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Intermolecular Dehydrative Coupling Reaction of Arylketones with Cyclic Alkenes Catalyzed by a Well-Defined Cationic Ruthenium-Hydride Complex: A Novel Ketone Olefination Method via Vinyl C–H Bond Activation

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Intermolecular Dehydrative Coupling Reaction of Arylketones with Cyclic Alkenes Catalyzed by a Well-Defined Cationic Ruthenium-Hydride Complex: A Novel Ketone Olefination Method via Vinyl C–H Bond Activation

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Summary: The cationic ruthenium-hydride complex $[(\eta^6\text{-}C_6H_6)(PCy_3)(CO)RuH]^+BF_4^-$ was found to be a highly effective catalyst for the intermolecular olefination reaction of arylketones with cycloalkenes. The preliminary mechanistic analysis revealed that electrophilic ruthenium-vinyl

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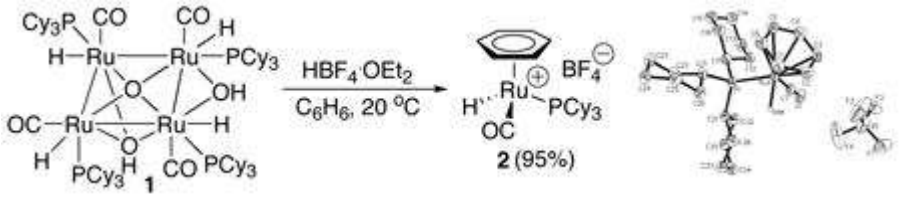
complex is the key species for mediating both vinyl C–H bond activation and the dehydrative olefination steps of the coupling reaction.

Wittig reaction constitutes one of the most versatile olefination methods whose synthetic prowess has been immensely demonstrated over the years in both laboratory-scale and industrial processes.[1] Despite its synthetic versatility, however, Wittig and related Peterson and Horner-Emmons olefination methods require stoichiometric amount of ylides (or carbanion equivalents), which pose debilitating problems of the formation and removal of byproducts especially for large-scale industrial applications. The Perkin and related Aldol-type condensation/dehydration reactions have also been commonly used as carbonyl olefination methods, but these also suffer from similar restricted functional group compatibility and the formation of copious amount of byproducts.[2] Considerable research progress has been achieved in the development of transition metal-based carbonyl olefination methods that are more functional group tolerant and environmentally compatible, including: Tebbe's and Petasis Ti reagents,[3] carbonyl-to-diazo coupling,[4] decarbonylative coupling reaction of aldehydes and alkynes,[5] and Pd-catalyzed coupling reactions.[6] From both synthetic and environmental points of view, the development of catalytic version of the carbonyl olefination methods from the intermolecular coupling of carbonyl compounds with unactivated olefins would be highly desirable, but still largely remains an elusive goal. Inspired by the recent progress on electrophilic C–H activation methods,[7] we have been exploring the coupling reactions of ketones and amines by using cationic ruthenium catalysts.[8] This report delineates a catalytic ketone olefination method that is transpired from the intermolecular dehydrative coupling reaction of arylketones and cyclic alkenes involving vinyl C–H bond activation.



(1)

We devised a convenient method to synthesize a cationic ruthenium-hydride complex from the protonation reaction of

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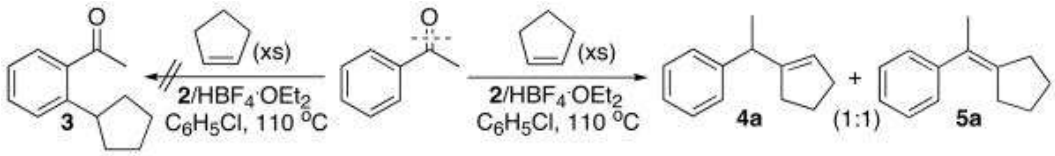
{[(PCy$_3$)(CO)RuH]$_4$(μ$_4$-O)(μ$_3$-OH)(μ$_2$-OH)} (**1**) (Eq 1).[9] Thus, the treatment of **1** (200 mg, 0.12 mmol) with $HBF_4{\cdot}OEt_2$ (64 μL) in C_6H_6 at room temperature cleanly led to the formation of the cationic ruthenium-hydride complex **2**, which was isolated as an ivory-colored solid in 95% yield. The ^{1}H NMR of **2** in CD_2Cl_2 showed the Ru–H signal at δ −10.39 (d, J_{PH} = 25.9 Hz), and a single phosphine peak was observed at δ 72.9 ppm by $^{31}P\{^1H\}$ NMR. The molecular structure of **2** as established from X-ray crystallography showed a three-legged piano stool geometry, which is capped by a η^6-benzene moiety.[10]

Having well-defined cationic ruthenium-hydride complex **2** in hand, we next explored its catalytic activity for the coupling reaction of arylketones and alkenes. We initially anticipated the formation of the *ortho*-C–H insertion product **3**, in light of the reported results on the chelate-directed coupling reaction of arylketones and alkenes.[11] Instead, the treatment of acetophenone with excess cyclopentene in the presence of **2**/$HBF_4{\cdot}OEt_2$ (5 mol %) in C_6H_5Cl cleanly produced a ~1:1 ratio of double bond isomers of the olefination products **4a** and **5a**, without forming any *ortho*-C–H insertion product **3** (Scheme 1).



Scheme 1

The preliminary survey of ruthenium catalysts showed that both *in-situ* formed **1**/$HBF_4{\cdot}OEt_2$ and the isolated catalyst **2**/$HBF_4{\cdot}OEt_2$ exhibited uniquely high activity for the coupling reaction (Table 1). The addition of $HBF_4{\cdot}OEt_2$ was found to be critical for giving the olefination products since the catalyst **2** alone exhibited a modest activity for the *ortho*-C–H insertion products (entries 5, 6).[12] One of the most remarkable feature of the coupling reaction is that a direct ketone olefination has been achieved from the intermolecular dehydrative coupling reaction of arylketones and unactivated alkenes without employing any reactive reagents.

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Table 1. Catalyst Survey for the Coupling Reaction of Acetophenone and Cyclopentene.[a]

entry	catalyst	additive	4a:5a	convn (%)[b]
1	**1**			0
2	**1**	$HBF_4{\cdot}OEt_2$	1:1	50
3	$RuHCl(CO)(PCy_3)_2$			0
4	$RuHCl(CO)(PCy_3)_2$	$HBF_4{\cdot}OEt_2$		6
5	**2**			12[c]
6	**2**	$HBF_4{\cdot}OEt_2$	1:1	60
7	$RuH_2(CO)(PPh_3)_3$	$HBF_4{\cdot}OEt_2$		8
8	$RuCl_2(PPh_3)_3$	$HBF_4{\cdot}OEt_2$		<5
9	$RuCl_3{\cdot}3H_2O$	$HBF_4{\cdot}OEt_2$		0
10	$Ru_3(CO)_{12}$	NH_4PF_6		0
11[d]	$[RuH(CO)(PCy_3)_2(S)_2]^+BF_4^-$	$HBF_4{\cdot}OEt_2$		0
12	$Re(CO)_3(THF)_2Br$	$HBF_4{\cdot}OEt_2$		<5
13	$Au(PPh_3)_3Cl$	$HBF_4{\cdot}OEt_2$		<5
14	$HBF_4{\cdot}OEt_2$			0
15	$Cy_3PH^+BF_4^-$			0

[a]Reaction conditions: acetophenone (0.1 mmol), cyclopentene (2.0 mmol), catalyst (10 mg, 5 mol %), additive (2 equiv to catalyst), C_6H_5Cl (2 mL), 110 °C, 15 h.
[b]Conversion was determined by GC based on acetophenone.
[c]Three different double bond isomers formed from dehydrogenation of **3**.
[d]S = CH_3CN.

The scope of the olefination reaction was explored by using **2**/$HBF_4{\cdot}OEt_2$ catalyst (Table 2). Arylketones with *para*-electron donating group was found to modestly promote the coupling reaction (entries 2, 3), while both terminal and internal olefins such as 1-hexene and 2-hexenes yielded the C–H insertion products **3** under the similar conditions. Both cyclopentene and cyclohexene were found to be suitable substrates, but sterically demanding cyclic alkenes such as cyclooctene and methylcyclopentene as well as trisubstituted olefins yielded <5% of the coupling products. A considerably higher conversion was achieved for naphthyl-substituted ketones (entries 8–11). In most cases, high selectivity for the olefination products of the type **4** and **5** was observed over the *ortho*-C–H insertion product of type **3**, where the formation of a nearly 1:1 ratio of the double bond isomers of **4** and **5** was observed on the crude product mixture. To obtain combined isolated yields, the hydrogenation reaction was performed on the crude product mixture. Thus, the treatment of a product mixture of **4** and **5** with H_2 (2 atm) at 110 °C in the presence of **2**/$HBF_4{\cdot}OEt_2$ (5 mol %) in C_6H_5Cl cleanly led to the olefin-hydrogenated product **6**, which was isolated by a column

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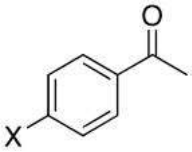
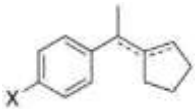
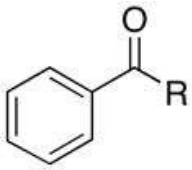
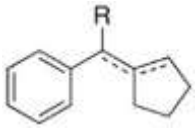
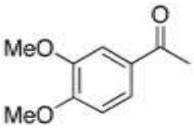
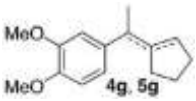
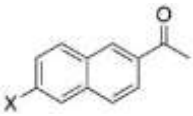
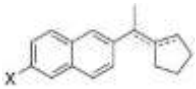
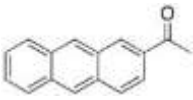
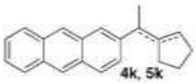
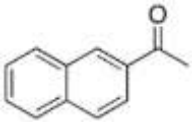
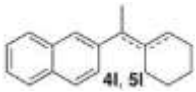
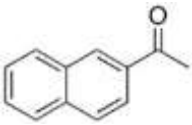
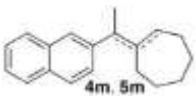
chromatography on silica gel. The isolated yield of **6** is listed in Table 1.

Table 2. Coupling Reaction of Arylketones and Cyclic Alkenes.[a]

entry	ketone	alkene	products		convn (%)[b]	yd (%)[c]
1				X = H (**4a**, **5a**)	60	52
2				X = Me (**4b**, **5b**)	65	55
3				X = OMe (**4c**, **5c**)	70	65
4				X = Cl (**4d**, **5d**)	36	30
5				R = Et (**4e**, **5e**)	42	34
6[d]				R = CH_2Ph (**4f**, **5f**)	30	23
7					53	45
8				X = H (**4h**, **5h**)	92	84
9				X = Me (**4i**, **5i**)	84	75
10				X = OMe (**4j**, **5j**)	97	86
11					92	84
12[e,f]					50	40[g]
13[e]					26	19

[a]Reaction conditions: ketone (0.7 mmol), alkene (14 mmol), **2** (20 mg, 5 mol %), $HBF_4{\cdot}OEt_2$ (10 μL, 2 equiv), C_6H_5Cl (2 mL), 110 °C, 15 h.
[b]Determined by GC based on ketone.
[c]Combined isolated yield of **4** and **5** determined from the hydrogenation product 6.
[d]Contained 28% of $PhCH_2CH_2Ph$.
[e]A 4:1 ratio of **4l** and **5l** was formed in the crude product mixture.
[f]10 mol % of **2** was used.
[g]A ~10% of *ortho*-C–H insertion product type **3** was also formed.

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The following experiments were performed to gain mechanistic insights on the olefination reaction. First, the deuterium-labeling pattern was examined from the treatment of acetophenone-d_8 (90 mg, 0.7 mmol) with excess cyclopentene (0.95 g, 14 mmol) and **2**/$HBF_4{\cdot}OEt_2$ (5 mol %). Extensive H/D exchange was found to occur on the methyl group of both **4a** and **5a** as well as on cyclopentene, without significant exchange on the ortho positions of the phenyl group as examined by ^1H and ^2H NMR.[12] The coupling reaction of acetophenone with a 1:1 mixture of 1-hexene and cyclopentene under the competitive conditions yielded the olefination products **4a** and **5a** predominantly over the C–H insertion product type **3** (**4a+5a:3** = 11:1). These results indicate that the vinyl C–H activation is rapid and reversible and that this step is favored over the arene *ortho*-C–H activation for cyclopentene case.

To discern the nature of catalytically relevant species, the reaction of **2** with cyclopentene was monitored by NMR. The treatment of **2** (20 mg, 35 μmol) with excess cyclopentene (24 mg, 10 equiv) in CD_2Cl_2 slowly formed a new cationic complex $[CpRu(CO)(PCy_3)(c\text{-}C_5H_8)]^+BF_4^-$ (**7**) within 3 h at 100 °C, along with $Cy_3PH^+BF_4^-$, free benzene and cyclopentane. The structure of **7** was tentatively assigned on the basis of NMR spectroscopic data. Trapping of **7** with PhCN resulted in a stable nitrile complex $[CpRu(CO)(PCy_3)(NCPh)]^+BF_4^-$ (**8**) (Scheme 2).[12] The formation of cyclopentadienyl complex **8** can be readily rationalized from the dehydrogenation of cyclopentene and the elimination of cyclopentane.

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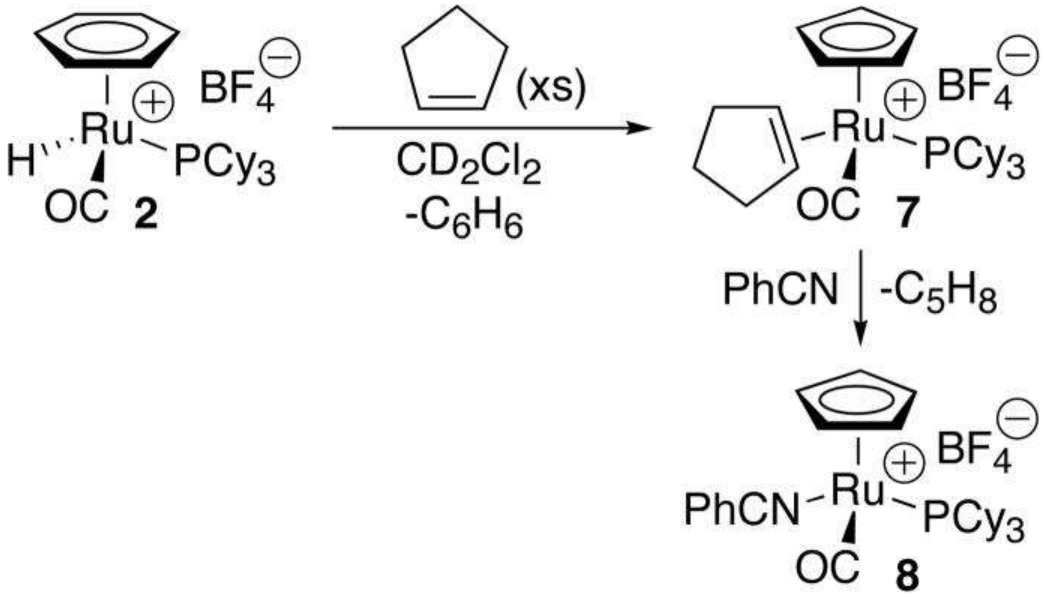

Scheme 2

Though details of the coupling reaction still remain to be established, we propose a mechanistic rationale that invokes both olefinic C–H bond activation and the dehydrative carbonyl olefination steps (Scheme 3). We propose that the electrophilic Ru-vinyl complex **9**, initially generated from the vinyl C–H activation of cycloalkene, is the key species for the coupling reaction. The dative coordination of ketone substrate followed by the alkenyl group migration to the electrophilic carbonyl carbon would yield the alcohol product after transfer of a hydrogen obtained from vinyl C–H activation of a coordinated alkene to the alkoxide ligand. While the formation of metal-vinyl species has been well documented in the C–H bond activation literature,[13] its synthetic utility has not been fully exploited in catalytic coupling reactions. The detailed mechanistic steps for the formation of the olefin products **4** and **5** from the alcohol are not clear at the present time, but it can be envisaged from an acid catalyzed reductive dehydration of the alcohol, in light of the well-known alcohol dehydration reactions.

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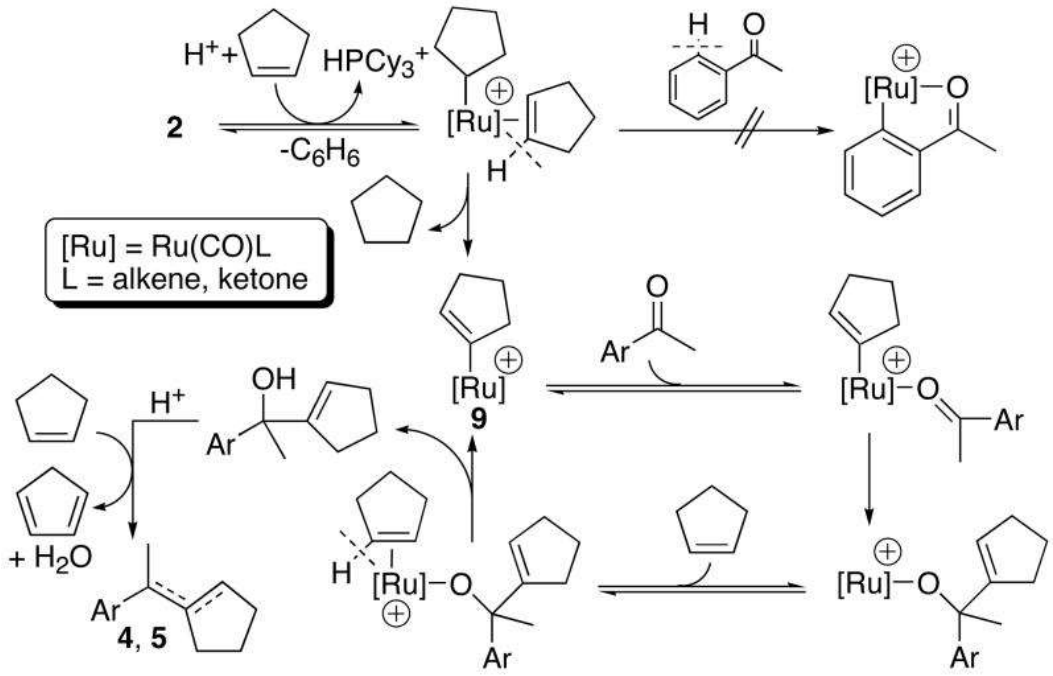

Scheme 3. A Mechanistic Rationale for the Ketone Olefination.

In summary, a novel catalytic ketone olefination method has been developed from the intermolecular coupling reaction of arylketones with cyclic alkenes. Electrophilic nature of the ruthenium catalyst **2** seems to be an essential feature for mediating both vinyl C–H bond activation and the subsequent dehydrative coupling steps of the reaction. The scope and synthetic efficacy of the catalytic method are currently being investigated.

Acknowledgments

Financial support from the National Institute of Health, General Medical Sciences (R15 GM55987) is gratefully acknowledged.

Footnotes

Supporting Information Available: Experimental procedures, spectroscopic data of organic products and X-ray crystallographic data of **2** (49 pages, print/PDF). This material is available free of charge via the Internet at http://pubs.acs.org.

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[12] See Supporting Information for the experimental details.

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Supplementary Material

Supporting Information

Intermolecular Dehydrative Coupling Reaction of Arylketones with Cyclic Alkenes Catalyzed by a Well-Defined Cationic Ruthenium-Hydride Complex: A Novel Ketone Olefination Method via Vinyl C-H Bond Activation

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General Information. All operations were carried out in an inert-atmosphere glove box or by using standard high vacuum and Schlenk techniques unless otherwise noted. Benzene, chlorobenzene, hexanes 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 substrates were received from commercial sources and used without further purification. The ^1H, ^2H, ^{13}C and ^{31}P NMR spectra were recorded on a Varian 300 or 400 MHz FT-NMR spectrometer. Mass spectra were recorded from a Agilent 6850 GC/MS spectrometer. The conversion of organic products was measured from a Hewlett-Packard HP 6890 GC spectrometer. Elemental analysis was performed at the Midwest Microlab, Indianapolis, IN.

Synthesis of $[(\eta^6\text{-}C_6H_6)RuH(CO)(PCy_3)]^+BF_4^-$ (2). In a glove box, complex **1** (200 mg, 0.12 mmol) was dissolved in benzene (10 mL) in a 25 mL Schlenk tube equipped with a Teflon screw-cap stopcock and a magnetic stirring bar. The tube was brought out of the box, and $HBF_4{\cdot}OEt_2$ (64 μL, 0.48 mmol) was added via syringe under N_2 stream. The color of the solution was changed from dark red to pale yellow immediately. After stirring for 1 h at room temperature, the solvent was removed under vacuum, and the residue was crashed by adding hexanes (10 mL). Filtering the resulting solid through a fritted funnel and recrystallization from CH_2Cl_2/hexanes yielded the product as a pale yellow powder (262 mg, 95% yield). Single crystals of **2** suitable for X-ray crystallography were obtained from a slow evaporation of benzene and hexanes solution.

For **2**: ^1H NMR (CD_2Cl_2, 400 MHz) δ 6.53 (s, C_6H_6), 2.0-1.2 (m, PCy_3), -10.39 (d, J_{PH} = 25.9 Hz, Ru-H); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 100 MHz), δ 196.4 (d, J_{CP} = 19.3 Hz, CO), 100.0 (C_6H_6), 38.4, 38.2, 30.2, 29.9, 27.4, 27.3 and 26.2 (PCy_3); $^{31}P\{^1H\}$ NMR (CD_2Cl_2, 162 MHz) δ 72.9 (PCy_3); IR (KBr) ν_{CO} = 1991 cm^{-1}; Anal. Calcd for

$C_{25}H_{40}BF_4OPRu$: C, 52.18; H, 7.01. Found: C, 51.73; H, 6.91.

