ru(1)-O(5)-Ru(2)	49.9(16)
O(6)-Ru(1)-O(5)-Ru(2)	-21.01(9)
P(1)-Ru(1)-O(5)-Ru(2)	160.74(8)
Ru(4)-Ru(1)-O(5)-Ru(2)	-66.61(7)
C(39)-Ru(3)-O(6)-Ru(4)	42.0(12)
O(7)-Ru(3)-O(6)-Ru(4)	56.11(8)
P(3)-Ru(3)-O(6)-Ru(4)	-121.33(6)
Ru(2)-Ru(3)-O(6)-Ru(4)	112.45(9)
C(39)-Ru(3)-O(6)-Ru(1)	-1.8(15)
O(7)-Ru(3)-O(6)-Ru(1)	12.3(5)
P(3)-Ru(3)-O(6)-Ru(1)	-165.2(6)
Ru(2)-Ru(3)-O(6)-Ru(1)	68.6(6)
Ru(4)-Ru(3)-O(6)-Ru(1)	-43.8(5)
C(39)-Ru(3)-O(6)-Ru(2)	-70.4(12)
O(7)-Ru(3)-O(6)-Ru(2)	-56.34(8)
P(3)-Ru(3)-O(6)-Ru(2)	126.22(6)
Ru(4)-Ru(3)-O(6)-Ru(2)	-112.45(9)
C(58)-Ru(4)-O(6)-Ru(3)	114.08(14)
O(7)-Ru(4)-O(6)-Ru(3)	-57.07(8)
P(4)-Ru(4)-O(6)-Ru(3)	-59.5(3)
Ru(1)-Ru(4)-O(6)-Ru(3)	-170.94(12)
C(58)-Ru(4)-O(6)-Ru(1)	-74.98(15)
O(7)-Ru(4)-O(6)-Ru(1)	113.87(10)
P(4)-Ru(4)-O(6)-Ru(1)	111.4(3)
Ru(3)-Ru(4)-O(6)-Ru(1)	170.94(12)
C(58)-Ru(4)-O(6)-Ru(2)	-170.07(15)
O(7)-Ru(4)-O(6)-Ru(2)	18.77(10)
P(4)-Ru(4)-O(6)-Ru(2)	16.3(4)
Ru(3)-Ru(4)-O(6)-Ru(2)	75.85(9)
Ru(1)-Ru(4)-O(6)-Ru(2)	-95.10(12)
C(1)-Ru(1)-O(6)-Ru(3)	138.5(6)
O(5)-Ru(1)-O(6)-Ru(3)	-46.3(6)
P(1)-Ru(1)-O(6)-Ru(3)	-33.7(10)
Ru(4)-Ru(1)-O(6)-Ru(3)	43.2(5)
Ru(2)-Ru(1)-O(6)-Ru(3)	-67.0(5)
C(1)-Ru(1)-O(6)-Ru(4)	95.26(14)
O(5)-Ru(1)-O(6)-Ru(4)	-89.59(10)
P(1)-Ru(1)-O(6)-Ru(4)	-77.0(5)
Ru(2)-Ru(1)-O(6)-Ru(4)	-110.22(11)
C(1)-Ru(1)-O(6)-Ru(2)	-154.52(14)
O(5)-Ru(1)-O(6)-Ru(2)	20.63(9)
P(1)-Ru(1)-O(6)-Ru(2)	33.3(5)
Ru(4)-Ru(1)-O(6)-Ru(2)	110.22(11)
C(20)-Ru(2)-O(6)-Ru(3)	-117.03(13)
O(5)-Ru(2)-O(6)-Ru(3)	146.61(10)
O(7)-Ru(2)-O(6)-Ru(3)	58.02(8)
P(2)-Ru(2)-O(6)-Ru(3)	49.0(4)
Ru(1)-Ru(2)-O(6)-Ru(3)	167.73(12)
C(20)-Ru(2)-O(6)-Ru(4)	166.03(14)
O(5)-Ru(2)-O(6)-Ru(4)	69.66(11)
O(7)-Ru(2)-O(6)-Ru(4)	-18.93(10)

P(2)-Ru(2)-O(6)-Ru(4)	-27.9(4)
Ru(3)-Ru(2)-O(6)-Ru(4)	-76.95(10)
Ru(1)-Ru(2)-O(6)-Ru(4)	90.78(12)
C(20)-Ru(2)-O(6)-Ru(1)	75.24(14)
O(5)-Ru(2)-O(6)-Ru(1)	-21.13(9)
O(7)-Ru(2)-O(6)-Ru(1)	-109.71(11)
P(2)-Ru(2)-O(6)-Ru(1)	-118.7(3)
Ru(3)-Ru(2)-O(6)-Ru(1)	-167.73(12)
C(20)-Ru(2)-O(7)-Ru(4)	49.4(9)
O(5)-Ru(2)-O(7)-Ru(4)	-64.73(11)
O(6)-Ru(2)-O(7)-Ru(4)	17.70(9)
P(2)-Ru(2)-O(7)-Ru(4)	-164.09(8)
Ru(3)-Ru(2)-O(7)-Ru(4)	71.67(8)
Ru(1)-Ru(2)-O(7)-Ru(4)	-21.52(8)
C(20)-Ru(2)-O(7)-Ru(3)	-22.3(9)
O(5)-Ru(2)-O(7)-Ru(3)	-136.40(8)
O(6)-Ru(2)-O(7)-Ru(3)	-53.97(8)
P(2)-Ru(2)-O(7)-Ru(3)	124.24(5)
Ru(1)-Ru(2)-O(7)-Ru(3)	-93.19(5)
C(58)-Ru(4)-O(7)-Ru(2)	-74.7(8)
O(6)-Ru(4)-O(7)-Ru(2)	-18.04(9)
P(4)-Ru(4)-O(7)-Ru(2)	161.40(8)
Ru(3)-Ru(4)-O(7)-Ru(2)	-71.45(8)
Ru(1)-Ru(4)-O(7)-Ru(2)	22.98(9)
C(58)-Ru(4)-O(7)-Ru(3)	-3.3(8)
O(6)-Ru(4)-O(7)-Ru(3)	53.41(8)
P(4)-Ru(4)-O(7)-Ru(3)	-127.15(5)
Ru(1)-Ru(4)-O(7)-Ru(3)	94.43(5)
C(39)-Ru(3)-O(7)-Ru(2)	-125.49(13)
O(6)-Ru(3)-O(7)-Ru(2)	56.21(8)
P(3)-Ru(3)-O(7)-Ru(2)	66.3(3)
Ru(4)-Ru(3)-O(7)-Ru(2)	110.33(8)
C(39)-Ru(3)-O(7)-Ru(4)	124.18(13)
O(6)-Ru(3)-O(7)-Ru(4)	-54.12(8)
P(3)-Ru(3)-O(7)-Ru(4)	-44.0(3)
Ru(2)-Ru(3)-O(7)-Ru(4)	-110.33(8)
O(6)-Ru(1)-C(1)-O(1)	113(5)
O(5)-Ru(1)-C(1)-O(1)	43(6)
P(1)-Ru(1)-C(1)-O(1)	-68(5)
Ru(4)-Ru(1)-C(1)-O(1)	159(5)
Ru(2)-Ru(1)-C(1)-O(1)	89(5)
C(14)-P(1)-C(2)-C(7)	50.4(3)
C(8)-P(1)-C(2)-C(7)	-56.4(4)
Ru(1)-P(1)-C(2)-C(7)	174.9(3)
C(14)-P(1)-C(2)-C(3)	-178.2(3)
C(8)-P(1)-C(2)-C(3)	75.0(3)
Ru(1)-P(1)-C(2)-C(3)	-53.7(3)
C(7)-C(2)-C(3)-C(4)	-59.1(4)
P(1)-C(2)-C(3)-C(4)	165.0(3)
C(2)-C(3)-C(4)-C(5)	57.1(5)
C(3)-C(4)-C(5)-C(6)	-53.8(5)
C(4)-C(5)-C(6)-C(7)	52.8(5)
C(3)-C(2)-C(7)-C(6)	58.1(5)
P(1)-C(2)-C(7)-C(6)	-168.7(3)
C(5)-C(6)-C(7)-C(2)	-55.4(5)
C(2)-P(1)-C(8)-C(9)	-63.0(3)