NMR Formation of $[(\eta^5\text{-}C_5H_5)Ru(CO)(PCy_3)(c\text{-}C_5H_8)]^+BF_4^-$ (7). In a glove box, complex **2** (20 mg, 35 μmol) and cyclopentene (24 mg, 10 equiv) were charged in CD_2Cl_2 (0.5 mL) in a J-Young NMR tube. The tube was brought out of the box, and was immersed in an oil bath set at 100 °C for 3 h. The formation of both free benzene (δ 7.38) and cyclopentane (δ 1.55) was also detected by ^{1}H NMR, while $Cy_3PH^+BF_4^-$ (δ 29.2) was detected by ^{31}P NMR. Both NMR and IR spectroscopic data were recorded at room temperature.

Selected spectroscopic data of **7**: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.39 (s, C_5H_5), 4.71 (m, =CH), 4.48 (t, J = 4.0 Hz, =CH); $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2) δ 206.3 (d, J_{CP} = 17.5 Hz, CO), 132.7 and 121.9 (=CH), 89.5 (C_5H_5); $^{31}P\{^1H\}$ NMR (162 MHz, CD_2Cl_2) δ 50.1 (s, PCy_3); IR (CD_2Cl_2) ν_{CO} = 1993 cm^{-1}.

Synthesis of $[(\eta^5\text{-}C_5H_5)Ru(CO)(PCy_3)(NCPh)]^+BF_4^-$ (8). In a glove box, complex **2** (0.20 mg, 0.35 mmol) and cyclopentene (0.48 g, 20 equiv) were charged in CH_2Cl_2 (3 mL) in a 25 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar. The tube was brought out of the box, and was stirred in an oil bath which was preset at 110 °C for 3 h. The reaction tube was immersed in a dry ice/acetone bath, and benzonitrile (0.18 g, 1.75 mmol, 5 equiv) was added via microsyringe to the reaction tube. After stirring for 1 h at room temperature, the solvent was removed under vacuum. *n*-Hexanes was added to the residue. The resulting solid was filtered through a fritted funnel, and washed it with hexanes (10-15 mL). Recrystallization from CH_2Cl_2/*n*-hexanes gave the complex **8** as an air-sensitive pale brown solid in 55 % yield (0.13 g; contained ~30 % of $Cy_3PH^+BF_4^-$).

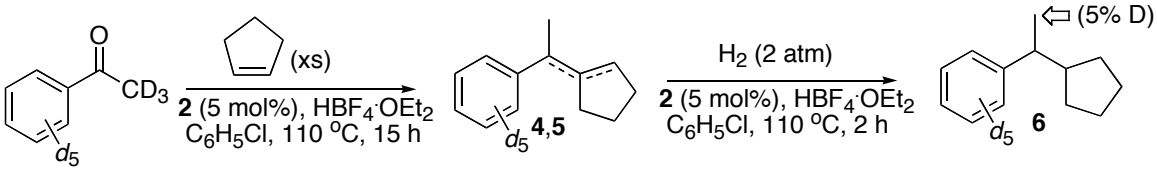
Selected spectroscopic data of **8**: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.6 (m, 5H, PhCN), 5.39 (s, C_5H_5), 2.2–1.2 (m, PCy_3); $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) δ 200.4 (d, J_{CP} = 1.4 Hz, CO), 196.8 (PhCN), 85.8 (C_5H_5); $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) δ 58.2 (s, PCy_3); IR (CH_2Cl_2) ν_{CO} = 1982, ν_{CN} = 2022 cm^{-1}.

Representative Procedure of the Catalytic Reaction. In a glove box, complex **2** (20 mg, 35 μmol), an arylketone (0.7 mmol) and an alkene (14 mmol) were dissolved in chlorobenzene (2 mL) in a 10 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar. The tube was brought out of the box, and $HBF_4{\cdot}OEt_2$ (10 μL, 70 μmol) was added to the reaction tube under a stream of N_2 gas. The tube was fully immersed in an oil bath set at 110 °C, and was stirred for 15 h. After the tube was cooled to room temperature, the solution was filtered through a short silica plug (hexanes/EtOAc = 2:1) in air, and the filtrate was analyzed by GC. To obtain the combined isolated yields, the product mixture **4** and **5** was subjected to the hydrogenation reaction. The treatment of the crude mixture with H_2 (2 atm) in the presence of **2** (20 mg, 5 mol %) at 110 °C for 2 h led to the clean formation of the hydrogenated product **6**. Analytically pure organic product **6** was obtained after a column chromatography on silica gel (hexanes/EtOAc).

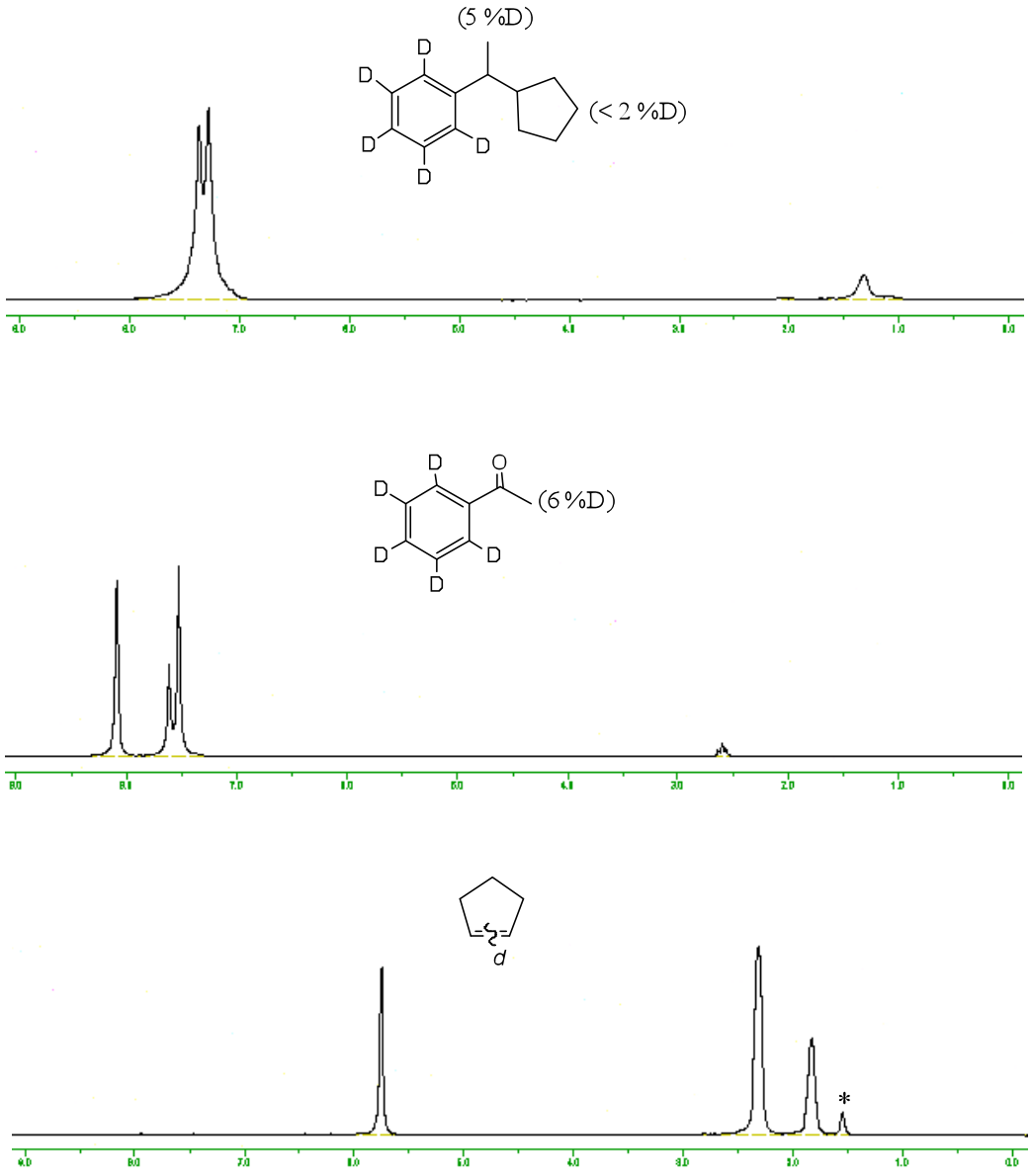
Deuterium Labeling Study. In a glove box, complex **2** (20 mg, 35 μmol), acetophenone-d_8 (89 mg, 0.70 mmol) and cyclopentene (0.94 g, 14 mmol) were dissolved in chlorobenzene (2 mL) in a 10 mL Schlenk tube equipped with a Teflon screw cap stopcock and a magnetic stirring bar. The tube was brought out of the box, and $HBF_4{\cdot}OEt_2$ (10 μL, 70 μmol) was added to the reaction tube via syringe under a stream of N_2 gas. The tube was fully immersed in an oil bath set at 110 °C, and was stirred for 15 h. After the tube was allowed to cool to room temperature, it was open to air and filtered through a small silica gel column (hexanes/EtOAc = 2:1). The filtrate was analyzed by

GC to determine the product conversion. Both unreacted cyclopentene-d_n and cyclopentane-d_n were collected separately via vacuum transfer. The products (**4a**-d_n, **5a**-d_n, after hydrogenation **6a**-d_n) and unreacted acetophenone-d_n were separated by column chromatography on silica gel (hexanes/EtOAc), and each was analyzed by both ^{1}H and ^{2}H NMR (Figure S1).

Figure S1. ^{2}H NMR Spectra of the Coupling Reaction of Acetophenone-d_8 and Cyclopentene.



^{2}H NMR (61 MHz, CH_2Cl_2)



* denotes cyclopentane.

Characterization Data of Organic Products

For **6a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.4-7.2 (m, 5H, Ar), 2.50 (dq, *J* = 9.4, 6.9 Hz, C*H*CH_3), 2.0 (m, CH_2C*H*CH_2), 1.8-1.0 (m, 8H, CH_2), 1.32 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 148.0, 127.6, 126.8 and 125.2 (Ar), 47.8 (*C*HCH_3), 46.3 (CH_2*C*H*C*H_2), 32.0, 31.6, 25.6 and 25.3 (CH_2), 21.7 (CH*C*H_3); GC-MS *m/z* = 174 (M^+).

For **6b**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (s, 4H, Ar), 2.49 (dq, *J* = 9.5, 6.9 Hz, C*H*CH_3), 2.41 (s, ArC*H*$_3$), 2.00 (m, CH_2C*H*CH_2), 1.8-1.0 (m, 8H, CH_2), 1.33 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 145.2, 135.2, 129.0 and 127.4 (Ar), 47.8 (*C*HCH_3), 46.0 (CH_2*C*HCH_2), 32.0, 31.7, 25.6 and 25.3 (CH_2), 27.8 (Ar*C*H_3), 21.2 (CH*C*H_3); GC-MS *m/z* = 188 (M^+).

For **6c**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 and 6.84 (d, *J* = 8.7 Hz, 4H, Ar), 3.80 (s, OCH_3), 2.40 (dq, *J* = 9.4, 6.9 Hz, C*H*CH_3), 1.9 (m, CH_2C*H*CH_2), 1.7-1.0 (m, 8H, CH_2), 1.24 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.7, 140.4, 128.3 and 113.7 (Ar), 55.4 (OCH_3), 50.0 (*C*HCH_3), 45.5 (CH_2*C*HCH_2), 32.0, 31.6, 25.6 and 25.3 (CH_2), 21.8 (CH*C*H_3); GC-MS *m/z* = 204 (M^+).

For **6d**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26, 7.12 (d, *J* = 8.4 Hz, 4H, Ar), 2.43 (dq, *J* = 9.4, 6.9 Hz, C*H*CH_3), 1.9 (m, CH_2C*H*CH_2), 1.7-1.0 (m, 8H, CH_2), 1.25 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 146.6, 128.8, 128.4 and 128.2 (Ar), 47.7 (*C*HCH_3), 45.8 (CH_2*C*HCH_2), 31.9, 31.6, 25.5 and 25.3 (CH_2), 21.6 (CH*C*H_3); GC-MS *m/z* = 208 (M^+).

For **6e**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.3-7.1 (m, Ar), 2.17 (dt, *J* = 3.5, 10.2 Hz, C*H*CH_2CH_3), 2.0 (m, CH_2C*H*CH_2), 1.9-0.9 (m, 8H, CH_2), 1.54 (t, *J* = 7.4 Hz, C*H*$_2$CH$_3$),

0.70 (t, J = 7.4 Hz, CH_2CH_3); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 145.9, 128.4, 128.2 and 125.8 (Ar), 54.4 ($CHCH_2CH_3$), 46.7 (CH_2CHCH_2), 32.0, 31.8, 25.5 and 25.1 (CH_2), 28.2 (CH_2CH_3), 12.4 (CH_2CH_3); GC-MS m/z = 188 (M^+).

For **6f**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.4-6.9 (m, 10H, Ar), 3.20-2.84 (m, CH_2Ar), 2.63 (td, J = 9.9, 4.2 Hz, CHAr), 2.2 (m, CH_2CHCH_2), 2.1-1.0 (m, 8H, CH_2); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 144.8, 141.1, 129.3, 128.6, 128.0, 125.9 and 125.7 (Ar), 54.8 ($CHAr$), 46.0 (CH_2CHCH_2), 42.4 (CH_2Ar), 32.1, 31.8, 25.6 and 25.2 (CH_2); GC-MS m/z = 250 (M^+).

For **6g**: ^1H NMR (400 MHz, $CDCl_3$) δ 6.8-6.7 (m, 3H, Ar), 3.87 and 3.84 (s, OCH_3), 2.36 (dq, J = 9.4, 6.9 Hz, $CHCH_3$), 1.9 (m, CH_2CHCH_2), 1.7-1.0 (m, 8H, CH_2), 1.23 (d, J = 6.9 Hz, $CHCH_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 148.6, 146.9, 140.8, 119.0, 110.9 and 110.5 (Ar), 55.8 and 55.7 (OCH_3), 47.8 ($CHCH_3$), 45.8 (CH_2CHCH_2), 31.8, 31.5, 25.4 and 25.1 (CH_2), 21.6 ($CHCH_3$); GC-MS m/z = 234 (M^+); Anal. Calcd for $C_{15}H_{22}O_2$: C, 76.88; H, 9.46. Found: C, 77.08; H, 9.18.

For **6h**: ^1H NMR (400 MHz, $CDCl_3$) δ 8.0-7.5 (m, 7H, Ar), 2.73 (dq, J = 9.8, 6.9 Hz, $CHCH_3$), 2.2 (m, CH_2CHCH_2), 2.1-1.1 (m, 8H, CH_2), 1.48 (d, J = 6.9 Hz, 3H, $CHCH_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 145.7, 133.8, 132.3, 127.8, 127.7, 126.2, 125.9, 125.6 and 125.1 (Ar), 47.6 ($CHCH_3$), 46.6 (CH_2CHCH_2), 32.1, 31.7, 25.6 and 25.4 (CH_2), 21.7 ($CHCH_3$); GC-MS m/z = 224 (M^+); Anal. Calcd for $C_{17}H_{20}$: C, 91.01; H, 8.99. Found: C, 90.91; H, 9.09.

For **6i**: ^1H NMR (400 MHz, $CDCl_3$) δ 7.8-7.4 (m, 6H, Ar), 2.64 (dq, J = 9.7, 6.9 Hz, $CHCH_3$), 2.57 (s, $ArCH_3$), 2.1 (m, CH_2CHCH_2), 2.1-0.9 (m, 8H, CH_2), 1.40 (d, J = 6.9 Hz, $CHCH_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 144.8, 134.6, 132.5, 132.0, 128.2,

127.5, 127.2, 126.7, 126.3 and 125.4 (Ar), 47.7 (*C*HCH$_3$), 46.5 (CH$_2$*C*HCH$_2$), 32.1, 31.7, 25.6 and 25.4 (CH$_2$), 21.8 and 21.7 (CH$_3$); GC-MS *m/z* = 238 (M$^+$); Anal. Calcd for $C_{18}H_{22}$: C, 90.70; H, 9.30. Found: C, 90.49; H, 9.12.

For **6j**: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.7-7.2 (m, 6H, Ar), 3.93 (s, OCH$_3$), 2.59 (dq, *J* = 9.6, 6.9 Hz, C*H*CH$_3$), 2.1 (m, CH$_2$C*H*CH$_2$), 2.0-1.0 (m, 8H, CH$_2$), 1.36 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 157.2, 143.5, 133.2, 129.2, 126.8, 125.5, 118.7 and 105.8 (Ar), 55.5 (OCH$_3$), 47.7 (*C*HCH$_3$), 46.3 (CH$_2$*C*HCH$_2$), 32.1, 31.7, 25.6 and 25.3 (CH$_2$), 21.8 (CH$_3$); GC-MS *m/z* = 254 (M$^+$); Anal. Calcd for $C_{18}H_{22}O$: C, 84.99; H, 8.72. Found: C, 85.01; H, 8.59.

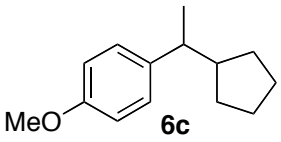
For **6k**: ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.4-7.4 (m, 9H, Ar), 2.65 (dq, *J* = 9.7, 6.9 Hz, C*H*CH$_3$), 2.1 (m, CH$_2$C*H*CH$_2$), 2.0-1.1 (m, 8H, CH$_2$), 1.38 (d, *J* = 6.9 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 145.0, 132.2, 132.0, 131.4, 131.0, 128.4, 128.2, 126.3, 126.0, 125.7, 125.3, 125.2 and 125.1 (Ar), 47.4 (*C*HCH$_3$), 46.7 (CH$_2$*C*HCH$_2$), 32.1, 31.7, 25.6 and 25.4 (CH$_2$), 21.4 (CH$_3$); GC-MS *m/z* = 274 (M$^+$); Anal. Calcd for $C_{21}H_{22}$: C, 91.92; H, 8.08. Found: C, 91.56; H, 8.09.

For **6l**: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.8-7.4 (m, 7H, Ar), 2.65 (quintet, *J* = 7.4 Hz, C*H*CH$_3$), 2.0-0.8 (m, cyclohexyl), 1.35 (d, *J* = 7.4 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 144.9, 133.8, 132.4, 127.8, 126.7, 126.2, 126.0 and 125.2 (Ar), 46.4 (*C*HCH$_3$), 44.4 (CH$_2$*C*HCH$_2$), 31.9, 30.9 and 26.8 (CH$_2$), 19.1 (CH$_3$); GC-MS *m/z* = 238 (M$^+$); Anal. Calcd for $C_{18}H_{22}$: C, 90.70; H, 9.30. Found: C, 90.51; H, 9.12.

For **6m**: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.8-7.4 (m, 7H, Ar), 2.81 (quintet, *J* = 7.0 Hz, C*H*CH$_3$), 1.9-1.2 (m, cycloheptyl), 1.35 (d, *J* = 7.0 Hz, CHC*H*$_3$); ^{13}C{^{1}H} NMR (100 MHz, CDCl$_3$) δ 145.1, 133.7, 132.2, 127.7, 126.9, 126.0, 125.9 and 125.2 (Ar), 46.1

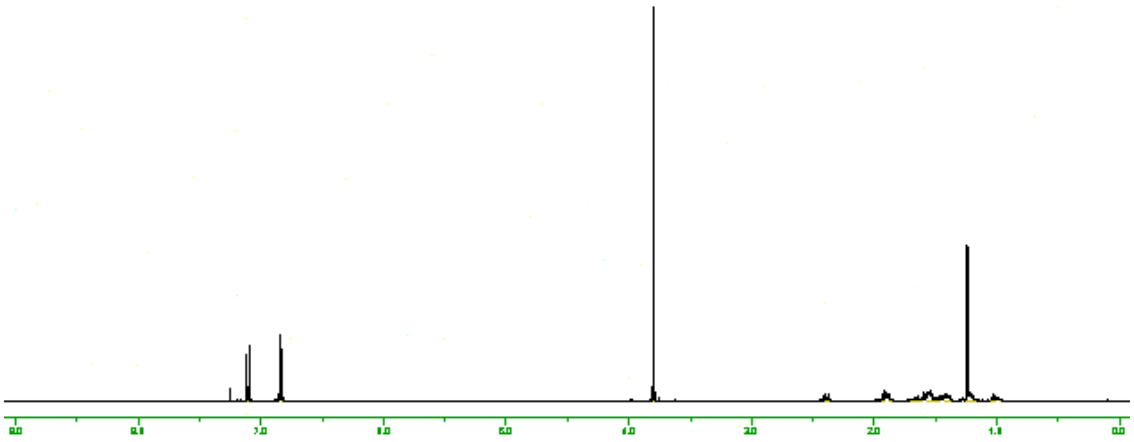
(*C*HCH$_3$), 45.6 (CH$_2$*C*HCH$_2$), 33.0, 31.3, 28.7, 28.5, 27.0 and 26.8 (CH$_2$), 18.6 (CH$_3$); GC-MS *m/z* = 252 (M^+); Anal. Calcd for $C_{19}H_{24}$: C, 90.42; H, 9.58. Found: C, 90.45; H, 9.55.

The ^{1}H and ^{13}C NMR Spectra of Selected Organic Products

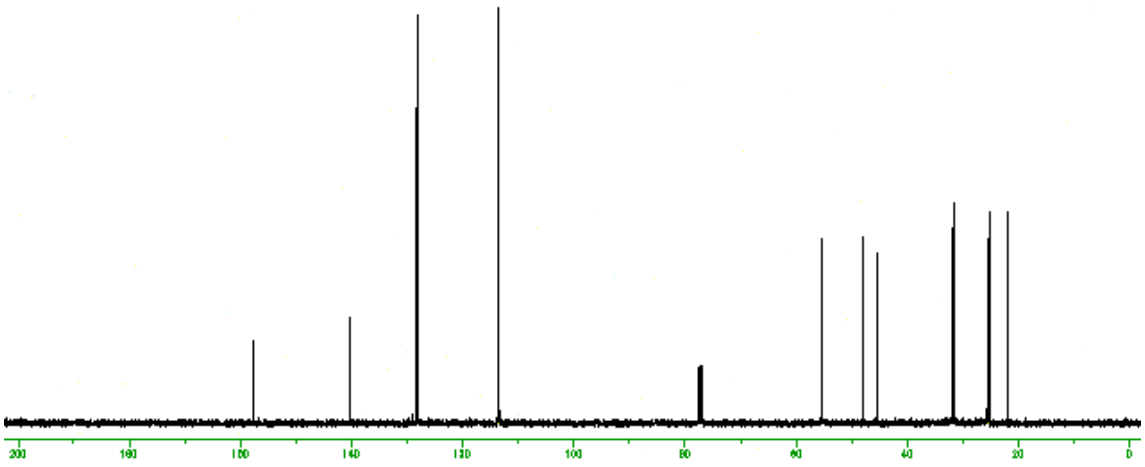


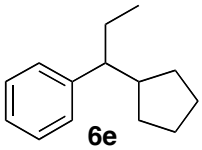
6c

^{1}H NMR (400 MHz, $CDCl_3$)



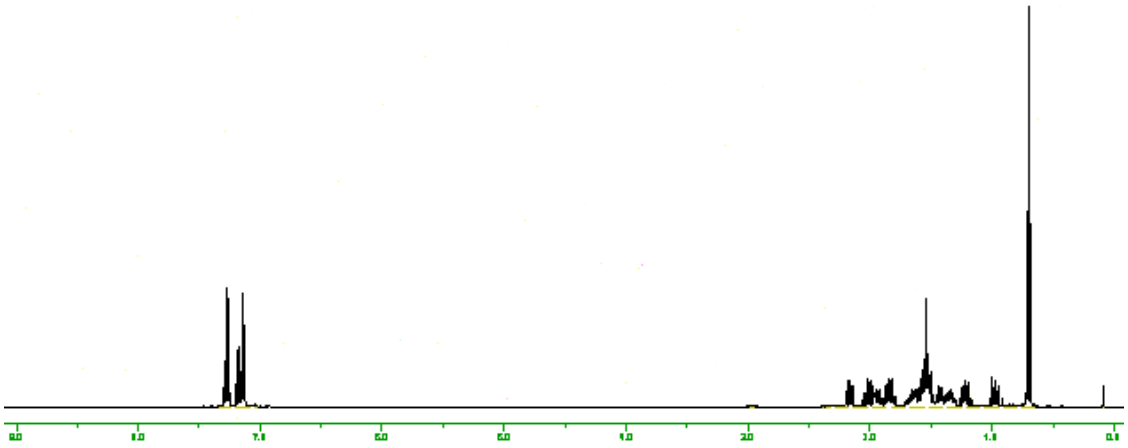
$^{13}C\{^{1}H$ NMR$\}$ (100 MHz, $CDCl_3$)



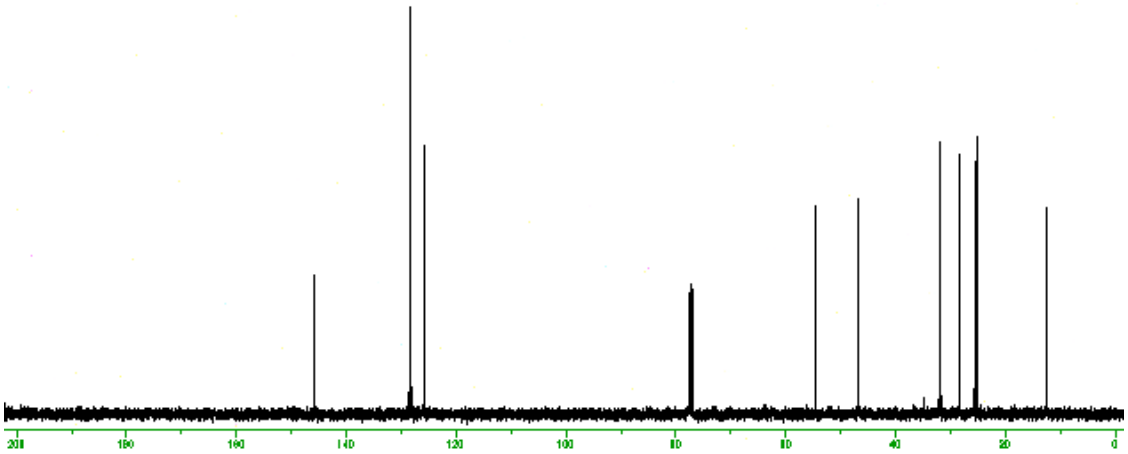


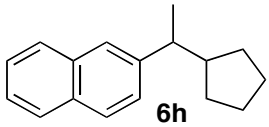
6e

^{1}H NMR (400 MHz, $CDCl_3$)



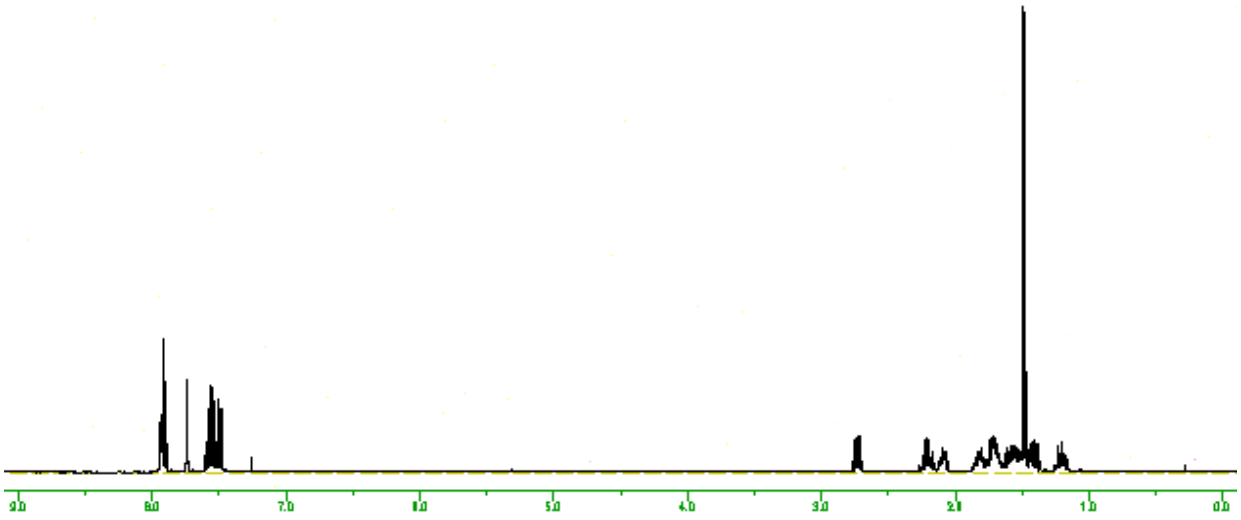
^{13}C{^{1}H NMR} (100 MHz, $CDCl_3$)



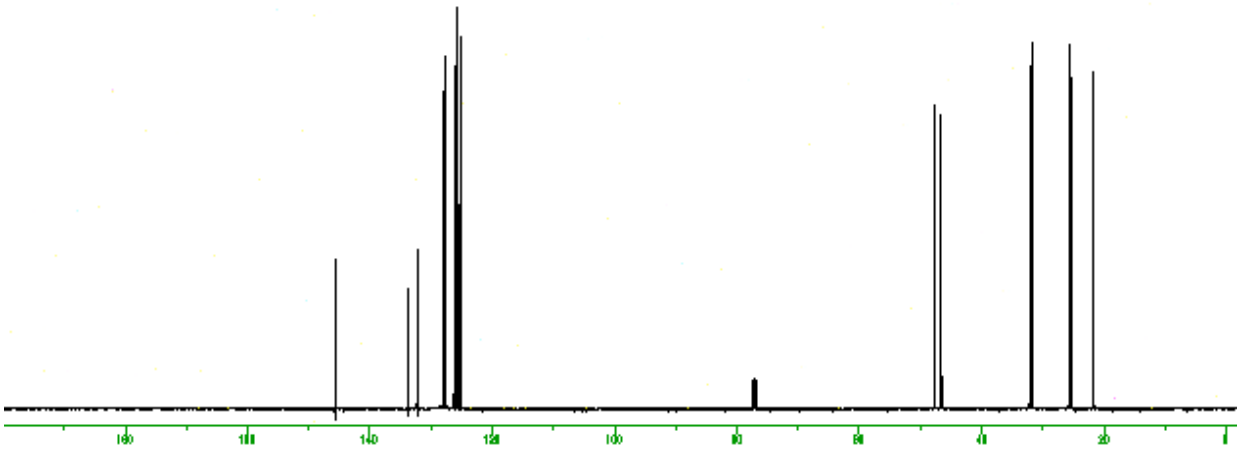


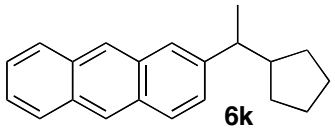
6h

^{1}H NMR (400 MHz, $CDCl_3$)



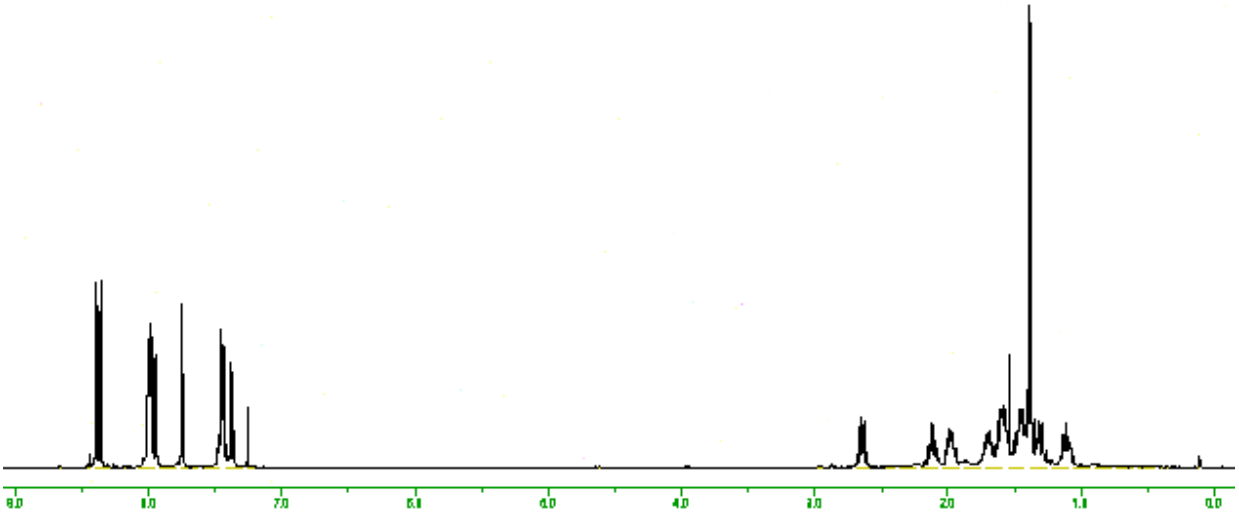
^{13}C{^{1}H NMR} (100 MHz, $CDCl_3$)



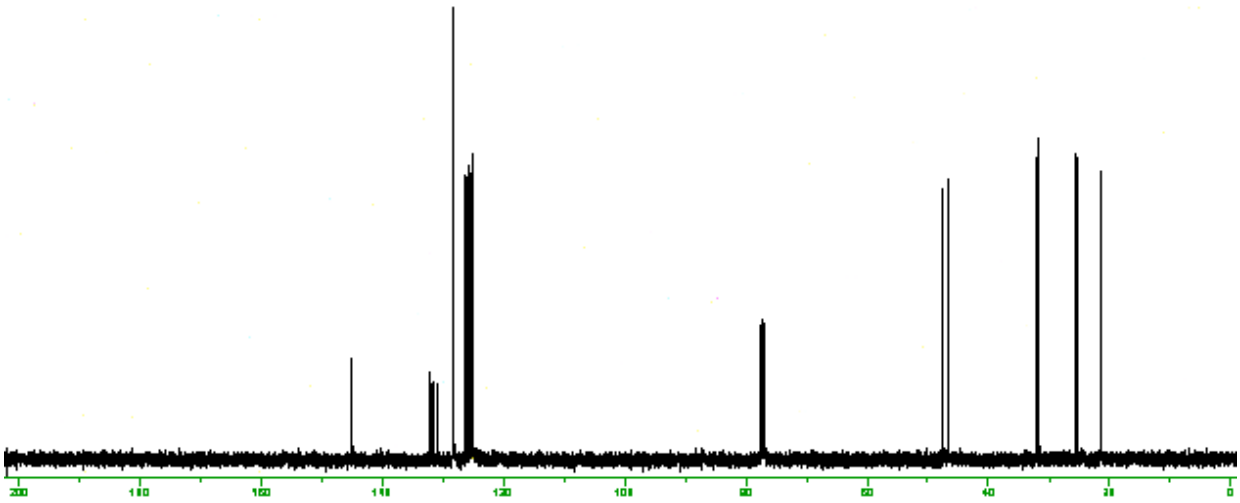


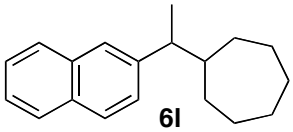
6k

^{1}H NMR (400 MHz, $CDCl_3$)



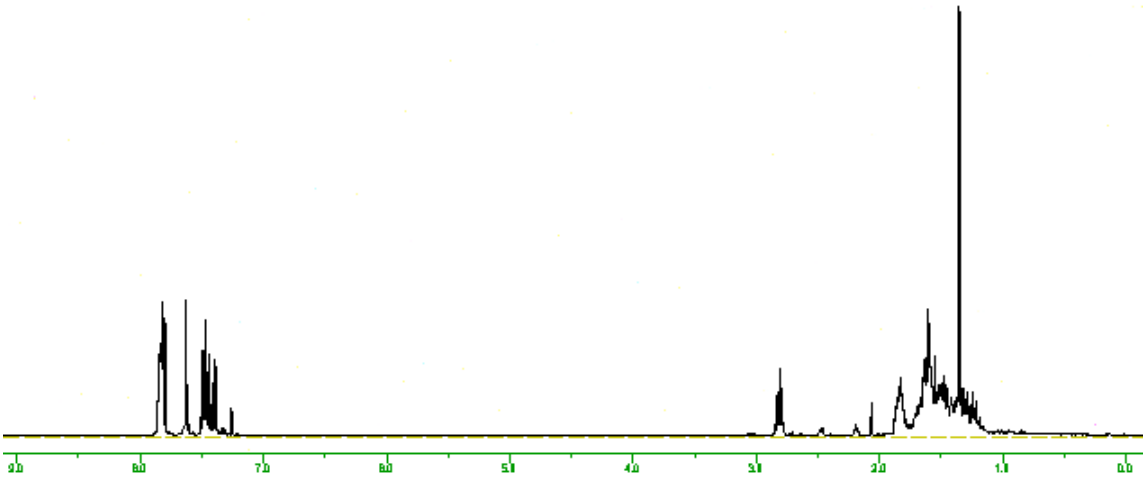
^{13}C{^{1}H NMR} (100 MHz, $CDCl_3$)



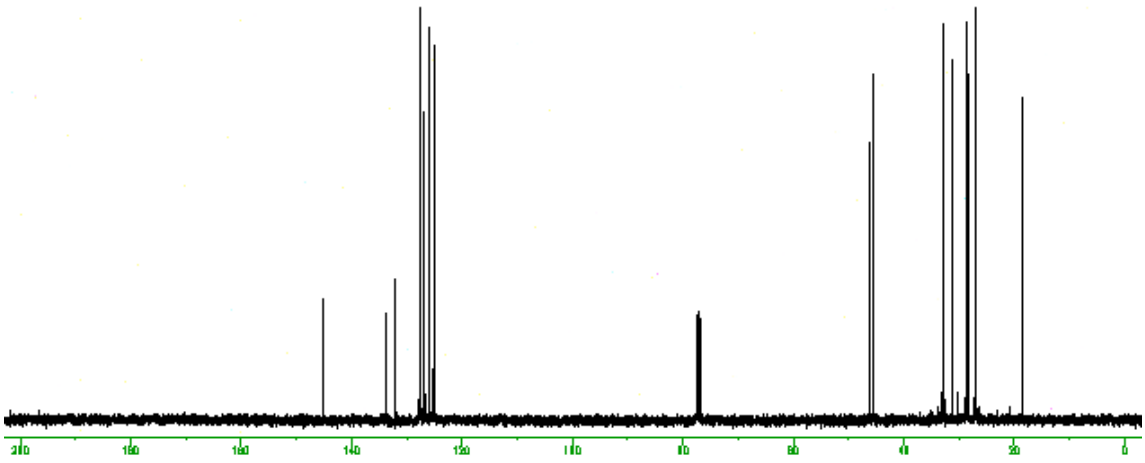


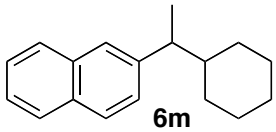
6l

^{1}H NMR (400 MHz, $CDCl_3$)



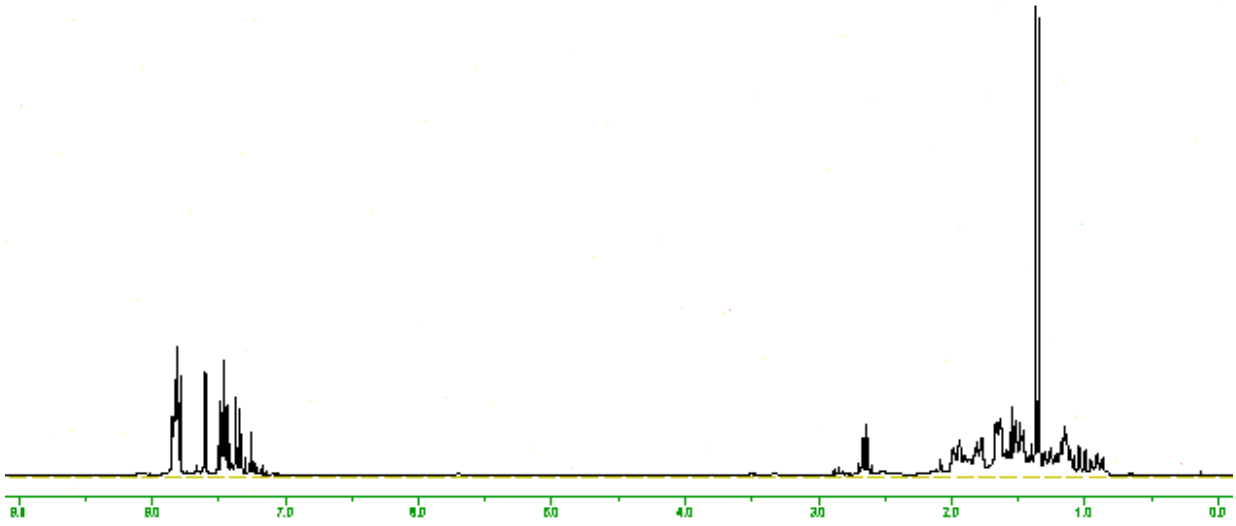
^{13}C{^{1}H NMR} (100 MHz, $CDCl_3$)





6m

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{^{1}H NMR} (100 MHz, $CDCl_3$)

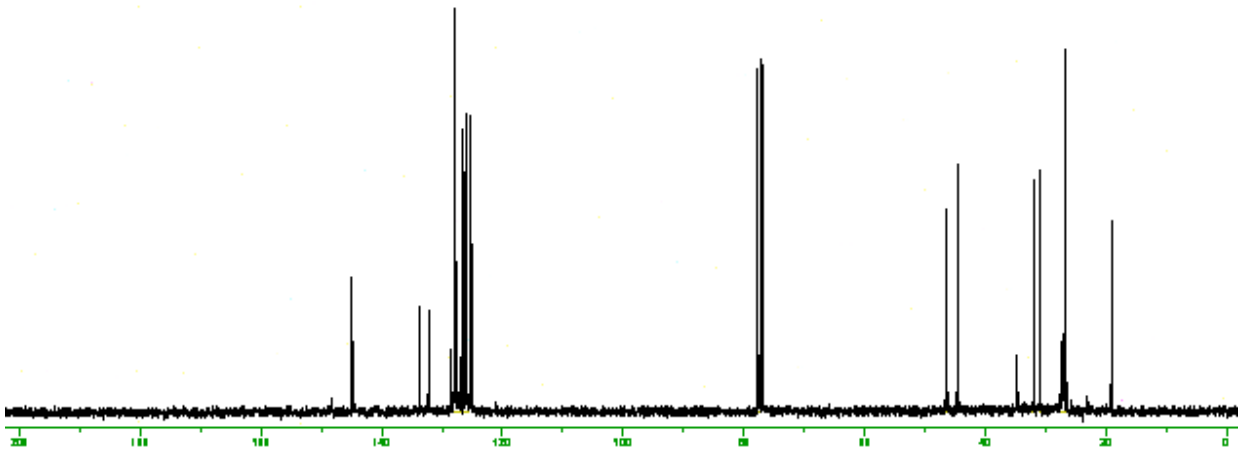


Table S2. Crystal data and structure refinement for **2**.