C(14)-P(1)-C(8)-C(9)	-171.4(3)
Ru(1)-P(1)-C(8)-C(9)	66.2(3)
C(2)-P(1)-C(8)-C(13)	67.5(4)
C(14)-P(1)-C(8)-C(13)	-40.9(3)
Ru(1)-P(1)-C(8)-C(13)	-163.3(3)
C(13)-C(8)-C(9)-C(10)	60.2(4)
P(1)-C(8)-C(9)-C(10)	-164.6(3)
C(8)-C(9)-C(10)-C(11)	-58.0(5)
C(9)-C(10)-C(11)-C(12)	54.1(5)
C(10)-C(11)-C(12)-C(13)	-53.9(5)
C(11)-C(12)-C(13)-C(8)	56.1(5)
C(9)-C(8)-C(13)-C(12)	-59.0(4)
P(1)-C(8)-C(13)-C(12)	168.2(3)
C(2)-P(1)-C(14)-C(15)	59.1(3)
C(8)-P(1)-C(14)-C(15)	173.7(3)
Ru(1)-P(1)-C(14)-C(15)	-64.9(3)
C(2)-P(1)-C(14)-C(19)	-177.2(3)
C(8)-P(1)-C(14)-C(19)	-62.6(3)
Ru(1)-P(1)-C(14)-C(19)	58.7(3)
C(19)-C(14)-C(15)-C(16)	54.0(4)
P(1)-C(14)-C(15)-C(16)	177.1(3)
C(14)-C(15)-C(16)-C(17)	-56.0(5)
C(15)-C(16)-C(17)-C(18)	57.0(5)
C(16)-C(17)-C(18)-C(19)	-56.7(5)
C(17)-C(18)-C(19)-C(14)	56.3(5)
C(15)-C(14)-C(19)-C(18)	-54.6(4)
P(1)-C(14)-C(19)-C(18)	-179.7(3)
O(5)-Ru(2)-C(20)-O(2)	-124(14)
O(6)-Ru(2)-C(20)-O(2)	153(14)
O(7)-Ru(2)-C(20)-O(2)	123(14)
P(2)-Ru(2)-C(20)-O(2)	-24(14)
Ru(3)-Ru(2)-C(20)-O(2)	103(14)
Ru(1)-Ru(2)-C(20)-O(2)	-166(100)
C(33)-P(2)-C(21)-C(26)	178.8(3)
C(27)-P(2)-C(21)-C(26)	-67.2(3)
Ru(2)-P(2)-C(21)-C(26)	59.5(3)
C(33)-P(2)-C(21)-C(22)	55.0(3)
C(27)-P(2)-C(21)-C(22)	169.0(3)
Ru(2)-P(2)-C(21)-C(22)	-64.3(3)
C(26)-C(21)-C(22)-C(23)	58.0(4)
P(2)-C(21)-C(22)-C(23)	-176.8(3)
C(21)-C(22)-C(23)-C(24)	-56.3(5)
C(22)-C(23)-C(24)-C(25)	54.1(5)
C(23)-C(24)-C(25)-C(26)	-54.4(5)
C(22)-C(21)-C(26)-C(25)	-58.1(5)
P(2)-C(21)-C(26)-C(25)	175.8(3)
C(24)-C(25)-C(26)-C(21)	57.1(5)
C(21)-P(2)-C(27)-C(28)	-52.7(4)
C(33)-P(2)-C(27)-C(28)	54.9(4)
Ru(2)-P(2)-C(27)-C(28)	-179.3(3)
C(21)-P(2)-C(27)-C(32)	177.6(3)
C(33)-P(2)-C(27)-C(32)	-74.8(4)
Ru(2)-P(2)-C(27)-C(32)	51.0(4)
C(32)-C(27)-C(28)-C(29)	-57.3(6)
P(2)-C(27)-C(28)-C(29)	171.4(4)
C(27)-C(28)-C(29)-C(30)	58.4(7)

C(28)-C(29)-C(30)-C(31)	-55.8(7)
C(29)-C(30)-C(31)-C(32)	53.6(6)
C(28)-C(27)-C(32)-C(31)	54.9(6)
P(2)-C(27)-C(32)-C(31)	-171.8(4)
C(30)-C(31)-C(32)-C(27)	-53.7(6)
C(21)-P(2)-C(33)-C(38)	173.3(3)
C(27)-P(2)-C(33)-C(38)	65.2(3)
Ru(2)-P(2)-C(33)-C(38)	-63.7(3)
C(21)-P(2)-C(33)-C(34)	42.6(4)
C(27)-P(2)-C(33)-C(34)	-65.4(4)
Ru(2)-P(2)-C(33)-C(34)	165.7(3)
C(38)-C(33)-C(34)-C(35)	60.0(5)
P(2)-C(33)-C(34)-C(35)	-167.1(3)
C(33)-C(34)-C(35)-C(36)	-58.4(5)
C(34)-C(35)-C(36)-C(37)	55.6(5)
C(35)-C(36)-C(37)-C(38)	-54.6(5)
C(36)-C(37)-C(38)-C(33)	56.5(5)
C(34)-C(33)-C(38)-C(37)	-58.8(4)
P(2)-C(33)-C(38)-C(37)	166.1(3)
O(6)-Ru(3)-C(39)-O(3)	-73(100)
O(7)-Ru(3)-C(39)-O(3)	-87(100)
P(3)-Ru(3)-C(39)-O(3)	90(100)
Ru(2)-Ru(3)-C(39)-O(3)	-139(100)
Ru(4)-Ru(3)-C(39)-O(3)	-35(100)
C(52)-P(3)-C(40)-C(41)	164.8(3)
C(46)-P(3)-C(40)-C(41)	56.6(3)
Ru(3)-P(3)-C(40)-C(41)	-70.3(3)
C(52)-P(3)-C(40)-C(45)	36.2(3)
C(46)-P(3)-C(40)-C(45)	-72.0(3)
Ru(3)-P(3)-C(40)-C(45)	161.1(3)
C(45)-C(40)-C(41)-C(42)	-55.7(4)
P(3)-C(40)-C(41)-C(42)	171.4(3)
C(40)-C(41)-C(42)-C(43)	56.6(5)
C(41)-C(42)-C(43)-C(44)	-55.8(5)
C(42)-C(43)-C(44)-C(45)	56.5(5)
C(43)-C(44)-C(45)-C(40)	-56.9(5)
C(41)-C(40)-C(45)-C(44)	55.8(5)
P(3)-C(40)-C(45)-C(44)	-175.0(3)
C(52)-P(3)-C(46)-C(51)	-62.7(3)
C(40)-P(3)-C(46)-C(51)	46.0(4)
Ru(3)-P(3)-C(46)-C(51)	170.4(3)
C(52)-P(3)-C(46)-C(47)	166.7(3)
C(40)-P(3)-C(46)-C(47)	-84.6(3)
Ru(3)-P(3)-C(46)-C(47)	39.7(3)
C(51)-C(46)-C(47)-C(48)	54.2(5)
P(3)-C(46)-C(47)-C(48)	-172.2(3)
C(46)-C(47)-C(48)-C(49)	-56.0(5)
C(47)-C(48)-C(49)-C(50)	56.9(5)
C(48)-C(49)-C(50)-C(51)	-57.5(5)
C(49)-C(50)-C(51)-C(46)	57.6(5)
C(47)-C(46)-C(51)-C(50)	-55.2(5)
P(3)-C(46)-C(51)-C(50)	172.4(3)
C(46)-P(3)-C(52)-C(57)	172.8(3)
C(40)-P(3)-C(52)-C(57)	58.7(3)
Ru(3)-P(3)-C(52)-C(57)	-61.7(3)
C(46)-P(3)-C(52)-C(53)	-62.4(3)