Identification code	yi1d5	
Empirical formula	C25 H40 B F4 O P Ru	
Formula weight	575.42	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.2618(7) Å	α = 110.465(2)°.
	b = 14.8597(8) Å	β = 97.596(2)°.
	c = 15.2625(9) Å	γ = 92.709(2)°.
Volume	2569.4(3) $Å^3$	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	5.914 mm^{-1}	
F(000)	1192	
Crystal size	0.13 x 0.07 x 0.05 mm^3	
Theta range for data collection	3.13 to 67.89°.	
Index ranges	-14<=h<=14, -17<=k<=16, 0<=l<=18	
Reflections collected	25850	
Independent reflections	8559 [R(int) = 0.0392]	
Completeness to theta = 67.89°	91.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7564 and 0.5136	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8559 / 0 / 640	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.1010	
R indices (all data)	R1 = 0.0483, wR2 = 0.1062	
Largest diff. peak and hole	1.573 and -0.609 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Ru(1)	798(1)	785(1)	-1646(1)	27(1)
P(1)	1006(1)	2391(1)	-1510(1)	26(1)
O(1)	1586(3)	1362(3)	436(3)	39(1)
C(1)	502(5)	-402(4)	-3133(4)	32(1)
C(2)	732(4)	-828(4)	-2438(4)	33(1)
C(3)	57(4)	-686(3)	-1735(4)	32(1)
C(4)	-826(5)	-111(4)	-1705(4)	36(1)
C(5)	-1028(4)	326(4)	-2373(4)	36(1)
C(6)	-363(5)	168(4)	-3095(4)	36(1)
C(7)	1314(4)	1172(4)	-349(4)	31(1)
C(11)	27(4)	3169(4)	-833(4)	30(1)
C(12)	-55(5)	3053(4)	122(4)	34(1)
C(13)	-712(5)	3847(4)	708(4)	41(1)
C(14)	-1856(5)	3813(4)	173(4)	43(1)
C(15)	-1824(5)	3815(4)	-817(4)	39(1)
C(16)	-1150(4)	3033(4)	-1374(4)	38(1)
C(21)	713(4)	2495(3)	-2688(3)	29(1)
C(22)	688(5)	3527(4)	-2700(4)	34(1)
C(23)	188(5)	3483(4)	-3690(4)	36(1)
C(24)	846(5)	2901(4)	-4436(4)	36(1)
C(25)	954(4)	1889(4)	-4403(4)	33(1)
C(26)	1437(4)	1943(4)	-3409(3)	31(1)
C(31)	2388(4)	3095(4)	-957(4)	29(1)
C(32)	2588(4)	3579(4)	125(4)	35(1)
C(33)	4474(4)	3203(4)	-921(4)	37(1)
C(34)	4666(5)	3694(4)	142(4)	38(1)
C(35)	3682(4)	4235(4)	478(4)	36(1)
C(36)	3378(4)	2531(4)	-1284(4)	32(1)
B(1)	2707(6)	-1368(5)	-486(4)	44(2)
F(1)	3533(3)	-1921(3)	-370(2)	57(1)
F(2)	2117(4)	-1819(3)	-1377(3)	92(2)

F(3)	2042(3)	-1298(3)	184(3)	72(1)
F(4)	3159(5)	-465(3)	-361(3)	86(2)
Ru(2)	4495(1)	895(1)	2358(1)	27(1)
P(2)	4528(1)	2472(1)	3397(1)	26(1)
O(1A)	3983(3)	1617(3)	761(2)	36(1)
C(1A)	5206(5)	169(4)	3391(4)	32(1)
C(2A)	4321(5)	-442(4)	2789(4)	32(1)
C(3A)	4299(5)	-740(4)	1797(4)	35(1)
C(4A)	5181(5)	-433(4)	1454(4)	33(1)
C(5A)	6106(5)	163(4)	2071(4)	38(1)
C(6A)	6109(5)	482(4)	3042(4)	35(1)
C(7A)	4184(4)	1362(4)	1377(3)	29(1)
C(11A)	3278(4)	3064(3)	3138(4)	30(1)
C(12A)	3348(5)	4165(4)	3654(4)	42(1)
C(13A)	2370(5)	4582(4)	3249(5)	46(1)
C(14A)	1267(5)	4110(4)	3311(4)	41(1)
C(15A)	1204(5)	3022(4)	2849(4)	40(1)
C(16A)	2180(4)	2610(4)	3254(4)	37(1)
C(21A)	4744(4)	2514(3)	4636(3)	27(1)
C(22A)	3823(4)	1949(4)	4872(3)	29(1)
C(23A)	4222(4)	1807(4)	5805(4)	32(1)
C(24A)	4575(5)	2762(4)	6612(4)	38(1)
C(25A)	5442(5)	3380(4)	6366(4)	38(1)
C(26A)	5037(5)	3507(4)	5429(4)	36(1)
C(31A)	5687(4)	3329(3)	3396(3)	29(1)
C(32A)	6832(4)	3039(4)	3665(4)	35(1)
C(33A)	7723(5)	3841(4)	3774(4)	40(1)
C(34A)	7674(5)	4081(4)	2880(4)	41(1)
C(35A)	6525(5)	4321(4)	2572(4)	40(1)
C(36A)	5634(5)	3515(4)	2470(4)	36(1)
B(2)	7564(5)	1082(4)	5480(4)	36(1)
F(5)	7960(3)	1521(2)	6446(2)	40(1)
F(6)	6587(3)	517(2)	5367(2)	45(1)
F(7)	8326(3)	492(2)	5035(2)	47(1)
F(8)	7371(3)	1775(3)	5089(2)	56(1)

Table S4. Bond lengths [Å] and angles [°] for **2**.

Ru(1)-C(7)	1.867(5)
Ru(1)-C(2)	2.268(5)
Ru(1)-C(3)	2.280(5)
Ru(1)-C(1)	2.305(5)
Ru(1)-C(4)	2.316(6)
Ru(1)-C(5)	2.319(5)
Ru(1)-C(6)	2.320(5)
Ru(1)-P(1)	2.3207(13)
Ru(1)-H(1M)	1.64(6)
P(1)-C(21)	1.848(5)
P(1)-C(11)	1.862(5)
P(1)-C(31)	1.876(5)
O(1)-C(7)	1.130(6)
C(1)-C(6)	1.382(8)
C(1)-C(2)	1.419(8)
C(1)-H(1A)	0.88(6)
C(2)-C(3)	1.406(7)
C(2)-H(2A)	0.87(6)
C(3)-C(4)	1.406(8)
C(3)-H(3A)	0.89(6)
C(4)-C(5)	1.390(8)
C(4)-H(4A)	0.93(6)
C(5)-C(6)	1.417(8)
C(5)-H(5A)	0.93(6)
C(6)-H(6A)	0.84(6)
C(11)-C(16)	1.532(7)
C(11)-C(12)	1.541(7)
C(11)-H(11A)	1.0000
C(12)-C(13)	1.543(7)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.516(8)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900

C(14)-C(15)	1.517(8)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.530(7)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(21)-C(26)	1.539(7)
C(21)-C(22)	1.541(7)
C(21)-H(21A)	1.0000
C(22)-C(23)	1.532(7)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.521(7)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.533(7)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.527(7)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(31)-C(32)	1.533(7)
C(31)-C(36)	1.546(7)
C(31)-H(31A)	1.0000
C(32)-C(35)	1.535(7)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.509(7)
C(33)-C(36)	1.549(7)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.528(7)

C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
B(1)-F(1)	1.366(7)
B(1)-F(4)	1.366(8)
B(1)-F(3)	1.370(8)
B(1)-F(2)	1.371(7)
Ru(2)-C(7A)	1.862(5)
Ru(2)-C(4A)	2.251(5)
Ru(2)-C(3A)	2.265(5)
Ru(2)-C(1A)	2.308(5)
Ru(2)-C(2A)	2.309(5)
Ru(2)-C(5A)	2.319(6)
Ru(2)-P(2)	2.3210(12)
Ru(2)-C(6A)	2.323(5)
Ru(2)-H(2M)	1.48(6)
P(2)-C(21A)	1.854(5)
P(2)-C(31A)	1.863(5)
P(2)-C(11A)	1.867(5)
O(1A)-C(7A)	1.133(6)
C(1A)-C(2A)	1.380(7)
C(1A)-C(6A)	1.418(8)
C(1A)-H(1AA)	0.91(6)
C(2A)-C(3A)	1.417(7)
C(2A)-H(2AA)	0.90(6)
C(3A)-C(4A)	1.387(8)
C(3A)-H(3AA)	1.05(6)
C(4A)-C(5A)	1.414(8)
C(4A)-H(4AA)	0.93(6)
C(5A)-C(6A)	1.388(8)
C(5A)-H(5AA)	0.87(6)
C(6A)-H(6AA)	0.88(6)
C(11A)-C(16A)	1.535(7)

C(11A)-C(12A)	1.540(7)
C(11A)-H(11B)	1.0000
C(12A)-C(13A)	1.532(8)
C(12A)-H(12C)	0.9900
C(12A)-H(12D)	0.9900
C(13A)-C(14A)	1.523(8)
C(13A)-H(13C)	0.9900
C(13A)-H(13D)	0.9900
C(14A)-C(15A)	1.514(7)
C(14A)-H(14C)	0.9900
C(14A)-H(14D)	0.9900
C(15A)-C(16A)	1.526(7)
C(15A)-H(15C)	0.9900
C(15A)-H(15D)	0.9900
C(16A)-H(16C)	0.9900
C(16A)-H(16D)	0.9900
C(21A)-C(22A)	1.530(7)
C(21A)-C(26A)	1.536(7)
C(21A)-H(21B)	1.0000
C(22A)-C(23A)	1.532(7)
C(22A)-H(22C)	0.9900
C(22A)-H(22D)	0.9900
C(23A)-C(24A)	1.516(7)
C(23A)-H(23C)	0.9900
C(23A)-H(23D)	0.9900
C(24A)-C(25A)	1.539(7)
C(24A)-H(24C)	0.9900
C(24A)-H(24D)	0.9900
C(25A)-C(26A)	1.528(7)
C(25A)-H(25C)	0.9900
C(25A)-H(25D)	0.9900
C(26A)-H(26C)	0.9900
C(26A)-H(26D)	0.9900
C(31A)-C(36A)	1.527(7)
C(31A)-C(32A)	1.533(7)
C(31A)-H(31B)	1.0000

C(32A)-C(33A)	1.527(7)
C(32A)-H(32C)	0.9900
C(32A)-H(32D)	0.9900
C(33A)-C(34A)	1.521(8)
C(33A)-H(33C)	0.9900
C(33A)-H(33D)	0.9900
C(34A)-C(35A)	1.525(8)
C(34A)-H(34C)	0.9900
C(34A)-H(34D)	0.9900
C(35A)-C(36A)	1.533(7)
C(35A)-H(35C)	0.9900
C(35A)-H(35D)	0.9900
C(36A)-H(36C)	0.9900
C(36A)-H(36D)	0.9900
B(2)-F(8)	1.373(7)
B(2)-F(6)	1.386(7)
B(2)-F(7)	1.391(7)
B(2)-F(5)	1.395(7)

C(7)-Ru(1)-C(2)	114.0(2)
C(7)-Ru(1)-C(3)	93.0(2)
C(2)-Ru(1)-C(3)	36.01(19)
C(7)-Ru(1)-C(1)	149.6(2)
C(2)-Ru(1)-C(1)	36.15(19)
C(3)-Ru(1)-C(1)	64.26(19)
C(7)-Ru(1)-C(4)	98.5(2)
C(2)-Ru(1)-C(4)	64.35(19)
C(3)-Ru(1)-C(4)	35.62(19)
C(1)-Ru(1)-C(4)	75.1(2)
C(7)-Ru(1)-C(5)	126.1(2)
C(2)-Ru(1)-C(5)	75.5(2)
C(3)-Ru(1)-C(5)	63.5(2)
C(1)-Ru(1)-C(5)	63.5(2)
C(4)-Ru(1)-C(5)	34.9(2)
C(7)-Ru(1)-C(6)	161.2(2)
C(2)-Ru(1)-C(6)	63.7(2)

C(3)-Ru(1)-C(6)	74.82(19)
C(1)-Ru(1)-C(6)	34.78(19)
C(4)-Ru(1)-C(6)	63.2(2)
C(5)-Ru(1)-C(6)	35.6(2)
C(7)-Ru(1)-P(1)	88.84(15)
C(2)-Ru(1)-P(1)	153.95(14)
C(3)-Ru(1)-P(1)	162.55(14)
C(1)-Ru(1)-P(1)	119.09(14)
C(4)-Ru(1)-P(1)	126.98(14)
C(5)-Ru(1)-P(1)	101.72(14)
C(6)-Ru(1)-P(1)	98.66(14)
C(7)-Ru(1)-H(1M)	88(2)
C(2)-Ru(1)-H(1M)	86(2)
C(3)-Ru(1)-H(1M)	115(2)
C(1)-Ru(1)-H(1M)	84(2)
C(4)-Ru(1)-H(1M)	150(2)
C(5)-Ru(1)-H(1M)	146(2)
C(6)-Ru(1)-H(1M)	110(2)
P(1)-Ru(1)-H(1M)	83(2)
C(21)-P(1)-C(11)	103.2(2)
C(21)-P(1)-C(31)	105.1(2)
C(11)-P(1)-C(31)	103.3(2)
C(21)-P(1)-Ru(1)	110.55(16)
C(11)-P(1)-Ru(1)	115.21(17)
C(31)-P(1)-Ru(1)	118.01(17)
C(6)-C(1)-C(2)	119.7(5)
C(6)-C(1)-Ru(1)	73.2(3)
C(2)-C(1)-Ru(1)	70.5(3)
C(6)-C(1)-H(1A)	121(4)
C(2)-C(1)-H(1A)	119(4)
Ru(1)-C(1)-H(1A)	130(4)
C(3)-C(2)-C(1)	119.4(5)
C(3)-C(2)-Ru(1)	72.5(3)
C(1)-C(2)-Ru(1)	73.4(3)
C(3)-C(2)-H(2A)	117(4)
C(1)-C(2)-H(2A)	124(4)

Ru(1)-C(2)-H(2A)	125(4)
C(2)-C(3)-C(4)	120.5(5)
C(2)-C(3)-Ru(1)	71.5(3)
C(4)-C(3)-Ru(1)	73.6(3)
C(2)-C(3)-H(3A)	116(4)
C(4)-C(3)-H(3A)	124(4)
Ru(1)-C(3)-H(3A)	123(4)
C(5)-C(4)-C(3)	119.7(5)
C(5)-C(4)-Ru(1)	72.6(3)
C(3)-C(4)-Ru(1)	70.8(3)
C(5)-C(4)-H(4A)	119(4)
C(3)-C(4)-H(4A)	122(4)
Ru(1)-C(4)-H(4A)	132(4)
C(4)-C(5)-C(6)	119.9(5)
C(4)-C(5)-Ru(1)	72.4(3)
C(6)-C(5)-Ru(1)	72.3(3)
C(4)-C(5)-H(5A)	129(4)
C(6)-C(5)-H(5A)	111(4)
Ru(1)-C(5)-H(5A)	125(4)
C(1)-C(6)-C(5)	120.7(5)
C(1)-C(6)-Ru(1)	72.0(3)
C(5)-C(6)-Ru(1)	72.2(3)
C(1)-C(6)-H(6A)	115(4)
C(5)-C(6)-H(6A)	124(4)
Ru(1)-C(6)-H(6A)	132(4)
O(1)-C(7)-Ru(1)	175.9(5)
C(16)-C(11)-C(12)	107.6(4)
C(16)-C(11)-P(1)	114.5(3)
C(12)-C(11)-P(1)	113.5(3)
C(16)-C(11)-H(11A)	106.9
C(12)-C(11)-H(11A)	106.9
P(1)-C(11)-H(11A)	106.9
C(11)-C(12)-C(13)	109.7(4)
C(11)-C(12)-H(12A)	109.7
C(13)-C(12)-H(12A)	109.7
C(11)-C(12)-H(12B)	109.7

C(13)-C(12)-H(12B)	109.7
H(12A)-C(12)-H(12B)	108.2
C(14)-C(13)-C(12)	111.2(5)
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13B)	109.4
C(12)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	112.4(5)
C(13)-C(14)-H(14A)	109.1
C(15)-C(14)-H(14A)	109.1
C(13)-C(14)-H(14B)	109.1
C(15)-C(14)-H(14B)	109.1
H(14A)-C(14)-H(14B)	107.9
C(14)-C(15)-C(16)	112.1(5)
C(14)-C(15)-H(15A)	109.2
C(16)-C(15)-H(15A)	109.2
C(14)-C(15)-H(15B)	109.2
C(16)-C(15)-H(15B)	109.2
H(15A)-C(15)-H(15B)	107.9
C(15)-C(16)-C(11)	109.8(4)
C(15)-C(16)-H(16A)	109.7
C(11)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16B)	109.7
C(11)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(26)-C(21)-C(22)	108.4(4)
C(26)-C(21)-P(1)	115.3(3)
C(22)-C(21)-P(1)	116.4(3)
C(26)-C(21)-H(21A)	105.2
C(22)-C(21)-H(21A)	105.2
P(1)-C(21)-H(21A)	105.2
C(23)-C(22)-C(21)	109.6(4)
C(23)-C(22)-H(22A)	109.7
C(21)-C(22)-H(22A)	109.7
C(23)-C(22)-H(22B)	109.7

C(21)-C(22)-H(22B)	109.7
H(22A)-C(22)-H(22B)	108.2
C(24)-C(23)-C(22)	111.2(4)
C(24)-C(23)-H(23A)	109.4
C(22)-C(23)-H(23A)	109.4
C(24)-C(23)-H(23B)	109.4
C(22)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0
C(23)-C(24)-C(25)	111.3(4)
C(23)-C(24)-H(24A)	109.4
C(25)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24B)	109.4
C(25)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
C(26)-C(25)-C(24)	111.1(4)
C(26)-C(25)-H(25A)	109.4
C(24)-C(25)-H(25A)	109.4
C(26)-C(25)-H(25B)	109.4
C(24)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0
C(25)-C(26)-C(21)	110.3(4)
C(25)-C(26)-H(26A)	109.6
C(21)-C(26)-H(26A)	109.6
C(25)-C(26)-H(26B)	109.6
C(21)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
C(32)-C(31)-C(36)	109.7(4)
C(32)-C(31)-P(1)	116.4(4)
C(36)-C(31)-P(1)	113.9(3)
C(32)-C(31)-H(31A)	105.2
C(36)-C(31)-H(31A)	105.2
P(1)-C(31)-H(31A)	105.2
C(31)-C(32)-C(35)	111.3(4)
C(31)-C(32)-H(32A)	109.4
C(35)-C(32)-H(32A)	109.4
C(31)-C(32)-H(32B)	109.4

C(35)-C(32)-H(32B)	109.4
H(32A)-C(32)-H(32B)	108.0
C(34)-C(33)-C(36)	111.9(4)
C(34)-C(33)-H(33A)	109.2
C(36)-C(33)-H(33A)	109.2
C(34)-C(33)-H(33B)	109.2
C(36)-C(33)-H(33B)	109.2
H(33A)-C(33)-H(33B)	107.9
C(33)-C(34)-C(35)	110.9(5)
C(33)-C(34)-H(34A)	109.5
C(35)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
C(35)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	108.0
C(34)-C(35)-C(32)	112.2(4)
C(34)-C(35)-H(35A)	109.2
C(32)-C(35)-H(35A)	109.2
C(34)-C(35)-H(35B)	109.2
C(32)-C(35)-H(35B)	109.2
H(35A)-C(35)-H(35B)	107.9
C(31)-C(36)-C(33)	110.8(4)
C(31)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	108.1
F(1)-B(1)-F(4)	109.3(6)
F(1)-B(1)-F(3)	108.6(5)
F(4)-B(1)-F(3)	109.0(5)
F(1)-B(1)-F(2)	107.7(5)
F(4)-B(1)-F(2)	111.8(6)
F(3)-B(1)-F(2)	110.3(6)
C(7A)-Ru(2)-C(4A)	94.0(2)
C(7A)-Ru(2)-C(3A)	110.9(2)
C(4A)-Ru(2)-C(3A)	35.8(2)
C(7A)-Ru(2)-C(1A)	166.9(2)

C(4A)-Ru(2)-C(1A)	74.79(19)
C(3A)-Ru(2)-C(1A)	63.71(19)
C(7A)-Ru(2)-C(2A)	144.9(2)
C(4A)-Ru(2)-C(2A)	64.04(19)
C(3A)-Ru(2)-C(2A)	36.08(19)
C(1A)-Ru(2)-C(2A)	34.79(19)
C(7A)-Ru(2)-C(5A)	103.8(2)
C(4A)-Ru(2)-C(5A)	36.0(2)
C(3A)-Ru(2)-C(5A)	64.4(2)
C(1A)-Ru(2)-C(5A)	63.1(2)
C(2A)-Ru(2)-C(5A)	75.0(2)
C(7A)-Ru(2)-P(2)	87.23(15)
C(4A)-Ru(2)-P(2)	157.17(15)
C(3A)-Ru(2)-P(2)	159.62(15)
C(1A)-Ru(2)-P(2)	100.47(13)
C(2A)-Ru(2)-P(2)	123.90(14)
C(5A)-Ru(2)-P(2)	121.75(15)
C(7A)-Ru(2)-C(6A)	133.0(2)
C(4A)-Ru(2)-C(6A)	63.75(19)
C(3A)-Ru(2)-C(6A)	75.69(19)
C(1A)-Ru(2)-C(6A)	35.65(19)
C(2A)-Ru(2)-C(6A)	63.62(19)
C(5A)-Ru(2)-C(6A)	34.8(2)
P(2)-Ru(2)-C(6A)	99.14(14)
C(7A)-Ru(2)-H(2M)	81(2)
C(4A)-Ru(2)-H(2M)	127(2)
C(3A)-Ru(2)-H(2M)	98(2)
C(1A)-Ru(2)-H(2M)	111(2)
C(2A)-Ru(2)-H(2M)	91(2)
C(5A)-Ru(2)-H(2M)	162(2)
P(2)-Ru(2)-H(2M)	76(2)
C(6A)-Ru(2)-H(2M)	146(2)
C(21A)-P(2)-C(31A)	102.8(2)
C(21A)-P(2)-C(11A)	111.7(2)
C(31A)-P(2)-C(11A)	102.9(2)
C(21A)-P(2)-Ru(2)	110.06(15)

C(31A)-P(2)-Ru(2)	115.70(16)
C(11A)-P(2)-Ru(2)	113.09(16)
C(2A)-C(1A)-C(6A)	121.5(5)
C(2A)-C(1A)-Ru(2)	72.6(3)
C(6A)-C(1A)-Ru(2)	72.7(3)
C(2A)-C(1A)-H(1AA)	121(4)
C(6A)-C(1A)-H(1AA)	117(4)
Ru(2)-C(1A)-H(1AA)	126(4)
C(1A)-C(2A)-C(3A)	119.3(5)
C(1A)-C(2A)-Ru(2)	72.6(3)
C(3A)-C(2A)-Ru(2)	70.3(3)
C(1A)-C(2A)-H(2AA)	123(4)
C(3A)-C(2A)-H(2AA)	118(4)
Ru(2)-C(2A)-H(2AA)	124(4)
C(4A)-C(3A)-C(2A)	119.2(5)
C(4A)-C(3A)-Ru(2)	71.6(3)
C(2A)-C(3A)-Ru(2)	73.7(3)
C(4A)-C(3A)-H(3AA)	108(3)
C(2A)-C(3A)-H(3AA)	132(3)
Ru(2)-C(3A)-H(3AA)	118(3)
C(3A)-C(4A)-C(5A)	121.5(5)
C(3A)-C(4A)-Ru(2)	72.7(3)
C(5A)-C(4A)-Ru(2)	74.6(3)
C(3A)-C(4A)-H(4AA)	117(4)
C(5A)-C(4A)-H(4AA)	121(4)
Ru(2)-C(4A)-H(4AA)	122(4)
C(6A)-C(5A)-C(4A)	119.2(5)
C(6A)-C(5A)-Ru(2)	72.8(3)
C(4A)-C(5A)-Ru(2)	69.4(3)
C(6A)-C(5A)-H(5AA)	122(4)
C(4A)-C(5A)-H(5AA)	117(4)
Ru(2)-C(5A)-H(5AA)	118(4)
C(5A)-C(6A)-C(1A)	119.2(5)
C(5A)-C(6A)-Ru(2)	72.4(3)
C(1A)-C(6A)-Ru(2)	71.6(3)
C(5A)-C(6A)-H(6AA)	127(4)

C(1A)-C(6A)-H(6AA)	113(4)
Ru(2)-C(6A)-H(6AA)	126(4)
O(1A)-C(7A)-Ru(2)	177.8(4)
C(16A)-C(11A)-C(12A)	108.5(4)
C(16A)-C(11A)-P(2)	115.3(3)
C(12A)-C(11A)-P(2)	115.9(4)
C(16A)-C(11A)-H(11B)	105.3
C(12A)-C(11A)-H(11B)	105.3
P(2)-C(11A)-H(11B)	105.3
C(13A)-C(12A)-C(11A)	110.6(5)
C(13A)-C(12A)-H(12C)	109.5
C(11A)-C(12A)-H(12C)	109.5
C(13A)-C(12A)-H(12D)	109.5
C(11A)-C(12A)-H(12D)	109.5
H(12C)-C(12A)-H(12D)	108.1
C(14A)-C(13A)-C(12A)	111.7(5)
C(14A)-C(13A)-H(13C)	109.3
C(12A)-C(13A)-H(13C)	109.3
C(14A)-C(13A)-H(13D)	109.3
C(12A)-C(13A)-H(13D)	109.3
H(13C)-C(13A)-H(13D)	107.9
C(15A)-C(14A)-C(13A)	110.8(5)
C(15A)-C(14A)-H(14C)	109.5
C(13A)-C(14A)-H(14C)	109.5
C(15A)-C(14A)-H(14D)	109.5
C(13A)-C(14A)-H(14D)	109.5
H(14C)-C(14A)-H(14D)	108.1
C(14A)-C(15A)-C(16A)	112.0(5)
C(14A)-C(15A)-H(15C)	109.2
C(16A)-C(15A)-H(15C)	109.2
C(14A)-C(15A)-H(15D)	109.2
C(16A)-C(15A)-H(15D)	109.2
H(15C)-C(15A)-H(15D)	107.9
C(15A)-C(16A)-C(11A)	110.6(4)
C(15A)-C(16A)-H(16C)	109.5
C(11A)-C(16A)-H(16C)	109.5

C(15A)-C(16A)-H(16D)	109.5
C(11A)-C(16A)-H(16D)	109.5
H(16C)-C(16A)-H(16D)	108.1
C(22A)-C(21A)-C(26A)	109.5(4)
C(22A)-C(21A)-P(2)	114.2(3)
C(26A)-C(21A)-P(2)	117.7(3)
C(22A)-C(21A)-H(21B)	104.7
C(26A)-C(21A)-H(21B)	104.7
P(2)-C(21A)-H(21B)	104.7
C(21A)-C(22A)-C(23A)	109.5(4)
C(21A)-C(22A)-H(22C)	109.8
C(23A)-C(22A)-H(22C)	109.8
C(21A)-C(22A)-H(22D)	109.8
C(23A)-C(22A)-H(22D)	109.8
H(22C)-C(22A)-H(22D)	108.2
C(24A)-C(23A)-C(22A)	111.7(4)
C(24A)-C(23A)-H(23C)	109.3
C(22A)-C(23A)-H(23C)	109.3
C(24A)-C(23A)-H(23D)	109.3
C(22A)-C(23A)-H(23D)	109.3
H(23C)-C(23A)-H(23D)	107.9
C(23A)-C(24A)-C(25A)	111.4(4)
C(23A)-C(24A)-H(24C)	109.3
C(25A)-C(24A)-H(24C)	109.3
C(23A)-C(24A)-H(24D)	109.3
C(25A)-C(24A)-H(24D)	109.3
H(24C)-C(24A)-H(24D)	108.0
C(26A)-C(25A)-C(24A)	111.3(5)
C(26A)-C(25A)-H(25C)	109.4
C(24A)-C(25A)-H(25C)	109.4
C(26A)-C(25A)-H(25D)	109.4
C(24A)-C(25A)-H(25D)	109.4
H(25C)-C(25A)-H(25D)	108.0
C(25A)-C(26A)-C(21A)	109.8(4)
C(25A)-C(26A)-H(26C)	109.7
C(21A)-C(26A)-H(26C)	109.7

C(25A)-C(26A)-H(26D)	109.7
C(21A)-C(26A)-H(26D)	109.7
H(26C)-C(26A)-H(26D)	108.2
C(36A)-C(31A)-C(32A)	109.9(4)
C(36A)-C(31A)-P(2)	113.7(4)
C(32A)-C(31A)-P(2)	113.3(3)
C(36A)-C(31A)-H(31B)	106.5
C(32A)-C(31A)-H(31B)	106.5
P(2)-C(31A)-H(31B)	106.5
C(33A)-C(32A)-C(31A)	109.9(4)
C(33A)-C(32A)-H(32C)	109.7
C(31A)-C(32A)-H(32C)	109.7
C(33A)-C(32A)-H(32D)	109.7
C(31A)-C(32A)-H(32D)	109.7
H(32C)-C(32A)-H(32D)	108.2
C(34A)-C(33A)-C(32A)	111.9(5)
C(34A)-C(33A)-H(33C)	109.2
C(32A)-C(33A)-H(33C)	109.2
C(34A)-C(33A)-H(33D)	109.2
C(32A)-C(33A)-H(33D)	109.2
H(33C)-C(33A)-H(33D)	107.9
C(33A)-C(34A)-C(35A)	111.5(5)
C(33A)-C(34A)-H(34C)	109.3
C(35A)-C(34A)-H(34C)	109.3
C(33A)-C(34A)-H(34D)	109.3
C(35A)-C(34A)-H(34D)	109.3
H(34C)-C(34A)-H(34D)	108.0
C(34A)-C(35A)-C(36A)	111.3(5)
C(34A)-C(35A)-H(35C)	109.4
C(36A)-C(35A)-H(35C)	109.4
C(34A)-C(35A)-H(35D)	109.4
C(36A)-C(35A)-H(35D)	109.4
H(35C)-C(35A)-H(35D)	108.0
C(31A)-C(36A)-C(35A)	110.3(4)
C(31A)-C(36A)-H(36C)	109.6
C(35A)-C(36A)-H(36C)	109.6

C(31A)-C(36A)-H(36D)	109.6
C(35A)-C(36A)-H(36D)	109.6
H(36C)-C(36A)-H(36D)	108.1
F(8)-B(2)-F(6)	109.8(5)
F(8)-B(2)-F(7)	110.2(5)
F(6)-B(2)-F(7)	108.7(5)
F(8)-B(2)-F(5)	109.8(5)
F(6)-B(2)-F(5)	108.4(5)
F(7)-B(2)-F(5)	109.9(5)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	29(1)	26(1)	28(1)	12(1)	4(1)	4(1)
P(1)	27(1)	26(1)	26(1)	10(1)	6(1)	4(1)
O(1)	45(2)	42(2)	31(2)	15(2)	3(2)	6(2)
C(1)	36(3)	32(3)	21(2)	4(2)	-1(2)	-1(2)
C(2)	32(3)	26(2)	35(3)	3(2)	4(2)	2(2)
C(3)	41(3)	22(2)	33(3)	13(2)	2(2)	-4(2)
C(4)	36(3)	34(3)	38(3)	11(2)	9(2)	1(2)
C(5)	27(3)	33(3)	43(3)	11(2)	-1(2)	0(2)
C(6)	41(3)	31(3)	32(3)	11(2)	-2(2)	-4(2)
C(7)	37(3)	27(3)	34(3)	18(2)	3(2)	5(2)
C(11)	33(3)	26(2)	33(3)	8(2)	10(2)	7(2)
C(12)	37(3)	33(3)	37(3)	15(2)	12(2)	9(2)
C(13)	50(3)	42(3)	37(3)	17(3)	21(3)	13(3)
C(14)	44(3)	44(3)	51(3)	22(3)	24(3)	17(3)
C(15)	35(3)	36(3)	45(3)	11(3)	12(2)	11(2)
C(16)	33(3)	37(3)	41(3)	9(2)	9(2)	5(2)
C(21)	35(3)	27(2)	27(2)	14(2)	4(2)	2(2)
C(22)	39(3)	29(3)	35(3)	14(2)	6(2)	4(2)
C(23)	38(3)	34(3)	41(3)	21(2)	5(2)	7(2)
C(24)	43(3)	43(3)	29(3)	21(2)	4(2)	4(2)
C(25)	34(3)	37(3)	30(3)	13(2)	8(2)	8(2)
C(26)	31(3)	30(3)	30(3)	11(2)	2(2)	3(2)
C(31)	26(3)	30(3)	31(3)	11(2)	4(2)	2(2)
C(32)	36(3)	33(3)	35(3)	10(2)	6(2)	4(2)
C(33)	32(3)	44(3)	35(3)	13(2)	5(2)	3(2)
C(34)	39(3)	34(3)	38(3)	11(2)	4(2)	0(2)
C(35)	36(3)	31(3)	38(3)	10(2)	4(2)	3(2)
C(36)	36(3)	31(3)	30(3)	11(2)	5(2)	5(2)
B(1)	65(5)	34(3)	24(3)	3(3)	-5(3)	13(3)
F(1)	45(2)	65(2)	47(2)	4(2)	0(2)	15(2)
F(2)	125(4)	59(3)	56(2)	-8(2)	-41(3)	43(3)

F(3)	53(2)	56(2)	89(3)	-2(2)	37(2)	-7(2)
F(4)	174(5)	38(2)	48(2)	16(2)	34(3)	-8(3)
Ru(2)	32(1)	25(1)	23(1)	9(1)	3(1)	6(1)
P(2)	31(1)	25(1)	24(1)	9(1)	6(1)	4(1)
O(1A)	44(2)	35(2)	29(2)	14(2)	0(2)	0(2)
C(1A)	44(3)	31(3)	25(3)	15(2)	0(2)	11(2)
C(2A)	34(3)	31(3)	37(3)	19(2)	6(2)	2(2)
C(3A)	40(3)	25(2)	34(3)	6(2)	-3(2)	1(2)
C(4A)	49(3)	27(3)	23(2)	8(2)	10(2)	17(2)
C(5A)	37(3)	40(3)	46(3)	26(3)	9(3)	14(2)
C(6A)	32(3)	32(3)	38(3)	13(2)	-5(2)	7(2)
C(7A)	26(3)	27(2)	29(3)	7(2)	1(2)	1(2)
C(11A)	32(3)	25(2)	33(3)	11(2)	5(2)	9(2)
C(12A)	35(3)	32(3)	52(3)	8(3)	6(3)	5(2)
C(13A)	44(3)	26(3)	67(4)	16(3)	6(3)	9(2)
C(14A)	35(3)	33(3)	54(4)	14(3)	5(3)	12(2)
C(15A)	29(3)	39(3)	48(3)	14(3)	2(2)	4(2)
C(16A)	35(3)	32(3)	43(3)	15(2)	1(2)	4(2)
C(21A)	39(3)	22(2)	19(2)	6(2)	4(2)	2(2)
C(22A)	29(3)	29(2)	31(3)	12(2)	10(2)	5(2)
C(23A)	32(3)	35(3)	34(3)	16(2)	11(2)	3(2)
C(24A)	46(3)	44(3)	28(3)	17(2)	10(2)	5(3)
C(25A)	49(3)	37(3)	27(3)	9(2)	5(2)	-3(2)
C(26A)	44(3)	32(3)	30(3)	10(2)	7(2)	-3(2)
C(31A)	35(3)	25(2)	29(3)	10(2)	8(2)	2(2)
C(32A)	35(3)	34(3)	44(3)	21(2)	10(2)	6(2)
C(33A)	34(3)	37(3)	48(3)	16(3)	9(3)	0(2)
C(34A)	47(3)	32(3)	46(3)	14(3)	18(3)	-4(2)
C(35A)	52(4)	35(3)	38(3)	16(2)	12(3)	1(3)
C(36A)	42(3)	38(3)	30(3)	14(2)	6(2)	5(2)
B(2)	35(3)	40(3)	33(3)	14(3)	3(2)	7(3)
F(5)	42(2)	40(2)	33(2)	11(1)	-6(1)	7(1)
F(6)	35(2)	56(2)	40(2)	13(2)	4(1)	-5(2)
F(7)	44(2)	56(2)	42(2)	16(2)	9(2)	12(2)
F(8)	74(3)	50(2)	49(2)	31(2)	-5(2)	6(2)

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

	x	y	z	U(eq)
H(1M)	2090(50)	830(50)	-1810(40)	59(19)
H(1A)	910(50)	-520(40)	-3590(40)	38
H(2A)	1280(50)	-1180(40)	-2420(40)	40
H(3A)	260(50)	-940(40)	-1300(40)	38
H(4A)	-1310(50)	-40(40)	-1270(40)	43
H(5A)	-1550(50)	750(40)	-2410(40)	43
H(6A)	-470(50)	370(40)	-3550(40)	43
H(11A)	321	3854	-686	37
H(12A)	696	3103	476	41
H(12B)	-431	2409	8	41
H(13A)	-780	3759	1313	49
H(13B)	-305	4488	858	49
H(14A)	-2218	4378	531	51
H(14B)	-2306	3224	128	51
H(15A)	-1496	4454	-772	46
H(15B)	-2588	3709	-1163	46
H(16A)	-1124	3072	-2005	45
H(16B)	-1507	2387	-1466	45
H(21A)	-56	2179	-2957	34
H(22A)	241	3901	-2229	41
H(22B)	1449	3856	-2528	41
H(23A)	-586	3185	-3845	43
H(23B)	180	4147	-3696	43
H(24A)	1592	3243	-4327	44
H(24B)	472	2844	-5071	44
H(25A)	217	1516	-4597	39
H(25B)	1438	1549	-4856	39
H(26A)	2196	2274	-3232	37
H(26B)	1477	1282	-3401	37
H(31A)	2413	3638	-1201	35
H(32A)	2606	3077	413	42

H(32B)	1971	3967	328	42
H(33A)	5098	2820	-1115	44
H(33B)	4455	3699	-1217	44
H(34A)	5342	4153	342	45
H(34B)	4781	3205	441	45
H(35A)	3630	4779	246	43
H(35B)	3804	4508	1179	43
H(36A)	3265	2248	-1984	38
H(36B)	3424	1996	-1039	38
H(2M)	3320(50)	1040(50)	2410(40)	58(19)
H(1AA)	5230(50)	400(40)	4030(40)	39
H(2AA)	3720(50)	-620(40)	2990(40)	38
H(3AA)	3670(50)	-1100(40)	1220(40)	43
H(4AA)	5120(50)	-600(40)	800(40)	39
H(5AA)	6580(50)	410(40)	1820(40)	45
H(6AA)	6620(50)	880(40)	3490(40)	42
H(11B)	3208	2964	2449	35
H(12C)	3345	4312	4338	50
H(12D)	4049	4469	3581	50
H(13C)	2418	5286	3603	55
H(13D)	2411	4481	2578	55
H(14C)	1178	4286	3984	49
H(14D)	656	4354	2992	49
H(15C)	1191	2846	2159	48
H(15D)	507	2731	2943	48
H(16C)	2119	1902	2923	44
H(16D)	2164	2742	3934	44
H(21B)	5410	2160	4685	33
H(22C)	3621	1313	4357	35
H(22D)	3159	2306	4931	35
H(23C)	3619	1453	5964	38
H(23D)	4854	1410	5727	38
H(24C)	4887	2641	7187	45
H(24D)	3920	3121	6751	45
H(25C)	5601	4021	6879	46
H(25D)	6138	3066	6320	46

H(26C)	5623	3880	5273	43
H(26D)	4378	3871	5489	43
H(31B)	5616	3961	3898	35
H(32C)	6865	2923	4268	42
H(32D)	6963	2434	3168	42
H(33C)	7626	4427	4311	48
H(33D)	8460	3636	3922	48
H(34C)	7874	3524	2364	49
H(34D)	8220	4639	2997	49
H(35C)	6502	4413	1958	49
H(35D)	6368	4933	3046	49
H(36C)	4895	3704	2300	43
H(36D)	5748	2917	1955	43

Table S7. Torsion angles [°] for **2**.

C(7)-Ru(1)-P(1)-C(21)	174.8(2)
C(2)-Ru(1)-P(1)-C(21)	22.4(4)
C(3)-Ru(1)-P(1)-C(21)	-89.0(5)
C(1)-Ru(1)-P(1)-C(21)	7.5(2)
C(4)-Ru(1)-P(1)-C(21)	-85.4(3)
C(5)-Ru(1)-P(1)-C(21)	-58.6(2)
C(6)-Ru(1)-P(1)-C(21)	-22.5(2)
C(7)-Ru(1)-P(1)-C(11)	-68.7(2)
C(2)-Ru(1)-P(1)-C(11)	138.9(4)
C(3)-Ru(1)-P(1)-C(11)	27.5(5)
C(1)-Ru(1)-P(1)-C(11)	124.0(2)
C(4)-Ru(1)-P(1)-C(11)	31.1(3)
C(5)-Ru(1)-P(1)-C(11)	57.9(2)
C(6)-Ru(1)-P(1)-C(11)	94.0(2)
C(7)-Ru(1)-P(1)-C(31)	53.8(2)
C(2)-Ru(1)-P(1)-C(31)	-98.5(4)
C(3)-Ru(1)-P(1)-C(31)	150.0(5)
C(1)-Ru(1)-P(1)-C(31)	-113.5(2)
C(4)-Ru(1)-P(1)-C(31)	153.6(3)
C(5)-Ru(1)-P(1)-C(31)	-179.5(2)
C(6)-Ru(1)-P(1)-C(31)	-143.5(2)
C(7)-Ru(1)-C(1)-C(6)	145.7(4)
C(2)-Ru(1)-C(1)-C(6)	131.0(5)
C(3)-Ru(1)-C(1)-C(6)	100.6(4)
C(4)-Ru(1)-C(1)-C(6)	64.3(3)
C(5)-Ru(1)-C(1)-C(6)	28.9(3)
P(1)-Ru(1)-C(1)-C(6)	-60.1(4)
C(7)-Ru(1)-C(1)-C(2)	14.6(6)
C(3)-Ru(1)-C(1)-C(2)	-30.4(3)
C(4)-Ru(1)-C(1)-C(2)	-66.7(3)
C(5)-Ru(1)-C(1)-C(2)	-102.1(4)
C(6)-Ru(1)-C(1)-C(2)	-131.0(5)
P(1)-Ru(1)-C(1)-C(2)	168.9(3)
C(6)-C(1)-C(2)-C(3)	1.8(7)

Ru(1)-C(1)-C(2)-C(3)	58.0(4)
C(6)-C(1)-C(2)-Ru(1)	-56.3(4)
C(7)-Ru(1)-C(2)-C(3)	58.9(4)
C(1)-Ru(1)-C(2)-C(3)	-129.2(5)
C(4)-Ru(1)-C(2)-C(3)	-29.2(3)
C(5)-Ru(1)-C(2)-C(3)	-64.5(3)
C(6)-Ru(1)-C(2)-C(3)	-100.5(4)
P(1)-Ru(1)-C(2)-C(3)	-151.7(3)
C(7)-Ru(1)-C(2)-C(1)	-171.9(3)
C(3)-Ru(1)-C(2)-C(1)	129.2(5)
C(4)-Ru(1)-C(2)-C(1)	100.0(4)
C(5)-Ru(1)-C(2)-C(1)	64.6(3)
C(6)-Ru(1)-C(2)-C(1)	28.7(3)
P(1)-Ru(1)-C(2)-C(1)	-22.5(5)
C(1)-C(2)-C(3)-C(4)	-1.3(8)
Ru(1)-C(2)-C(3)-C(4)	57.2(4)
C(1)-C(2)-C(3)-Ru(1)	-58.5(4)
C(7)-Ru(1)-C(3)-C(2)	-128.4(3)
C(1)-Ru(1)-C(3)-C(2)	30.5(3)
C(4)-Ru(1)-C(3)-C(2)	131.0(5)
C(5)-Ru(1)-C(3)-C(2)	102.3(4)
C(6)-Ru(1)-C(3)-C(2)	66.0(3)
P(1)-Ru(1)-C(3)-C(2)	136.0(4)
C(7)-Ru(1)-C(3)-C(4)	100.5(3)
C(2)-Ru(1)-C(3)-C(4)	-131.0(5)
C(1)-Ru(1)-C(3)-C(4)	-100.5(4)
C(5)-Ru(1)-C(3)-C(4)	-28.7(3)
C(6)-Ru(1)-C(3)-C(4)	-65.0(3)
P(1)-Ru(1)-C(3)-C(4)	4.9(7)
C(2)-C(3)-C(4)-C(5)	-0.5(8)
Ru(1)-C(3)-C(4)-C(5)	55.7(5)
C(2)-C(3)-C(4)-Ru(1)	-56.2(4)
C(7)-Ru(1)-C(4)-C(5)	145.6(3)
C(2)-Ru(1)-C(4)-C(5)	-101.8(4)
C(3)-Ru(1)-C(4)-C(5)	-131.3(5)
C(1)-Ru(1)-C(4)-C(5)	-64.8(3)