C(40)-P(3)-C(52)-C(53)	-176.6(3)
Ru(3)-P(3)-C(52)-C(53)	63.1(3)
C(57)-C(52)-C(53)-C(54)	-58.1(5)
P(3)-C(52)-C(53)-C(54)	175.1(3)
C(52)-C(53)-C(54)-C(55)	56.2(5)
C(53)-C(54)-C(55)-C(56)	-53.2(6)
C(54)-C(55)-C(56)-C(57)	54.0(5)
C(55)-C(56)-C(57)-C(52)	-57.5(5)
C(53)-C(52)-C(57)-C(56)	59.0(4)
P(3)-C(52)-C(57)-C(56)	-173.5(3)
O(6)-Ru(4)-C(58)-O(4)	-149(15)
O(7)-Ru(4)-C(58)-O(4)	-95(15)
P(4)-Ru(4)-C(58)-O(4)	30(15)
Ru(3)-Ru(4)-C(58)-O(4)	-98(15)
Ru(1)-Ru(4)-C(58)-O(4)	167(100)
C(71)-P(4)-C(59)-C(64)	179.9(3)
C(65)-P(4)-C(59)-C(64)	-65.3(3)
Ru(4)-P(4)-C(59)-C(64)	60.3(3)
C(71)-P(4)-C(59)-C(60)	56.3(3)
C(65)-P(4)-C(59)-C(60)	171.1(3)
Ru(4)-P(4)-C(59)-C(60)	-63.3(3)
C(64)-C(59)-C(60)-C(61)	56.1(5)
P(4)-C(59)-C(60)-C(61)	-179.7(3)
C(59)-C(60)-C(61)-C(62)	-54.6(6)
C(60)-C(61)-C(62)-C(63)	54.1(6)
C(61)-C(62)-C(63)-C(64)	-55.0(5)
C(62)-C(63)-C(64)-C(59)	57.2(5)
C(60)-C(59)-C(64)-C(63)	-57.3(5)
P(4)-C(59)-C(64)-C(63)	177.4(3)
C(71)-P(4)-C(65)-C(70)	-63.6(4)
C(59)-P(4)-C(65)-C(70)	-171.4(3)
Ru(4)-P(4)-C(65)-C(70)	62.7(3)
C(71)-P(4)-C(65)-C(66)	68.6(4)
C(59)-P(4)-C(65)-C(66)	-39.1(4)
Ru(4)-P(4)-C(65)-C(66)	-165.0(3)
C(70)-C(65)-C(66)-C(67)	-58.3(5)
P(4)-C(65)-C(66)-C(67)	168.2(4)
C(65)-C(66)-C(67)-C(68)	57.2(6)
C(66)-C(67)-C(68)-C(69)	-54.5(7)
C(67)-C(68)-C(69)-C(70)	52.4(7)
C(66)-C(65)-C(70)-C(69)	57.3(5)
P(4)-C(65)-C(70)-C(69)	-165.5(4)
C(68)-C(69)-C(70)-C(65)	-54.3(7)
C(65)-P(4)-C(71)-C(76)	76.3(3)
C(59)-P(4)-C(71)-C(76)	-174.6(3)
Ru(4)-P(4)-C(71)-C(76)	-52.1(3)
C(65)-P(4)-C(71)-C(72)	-55.8(4)
C(59)-P(4)-C(71)-C(72)	53.3(4)
Ru(4)-P(4)-C(71)-C(72)	175.9(3)
C(76)-C(71)-C(72)-C(73)	57.2(5)
P(4)-C(71)-C(72)-C(73)	-168.4(3)
C(71)-C(72)-C(73)-C(74)	-55.3(6)
C(72)-C(73)-C(74)-C(75)	53.5(6)
C(73)-C(74)-C(75)-C(76)	-53.4(6)
C(72)-C(71)-C(76)-C(75)	-57.9(5)
P(4)-C(71)-C(76)-C(75)	166.7(3)

C(74)-C(75)-C(76)-C(71)	55.9(5)

Symmetry transformations used to generate equivalent atoms:

Table S8. Crystal data and structure refinement for **3**.

Identification code	yi02	
Empirical formula	C_{56} $H_{99.4}$ $Cl_{0.60}$ $O_{2.40}$ P_3 Ru_2	
Formula weight	1127.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.4965(7) Å	α= 90°.
	b = 23.4569(12) Å	β= 105.5630(10)°.
	c = 17.5553(9) Å	γ = 90°.
Volume	5750.7(5) $Å^3$	
Z	4	
Density (calculated)	1.302 Mg/m^3	
Absorption coefficient	0.675 mm^{-1}	
F(000)	2391	
Crystal size	0.32 x 0.26 x 0.24 mm^3	
Theta range for data collection	1.70 to 26.44°.	
Index ranges	-18<=h<=17, 0<=k<=29, 0<=l<=21	
Reflections collected	36735	
Independent reflections	11714 [R(int) = 0.0511]	
Completeness to theta = 26.44°	99.0 %	
Absorption correction	Multi-scan with SADABS	
Max. and min. transmission	0.8548 and 0.8130	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11714 / 0 / 587	
Goodness-of-fit on F^2	0.951	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0924	
R indices (all data)	R1 = 0.0666, wR2 = 0.1036	
Largest diff. peak and hole	1.384 and -0.873 e.$Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl	9427(2)	2806(1)	1889(1)	28(1)
Ru(1)	9627(1)	2044(1)	961(1)	21(1)
Ru(2)	8312(1)	3008(1)	626(1)	28(1)
O(3)	9322(9)	2744(5)	1606(5)	41(3)
P(1)	8687(1)	1395(1)	1464(1)	23(1)
P(2)	10973(1)	2518(1)	749(1)	24(1)
P(3)	7732(1)	3810(1)	1119(1)	27(1)
O(1)	9756(2)	1184(1)	-247(1)	42(1)
O(2)	6946(3)	3175(2)	-946(2)	89(1)
C(1)	9707(2)	1519(1)	224(2)	27(1)
C(2)	7477(3)	3109(2)	-333(2)	56(1)
C(3)	9188(2)	658(1)	1486(2)	28(1)
C(4)	10175(3)	574(1)	2066(2)	38(1)
C(5)	10623(3)	17(2)	1891(3)	47(1)
C(6)	9985(3)	-488(2)	1932(2)	45(1)
C(7)	8987(3)	-404(1)	1398(2)	44(1)
C(8)	8546(3)	159(1)	1557(2)	40(1)
C(9)	7422(2)	1271(1)	901(2)	27(1)
C(10)	7355(3)	1108(2)	45(2)	37(1)
C(11)	6322(3)	973(2)	-412(2)	51(1)
C(12)	5661(3)	1468(2)	-375(3)	66(1)
C(13)	5725(3)	1633(2)	469(2)	64(1)
C(14)	6755(3)	1768(2)	916(2)	45(1)
C(15)	8569(2)	1590(1)	2456(2)	28(1)
C(16)	7942(3)	1208(2)	2823(2)	38(1)
C(17)	7734(3)	1500(2)	3530(2)	48(1)
C(18)	8640(3)	1683(2)	4141(2)	56(1)
C(19)	9296(3)	2025(2)	3784(2)	53(1)
C(20)	9509(3)	1715(2)	3086(2)	39(1)
C(21)	11955(3)	2047(2)	602(2)	46(1)
C(22)	12018(4)	1917(2)	-181(3)	75(2)
C(23)	12930(3)	1601(2)	-226(2)	51(1)
C(24)	13153(4)	1103(2)	341(3)	66(1)
C(25)	13050(5)	1217(3)	1111(4)	101(2)
C(26)	12174(3)	1543(2)	1160(2)	40(1)
C(27)	11582(3)	2963(1)	1609(2)	29(1)
C(28)	11832(3)	2657(2)	2411(2)	40(1)
C(29)	12123(3)	3089(2)	3083(2)	50(1)
C(30)	12957(3)	3454(2)	3011(2)	54(1)
C(31)	12765(3)	3730(2)	2200(2)	51(1)
C(32)	12476(3)	3291(2)	1543(2)	41(1)
C(33)	10780(3)	3030(1)	-102(2)	28(1)
C(34)	10088(3)	2777(1)	-844(2)	31(1)
C(35)	9896(3)	3186(2)	-1545(2)	37(1)
C(36)	9533(3)	3757(2)	-1351(2)	43(1)
C(37)	10222(3)	4012(2)	-621(2)	51(1)
C(38)	10415(3)	3609(2)	80(2)	47(1)
C(39)	6726(2)	3652(1)	1558(2)	27(1)
C(40)	5842(2)	3420(2)	946(2)	31(1)
C(41)	5038(3)	3279(2)	1313(2)	41(1)
C(42)	5355(3)	2860(2)	1998(2)	40(1)

C(43)	6229(3)	3077(2)	2604(2)	38(1)
C(44)	7039(3)	3224(1)	2245(2)	32(1)
C(45)	8612(2)	4172(1)	1947(2)	29(1)
C(46)	8229(3)	4602(2)	2445(2)	43(1)
C(47)	9025(3)	4800(2)	3155(2)	49(1)
C(48)	9863(3)	5050(2)	2914(3)	53(1)
C(49)	10240(3)	4634(2)	2403(2)	52(1)
C(50)	9449(3)	4437(2)	1696(2)	41(1)
C(51)	7193(2)	4335(1)	335(2)	28(1)
C(52)	6647(3)	4847(1)	548(2)	37(1)
C(53)	6084(3)	5141(2)	-213(2)	47(1)
C(54)	6742(3)	5336(2)	-706(2)	56(1)
C(55)	7312(3)	4845(2)	-894(2)	51(1)
C(56)	7874(3)	4538(2)	-144(2)	42(1)

Table S10. Bond lengths [Å] and angles [°] for **3**.

Ru(1)-C(1)	1.812(3)	C(19)-C(20)	1.528(5)
Ru(1)-O(3)	2.108(10)	C(21)-C(22)	1.434(5)
Ru(1)-P(2)	2.3608(9)	C(21)-C(26)	1.515(5)
Ru(1)-P(1)	2.3670(9)	C(22)-C(23)	1.536(6)
Ru(1)-Ru(2)	2.9129(4)	C(23)-C(24)	1.511(6)
Ru(2)-C(2)	1.806(4)	C(24)-C(25)	1.425(6)
Ru(2)-O(3)	2.034(10)	C(25)-C(26)	1.503(6)
Ru(2)-P(3)	2.3223(9)	C(27)-C(28)	1.534(4)
P(1)-C(15)	1.852(3)	C(27)-C(32)	1.538(5)
P(1)-C(9)	1.857(3)	C(28)-C(29)	1.525(5)
P(1)-C(3)	1.870(3)	C(29)-C(30)	1.514(5)
P(2)-C(27)	1.852(3)	C(30)-C(31)	1.520(5)
P(2)-C(21)	1.875(4)	C(31)-C(32)	1.518(5)
P(2)-C(33)	1.877(3)	C(33)-C(38)	1.523(5)
P(3)-C(51)	1.854(3)	C(33)-C(34)	1.534(4)
P(3)-C(39)	1.860(3)	C(34)-C(35)	1.526(4)
P(3)-C(45)	1.861(3)	C(35)-C(36)	1.510(5)
O(1)-C(1)	1.158(4)	C(36)-C(37)	1.520(5)
O(2)-C(2)	1.153(4)	C(37)-C(38)	1.517(5)
C(3)-C(8)	1.521(5)	C(39)-C(40)	1.533(5)
C(3)-C(4)	1.530(5)	C(39)-C(44)	1.542(4)
C(4)-C(5)	1.528(5)	C(40)-C(41)	1.511(5)
C(5)-C(6)	1.514(5)	C(41)-C(42)	1.526(5)
C(6)-C(7)	1.510(5)	C(42)-C(43)	1.507(5)
C(7)-C(8)	1.526(5)	C(43)-C(44)	1.514(5)
C(9)-C(14)	1.519(5)	C(45)-C(50)	1.530(5)
C(9)-C(10)	1.529(4)	C(45)-C(46)	1.535(5)
C(10)-C(11)	1.529(5)	C(46)-C(47)	1.526(5)
C(11)-C(12)	1.519(6)	C(47)-C(48)	1.507(6)
C(12)-C(13)	1.509(6)	C(48)-C(49)	1.522(6)
C(13)-C(14)	1.521(5)	C(49)-C(50)	1.517(5)
C(15)-C(20)	1.535(5)	C(51)-C(56)	1.534(5)
C(15)-C(16)	1.536(5)	C(51)-C(52)	1.538(4)
C(16)-C(17)	1.516(5)	C(52)-C(53)	1.530(5)
C(17)-C(18)	1.518(5)	C(53)-C(54)	1.521(5)
C(18)-C(19)	1.503(6)	C(54)-C(55)	1.505(6)
C(55)-C(56)	1.528(5)		
C(1)-Ru(1)-O(3)	167.4(3)	Ru(2)-O(3)-Ru(1)	89.4(3)
C(1)-Ru(1)-P(2)	89.63(11)	C(15)-P(1)-C(9)	102.23(15)
O(3)-Ru(1)-P(2)	91.1(4)	C(15)-P(1)-C(3)	110.02(15)
C(1)-Ru(1)-P(1)	89.01(10)	C(9)-P(1)-C(3)	100.93(14)
O(3)-Ru(1)-P(1)	94.4(4)	C(15)-P(1)-Ru(1)	113.52(10)
P(2)-Ru(1)-P(1)	160.88(3)	C(9)-P(1)-Ru(1)	119.12(11)
C(1)-Ru(1)-Ru(2)	123.17(10)	C(3)-P(1)-Ru(1)	110.05(11)
O(3)-Ru(1)-Ru(2)	44.3(3)	C(27)-P(2)-C(21)	103.34(18)
P(2)-Ru(1)-Ru(2)	97.25(2)	C(27)-P(2)-C(33)	103.02(14)
P(1)-Ru(1)-Ru(2)	99.44(2)	C(21)-P(2)-C(33)	102.94(16)
C(2)-Ru(2)-O(3)	168.2(3)	C(27)-P(2)-Ru(1)	111.75(11)
C(2)-Ru(2)-P(3)	91.25(12)	C(21)-P(2)-Ru(1)	115.73(13)
O(3)-Ru(2)-P(3)	100.5(3)	C(33)-P(2)-Ru(1)	118.26(12)
C(2)-Ru(2)-Ru(1)	121.91(11)	C(51)-P(3)-C(39)	102.67(15)
O(3)-Ru(2)-Ru(1)	46.4(3)	C(51)-P(3)-C(45)	109.96(15)
P(3)-Ru(2)-Ru(1)	146.79(2)	C(39)-P(3)-C(45)	102.54(15)