C(6)-Ru(1)-C(4)-C(5)	-29.7(3)
P(1)-Ru(1)-C(4)-C(5)	50.6(4)
C(7)-Ru(1)-C(4)-C(3)	-83.1(3)
C(2)-Ru(1)-C(4)-C(3)	29.5(3)
C(1)-Ru(1)-C(4)-C(3)	66.4(3)
C(5)-Ru(1)-C(4)-C(3)	131.3(5)
C(6)-Ru(1)-C(4)-C(3)	101.6(4)
P(1)-Ru(1)-C(4)-C(3)	-178.2(2)
C(3)-C(4)-C(5)-C(6)	1.8(8)
Ru(1)-C(4)-C(5)-C(6)	56.6(5)
C(3)-C(4)-C(5)-Ru(1)	-54.8(5)
C(7)-Ru(1)-C(5)-C(4)	-43.7(4)
C(2)-Ru(1)-C(5)-C(4)	65.7(3)
C(3)-Ru(1)-C(5)-C(4)	29.3(3)
C(1)-Ru(1)-C(5)-C(4)	102.2(4)
C(6)-Ru(1)-C(5)-C(4)	130.5(5)
P(1)-Ru(1)-C(5)-C(4)	-140.9(3)
C(7)-Ru(1)-C(5)-C(6)	-174.3(3)
C(2)-Ru(1)-C(5)-C(6)	-64.9(3)
C(3)-Ru(1)-C(5)-C(6)	-101.3(4)
C(1)-Ru(1)-C(5)-C(6)	-28.3(3)
C(4)-Ru(1)-C(5)-C(6)	-130.5(5)
P(1)-Ru(1)-C(5)-C(6)	88.5(3)
C(2)-C(1)-C(6)-C(5)	-0.5(8)
Ru(1)-C(1)-C(6)-C(5)	-55.4(5)
C(2)-C(1)-C(6)-Ru(1)	55.0(4)
C(4)-C(5)-C(6)-C(1)	-1.3(8)
Ru(1)-C(5)-C(6)-C(1)	55.4(5)
C(4)-C(5)-C(6)-Ru(1)	-56.7(5)
C(7)-Ru(1)-C(6)-C(1)	-117.4(7)
C(2)-Ru(1)-C(6)-C(1)	-29.7(3)
C(3)-Ru(1)-C(6)-C(1)	-66.5(3)
C(4)-Ru(1)-C(6)-C(1)	-102.8(4)
C(5)-Ru(1)-C(6)-C(1)	-131.9(5)
P(1)-Ru(1)-C(6)-C(1)	130.0(3)
C(7)-Ru(1)-C(6)-C(5)	14.6(8)

C(2)-Ru(1)-C(6)-C(5)	102.2(4)
C(3)-Ru(1)-C(6)-C(5)	65.4(3)
C(1)-Ru(1)-C(6)-C(5)	131.9(5)
C(4)-Ru(1)-C(6)-C(5)	29.1(3)
P(1)-Ru(1)-C(6)-C(5)	-98.1(3)
C(2)-Ru(1)-C(7)-O(1)	-45(7)
C(3)-Ru(1)-C(7)-O(1)	-15(7)
C(1)-Ru(1)-C(7)-O(1)	-55(7)
C(4)-Ru(1)-C(7)-O(1)	21(7)
C(5)-Ru(1)-C(7)-O(1)	44(7)
C(6)-Ru(1)-C(7)-O(1)	34(7)
P(1)-Ru(1)-C(7)-O(1)	148(7)
C(21)-P(1)-C(11)-C(16)	44.7(4)
C(31)-P(1)-C(11)-C(16)	154.0(4)
Ru(1)-P(1)-C(11)-C(16)	-75.9(4)
C(21)-P(1)-C(11)-C(12)	168.8(4)
C(31)-P(1)-C(11)-C(12)	-81.9(4)
Ru(1)-P(1)-C(11)-C(12)	48.2(4)
C(16)-C(11)-C(12)-C(13)	-62.3(5)
P(1)-C(11)-C(12)-C(13)	169.9(4)
C(11)-C(12)-C(13)-C(14)	57.6(6)
C(12)-C(13)-C(14)-C(15)	-51.8(6)
C(13)-C(14)-C(15)-C(16)	51.8(6)
C(14)-C(15)-C(16)-C(11)	-57.3(6)
C(12)-C(11)-C(16)-C(15)	62.0(6)
P(1)-C(11)-C(16)-C(15)	-170.8(4)
C(11)-P(1)-C(21)-C(26)	178.2(4)
C(31)-P(1)-C(21)-C(26)	70.2(4)
Ru(1)-P(1)-C(21)-C(26)	-58.1(4)
C(11)-P(1)-C(21)-C(22)	49.6(4)
C(31)-P(1)-C(21)-C(22)	-58.4(4)
Ru(1)-P(1)-C(21)-C(22)	173.3(3)
C(26)-C(21)-C(22)-C(23)	60.7(5)
P(1)-C(21)-C(22)-C(23)	-167.4(4)
C(21)-C(22)-C(23)-C(24)	-58.6(6)
C(22)-C(23)-C(24)-C(25)	54.9(6)

C(23)-C(24)-C(25)-C(26)	-54.2(6)
C(24)-C(25)-C(26)-C(21)	57.5(6)
C(22)-C(21)-C(26)-C(25)	-60.5(5)
P(1)-C(21)-C(26)-C(25)	167.0(3)
C(21)-P(1)-C(31)-C(32)	149.3(4)
C(11)-P(1)-C(31)-C(32)	41.5(4)
Ru(1)-P(1)-C(31)-C(32)	-86.9(4)
C(21)-P(1)-C(31)-C(36)	-81.5(4)
C(11)-P(1)-C(31)-C(36)	170.7(4)
Ru(1)-P(1)-C(31)-C(36)	42.2(4)
C(36)-C(31)-C(32)-C(35)	56.1(6)
P(1)-C(31)-C(32)-C(35)	-172.7(4)
C(36)-C(33)-C(34)-C(35)	-54.8(6)
C(33)-C(34)-C(35)-C(32)	54.6(6)
C(31)-C(32)-C(35)-C(34)	-55.9(6)
C(32)-C(31)-C(36)-C(33)	-56.2(5)
P(1)-C(31)-C(36)-C(33)	171.3(3)
C(34)-C(33)-C(36)-C(31)	56.4(6)
C(7A)-Ru(2)-P(2)-C(21A)	176.6(2)
C(4A)-Ru(2)-P(2)-C(21A)	-89.8(4)
C(3A)-Ru(2)-P(2)-C(21A)	23.1(5)
C(1A)-Ru(2)-P(2)-C(21A)	-14.2(2)
C(2A)-Ru(2)-P(2)-C(21A)	14.0(2)
C(5A)-Ru(2)-P(2)-C(21A)	-78.9(2)
C(6A)-Ru(2)-P(2)-C(21A)	-50.3(2)
C(7A)-Ru(2)-P(2)-C(31A)	-67.5(2)
C(4A)-Ru(2)-P(2)-C(31A)	26.1(4)
C(3A)-Ru(2)-P(2)-C(31A)	139.0(4)
C(1A)-Ru(2)-P(2)-C(31A)	101.7(2)
C(2A)-Ru(2)-P(2)-C(31A)	129.9(2)
C(5A)-Ru(2)-P(2)-C(31A)	37.0(2)
C(6A)-Ru(2)-P(2)-C(31A)	65.6(2)
C(7A)-Ru(2)-P(2)-C(11A)	50.8(2)
C(4A)-Ru(2)-P(2)-C(11A)	144.5(4)
C(3A)-Ru(2)-P(2)-C(11A)	-102.7(4)
C(1A)-Ru(2)-P(2)-C(11A)	-139.9(2)

C(2A)-Ru(2)-P(2)-C(11A)	-111.8(2)
C(5A)-Ru(2)-P(2)-C(11A)	155.4(2)
C(6A)-Ru(2)-P(2)-C(11A)	-176.1(2)
C(7A)-Ru(2)-C(1A)-C(2A)	-98.1(9)
C(4A)-Ru(2)-C(1A)-C(2A)	-66.2(3)
C(3A)-Ru(2)-C(1A)-C(2A)	-29.7(3)
C(5A)-Ru(2)-C(1A)-C(2A)	-102.8(4)
P(2)-Ru(2)-C(1A)-C(2A)	136.7(3)
C(6A)-Ru(2)-C(1A)-C(2A)	-132.1(5)
C(7A)-Ru(2)-C(1A)-C(6A)	34.0(10)
C(4A)-Ru(2)-C(1A)-C(6A)	66.0(3)
C(3A)-Ru(2)-C(1A)-C(6A)	102.5(4)
C(2A)-Ru(2)-C(1A)-C(6A)	132.1(5)
C(5A)-Ru(2)-C(1A)-C(6A)	29.3(3)
P(2)-Ru(2)-C(1A)-C(6A)	-91.1(3)
C(6A)-C(1A)-C(2A)-C(3A)	-1.8(8)
Ru(2)-C(1A)-C(2A)-C(3A)	54.4(4)
C(6A)-C(1A)-C(2A)-Ru(2)	-56.2(4)
C(7A)-Ru(2)-C(2A)-C(1A)	157.0(4)
C(4A)-Ru(2)-C(2A)-C(1A)	100.9(4)
C(3A)-Ru(2)-C(2A)-C(1A)	131.1(5)
C(5A)-Ru(2)-C(2A)-C(1A)	64.1(3)
P(2)-Ru(2)-C(2A)-C(1A)	-54.3(4)
C(6A)-Ru(2)-C(2A)-C(1A)	28.8(3)
C(7A)-Ru(2)-C(2A)-C(3A)	25.9(5)
C(4A)-Ru(2)-C(2A)-C(3A)	-30.2(3)
C(1A)-Ru(2)-C(2A)-C(3A)	-131.1(5)
C(5A)-Ru(2)-C(2A)-C(3A)	-66.9(3)
P(2)-Ru(2)-C(2A)-C(3A)	174.6(3)
C(6A)-Ru(2)-C(2A)-C(3A)	-102.3(4)
C(1A)-C(2A)-C(3A)-C(4A)	1.7(8)
Ru(2)-C(2A)-C(3A)-C(4A)	57.2(4)
C(1A)-C(2A)-C(3A)-Ru(2)	-55.5(4)
C(7A)-Ru(2)-C(3A)-C(4A)	66.2(4)
C(1A)-Ru(2)-C(3A)-C(4A)	-100.7(3)
C(2A)-Ru(2)-C(3A)-C(4A)	-129.3(5)

C(5A)-Ru(2)-C(3A)-C(4A)	-29.6(3)
P(2)-Ru(2)-C(3A)-C(4A)	-142.3(4)
C(6A)-Ru(2)-C(3A)-C(4A)	-64.7(3)
C(7A)-Ru(2)-C(3A)-C(2A)	-164.4(3)
C(4A)-Ru(2)-C(3A)-C(2A)	129.3(5)
C(1A)-Ru(2)-C(3A)-C(2A)	28.7(3)
C(5A)-Ru(2)-C(3A)-C(2A)	99.8(3)
P(2)-Ru(2)-C(3A)-C(2A)	-12.9(6)
C(6A)-Ru(2)-C(3A)-C(2A)	64.6(3)
C(2A)-C(3A)-C(4A)-C(5A)	0.6(8)
Ru(2)-C(3A)-C(4A)-C(5A)	58.9(4)
C(2A)-C(3A)-C(4A)-Ru(2)	-58.3(4)
C(7A)-Ru(2)-C(4A)-C(3A)	-121.0(3)
C(1A)-Ru(2)-C(4A)-C(3A)	65.9(3)
C(2A)-Ru(2)-C(4A)-C(3A)	30.4(3)
C(5A)-Ru(2)-C(4A)-C(3A)	130.8(5)
P(2)-Ru(2)-C(4A)-C(3A)	146.7(3)
C(6A)-Ru(2)-C(4A)-C(3A)	102.3(3)
C(7A)-Ru(2)-C(4A)-C(5A)	108.2(3)
C(3A)-Ru(2)-C(4A)-C(5A)	-130.8(5)
C(1A)-Ru(2)-C(4A)-C(5A)	-64.9(3)
C(2A)-Ru(2)-C(4A)-C(5A)	-100.4(3)
P(2)-Ru(2)-C(4A)-C(5A)	15.9(5)
C(6A)-Ru(2)-C(4A)-C(5A)	-28.5(3)
C(3A)-C(4A)-C(5A)-C(6A)	-2.9(8)
Ru(2)-C(4A)-C(5A)-C(6A)	55.1(5)
C(3A)-C(4A)-C(5A)-Ru(2)	-57.9(4)
C(7A)-Ru(2)-C(5A)-C(6A)	151.1(3)
C(4A)-Ru(2)-C(5A)-C(6A)	-131.4(5)
C(3A)-Ru(2)-C(5A)-C(6A)	-102.1(4)
C(1A)-Ru(2)-C(5A)-C(6A)	-30.0(3)
C(2A)-Ru(2)-C(5A)-C(6A)	-65.1(3)
P(2)-Ru(2)-C(5A)-C(6A)	55.7(4)
C(7A)-Ru(2)-C(5A)-C(4A)	-77.4(3)
C(3A)-Ru(2)-C(5A)-C(4A)	29.4(3)
C(1A)-Ru(2)-C(5A)-C(4A)	101.5(4)

C(2A)-Ru(2)-C(5A)-C(4A)	66.3(3)
P(2)-Ru(2)-C(5A)-C(4A)	-172.8(3)
C(6A)-Ru(2)-C(5A)-C(4A)	131.4(5)
C(4A)-C(5A)-C(6A)-C(1A)	2.8(8)
Ru(2)-C(5A)-C(6A)-C(1A)	56.2(4)
C(4A)-C(5A)-C(6A)-Ru(2)	-53.5(4)
C(2A)-C(1A)-C(6A)-C(5A)	-0.5(8)
Ru(2)-C(1A)-C(6A)-C(5A)	-56.6(5)
C(2A)-C(1A)-C(6A)-Ru(2)	56.1(4)
C(7A)-Ru(2)-C(6A)-C(5A)	-39.9(4)
C(4A)-Ru(2)-C(6A)-C(5A)	29.4(3)
C(3A)-Ru(2)-C(6A)-C(5A)	65.5(3)
C(1A)-Ru(2)-C(6A)-C(5A)	130.1(5)
C(2A)-Ru(2)-C(6A)-C(5A)	102.0(4)
P(2)-Ru(2)-C(6A)-C(5A)	-134.6(3)
C(7A)-Ru(2)-C(6A)-C(1A)	-170.0(3)
C(4A)-Ru(2)-C(6A)-C(1A)	-100.7(3)
C(3A)-Ru(2)-C(6A)-C(1A)	-64.6(3)
C(2A)-Ru(2)-C(6A)-C(1A)	-28.2(3)
C(5A)-Ru(2)-C(6A)-C(1A)	-130.1(5)
P(2)-Ru(2)-C(6A)-C(1A)	95.2(3)
C(4A)-Ru(2)-C(7A)-O(1A)	40(12)
C(3A)-Ru(2)-C(7A)-O(1A)	8(12)
C(1A)-Ru(2)-C(7A)-O(1A)	71(12)
C(2A)-Ru(2)-C(7A)-O(1A)	-8(12)
C(5A)-Ru(2)-C(7A)-O(1A)	75(12)
P(2)-Ru(2)-C(7A)-O(1A)	-163(12)
C(6A)-Ru(2)-C(7A)-O(1A)	97(12)
C(21A)-P(2)-C(11A)-C(16A)	-60.6(4)
C(31A)-P(2)-C(11A)-C(16A)	-170.2(4)
Ru(2)-P(2)-C(11A)-C(16A)	64.2(4)
C(21A)-P(2)-C(11A)-C(12A)	67.7(5)
C(31A)-P(2)-C(11A)-C(12A)	-41.9(4)
Ru(2)-P(2)-C(11A)-C(12A)	-167.5(4)
C(16A)-C(11A)-C(12A)-C(13A)	-58.7(6)
P(2)-C(11A)-C(12A)-C(13A)	169.7(4)

C(11A)-C(12A)-C(13A)-C(14A)	57.2(7)
C(12A)-C(13A)-C(14A)-C(15A)	-54.1(7)
C(13A)-C(14A)-C(15A)-C(16A)	54.4(7)
C(14A)-C(15A)-C(16A)-C(11A)	-57.7(6)
C(12A)-C(11A)-C(16A)-C(15A)	58.8(6)
P(2)-C(11A)-C(16A)-C(15A)	-169.3(4)
C(31A)-P(2)-C(21A)-C(22A)	173.8(4)
C(11A)-P(2)-C(21A)-C(22A)	64.1(4)
Ru(2)-P(2)-C(21A)-C(22A)	-62.4(4)
C(31A)-P(2)-C(21A)-C(26A)	43.4(4)
C(11A)-P(2)-C(21A)-C(26A)	-66.3(5)
Ru(2)-P(2)-C(21A)-C(26A)	167.2(4)
C(26A)-C(21A)-C(22A)-C(23A)	-60.5(5)
P(2)-C(21A)-C(22A)-C(23A)	165.1(3)
C(21A)-C(22A)-C(23A)-C(24A)	57.7(5)
C(22A)-C(23A)-C(24A)-C(25A)	-54.1(6)
C(23A)-C(24A)-C(25A)-C(26A)	53.6(6)
C(24A)-C(25A)-C(26A)-C(21A)	-56.8(6)
C(22A)-C(21A)-C(26A)-C(25A)	60.5(6)
P(2)-C(21A)-C(26A)-C(25A)	-166.9(4)
C(21A)-P(2)-C(31A)-C(36A)	-173.8(4)
C(11A)-P(2)-C(31A)-C(36A)	-57.6(4)
Ru(2)-P(2)-C(31A)-C(36A)	66.2(4)
C(21A)-P(2)-C(31A)-C(32A)	59.7(4)
C(11A)-P(2)-C(31A)-C(32A)	175.9(4)
Ru(2)-P(2)-C(31A)-C(32A)	-60.2(4)
C(36A)-C(31A)-C(32A)-C(33A)	59.0(6)
P(2)-C(31A)-C(32A)-C(33A)	-172.6(4)
C(31A)-C(32A)-C(33A)-C(34A)	-56.7(6)
C(32A)-C(33A)-C(34A)-C(35A)	54.2(6)
C(33A)-C(34A)-C(35A)-C(36A)	-53.8(6)
C(32A)-C(31A)-C(36A)-C(35A)	-59.1(6)
P(2)-C(31A)-C(36A)-C(35A)	172.7(4)
C(34A)-C(35A)-C(36A)-C(31A)	56.5(6)

Symmetry transformations used to generate equivalent atoms:

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_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C25 H40 B F4 O P Ru'
_chemical_formula_weight          575.42

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 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0181   0.0091
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B'  'B'   0.0090   0.0039
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0492   0.0322
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'F'  'F'   0.0727   0.0534
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 'P'  'P'   0.2955   0.4335
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ru'  'Ru'   0.0552   3.2960
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'P -1'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                    12.2618(7)
_cell_length_b                    14.8597(8)
_cell_length_c                    15.2625(9)
_cell_angle_alpha                 110.465(2)
_cell_angle_beta                  97.596(2)
_cell_angle_gamma                 92.709(2)
_cell_volume                      2569.4(3)
_cell_formula_units_Z             4
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     6891
_cell_measurement_theta_min       3
_cell_measurement_theta_max       67

_exptl_crystal_description        'block'
_exptl_crystal_colour             'colorless'
_exptl_crystal_size_max           0.13
_exptl_crystal_size_mid           0.07
_exptl_crystal_size_min           0.05
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.488
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_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1192
_exptl_absorpt_coefficient_mu     5.914
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_correction_T_min   0.5136
_exptl_absorpt_correction_T_max   0.7564
_exptl_absorpt_process_details
;
 TWINABS. Program for empirical absorption correction of
 area-detector data for twinned crystals.
 University of Goetingen. Germany.  Sheldrick, G. M. 2007
;

_exptl_special_details
;
 Quasi-merohedral twin with 3:1 components ratio grown
 together with 180 deg rotation around reciprocal [0 1 0]
 vector; about 2/3 of all reflections are overlapped
;