C(51)-P(3)-Ru(2)	112.56(11)	C(32)-C(27)-P(2)	116.6(2)
C(39)-P(3)-Ru(2)	113.27(10)	C(29)-C(28)-C(27)	110.4(3)
C(45)-P(3)-Ru(2)	114.76(11)	C(30)-C(29)-C(28)	111.9(3)
O(1)-C(1)-Ru(1)	179.8(4)	C(29)-C(30)-C(31)	111.7(3)
O(2)-C(2)-Ru(2)	179.8(6)	C(32)-C(31)-C(30)	111.5(3)
C(8)-C(3)-C(4)	109.2(3)	C(31)-C(32)-C(27)	110.4(3)
C(8)-C(3)-P(1)	118.0(2)	C(38)-C(33)-C(34)	109.7(3)
C(4)-C(3)-P(1)	114.9(2)	C(38)-C(33)-P(2)	113.0(2)
C(5)-C(4)-C(3)	110.4(3)	C(34)-C(33)-P(2)	110.7(2)
C(6)-C(5)-C(4)	111.2(3)	C(35)-C(34)-C(33)	112.3(3)
C(7)-C(6)-C(5)	111.4(3)	C(36)-C(35)-C(34)	112.0(3)
C(6)-C(7)-C(8)	112.2(3)	C(35)-C(36)-C(37)	110.4(3)
C(3)-C(8)-C(7)	110.9(3)	C(38)-C(37)-C(36)	112.1(3)
C(14)-C(9)-C(10)	109.6(3)	C(37)-C(38)-C(33)	112.7(3)
C(14)-C(9)-P(1)	114.5(2)	C(40)-C(39)-C(44)	109.5(3)
C(10)-C(9)-P(1)	110.8(2)	C(40)-C(39)-P(3)	112.4(2)
C(9)-C(10)-C(11)	111.3(3)	C(44)-C(39)-P(3)	110.8(2)
C(12)-C(11)-C(10)	111.0(3)	C(41)-C(40)-C(39)	111.9(3)
C(13)-C(12)-C(11)	111.4(4)	C(40)-C(41)-C(42)	112.0(3)
C(12)-C(13)-C(14)	110.7(4)	C(43)-C(42)-C(41)	110.9(3)
C(9)-C(14)-C(13)	111.9(3)	C(42)-C(43)-C(44)	112.5(3)
C(20)-C(15)-C(16)	108.6(3)	C(43)-C(44)-C(39)	112.0(3)
C(20)-C(15)-P(1)	115.9(2)	C(50)-C(45)-C(46)	109.4(3)
C(16)-C(15)-P(1)	117.7(2)	C(50)-C(45)-P(3)	113.1(2)
C(17)-C(16)-C(15)	110.5(3)	C(46)-C(45)-P(3)	117.9(2)
C(16)-C(17)-C(18)	112.4(3)	C(47)-C(46)-C(45)	110.8(3)
C(19)-C(18)-C(17)	112.4(3)	C(48)-C(47)-C(46)	112.3(3)
C(18)-C(19)-C(20)	111.5(3)	C(47)-C(48)-C(49)	111.1(3)
C(19)-C(20)-C(15)	109.7(3)	C(50)-C(49)-C(48)	111.4(3)
C(22)-C(21)-C(26)	113.5(3)	C(49)-C(50)-C(45)	111.8(3)
C(22)-C(21)-P(2)	120.2(3)	C(56)-C(51)-C(52)	109.8(3)
C(26)-C(21)-P(2)	114.0(3)	C(56)-C(51)-P(3)	114.1(2)
C(21)-C(22)-C(23)	115.4(4)	C(52)-C(51)-P(3)	118.6(2)
C(24)-C(23)-C(22)	112.0(4)	C(53)-C(52)-C(51)	109.2(3)
C(25)-C(24)-C(23)	114.9(4)	C(54)-C(53)-C(52)	111.3(3)
C(24)-C(25)-C(26)	117.1(5)	C(55)-C(54)-C(53)	111.1(3)
C(25)-C(26)-C(21)	113.1(3)	C(54)-C(55)-C(56)	111.6(3)
C(28)-C(27)-C(32)	107.8(3)	C(55)-C(56)-C(51)	110.2(3)
C(28)-C(27)-P(2)	115.4(2)		