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      1.54178
_diffrn_radiation_type            CuK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker APEX2 CCD detector'
_diffrn_measurement_method        '\w scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             25850
_diffrn_reflns_av_R_equivalents   0.0392
_diffrn_reflns_av_sigmaI/netI     0.0309
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_diffrn_reflns_theta_max          67.89
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_reflns_number_gt                 7715
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'APEX2-2008.5-0 (Bruker, 2008)'
_computing_cell_refinement        'SAINT v7.56A (Bruker, 2008)'
_computing_data_reduction         'TWINABS-2008/2 (Bruker, 2008)'
_computing_structure_solution     'XS/SHELXTL-2008/1 (Bruker, 2008)'
_computing_structure_refinement   'SHELXL-2008/4(Bruker, 2008)'
_computing_molecular_graphics     'XP v5.1 (Bruker, 1998)'
_computing_publication_material   'XCIF-2008/2 (Bruker, 2008)'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0629P)^2^+4.4408P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          8559
_refine_ls_number_parameters      640
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0483
_refine_ls_R_factor_gt            0.0408
_refine_ls_wR_factor_ref          0.1062
_refine_ls_wR_factor_gt           0.1010
_refine_ls_goodness_of_fit_ref    1.002
_refine_ls_restrained_S_all       1.002
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
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 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Ru1 Ru 0.07980(3) 0.07850(3) -0.16458(3) 0.02716(11) Uani 1 1 d . . .
H1M H 0.209(5) 0.083(5) -0.181(4) 0.059(19) Uiso 1 1 d . . .
P1 P 0.10055(10) 0.23910(9) -0.15102(9) 0.0261(3) Uani 1 1 d . . .
O1 O 0.1586(3) 0.1362(3) 0.0436(3) 0.0390(9) Uani 1 1 d . . .
C1 C 0.0502(5) -0.0402(4) -0.3133(4) 0.0318(11) Uani 1 1 d . . .
H1A H 0.091(5) -0.052(4) -0.359(4) 0.038 Uiso 1 1 d . . .
C2 C 0.0732(4) -0.0828(4) -0.2438(4) 0.0333(11) Uani 1 1 d . . .
H2A H 0.128(5) -0.118(4) -0.242(4) 0.040 Uiso 1 1 d . . .
C3 C 0.0057(4) -0.0686(3) -0.1735(4) 0.0317(11) Uani 1 1 d . . .
H3A H 0.026(5) -0.094(4) -0.130(4) 0.038 Uiso 1 1 d . . .
C4 C -0.0826(5) -0.0111(4) -0.1705(4) 0.0360(12) Uani 1 1 d . . .
H4A H -0.131(5) -0.004(4) -0.127(4) 0.043 Uiso 1 1 d . . .
C5 C -0.1028(4) 0.0326(4) -0.2373(4) 0.0356(12) Uani 1 1 d . . .
H5A H -0.155(5) 0.075(4) -0.241(4) 0.043 Uiso 1 1 d . . .
C6 C -0.0363(5) 0.0168(4) -0.3095(4) 0.0358(12) Uani 1 1 d . . .
H6A H -0.047(5) 0.037(4) -0.355(4) 0.043 Uiso 1 1 d . . .
C7 C 0.1314(4) 0.1172(4) -0.0349(4) 0.0313(11) Uani 1 1 d . . .
C11 C 0.0027(4) 0.3169(4) -0.0833(4) 0.0305(11) Uani 1 1 d . . .
H11A H 0.0321 0.3854 -0.0686 0.037 Uiso 1 1 calc R . .
C12 C -0.0055(5) 0.3053(4) 0.0122(4) 0.0343(12) Uani 1 1 d . . .
H12A H 0.0696 0.3103 0.0476 0.041 Uiso 1 1 calc R . .
H12B H -0.0431 0.2409 0.0008 0.041 Uiso 1 1 calc R . .
C13 C -0.0712(5) 0.3847(4) 0.0708(4) 0.0410(13) Uani 1 1 d . . .
H13A H -0.0780 0.3759 0.1313 0.049 Uiso 1 1 calc R . .
H13B H -0.0305 0.4488 0.0858 0.049 Uiso 1 1 calc R . .
C14 C -0.1856(5) 0.3813(4) 0.0173(4) 0.0428(14) Uani 1 1 d . . .
H14A H -0.2218 0.4378 0.0531 0.051 Uiso 1 1 calc R . .
H14B H -0.2306 0.3224 0.0128 0.051 Uiso 1 1 calc R . .
C15 C -0.1824(5) 0.3815(4) -0.0817(4) 0.0387(13) Uani 1 1 d . . .
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H15A H -0.1496 0.4454 -0.0772 0.046 Uiso 1 1 calc R . .
H15B H -0.2588 0.3709 -0.1163 0.046 Uiso 1 1 calc R . .
C16 C -0.1150(4) 0.3033(4) -0.1374(4) 0.0378(12) Uani 1 1 d . . .
H16A H -0.1124 0.3072 -0.2005 0.045 Uiso 1 1 calc R . .
H16B H -0.1507 0.2387 -0.1466 0.045 Uiso 1 1 calc R . .
C21 C 0.0713(4) 0.2495(3) -0.2688(3) 0.0286(10) Uani 1 1 d . . .
H21A H -0.0056 0.2179 -0.2957 0.034 Uiso 1 1 calc R . .
C22 C 0.0688(5) 0.3527(4) -0.2700(4) 0.0339(12) Uani 1 1 d . . .
H22A H 0.0241 0.3901 -0.2229 0.041 Uiso 1 1 calc R . .
H22B H 0.1449 0.3856 -0.2528 0.041 Uiso 1 1 calc R . .
C23 C 0.0188(5) 0.3483(4) -0.3690(4) 0.0360(12) Uani 1 1 d . . .
H23A H -0.0586 0.3185 -0.3845 0.043 Uiso 1 1 calc R . .
H23B H 0.0180 0.4147 -0.3696 0.043 Uiso 1 1 calc R . .
C24 C 0.0846(5) 0.2901(4) -0.4436(4) 0.0365(12) Uani 1 1 d . . .
H24A H 0.1592 0.3243 -0.4327 0.044 Uiso 1 1 calc R . .
H24B H 0.0472 0.2844 -0.5071 0.044 Uiso 1 1 calc R . .
C25 C 0.0954(4) 0.1889(4) -0.4403(4) 0.0329(11) Uani 1 1 d . . .
H25A H 0.0217 0.1516 -0.4597 0.039 Uiso 1 1 calc R . .
H25B H 0.1438 0.1549 -0.4856 0.039 Uiso 1 1 calc R . .
C26 C 0.1437(4) 0.1943(4) -0.3409(3) 0.0306(11) Uani 1 1 d . . .
H26A H 0.2196 0.2274 -0.3232 0.037 Uiso 1 1 calc R . .
H26B H 0.1477 0.1282 -0.3401 0.037 Uiso 1 1 calc R . .
C31 C 0.2388(4) 0.3095(4) -0.0957(4) 0.0293(11) Uani 1 1 d . . .
H31A H 0.2413 0.3638 -0.1201 0.035 Uiso 1 1 calc R . .
C32 C 0.2588(4) 0.3579(4) 0.0125(4) 0.0352(12) Uani 1 1 d . . .
H32A H 0.2606 0.3077 0.0413 0.042 Uiso 1 1 calc R . .
H32B H 0.1971 0.3967 0.0328 0.042 Uiso 1 1 calc R . .
C33 C 0.4474(4) 0.3203(4) -0.0921(4) 0.0371(12) Uani 1 1 d . . .
H33A H 0.5098 0.2820 -0.1115 0.044 Uiso 1 1 calc R . .
H33B H 0.4455 0.3699 -0.1217 0.044 Uiso 1 1 calc R . .
C34 C 0.4666(5) 0.3694(4) 0.0142(4) 0.0376(12) Uani 1 1 d . . .
H34A H 0.5342 0.4153 0.0342 0.045 Uiso 1 1 calc R . .
H34B H 0.4781 0.3205 0.0441 0.045 Uiso 1 1 calc R . .
C35 C 0.3682(4) 0.4235(4) 0.0478(4) 0.0359(12) Uani 1 1 d . . .
H35A H 0.3630 0.4779 0.0246 0.043 Uiso 1 1 calc R . .
H35B H 0.3804 0.4508 0.1179 0.043 Uiso 1 1 calc R . .
C36 C 0.3378(4) 0.2531(4) -0.1284(4) 0.0320(11) Uani 1 1 d . . .
H36A H 0.3265 0.2248 -0.1984 0.038 Uiso 1 1 calc R . .
H36B H 0.3424 0.1996 -0.1039 0.038 Uiso 1 1 calc R . .
B1 B 0.2707(6) -0.1368(5) -0.0486(4) 0.0441(17) Uani 1 1 d . . .
F1 F 0.3533(3) -0.1921(3) -0.0370(2) 0.0569(10) Uani 1 1 d . . .
F2 F 0.2117(4) -0.1819(3) -0.1377(3) 0.0920(18) Uani 1 1 d . . .
F3 F 0.2042(3) -0.1298(3) 0.0184(3) 0.0717(13) Uani 1 1 d . . .
F4 F 0.3159(5) -0.0465(3) -0.0361(3) 0.0858(16) Uani 1 1 d . . .
Ru2 Ru 0.44951(3) 0.08949(3) 0.23576(2) 0.02687(10) Uani 1 1 d . . .
H2M H 0.332(5) 0.104(5) 0.241(4) 0.058(19) Uiso 1 1 d . . .
P2 P 0.45276(11) 0.24725(9) 0.33967(9) 0.0263(3) Uani 1 1 d . . .
O1A O 0.3983(3) 0.1617(3) 0.0761(2) 0.0361(8) Uani 1 1 d . . .
C1A C 0.5206(5) 0.0169(4) 0.3391(4) 0.0322(12) Uani 1 1 d . . .
H1AA H 0.523(5) 0.040(4) 0.403(4) 0.039 Uiso 1 1 d . . .
C2A C 0.4321(5) -0.0442(4) 0.2789(4) 0.0319(11) Uani 1 1 d . . .
H2AA H 0.372(5) -0.062(4) 0.299(4) 0.038 Uiso 1 1 d . . .
C3A C 0.4299(5) -0.0740(4) 0.1797(4) 0.0354(12) Uani 1 1 d . . .
H3AA H 0.367(5) -0.110(4) 0.122(4) 0.043 Uiso 1 1 d . . .
C4A C 0.5181(5) -0.0433(4) 0.1454(4) 0.0326(12) Uani 1 1 d . . .
H4AA H 0.512(5) -0.060(4) 0.080(4) 0.039 Uiso 1 1 d . . .
C5A C 0.6106(5) 0.0163(4) 0.2071(4) 0.0378(12) Uani 1 1 d . . .
H5AA H 0.658(5) 0.041(4) 0.182(4) 0.045 Uiso 1 1 d . . .
C6A C 0.6109(5) 0.0482(4) 0.3042(4) 0.0351(12) Uani 1 1 d . . .
H6AA H 0.662(5) 0.088(4) 0.349(4) 0.042 Uiso 1 1 d . . .
C7A C 0.4184(4) 0.1362(4) 0.1377(3) 0.0287(11) Uani 1 1 d . . .
C11A C 0.3278(4) 0.3064(3) 0.3138(4) 0.0295(11) Uani 1 1 d . . .
H11B H 0.3208 0.2964 0.2449 0.035 Uiso 1 1 calc R . .
C12A C 0.3348(5) 0.4165(4) 0.3654(4) 0.0416(13) Uani 1 1 d . . .
```

```
H12C H 0.3345 0.4312 0.4338 0.050 Uiso 1 1 calc R . .
H12D H 0.4049 0.4469 0.3581 0.050 Uiso 1 1 calc R . .
C13A C 0.2370(5) 0.4582(4) 0.3249(5) 0.0457(14) Uani 1 1 d . . .
H13C H 0.2418 0.5286 0.3603 0.055 Uiso 1 1 calc R . .
H13D H 0.2411 0.4481 0.2578 0.055 Uiso 1 1 calc R . .
C14A C 0.1267(5) 0.4110(4) 0.3311(4) 0.0412(13) Uani 1 1 d . . .
H14C H 0.1178 0.4286 0.3984 0.049 Uiso 1 1 calc R . .
H14D H 0.0656 0.4354 0.2992 0.049 Uiso 1 1 calc R . .
C15A C 0.1204(5) 0.3022(4) 0.2849(4) 0.0398(13) Uani 1 1 d . . .
H15C H 0.1191 0.2846 0.2159 0.048 Uiso 1 1 calc R . .
H15D H 0.0507 0.2731 0.2943 0.048 Uiso 1 1 calc R . .
C16A C 0.2180(4) 0.2610(4) 0.3254(4) 0.0369(12) Uani 1 1 d . . .
H16C H 0.2119 0.1902 0.2923 0.044 Uiso 1 1 calc R . .
H16D H 0.2164 0.2742 0.3934 0.044 Uiso 1 1 calc R . .
C21A C 0.4744(4) 0.2514(3) 0.4636(3) 0.0272(10) Uani 1 1 d . . .
H21B H 0.5410 0.2160 0.4685 0.033 Uiso 1 1 calc R . .
C22A C 0.3823(4) 0.1949(4) 0.4872(3) 0.0289(11) Uani 1 1 d . . .
H22C H 0.3621 0.1313 0.4357 0.035 Uiso 1 1 calc R . .
H22D H 0.3159 0.2306 0.4931 0.035 Uiso 1 1 calc R . .
C23A C 0.4222(4) 0.1807(4) 0.5805(4) 0.0320(11) Uani 1 1 d . . .
H23C H 0.3619 0.1453 0.5964 0.038 Uiso 1 1 calc R . .
H23D H 0.4854 0.1410 0.5727 0.038 Uiso 1 1 calc R . .
C24A C 0.4575(5) 0.2762(4) 0.6612(4) 0.0378(12) Uani 1 1 d . . .
H24C H 0.4887 0.2641 0.7187 0.045 Uiso 1 1 calc R . .
H24D H 0.3920 0.3121 0.6751 0.045 Uiso 1 1 calc R . .
C25A C 0.5442(5) 0.3380(4) 0.6366(4) 0.0385(13) Uani 1 1 d . . .
H25C H 0.5601 0.4021 0.6879 0.046 Uiso 1 1 calc R . .
H25D H 0.6138 0.3066 0.6320 0.046 Uiso 1 1 calc R . .
C26A C 0.5037(5) 0.3507(4) 0.5429(4) 0.0358(12) Uani 1 1 d . . .
H26C H 0.5623 0.3880 0.5273 0.043 Uiso 1 1 calc R . .
H26D H 0.4378 0.3871 0.5489 0.043 Uiso 1 1 calc R . .
C31A C 0.5687(4) 0.3329(3) 0.3396(3) 0.0293(11) Uani 1 1 d . . .
H31B H 0.5616 0.3961 0.3898 0.035 Uiso 1 1 calc R . .
C32A C 0.6832(4) 0.3039(4) 0.3665(4) 0.0350(12) Uani 1 1 d . . .
H32C H 0.6865 0.2923 0.4268 0.042 Uiso 1 1 calc R . .
H32D H 0.6963 0.2434 0.3168 0.042 Uiso 1 1 calc R . .
C33A C 0.7723(5) 0.3841(4) 0.3774(4) 0.0397(13) Uani 1 1 d . . .
H33C H 0.7626 0.4427 0.4311 0.048 Uiso 1 1 calc R . .
H33D H 0.8460 0.3636 0.3922 0.048 Uiso 1 1 calc R . .
C34A C 0.7674(5) 0.4081(4) 0.2880(4) 0.0408(13) Uani 1 1 d . . .
H34C H 0.7874 0.3524 0.2364 0.049 Uiso 1 1 calc R . .
H34D H 0.8220 0.4639 0.2997 0.049 Uiso 1 1 calc R . .
C35A C 0.6525(5) 0.4321(4) 0.2572(4) 0.0405(13) Uani 1 1 d . . .
H35C H 0.6502 0.4413 0.1958 0.049 Uiso 1 1 calc R . .
H35D H 0.6368 0.4933 0.3046 0.049 Uiso 1 1 calc R . .
C36A C 0.5634(5) 0.3515(4) 0.2470(4) 0.0362(12) Uani 1 1 d . . .
H36C H 0.4895 0.3704 0.2300 0.043 Uiso 1 1 calc R . .
H36D H 0.5748 0.2917 0.1955 0.043 Uiso 1 1 calc R . .
B2 B 0.7564(5) 0.1082(4) 0.5480(4) 0.0356(13) Uani 1 1 d . . .
F5 F 0.7960(3) 0.1521(2) 0.6446(2) 0.0401(7) Uani 1 1 d . . .
F6 F 0.6587(3) 0.0517(2) 0.5367(2) 0.0453(8) Uani 1 1 d . . .
F7 F 0.8326(3) 0.0492(2) 0.5035(2) 0.0473(8) Uani 1 1 d . . .
F8 F 0.7371(3) 0.1775(3) 0.5089(2) 0.0560(9) Uani 1 1 d . . .

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P1 0.0270(6) 0.0259(6) 0.0263(6) 0.0100(5) 0.0055(5) 0.0036(5)
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O1 0.045(2) 0.042(2) 0.031(2) 0.0152(17) 0.0032(17) 0.0056(17)
C1 0.036(3) 0.032(3) 0.021(2) 0.004(2) -0.001(2) -0.001(2)
C2 0.032(3) 0.026(2) 0.035(3) 0.003(2) 0.004(2) 0.002(2)
C3 0.041(3) 0.022(2) 0.033(3) 0.013(2) 0.002(2) -0.004(2)
C4 0.036(3) 0.034(3) 0.038(3) 0.011(2) 0.009(2) 0.001(2)
C5 0.027(3) 0.033(3) 0.043(3) 0.011(2) -0.001(2) 0.000(2)
C6 0.041(3) 0.031(3) 0.032(3) 0.011(2) -0.002(2) -0.004(2)
C7 0.037(3) 0.027(3) 0.034(3) 0.018(2) 0.003(2) 0.005(2)
C11 0.033(3) 0.026(2) 0.033(3) 0.008(2) 0.010(2) 0.007(2)
C12 0.037(3) 0.033(3) 0.037(3) 0.015(2) 0.012(2) 0.009(2)
C13 0.050(3) 0.042(3) 0.037(3) 0.017(3) 0.021(3) 0.013(3)
C14 0.044(3) 0.044(3) 0.051(3) 0.022(3) 0.024(3) 0.017(3)
C15 0.035(3) 0.036(3) 0.045(3) 0.011(3) 0.012(2) 0.011(2)
C16 0.033(3) 0.037(3) 0.041(3) 0.009(2) 0.009(2) 0.005(2)
C21 0.035(3) 0.027(2) 0.027(2) 0.014(2) 0.004(2) 0.002(2)
C22 0.039(3) 0.029(3) 0.035(3) 0.014(2) 0.006(2) 0.004(2)
C23 0.038(3) 0.034(3) 0.041(3) 0.021(2) 0.005(2) 0.007(2)
C24 0.043(3) 0.043(3) 0.029(3) 0.021(2) 0.004(2) 0.004(2)
C25 0.034(3) 0.037(3) 0.030(3) 0.013(2) 0.008(2) 0.008(2)
C26 0.031(3) 0.030(3) 0.030(3) 0.011(2) 0.002(2) 0.003(2)
C31 0.026(3) 0.030(3) 0.031(3) 0.011(2) 0.004(2) 0.002(2)
C32 0.036(3) 0.033(3) 0.035(3) 0.010(2) 0.006(2) 0.004(2)
C33 0.032(3) 0.044(3) 0.035(3) 0.013(2) 0.005(2) 0.003(2)
C34 0.039(3) 0.034(3) 0.038(3) 0.011(2) 0.004(2) 0.000(2)
C35 0.036(3) 0.031(3) 0.038(3) 0.010(2) 0.004(2) 0.003(2)
C36 0.036(3) 0.031(3) 0.030(3) 0.011(2) 0.005(2) 0.005(2)
B1 0.065(5) 0.034(3) 0.024(3) 0.003(3) -0.005(3) 0.013(3)
F1 0.045(2) 0.065(2) 0.047(2) 0.0040(18) -0.0002(16) 0.0147(17)
F2 0.125(4) 0.059(3) 0.056(2) -0.008(2) -0.041(3) 0.043(3)
F3 0.053(2) 0.056(2) 0.089(3) -0.002(2) 0.037(2) -0.0072(18)
F4 0.174(5) 0.038(2) 0.048(2) 0.0160(18) 0.034(3) -0.008(3)
Ru2 0.0320(2) 0.02549(19) 0.02304(18) 0.00865(16) 0.00315(14) 0.00629(16)
P2 0.0314(7) 0.0246(6) 0.0239(6) 0.0092(5) 0.0059(5) 0.0043(5)
O1A 0.044(2) 0.035(2) 0.0291(19) 0.0145(16) 0.0004(16) -0.0004(16)
C1A 0.044(3) 0.031(3) 0.025(3) 0.015(2) 0.000(2) 0.011(2)
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C3A 0.040(3) 0.025(2) 0.034(3) 0.006(2) -0.003(2) 0.001(2)
C4A 0.049(3) 0.027(3) 0.023(2) 0.008(2) 0.010(2) 0.017(2)
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C6A 0.032(3) 0.032(3) 0.038(3) 0.013(2) -0.005(2) 0.007(2)
C7A 0.026(3) 0.027(2) 0.029(3) 0.007(2) 0.001(2) 0.001(2)
C11A 0.032(3) 0.025(2) 0.033(3) 0.011(2) 0.005(2) 0.009(2)
C12A 0.035(3) 0.032(3) 0.052(3) 0.008(3) 0.006(3) 0.005(2)
C13A 0.044(3) 0.026(3) 0.067(4) 0.016(3) 0.006(3) 0.009(2)
C14A 0.035(3) 0.033(3) 0.054(4) 0.014(3) 0.005(3) 0.012(2)
C15A 0.029(3) 0.039(3) 0.048(3) 0.014(3) 0.002(2) 0.004(2)
C16A 0.035(3) 0.032(3) 0.043(3) 0.015(2) 0.001(2) 0.004(2)
C21A 0.039(3) 0.022(2) 0.019(2) 0.0056(19) 0.004(2) 0.002(2)
C22A 0.029(3) 0.029(2) 0.031(3) 0.012(2) 0.010(2) 0.005(2)
C23A 0.032(3) 0.035(3) 0.034(3) 0.016(2) 0.011(2) 0.003(2)
C24A 0.046(3) 0.044(3) 0.028(3) 0.017(2) 0.010(2) 0.005(3)
C25A 0.049(3) 0.037(3) 0.027(3) 0.009(2) 0.005(2) -0.003(2)
C26A 0.044(3) 0.032(3) 0.030(3) 0.010(2) 0.007(2) -0.003(2)
C31A 0.035(3) 0.025(2) 0.029(3) 0.010(2) 0.008(2) 0.002(2)
C32A 0.035(3) 0.034(3) 0.044(3) 0.021(2) 0.010(2) 0.006(2)
C33A 0.034(3) 0.037(3) 0.048(3) 0.016(3) 0.009(3) 0.000(2)
C34A 0.047(3) 0.032(3) 0.046(3) 0.014(3) 0.018(3) -0.004(2)
C35A 0.052(4) 0.035(3) 0.038(3) 0.016(2) 0.012(3) 0.001(3)
C36A 0.042(3) 0.038(3) 0.030(3) 0.014(2) 0.006(2) 0.005(2)
B2 0.035(3) 0.040(3) 0.033(3) 0.014(3) 0.003(2) 0.007(3)
F5 0.0420(18) 0.0404(17) 0.0332(16) 0.0113(14) -0.0056(14) 0.0072(14)
F6 0.0354(18) 0.056(2) 0.0401(18) 0.0133(15) 0.0045(14) -0.0052(15)
F7 0.0440(19) 0.056(2) 0.0417(18) 0.0156(16) 0.0094(15) 0.0121(16)
F8 0.074(3) 0.050(2) 0.049(2) 0.0308(17) -0.0053(18) 0.0055(18)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Ru1 H1M 1.64(6) . ?
P1 C21 1.848(5) . ?
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C22 H22A 0.9900 . ?
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C13 C14 H14B 109.1 . . ?
C15 C14 H14B 109.1 . . ?
H14A C14 H14B 107.9 . . ?
C14 C15 C16 112.1(5) . . ?
C14 C15 H15A 109.2 . . ?
C16 C15 H15A 109.2 . . ?
C14 C15 H15B 109.2 . . ?
C16 C15 H15B 109.2 . . ?
H15A C15 H15B 107.9 . . ?
C15 C16 C11 109.8(4) . . ?
C15 C16 H16A 109.7 . . ?
C11 C16 H16A 109.7 . . ?
C15 C16 H16B 109.7 . . ?
C11 C16 H16B 109.7 . . ?
H16A C16 H16B 108.2 . . ?
C26 C21 C22 108.4(4) . . ?
C26 C21 P1 115.3(3) . . ?
C22 C21 P1 116.4(3) . . ?
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C22 C21 H21A 105.2 . . ?
P1 C21 H21A 105.2 . . ?
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C21 C22 H22A 109.7 . . ?
C23 C22 H22B 109.7 . . ?
C21 C22 H22B 109.7 . . ?
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C22 C23 H23B 109.4 . . ?
H23A C23 H23B 108.0 . . ?
C23 C24 C25 111.3(4) . . ?
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C25 C26 H26B 109.6 . . ?
C21 C26 H26B 109.6 . . ?
H26A C26 H26B 108.1 . . ?
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P1 C31 H31A 105.2 . . ?
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C35 C32 H32B 109.4 . . ?
H32A C32 H32B 108.0 . . ?
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C36 C33 H33A 109.2 . . ?
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C36 C33 H33B 109.2 . . ?
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C35 C34 H34A 109.5 . . ?
C33 C34 H34B 109.5 . . ?
C35 C34 H34B 109.5 . . ?
H34A C34 H34B 108.0 . . ?
C34 C35 C32 112.2(4) . . ?
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C32 C35 H35A 109.2 . . ?
C34 C35 H35B 109.2 . . ?
C32 C35 H35B 109.2 . . ?
H35A C35 H35B 107.9 . . ?
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C31 C36 H36B 109.5 . . ?
C33 C36 H36B 109.5 . . ?
H36A C36 H36B 108.1 . . ?
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F1 B1 F3 108.6(5) . . ?
F4 B1 F3 109.0(5) . . ?
F1 B1 F2 107.7(5) . . ?
F4 B1 F2 111.8(6) . . ?
F3 B1 F2 110.3(6) . . ?
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C7A Ru2 C3A 110.9(2) . . ?
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C7A Ru2 C1A 166.9(2) . . ?
C4A Ru2 C1A 74.79(19) . . ?
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C2A Ru2 C5A 75.0(2) . . ?
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C3A Ru2 P2 159.62(15) . . ?
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Ru2 C3A H3AA 118(3) . . ?
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C4A C5A Ru2 69.4(3) . . ?
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C15A C14A H14D 109.5 . . ?
C13A C14A H14D 109.5 . . ?
H14C C14A H14D 108.1 . . ?
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C14A C15A H15D 109.2 . . ?
C16A C15A H15D 109.2 . . ?
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C11A C16A H16D 109.5 . . ?
H16C C16A H16D 108.1 . . ?
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C26A C21A P2 117.7(3) . . ?
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C26A C21A H21B 104.7 . . ?
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C22A C23A H23C 109.3 . . ?
C24A C23A H23D 109.3 . . ?
C22A C23A H23D 109.3 . . ?
H23C C23A H23D 107.9 . . ?
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H24C C24A H24D 108.0 . . ?
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C24A C25A H25C 109.4 . . ?
C26A C25A H25D 109.4 . . ?
C24A C25A H25D 109.4 . . ?
H25C C25A H25D 108.0 . . ?
C25A C26A C21A 109.8(4) . . ?
C25A C26A H26C 109.7 . . ?
C21A C26A H26C 109.7 . . ?
C25A C26A H26D 109.7 . . ?
C21A C26A H26D 109.7 . . ?
H26C C26A H26D 108.2 . . ?
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C32A C31A H31B 106.5 . . ?
P2 C31A H31B 106.5 . . ?
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C31A C32A H32C 109.7 . . ?
C33A C32A H32D 109.7 . . ?
C31A C32A H32D 109.7 . . ?
H32C C32A H32D 108.2 . . ?
C34A C33A C32A 111.9(5) . . ?
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C32A C33A H33D 109.2 . . ?
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C35A C34A H34D 109.3 . . ?
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C36A C35A H35D 109.4 . . ?
H35C C35A H35D 108.0 . . ?
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H36C C36A H36D 108.1 . . ?
F8 B2 F6 109.8(5) . . ?
F8 B2 F7 110.2(5) . . ?
F6 B2 F7 108.7(5) . . ?
F8 B2 F5 109.8(5) . . ?
F6 B2 F5 108.4(5) . . ?
F7 B2 F5 109.9(5) . . ?