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2$x 10^3) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl	29(1)	26(1)	29(1)	0(1)	6(1)	5(1)
Ru(1)	22(1)	18(1)	23(1)	-1(1)	6(1)	0(1)
Ru(2)	31(1)	27(1)	24(1)	0(1)	4(1)	10(1)
O(3)	61(6)	45(5)	15(5)	-12(4)	4(5)	-1(4)
P(1)	22(1)	20(1)	24(1)	1(1)	4(1)	0(1)
P(2)	23(1)	26(1)	22(1)	1(1)	6(1)	0(1)
P(3)	30(1)	25(1)	25(1)	1(1)	7(1)	7(1)
O(1)	48(2)	41(2)	41(2)	-17(1)	17(1)	0(1)
O(2)	110(3)	82(2)	44(2)	-22(2)	-31(2)	53(2)
C(1)	24(2)	26(2)	30(2)	3(1)	5(2)	-1(1)
C(2)	70(3)	47(2)	38(2)	-12(2)	-6(2)	39(2)
C(3)	27(2)	23(2)	32(2)	3(1)	4(2)	1(1)
C(4)	33(2)	26(2)	49(2)	7(2)	0(2)	0(2)
C(5)	33(2)	40(2)	64(3)	10(2)	5(2)	11(2)
C(6)	47(3)	26(2)	58(3)	3(2)	8(2)	10(2)
C(7)	45(3)	22(2)	58(2)	1(2)	5(2)	-4(2)
C(8)	33(2)	25(2)	59(2)	6(2)	8(2)	-1(2)
C(9)	24(2)	26(2)	31(2)	0(1)	6(2)	-1(1)
C(10)	29(2)	44(2)	34(2)	-6(2)	3(2)	-1(2)
C(11)	39(3)	65(3)	40(2)	-16(2)	-7(2)	-4(2)
C(12)	35(3)	94(4)	54(3)	-14(3)	-13(2)	13(3)
C(13)	28(2)	96(4)	57(3)	-20(3)	-6(2)	18(2)
C(14)	34(2)	53(2)	43(2)	-9(2)	0(2)	15(2)
C(15)	28(2)	28(2)	28(2)	1(1)	8(2)	-1(2)
C(16)	40(2)	42(2)	34(2)	2(2)	14(2)	-7(2)
C(17)	48(3)	62(3)	40(2)	3(2)	23(2)	2(2)
C(18)	67(3)	75(3)	26(2)	0(2)	15(2)	9(3)
C(19)	63(3)	59(3)	30(2)	-10(2)	4(2)	-2(2)
C(20)	38(2)	48(2)	26(2)	-5(2)	3(2)	-4(2)
C(21)	47(3)	50(2)	47(2)	16(2)	24(2)	21(2)
C(22)	84(4)	93(4)	58(3)	22(3)	37(3)	48(3)
C(23)	41(3)	68(3)	49(2)	-3(2)	23(2)	16(2)
C(24)	65(3)	75(3)	58(3)	4(2)	19(3)	41(3)
C(25)	117(5)	97(4)	109(5)	53(4)	66(4)	75(4)
C(26)	39(2)	42(2)	41(2)	9(2)	15(2)	15(2)
C(27)	29(2)	33(2)	24(2)	-2(1)	8(2)	-9(2)
C(28)	48(3)	42(2)	28(2)	4(2)	6(2)	-18(2)
C(29)	68(3)	55(3)	24(2)	4(2)	7(2)	-24(2)
C(30)	59(3)	62(3)	32(2)	-2(2)	-2(2)	-27(2)
C(31)	60(3)	56(3)	34(2)	-5(2)	8(2)	-35(2)
C(32)	38(2)	55(2)	30(2)	1(2)	9(2)	-19(2)
C(33)	32(2)	30(2)	24(2)	2(1)	10(2)	-1(2)
C(34)	31(2)	35(2)	28(2)	1(1)	9(2)	3(2)
C(35)	39(2)	47(2)	28(2)	5(2)	11(2)	4(2)
C(36)	52(3)	44(2)	34(2)	12(2)	12(2)	13(2)
C(37)	69(3)	32(2)	48(2)	7(2)	10(2)	13(2)
C(38)	69(3)	34(2)	33(2)	-2(2)	4(2)	11(2)
C(39)	32(2)	22(2)	30(2)	0(1)	11(2)	2(1)
C(40)	30(2)	34(2)	30(2)	5(1)	7(2)	5(2)
C(41)	37(2)	46(2)	42(2)	8(2)	13(2)	5(2)
C(42)	43(2)	41(2)	40(2)	4(2)	19(2)	2(2)

C(43)	51(3)	34(2)	30(2)	4(2)	15(2)	7(2)
C(44)	38(2)	30(2)	26(2)	4(1)	7(2)	1(2)
C(45)	29(2)	28(2)	28(2)	0(1)	6(2)	5(2)
C(46)	38(2)	42(2)	49(2)	-16(2)	13(2)	-2(2)
C(47)	52(3)	48(2)	46(2)	-18(2)	12(2)	3(2)
C(48)	47(3)	52(3)	55(3)	-10(2)	3(2)	-8(2)
C(49)	34(2)	67(3)	53(3)	-10(2)	8(2)	-10(2)
C(50)	34(2)	52(2)	38(2)	-4(2)	10(2)	-5(2)
C(51)	30(2)	27(2)	29(2)	4(1)	9(2)	6(2)
C(52)	44(2)	30(2)	40(2)	9(2)	17(2)	13(2)
C(53)	43(3)	42(2)	57(2)	18(2)	16(2)	17(2)
C(54)	60(3)	51(3)	57(3)	31(2)	17(2)	15(2)
C(55)	46(3)	69(3)	42(2)	24(2)	18(2)	11(2)
C(56)	44(3)	47(2)	40(2)	17(2)	19(2)	10(2)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **3**.

	x	y	z	U(eq)
H(3)	9557	2879	2133	50
H(3)	9303	610	953	34
H(4A)	10596	897	2022	46
H(4B)	10111	566	2614	46
H(5A)	10727	36	1357	57
H(5B)	11253	-36	2278	57
H(6A)	10267	-838	1773	54
H(6B)	9951	-538	2483	54
H(7A)	8575	-722	1478	52
H(7B)	9012	-414	840	52
H(8A)	7912	208	1173	48
H(8B)	8452	153	2095	48
H(9)	7184	939	1150	33
H(10A)	7763	771	37	44
H(10B)	7596	1427	-218	44
H(11A)	6295	891	-970	62
H(11B)	6104	628	-184	62
H(12A)	5836	1800	-656	79
H(12B)	4993	1361	-646	79
H(13A)	5485	1316	735	77
H(13B)	5317	1971	474	77
H(14A)	6973	2106	676	54
H(14B)	6783	1862	1471	54
H(15)	8227	1964	2373	33
H(16A)	7333	1124	2423	45
H(16B)	8275	842	2992	45
H(17A)	7368	1236	3779	57
H(17B)	7329	1840	3346	57
H(18A)	8464	1914	4553	67
H(18B)	8983	1340	4399	67
H(19A)	9903	2099	4192	63
H(19B)	8995	2398	3603	63
H(20A)	9847	1353	3269	46
H(20B)	9929	1953	2855	46
H(21)	12533	2292	807	55
H(22A)	11978	2279	-480	90
H(22B)	11457	1683	-449	90
H(23A)	12848	1461	-772	61
H(23B)	13476	1870	-101	61
H(24A)	12726	782	110	79
H(24B)	13820	979	392	79
H(25A)	13620	1432	1408	121
H(25B)	13052	848	1385	121
H(26A)	12268	1680	1709	48
H(26B)	11617	1281	1037	48
H(27)	11106	3262	1647	34
H(28A)	11271	2437	2465	48
H(28B)	12365	2387	2440	48
H(29A)	11570	3337	3079	60
H(29B)	12303	2883	3594	60