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C4 Ru1 P1 C21 -85.4(3) . . . . ?
C5 Ru1 P1 C21 -58.6(2) . . . . ?
C6 Ru1 P1 C21 -22.5(2) . . . . ?
C7 Ru1 P1 C11 -68.7(2) . . . . ?
C2 Ru1 P1 C11 138.9(4) . . . . ?
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C5 Ru1 P1 C31 -179.5(2) . . . . ?
C6 Ru1 P1 C31 -143.5(2) . . . . ?
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C2 Ru1 C1 C6 131.0(5) . . . . ?
C3 Ru1 C1 C6 100.6(4) . . . . ?
C4 Ru1 C1 C6 64.3(3) . . . . ?
C5 Ru1 C1 C6 28.9(3) . . . . ?
P1 Ru1 C1 C6 -60.1(4) . . . . ?
C7 Ru1 C1 C2 14.6(6) . . . . ?
C3 Ru1 C1 C2 -30.4(3) . . . . ?
C4 Ru1 C1 C2 -66.7(3) . . . . ?
C5 Ru1 C1 C2 -102.1(4) . . . . ?
C6 Ru1 C1 C2 -131.0(5) . . . . ?
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C6 C1 C2 C3 1.8(7) . . . . ?
Ru1 C1 C2 C3 58.0(4) . . . . ?
C6 C1 C2 Ru1 -56.3(4) . . . . ?
C7 Ru1 C2 C3 58.9(4) . . . . ?
C1 Ru1 C2 C3 -129.2(5) . . . . ?
C4 Ru1 C2 C3 -29.2(3) . . . . ?
C5 Ru1 C2 C3 -64.5(3) . . . . ?
C6 Ru1 C2 C3 -100.5(4) . . . . ?
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C7 Ru1 C2 C1 -171.9(3) . . . . ?
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C6 Ru1 C2 C1 28.7(3) . . . . ?
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C1 C2 C3 Ru1 -58.5(4) . . . . ?
C7 Ru1 C3 C2 -128.4(3) . . . . ?
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C4 Ru1 C3 C2 131.0(5) . . . . ?
C5 Ru1 C3 C2 102.3(4) . . . . ?
C6 Ru1 C3 C2 66.0(3) . . . . ?
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C1 Ru1 C3 C4 -100.5(4) . . . . ?
C5 Ru1 C3 C4 -28.7(3) . . . . ?
C6 Ru1 C3 C4 -65.0(3) . . . . ?
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C2 C3 C4 C5 -0.5(8) . . . . ?
Ru1 C3 C4 C5 55.7(5) . . . . ?
C2 C3 C4 Ru1 -56.2(4) . . . . ?
C7 Ru1 C4 C5 145.6(3) . . . . ?
C2 Ru1 C4 C5 -101.8(4) . . . . ?
C3 Ru1 C4 C5 -131.3(5) . . . . ?
C1 Ru1 C4 C5 -64.8(3) . . . . ?
C6 Ru1 C4 C5 -29.7(3) . . . . ?
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C7 Ru1 C4 C3 -83.1(3) . . . . ?
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C1 Ru1 C4 C3 66.4(3) . . . . ?
C5 Ru1 C4 C3 131.3(5) . . . . ?
C6 Ru1 C4 C3 101.6(4) . . . . ?
P1 Ru1 C4 C3 -178.2(2) . . . . ?
C3 C4 C5 C6 1.8(8) . . . . ?
Ru1 C4 C5 C6 56.6(5) . . . . ?
C3 C4 C5 Ru1 -54.8(5) . . . . ?
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C3 Ru1 C5 C4 29.3(3) . . . . ?
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C3 Ru1 C5 C6 -101.3(4) . . . . ?
C1 Ru1 C5 C6 -28.3(3) . . . . ?
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C7 Ru1 C6 C1 -117.4(7) . . . . ?
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C3 Ru1 C6 C1 -66.5(3) . . . . ?
C4 Ru1 C6 C1 -102.8(4) . . . . ?
C5 Ru1 C6 C1 -131.9(5) . . . . ?
P1 Ru1 C6 C1 130.0(3) . . . . ?
C7 Ru1 C6 C5 14.6(8) . . . . ?
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C3 Ru1 C6 C5 65.4(3) . . . . ?
C1 Ru1 C6 C5 131.9(5) . . . . ?
C4 Ru1 C6 C5 29.1(3) . . . . ?
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C3 Ru1 C7 O1 -15(7) . . . . ?
C1 Ru1 C7 O1 -55(7) . . . . ?
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P1 Ru1 C7 O1 148(7) . . . . ?
C21 P1 C11 C16 44.7(4) . . . . ?
C31 P1 C11 C16 154.0(4) . . . . ?
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Ru1 P1 C21 C26 -58.1(4) . . . . ?
C11 P1 C21 C22 49.6(4) . . . . ?
C31 P1 C21 C22 -58.4(4) . . . . ?
Ru1 P1 C21 C22 173.3(3) . . . . ?
C26 C21 C22 C23 60.7(5) . . . . ?
P1 C21 C22 C23 -167.4(4) . . . . ?
C21 C22 C23 C24 -58.6(6) . . . . ?
C22 C23 C24 C25 54.9(6) . . . . ?
C23 C24 C25 C26 -54.2(6) . . . . ?
C24 C25 C26 C21 57.5(6) . . . . ?
C22 C21 C26 C25 -60.5(5) . . . . ?
P1 C21 C26 C25 167.0(3) . . . . ?
C21 P1 C31 C32 149.3(4) . . . . ?
C11 P1 C31 C32 41.5(4) . . . . ?
Ru1 P1 C31 C32 -86.9(4) . . . . ?
C21 P1 C31 C36 -81.5(4) . . . . ?
C11 P1 C31 C36 170.7(4) . . . . ?
Ru1 P1 C31 C36 42.2(4) . . . . ?
C36 C31 C32 C35 56.1(6) . . . . ?
P1 C31 C32 C35 -172.7(4) . . . . ?
C36 C33 C34 C35 -54.8(6) . . . . ?
C33 C34 C35 C32 54.6(6) . . . . ?
C31 C32 C35 C34 -55.9(6) . . . . ?
C32 C31 C36 C33 -56.2(5) . . . . ?
P1 C31 C36 C33 171.3(3) . . . . ?
C34 C33 C36 C31 56.4(6) . . . . ?
C7A Ru2 P2 C21A 176.6(2) . . . . ?
C4A Ru2 P2 C21A -89.8(4) . . . . ?
C3A Ru2 P2 C21A 23.1(5) . . . . ?
C1A Ru2 P2 C21A -14.2(2) . . . . ?
C2A Ru2 P2 C21A 14.0(2) . . . . ?
C5A Ru2 P2 C21A -78.9(2) . . . . ?
C6A Ru2 P2 C21A -50.3(2) . . . . ?
C7A Ru2 P2 C31A -67.5(2) . . . . ?
C4A Ru2 P2 C31A 26.1(4) . . . . ?
C3A Ru2 P2 C31A 139.0(4) . . . . ?
C1A Ru2 P2 C31A 101.7(2) . . . . ?
C2A Ru2 P2 C31A 129.9(2) . . . . ?
C5A Ru2 P2 C31A 37.0(2) . . . . ?
C6A Ru2 P2 C31A 65.6(2) . . . . ?
C7A Ru2 P2 C11A 50.8(2) . . . . ?
C4A Ru2 P2 C11A 144.5(4) . . . . ?
C3A Ru2 P2 C11A -102.7(4) . . . . ?
C1A Ru2 P2 C11A -139.9(2) . . . . ?
C2A Ru2 P2 C11A -111.8(2) . . . . ?
C5A Ru2 P2 C11A 155.4(2) . . . . ?
C6A Ru2 P2 C11A -176.1(2) . . . . ?
C7A Ru2 C1A C2A -98.1(9) . . . . ?
C4A Ru2 C1A C2A -66.2(3) . . . . ?
C3A Ru2 C1A C2A -29.7(3) . . . . ?
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C5A Ru2 C1A C2A -102.8(4) . . . . ?
P2 Ru2 C1A C2A 136.7(3) . . . . ?
C6A Ru2 C1A C2A -132.1(5) . . . . ?
C7A Ru2 C1A C6A 34.0(10) . . . . ?
C4A Ru2 C1A C6A 66.0(3) . . . . ?
C3A Ru2 C1A C6A 102.5(4) . . . . ?
C2A Ru2 C1A C6A 132.1(5) . . . . ?
C5A Ru2 C1A C6A 29.3(3) . . . . ?
P2 Ru2 C1A C6A -91.1(3) . . . . ?
C6A C1A C2A C3A -1.8(8) . . . . ?
Ru2 C1A C2A C3A 54.4(4) . . . . ?
C6A C1A C2A Ru2 -56.2(4) . . . . ?
C7A Ru2 C2A C1A 157.0(4) . . . . ?
C4A Ru2 C2A C1A 100.9(4) . . . . ?
C3A Ru2 C2A C1A 131.1(5) . . . . ?
C5A Ru2 C2A C1A 64.1(3) . . . . ?
P2 Ru2 C2A C1A -54.3(4) . . . . ?
C6A Ru2 C2A C1A 28.8(3) . . . . ?
C7A Ru2 C2A C3A 25.9(5) . . . . ?
C4A Ru2 C2A C3A -30.2(3) . . . . ?
C1A Ru2 C2A C3A -131.1(5) . . . . ?
C5A Ru2 C2A C3A -66.9(3) . . . . ?
P2 Ru2 C2A C3A 174.6(3) . . . . ?
C6A Ru2 C2A C3A -102.3(4) . . . . ?
C1A C2A C3A C4A 1.7(8) . . . . ?
Ru2 C2A C3A C4A 57.2(4) . . . . ?
C1A C2A C3A Ru2 -55.5(4) . . . . ?
C7A Ru2 C3A C4A 66.2(4) . . . . ?
C1A Ru2 C3A C4A -100.7(3) . . . . ?
C2A Ru2 C3A C4A -129.3(5) . . . . ?
C5A Ru2 C3A C4A -29.6(3) . . . . ?
P2 Ru2 C3A C4A -142.3(4) . . . . ?
C6A Ru2 C3A C4A -64.7(3) . . . . ?
C7A Ru2 C3A C2A -164.4(3) . . . . ?
C4A Ru2 C3A C2A 129.3(5) . . . . ?
C1A Ru2 C3A C2A 28.7(3) . . . . ?
C5A Ru2 C3A C2A 99.8(3) . . . . ?
P2 Ru2 C3A C2A -12.9(6) . . . . ?
C6A Ru2 C3A C2A 64.6(3) . . . . ?
C2A C3A C4A C5A 0.6(8) . . . . ?
Ru2 C3A C4A C5A 58.9(4) . . . . ?
C2A C3A C4A Ru2 -58.3(4) . . . . ?
C7A Ru2 C4A C3A -121.0(3) . . . . ?
C1A Ru2 C4A C3A 65.9(3) . . . . ?
C2A Ru2 C4A C3A 30.4(3) . . . . ?
C5A Ru2 C4A C3A 130.8(5) . . . . ?
P2 Ru2 C4A C3A 146.7(3) . . . . ?
C6A Ru2 C4A C3A 102.3(3) . . . . ?
C7A Ru2 C4A C5A 108.2(3) . . . . ?
C3A Ru2 C4A C5A -130.8(5) . . . . ?
C1A Ru2 C4A C5A -64.9(3) . . . . ?
C2A Ru2 C4A C5A -100.4(3) . . . . ?
P2 Ru2 C4A C5A 15.9(5) . . . . ?
C6A Ru2 C4A C5A -28.5(3) . . . . ?
C3A C4A C5A C6A -2.9(8) . . . . ?
Ru2 C4A C5A C6A 55.1(5) . . . . ?
C3A C4A C5A Ru2 -57.9(4) . . . . ?
C7A Ru2 C5A C6A 151.1(3) . . . . ?
C4A Ru2 C5A C6A -131.4(5) . . . . ?
C3A Ru2 C5A C6A -102.1(4) . . . . ?
C1A Ru2 C5A C6A -30.0(3) . . . . ?
C2A Ru2 C5A C6A -65.1(3) . . . . ?
P2 Ru2 C5A C6A 55.7(4) . . . . ?
C7A Ru2 C5A C4A -77.4(3) . . . . ?
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C3A Ru2 C5A C4A 29.4(3) . . . . ?
C1A Ru2 C5A C4A 101.5(4) . . . . ?
C2A Ru2 C5A C4A 66.3(3) . . . . ?
P2 Ru2 C5A C4A -172.8(3) . . . . ?
C6A Ru2 C5A C4A 131.4(5) . . . . ?
C4A C5A C6A C1A 2.8(8) . . . . ?
Ru2 C5A C6A C1A 56.2(4) . . . . ?
C4A C5A C6A Ru2 -53.5(4) . . . . ?
C2A C1A C6A C5A -0.5(8) . . . . ?
Ru2 C1A C6A C5A -56.6(5) . . . . ?
C2A C1A C6A Ru2 56.1(4) . . . . ?
C7A Ru2 C6A C5A -39.9(4) . . . . ?
C4A Ru2 C6A C5A 29.4(3) . . . . ?
C3A Ru2 C6A C5A 65.5(3) . . . . ?
C1A Ru2 C6A C5A 130.1(5) . . . . ?
C2A Ru2 C6A C5A 102.0(4) . . . . ?
P2 Ru2 C6A C5A -134.6(3) . . . . ?
C7A Ru2 C6A C1A -170.0(3) . . . . ?
C4A Ru2 C6A C1A -100.7(3) . . . . ?
C3A Ru2 C6A C1A -64.6(3) . . . . ?
C2A Ru2 C6A C1A -28.2(3) . . . . ?
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P2 Ru2 C6A C1A 95.2(3) . . . . ?
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P2 Ru2 C7A O1A -163(12) . . . . ?
C6A Ru2 C7A O1A 97(12) . . . . ?
C21A P2 C11A C16A -60.6(4) . . . . ?
C31A P2 C11A C16A -170.2(4) . . . . ?
Ru2 P2 C11A C16A 64.2(4) . . . . ?
C21A P2 C11A C12A 67.7(5) . . . . ?
C31A P2 C11A C12A -41.9(4) . . . . ?
Ru2 P2 C11A C12A -167.5(4) . . . . ?
C16A C11A C12A C13A -58.7(6) . . . . ?
P2 C11A C12A C13A 169.7(4) . . . . ?
C11A C12A C13A C14A 57.2(7) . . . . ?
C12A C13A C14A C15A -54.1(7) . . . . ?
C13A C14A C15A C16A 54.4(7) . . . . ?
C14A C15A C16A C11A -57.7(6) . . . . ?
C12A C11A C16A C15A 58.8(6) . . . . ?
P2 C11A C16A C15A -169.3(4) . . . . ?
C31A P2 C21A C22A 173.8(4) . . . . ?
C11A P2 C21A C22A 64.1(4) . . . . ?
Ru2 P2 C21A C22A -62.4(4) . . . . ?
C31A P2 C21A C26A 43.4(4) . . . . ?
C11A P2 C21A C26A -66.3(5) . . . . ?
Ru2 P2 C21A C26A 167.2(4) . . . . ?
C26A C21A C22A C23A -60.5(5) . . . . ?
P2 C21A C22A C23A 165.1(3) . . . . ?
C21A C22A C23A C24A 57.7(5) . . . . ?
C22A C23A C24A C25A -54.1(6) . . . . ?
C23A C24A C25A C26A 53.6(6) . . . . ?
C24A C25A C26A C21A -56.8(6) . . . . ?
C22A C21A C26A C25A 60.5(6) . . . . ?
P2 C21A C26A C25A -166.9(4) . . . . ?
C21A P2 C31A C36A -173.8(4) . . . . ?
C11A P2 C31A C36A -57.6(4) . . . . ?
Ru2 P2 C31A C36A 66.2(4) . . . . ?
C21A P2 C31A C32A 59.7(4) . . . . ?
C11A P2 C31A C32A 175.9(4) . . . . ?
Ru2 P2 C31A C32A -60.2(4) . . . . ?
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C36A C31A C32A C33A 59.0(6) . . . . ?
P2 C31A C32A C33A -172.6(4) . . . . ?
C31A C32A C33A C34A -56.7(6) . . . . ?
C32A C33A C34A C35A 54.2(6) . . . . ?
C33A C34A C35A C36A -53.8(6) . . . . ?
C32A C31A C36A C35A -59.1(6) . . . . ?
P2 C31A C36A C35A 172.7(4) . . . . ?
C34A C35A C36A C31A 56.5(6) . . . . ?

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_diffrn_reflns_theta_full              67.89
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_refine_diff_density_max    1.573
_refine_diff_density_min   -0.609
_refine_diff_density_rms    0.085
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