H(30A)	13540	3216	3105	65
H(30B)	13075	3755	3421	65
H(31A)	12247	4016	2140	61
H(31B)	13348	3931	2156	61
H(32A)	13010	3021	1578	49
H(32B)	12339	3485	1024	49
H(33)	11411	3090	-219	34
H(34A)	10361	2419	-988	37
H(34B)	9474	2684	-727	37
H(35A)	10495	3244	-1705	45
H(35B)	9417	3015	-1998	45
H(36A)	8895	3709	-1256	52
H(36B)	9465	4019	-1805	52
H(37A)	10834	4104	-742	61
H(37B)	9950	4372	-481	61
H(38A)	9817	3555	241	56
H(38B)	10894	3784	529	56
H(39)	6540	4015	1775	33
H(40A)	5616	3708	524	38
H(40B)	6022	3073	699	38
H(41A)	4497	3113	904	49
H(41B)	4810	3634	1507	49
H(42A)	4827	2804	2250	48
H(42B)	5500	2487	1794	48
H(43A)	6450	2782	3016	45
H(43B)	6053	3420	2861	45
H(44A)	7272	2871	2049	38
H(44B)	7576	3389	2659	38
H(45)	8904	3859	2321	35
H(46A)	7956	4935	2115	51
H(46B)	7711	4423	2632	51
H(47A)	8767	5090	3451	59
H(47B)	9249	4472	3512	59
H(48A)	10381	5143	3393	64
H(48B)	9662	5407	2615	64
H(49A)	10751	4820	2216	63
H(49B)	10522	4298	2725	63
H(50A)	9712	4153	1393	50
H(50B)	9215	4767	1345	50
H(51)	6691	4113	-54	34
H(52A)	6202	4715	852	44
H(52B)	7104	5119	880	44
H(53A)	5601	4874	-527	56
H(53B)	5741	5475	-77	56
H(54A)	6355	5508	-1205	67
H(54B)	7185	5631	-413	67
H(55A)	7763	4988	-1185	61
H(55B)	6873	4571	-1240	61
H(56A)	8357	4800	181	51
H(56B)	8215	4207	-289	51

Table S13. Torsion angles [°] for **3**.

C(1)-Ru(1)-Ru(2)-C(2)	2.5(2)	P(3)-Ru(2)-C(2)-O(2)	67(100)
O(3)-Ru(1)-Ru(2)-C(2)	-179.0(5)	Ru(1)-Ru(2)-C(2)-O(2)	-114(100)
P(2)-Ru(1)-Ru(2)-C(2)	96.9(2)	C(15)-P(1)-C(3)-C(8)	71.7(3)
P(1)-Ru(1)-Ru(2)-C(2)	-92.5(2)	C(9)-P(1)-C(3)-C(8)	-35.7(3)
C(1)-Ru(1)-Ru(2)-O(3)	-178.4(5)	Ru(1)-P(1)-C(3)-C(8)	-162.5(2)
P(2)-Ru(1)-Ru(2)-O(3)	-84.1(5)	C(15)-P(1)-C(3)-C(4)	-59.4(3)
P(1)-Ru(1)-Ru(2)-O(3)	86.5(5)	C(9)-P(1)-C(3)-C(4)	-166.9(3)
C(1)-Ru(1)-Ru(2)-P(3)	178.96(13)	Ru(1)-P(1)-C(3)-C(4)	66.4(3)
O(3)-Ru(1)-Ru(2)-P(3)	-2.6(5)	C(8)-C(3)-C(4)-C(5)	59.1(4)
P(2)-Ru(1)-Ru(2)-P(3)	-86.71(5)	P(1)-C(3)-C(4)-C(5)	-165.6(3)
P(1)-Ru(1)-Ru(2)-P(3)	83.93(5)	C(3)-C(4)-C(5)-C(6)	-57.8(4)
C(2)-Ru(2)-O(3)-Ru(1)	4(2)	C(4)-C(5)-C(6)-C(7)	54.4(5)
P(3)-Ru(2)-O(3)-Ru(1)	178.5(3)	C(5)-C(6)-C(7)-C(8)	-53.4(5)
C(1)-Ru(1)-O(3)-Ru(2)	6(2)	C(4)-C(3)-C(8)-C(7)	-57.8(4)
P(2)-Ru(1)-O(3)-Ru(2)	99.3(4)	P(1)-C(3)-C(8)-C(7)	168.5(3)
P(1)-Ru(1)-O(3)-Ru(2)	-99.1(4)	C(6)-C(7)-C(8)-C(3)	55.6(4)
C(1)-Ru(1)-P(1)-C(15)	165.04(15)	C(15)-P(1)-C(9)-C(14)	54.8(3)
O(3)-Ru(1)-P(1)-C(15)	-27.1(3)	C(3)-P(1)-C(9)-C(14)	168.3(3)
P(2)-Ru(1)-P(1)-C(15)	79.05(15)	Ru(1)-P(1)-C(9)-C(14)	-71.2(3)
Ru(2)-Ru(1)-P(1)-C(15)	-71.46(12)	C(15)-P(1)-C(9)-C(10)	179.4(2)
C(1)-Ru(1)-P(1)-C(9)	-74.50(16)	C(3)-P(1)-C(9)-C(10)	-67.1(3)
O(3)-Ru(1)-P(1)-C(9)	93.3(3)	Ru(1)-P(1)-C(9)-C(10)	53.3(3)
P(2)-Ru(1)-P(1)-C(9)	-160.49(13)	C(14)-C(9)-C(10)-C(11)	-56.0(4)
Ru(2)-Ru(1)-P(1)-C(9)	49.00(12)	P(1)-C(9)-C(10)-C(11)	176.7(3)
C(1)-Ru(1)-P(1)-C(3)	41.24(15)	C(9)-C(10)-C(11)-C(12)	55.8(5)
O(3)-Ru(1)-P(1)-C(3)	-150.9(3)	C(10)-C(11)-C(12)-C(13)	-55.6(5)
P(2)-Ru(1)-P(1)-C(3)	-44.75(15)	C(11)-C(12)-C(13)-C(14)	55.8(6)
Ru(2)-Ru(1)-P(1)-C(3)	164.74(11)	C(10)-C(9)-C(14)-C(13)	56.7(4)
C(1)-Ru(1)-P(2)-C(27)	-157.58(16)	P(1)-C(9)-C(14)-C(13)	-178.0(3)
O(3)-Ru(1)-P(2)-C(27)	35.0(3)	C(12)-C(13)-C(14)-C(9)	-57.0(5)
P(1)-Ru(1)-P(2)-C(27)	-71.70(15)	C(9)-P(1)-C(15)-C(20)	179.2(2)
Ru(2)-Ru(1)-P(2)-C(27)	79.00(12)	C(3)-P(1)-C(15)-C(20)	72.6(3)
C(1)-Ru(1)-P(2)-C(21)	-39.68(17)	Ru(1)-P(1)-C(15)-C(20)	-51.2(3)
O(3)-Ru(1)-P(2)-C(21)	152.9(3)	C(9)-P(1)-C(15)-C(16)	48.2(3)
P(1)-Ru(1)-P(2)-C(21)	46.21(18)	C(3)-P(1)-C(15)-C(16)	-58.4(3)
Ru(2)-Ru(1)-P(2)-C(21)	-163.09(14)	Ru(1)-P(1)-C(15)-C(16)	177.8(2)
C(1)-Ru(1)-P(2)-C(33)	83.09(15)	C(20)-C(15)-C(16)-C(17)	59.2(4)
O(3)-Ru(1)-P(2)-C(33)	-84.3(3)	P(1)-C(15)-C(16)-C(17)	-166.5(3)
P(1)-Ru(1)-P(2)-C(33)	168.98(13)	C(15)-C(16)-C(17)-C(18)	-54.8(4)
Ru(2)-Ru(1)-P(2)-C(33)	-40.33(12)	C(16)-C(17)-C(18)-C(19)	51.6(5)
C(2)-Ru(2)-P(3)-C(51)	-25.9(2)	C(17)-C(18)-C(19)-C(20)	-53.0(5)
O(3)-Ru(2)-P(3)-C(51)	155.2(4)	C(18)-C(19)-C(20)-C(15)	58.1(4)
Ru(1)-Ru(2)-P(3)-C(51)	157.10(12)	C(16)-C(15)-C(20)-C(19)	-60.7(4)
C(2)-Ru(2)-P(3)-C(39)	90.0(2)	P(1)-C(15)-C(20)-C(19)	164.2(3)
O(3)-Ru(2)-P(3)-C(39)	-88.9(4)	C(27)-P(2)-C(21)-C(22)	-140.1(4)
Ru(1)-Ru(2)-P(3)-C(39)	-86.97(12)	C(33)-P(2)-C(21)-C(22)	-33.1(4)
C(2)-Ru(2)-P(3)-C(45)	-152.7(2)	Ru(1)-P(2)-C(21)-C(22)	97.5(4)
O(3)-Ru(2)-P(3)-C(45)	28.4(4)	C(27)-P(2)-C(21)-C(26)	80.1(3)
Ru(1)-Ru(2)-P(3)-C(45)	30.33(14)	C(33)-P(2)-C(21)-C(26)	-173.0(3)
O(3)-Ru(1)-C(1)-O(1)	-52(100)	Ru(1)-P(2)-C(21)-C(26)	-42.4(3)
P(2)-Ru(1)-C(1)-O(1)	-146(100)	C(26)-C(21)-C(22)-C(23)	-48.5(6)
P(1)-Ru(1)-C(1)-O(1)	53(100)	P(2)-C(21)-C(22)-C(23)	171.5(3)
Ru(2)-Ru(1)-C(1)-O(1)	-47(100)	C(21)-C(22)-C(23)-C(24)	47.1(6)
O(3)-Ru(2)-C(2)-O(2)	-118(100)	C(22)-C(23)-C(24)-C(25)	-43.7(7)

C(23)-C(24)-C(25)-C(26)	44.0(8)	Ru(2)-P(3)-C(39)-C(44)	59.4(2)
C(24)-C(25)-C(26)-C(21)	-43.9(7)	C(44)-C(39)-C(40)-C(41)	55.0(4)
C(22)-C(21)-C(26)-C(25)	45.4(6)	P(3)-C(39)-C(40)-C(41)	178.6(2)
P(2)-C(21)-C(26)-C(25)	-172.0(4)	C(39)-C(40)-C(41)-C(42)	-56.0(4)
C(21)-P(2)-C(27)-C(28)	-73.5(3)	C(40)-C(41)-C(42)-C(43)	54.4(4)
C(33)-P(2)-C(27)-C(28)	179.5(3)	C(41)-C(42)-C(43)-C(44)	-53.9(4)
Ru(1)-P(2)-C(27)-C(28)	51.6(3)	C(42)-C(43)-C(44)-C(39)	54.9(4)
C(21)-P(2)-C(27)-C(32)	54.6(3)	C(40)-C(39)-C(44)-C(43)	-54.2(4)
C(33)-P(2)-C(27)-C(32)	-52.3(3)	P(3)-C(39)-C(44)-C(43)	-178.8(2)
Ru(1)-P(2)-C(27)-C(32)	179.7(2)	C(51)-P(3)-C(45)-C(50)	-61.8(3)
C(32)-C(27)-C(28)-C(29)	60.1(4)	C(39)-P(3)-C(45)-C(50)	-170.5(2)
P(2)-C(27)-C(28)-C(29)	-167.5(3)	Ru(2)-P(3)-C(45)-C(50)	66.3(3)
C(27)-C(28)-C(29)-C(30)	-57.0(5)	C(51)-P(3)-C(45)-C(46)	67.6(3)
C(28)-C(29)-C(30)-C(31)	52.6(5)	C(39)-P(3)-C(45)-C(46)	-41.1(3)
C(29)-C(30)-C(31)-C(32)	-53.0(5)	Ru(2)-P(3)-C(45)-C(46)	-164.3(2)
C(30)-C(31)-C(32)-C(27)	57.7(5)	C(50)-C(45)-C(46)-C(47)	-56.0(4)
C(28)-C(27)-C(32)-C(31)	-60.7(4)	P(3)-C(45)-C(46)-C(47)	172.9(3)
P(2)-C(27)-C(32)-C(31)	167.6(3)	C(45)-C(46)-C(47)-C(48)	56.1(4)
C(27)-P(2)-C(33)-C(38)	-44.1(3)	C(46)-C(47)-C(48)-C(49)	-54.6(5)
C(21)-P(2)-C(33)-C(38)	-151.4(3)	C(47)-C(48)-C(49)-C(50)	54.2(5)
Ru(1)-P(2)-C(33)-C(38)	79.7(3)	C(48)-C(49)-C(50)-C(45)	-56.1(5)
C(27)-P(2)-C(33)-C(34)	-167.6(2)	C(46)-C(45)-C(50)-C(49)	56.7(4)
C(21)-P(2)-C(33)-C(34)	85.2(3)	P(3)-C(45)-C(50)-C(49)	-169.7(3)
Ru(1)-P(2)-C(33)-C(34)	-43.8(3)	C(39)-P(3)-C(51)-C(56)	-179.1(3)
C(38)-C(33)-C(34)-C(35)	53.5(4)	C(45)-P(3)-C(51)-C(56)	72.4(3)
P(2)-C(33)-C(34)-C(35)	178.8(2)	Ru(2)-P(3)-C(51)-C(56)	-56.9(3)
C(33)-C(34)-C(35)-C(36)	-55.4(4)	C(39)-P(3)-C(51)-C(52)	49.0(3)
C(34)-C(35)-C(36)-C(37)	54.9(4)	C(45)-P(3)-C(51)-C(52)	-59.5(3)
C(35)-C(36)-C(37)-C(38)	-54.9(5)	Ru(2)-P(3)-C(51)-C(52)	171.2(2)
C(36)-C(37)-C(38)-C(33)	55.4(5)	C(56)-C(51)-C(52)-C(53)	58.9(4)
C(34)-C(33)-C(38)-C(37)	-53.6(4)	P(3)-C(51)-C(52)-C(53)	-167.4(3)
P(2)-C(33)-C(38)-C(37)	-177.6(3)	C(51)-C(52)-C(53)-C(54)	-58.0(4)
C(51)-P(3)-C(39)-C(40)	58.2(3)	C(52)-C(53)-C(54)-C(55)	56.4(5)
C(45)-P(3)-C(39)-C(40)	172.4(2)	C(53)-C(54)-C(55)-C(56)	-55.3(5)
Ru(2)-P(3)-C(39)-C(40)	-63.4(2)	C(54)-C(55)-C(56)-C(51)	56.5(5)
C(51)-P(3)-C(39)-C(44)	-178.9(2)	C(52)-C(51)-C(56)-C(55)	-58.2(4)
C(45)-P(3)-C(39)-C(44)	-64.8(2)	P(3)-C(51)-C(56)-C(55)	165.8(3)

Symmetry transformations used to generate equivalent atoms: