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communication

Stoichiometric and Catalytic Cross Dimerization between Butadiene and Methyl Acrylate Promoted by Ruthenium(0) Complex

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Experimental

General procedures

All manipulations were carried out under dry nitrogen using standard Schlenk and vacuum line techniques. Benzene, hexane and Et_2O were dried over anhydrous calcium chloride and then distilled from sodium wire under nitrogen with benzophenone ketyl as an indicator. MeCN was dried over calcium chloride and distilled over calcium hydride under nitrogen. Ru(*cisoid*-η^4-butadiene)(η^4-1,5-COD)(MeCN) (**1a**) was prepared according to the reported method.[1] Methyl acrylate was dried over anhydrous $MgSO_4$ and purified by the valve-to-valve distillation under reduced pressure. Butadiene was purchased from Deuterated solvents for use in NMR experiments were purchased from Kanto Chemical and dried with sodium wire for C_6D_6, and was directly vacuum transferred into an NMR tube. NMR spectra were recorded on a JEOL LA-300 spectrometer (300.4 MHz for ^{1}H) with chemical shifts reported in ppm downfield from TMS for ^{1}H and from 85% H_3PO_4 in D_2O for ^{31}P NMR. IR spectra were recorded on a JASCO FT/IR-4100 spectrometer using KBr disks. GLC analysis was performed on a Shimadzu GC-14B with FID detector equipped with a capillary column (TC-wax, 0.25 mmf x 30 m). GLC conditions: injector: 220 ˚C, detector 220 ˚C, Initial temp.: 50 ˚C, Initial time: 5 min, program rate: 5 ˚C/min, final temp.: 220 ˚C. GC-MS spectra were performed on a Shimadzu QP2010 equipped with a capillary column (TC-wax, 0.25 mmf x 30 m). Elemental analysis was performed on a Perkin-Elmer 2400 Series II CHN spectrometer.

Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(MeCN) (2a). Methyl acrylate (30.0 μL, 0.333 mmol) was added to a benzene solution (6 mL) of **1a** (98.8 mg, 0.325 mmol) at 6 ˚C by a hypodermic syringe. The reaction mixture was stirred for 3 h at 6 ˚C and then allowed to rise to room temperature. After removal of all volatile matters, of Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(MeCN) (**2a**) was obtained as brown oil in 97% yield (122.5 mg, 0.314 mmol). This compound was characterized by spectroscopic method. ^{1}H NMR (300 MHz, C_6D_6, r.t.): δ 0.82 (s, 3H, NC*Me*), 0.99 (t, $J_{H\text{-}H}$ = 7.2 Hz, 3H, 7-*Me*), 1.22 (q, $J_{H\text{-}H}$ = 7.0 Hz, 1H, 5-C*H*), 1.30 (dqui, $J_{H\text{-}H}$ = 13.8, 7.0 Hz, 1H, 6-CH_2), 1.39 (d, $J_{H\text{-}H}$ = 7.1 Hz, 1H, 2-C*H*), 1.48 (dqui, $J_{H\text{-}H}$ = 13.8, 7.0 Hz, 1H, 6-CH_2), 1.95-2.1 (m, 4H,

COD), 2.15-2.3 (m, 2H, COD), 2.4-2.55 (m, 2H, COD), 3.0-3.1 (m, 1H, COD), 3.3-3.45 (m, 2H, COD), 3.49 (s, 3H, O*Me*), 4.52-4.57 (m, 1H, COD), 4.86 (dd, $J_{H\text{-}H}$ = 7.0, 5.1 Hz, 1H, 4-C*H*), 6.10 (dd, $J_{H\text{-}H}$ = 7.1, 5.1 Hz, 1H, 3-C*H*).

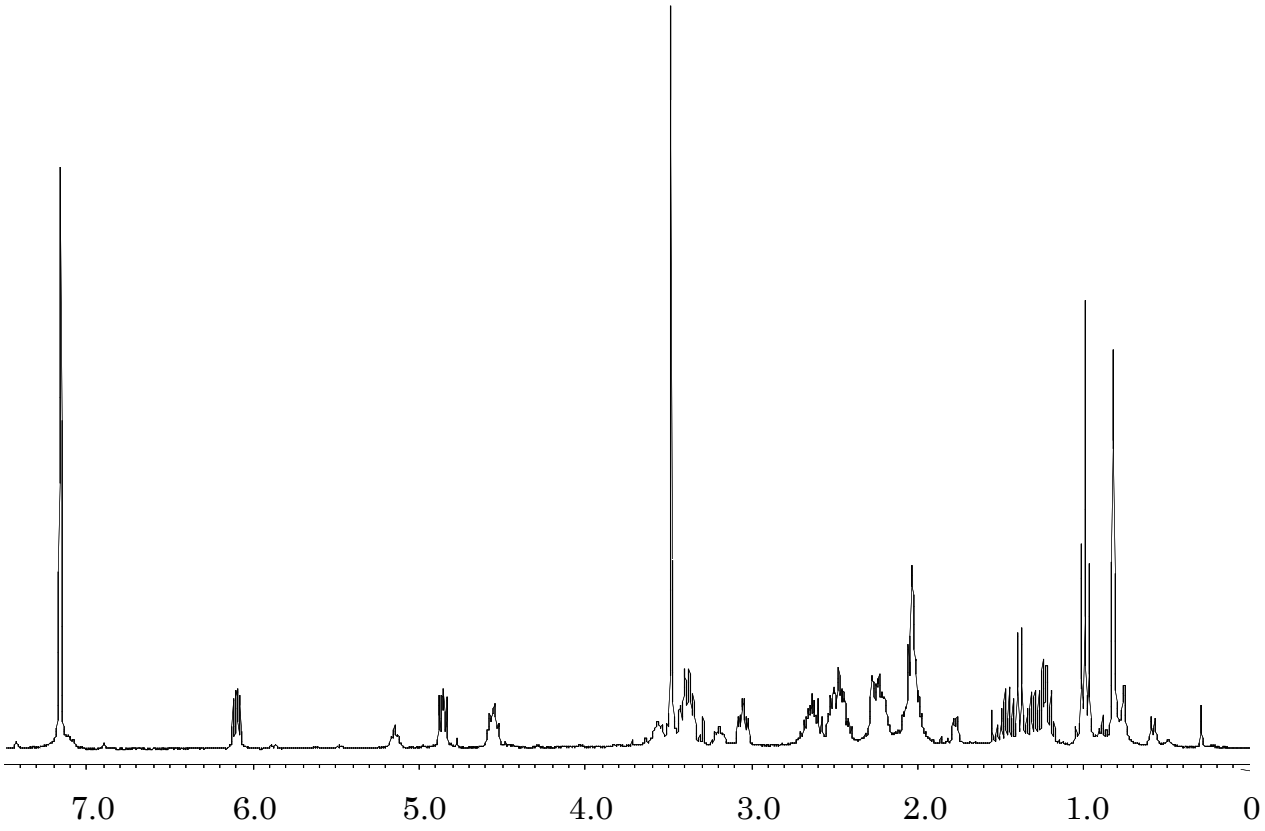


Figure S1. ^{1}H NMR Spectrum of 2a in benzene-d_6 at room temperature.

Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(PPh_3) (2b). To a benzene solution (6 mL) of **1a** (127.3 mg, 0.418 mmol), methyl acrylate (38.0 μL, 0.420 mmol) was added by a hypodermic syringe and the reaction mixture was stirred at 6 ˚C for 3 h. Then, PPh_3 (109.7 mg, 0.4182 mmol) was added to the solution. The solution was stirred for 3 h at room temperature. After removal of all volatile matters, yellow powder was obtained. Recrystallization of the powder from cold Et_2O gave Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(PPh_3) (**2b**) as dark

yellow blocks in 36% yield. (92.3 mg, 0.150 mmol). ^{1}H NMR (300 MHz, C_6D_6, r.t.): δ –0.59 (m, 1H, 5-C*H*), 0.36 (t, $J_{H\text{-}H}$ = $J_{H\text{-}P}$ = 7.5 Hz, 1H, 2-C*H*), 0.69 (t, $J_{H\text{-}H}$ = 7.2 Hz, 3H, 7-*Me*), 0.92-1.02 (m, 1H, 6-CH_2), 1.20-1.27 (m, 1H, 6-CH_2), 1.38-1.50 (m, 1H, COD), 1.8-2.5 (m, 8H, COD), 3.2 (m, 1H, COD), 3.44 (s, 3H, O*Me*), 3.85 (m, 1H, COD), 4.7 (m, 1H, COD), 4.91 (t, $J_{H\text{-}H}$ = 7.5 Hz, 1H, 4-C*H*), 6.27 (t, $J_{H\text{-}H}$ = 7.5 Hz, 1H, 3-C*H*), 6.98-7.04 (m, 9H, P*Ph*), 7.29 (t, *J* = 8.1 Hz, 6H, P*Ph*). ^{13}C{^{1}H} NMR (75.5 MHz, C_6D_6, r.t.): δ 18.0 (s), 24.3 (s), 28.1 (s), 28.3 (s), 30.1 (s), 31.7 (s), 34.9 (s), 43.1 (d, $J_{C\text{-}P}$ = 5 Hz), 50.3 (s), 64.1 (s), 70.8 (d, $J_{C\text{-}P}$ = 5 Hz), 72.2 (d, $J_{C\text{-}P}$ = 5 Hz), 72.8 (d, $J_{C\text{-}P}$ = 4 Hz), 74.1 (d, $J_{C\text{-}P}$ = 4 Hz), 84.9 (s), 94.0 (s), 128.8 (partly obscured by the solvent signals), 134.3 (d, $J_{C\text{-}P}$ = 8 Hz), 138.3 (d, $J_{C\text{-}P}$ = 33 Hz), 175.8 (s). ^{31}P{^{1}H} NMR (121.6 MHz, C_6D_6, r.t.): δ 51.8 (s). IR (KBr, cm^{-1}): 3021 (m), 2921 (m), 2871 (m), 2827 (m), 1691 (vs), 1586 (w), 1457 (s), 1432 (s), 1316 (m), 1160 (s). Anal. Calcd for $C_{34}H_{39}O_2PRu$: C, 66.76; H, 6.43. Found: C, 66.64; H, 6.52.

Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(CO) (2c). To a reaction mixture of **1a** (94.0 mg, 0.310 mmol) with methyl acrylate (27.8 μL, 0.309 mmol), CO gas (0.1 MPa) was bubbled to the solution and then the mixture was stirred at room temperature for 3 h. After removal of all volatile matters, off yellow powder was obtained. Recrystallization of the powder from cold Et_2O gave Ru{*cisoid*-η^4-(2*E*,4*E*)-(methyl hepta-2,4-dienoate)}(η^4-1,5-COD)(CO) (**2c**) as yellow needles in 53% yield. (62.3 mg, 0.165 mmol). This compound was characterized by spectroscopic method. ^{1}H NMR (300 MHz, C_6D_6, r.t.): δ 0.75 (obscured by the adjacent signal, 5-C*H*), 0.77-0.79 (obscured by the adjacent signal, 1H, 6-CH_2), 0.78 (d, $J_{H\text{-}H}$ = 7.2 Hz, 3H, 7-*Me*), 1.03-1.05 (m, 1H, 6-CH_2), 1.12 (d, $J_{H\text{-}H}$ = 6.9 Hz, 1H, 2-C*H*), 1.5-1.8 (m, 2H, COD), 1.8-2.1 (m, 4H, COD), 2.1-2.3 (m, 1H, COD), 2.4-2.6 (m, 1H, COD), 3.0-3.2 (m, 2H, COD), 3.31 (s, 3H, O*Me*), 3.4-3.5 (m, 1H, COD), 4.4-4.5 (m, 1H, COD), 4.64 (t, $J_{H\text{-}H}$ = 6.9 Hz, 4-C*H*), 5.94 (dd, $J_{H\text{-}H}$ = 6.9, 5.1 Hz, 1H, 3-C*H*). IR (KBr, cm^{-1}): 2964 (m), 2835 (w), 1976 (s), 1739 (m), 1699 (m), 1436 (w).

Iodolysis of 2a. Complex **2a** (10.2 mg, 0.034 mmol) was dissolved in C_6D_6 (600 μL) and then excess iodine was added to the solution. After 10 min at room temperature, the sample was characterized by NMR, GC and GC-MS. The product was characterized as (*2E,4E*)-methyl hepta-2,4-dienoate in 80% yield on the basis of the

spectroscopic data. ^{1}H NMR (300 MHz, C_6D_6, r.t.): δ 0.72 (t, J_{H-H} = 7.4 Hz, 3H, 7-*Me*), 1.74 (m, 2H, 6-C*H*$_2$), 3.45 (s, 3H, O*Me*), 5.64 (dt, J_{H-H} = 15.0, 6.6 Hz, 1H, 5-C*H*), 5.83 (dd, J_{H-H} = 15.0, 10.9 Hz, 1H, 4-C*H*), 5.86 (d, J_{H-H} = 15.4 Hz, 1H, 2-C*H*), 7.44 (dd, J_{H-H} = 15.4, 10.9 Hz, 1H, 3-C*H*). *lit.*[2]: ^{1}H NMR (200 MHz, C_6D_6): δ 0.73 (t, 3H), 1.80 (m, 2H), 5.66 (dt, *J* = 15.0, 7.0 Hz, 1H), 5.78 (dd, *J* = 15.0, 10.8 Hz, 1H), 5.83 (d, *J* = 15.4 Hz, 1H), 7.45 (dd, *J* = 15.4, 10.9 Hz, 1H). GC: (retention time) = 19.10 min. GC-MS (m/e) = 140 (M^+), 111, 109, 81.

Iodolysis of 2b. Similar to **2a**, iodolysis of **2b** (8.3 mg, 0.014 mmol) produced (*2E,4E*)-methyl hepta-2,4-dienoate in 81% yield.

Iodolysis of 2c. Similar to **2a**, iodolysis of **2c** (5.4 mg, 0.017 mmol) produced) produced (*2E,4E*)-methyl hepta-2,4-dienoate in 78% yield.

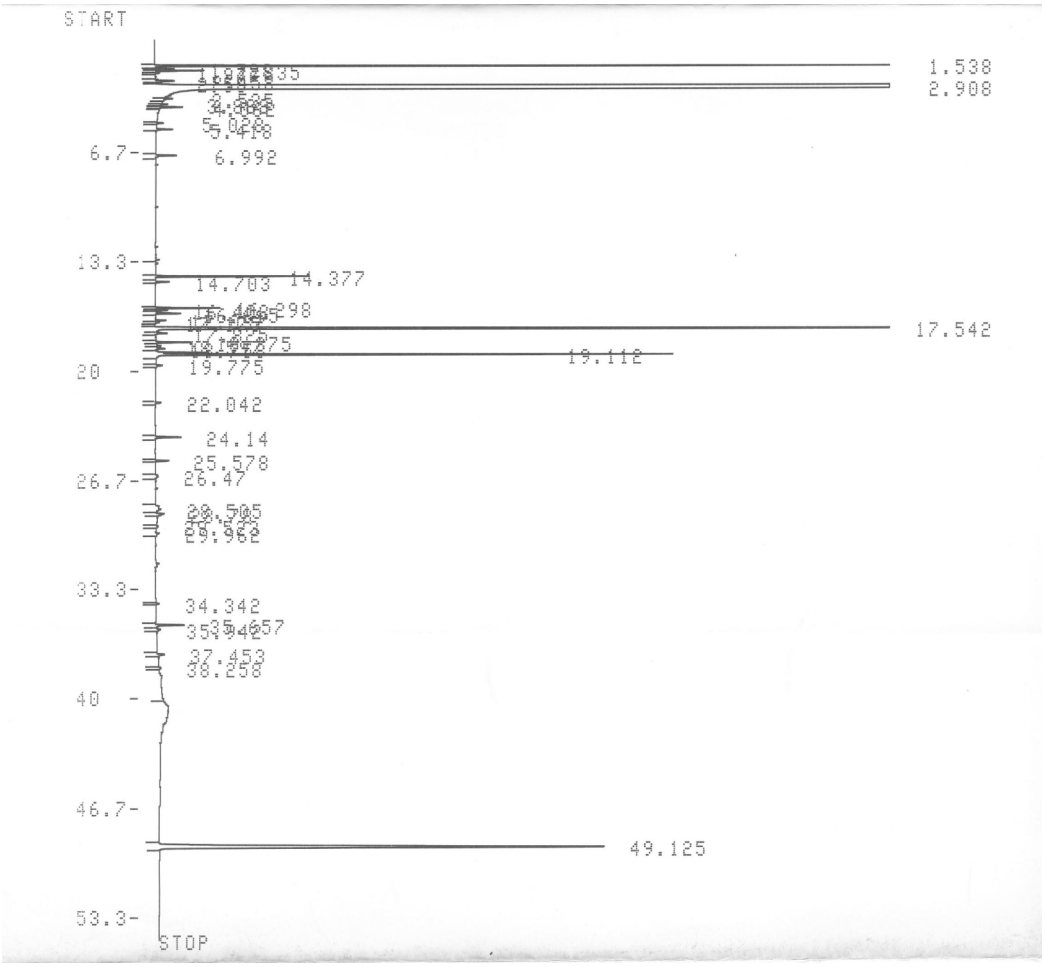
Treatment of 2b with butadiene. Complex **2b** (11.6 mg, 0.019 mmol) in C_6D_6 (600 μL) was exposed to excess amount of butadiene for 1 day at room temperature. Ru(*cisoid*-η^4-butadiene)(η^4-1,5-COD)(PPh_3) (**2b**) and (*2E,4E*)-methyl hepta-2,4-dienoate were produced in 80% and 49% yields, respectively. ^{1}H NMR spectrum of **2b**: ^{1}H NMR (300 MHz, C_6D_6, r.t.): δ –1.00 (m, 2H, *endo*-C*H*$_2$ in butadiene), 1.43 (m, 2H, *exo*-C*H*$_2$ in butadiene), 1.43-2.20 (m, 8H, COD), 2.88 (m, 2H, COD), 3.39 (m, 2H, COD), 5.14 (m, 2H, 2- and 3-C*H* in butadiene), 6.97-7.0 (m, 9H, P*Ph*), 7.75 (dd, *J* = 8.4, 1.2 Hz, 6H). ^{31}P{^{1}H} NMR (121.6 MHz, C_6D_6, r.t.): δ 64.4(s).

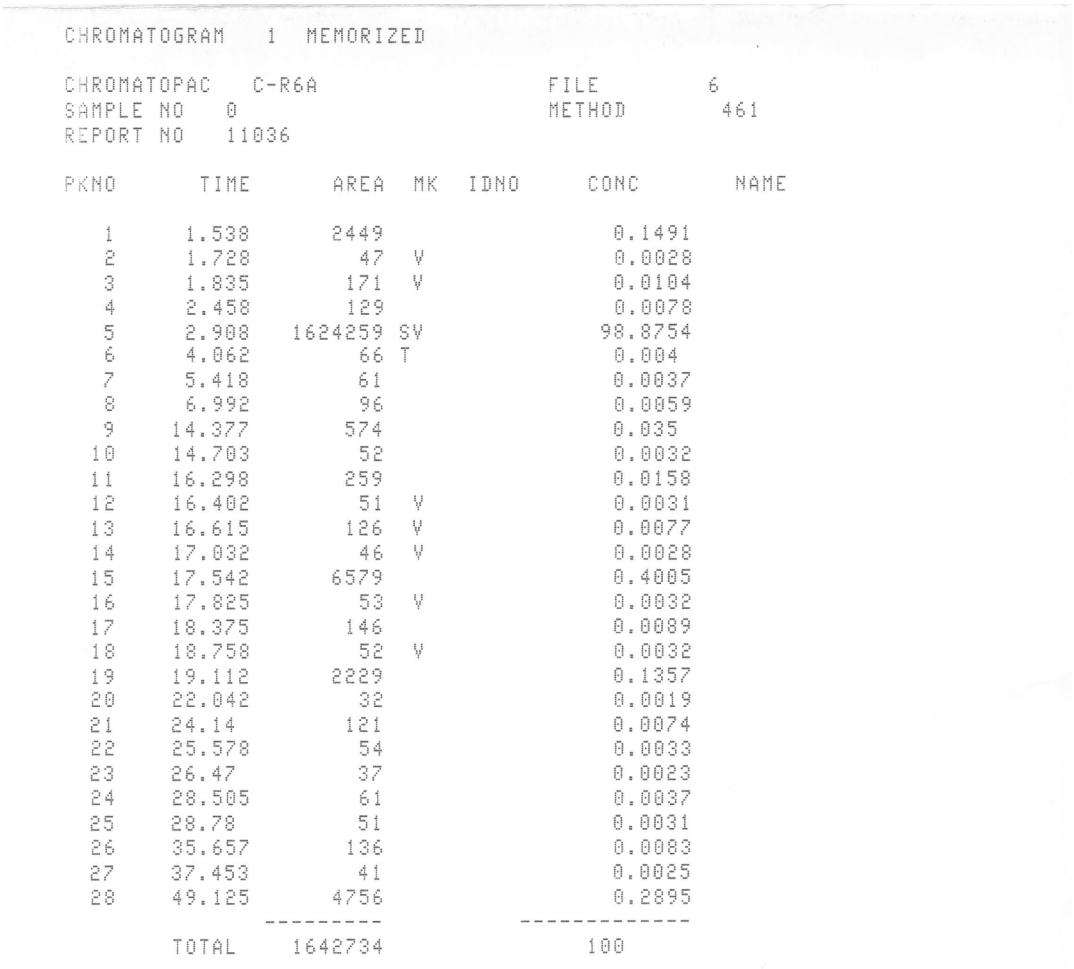
Treatment of 2a with butadiene. Similar to **2b**, treatment of **2a** (5.3 mg, 0.014 mmol) with excess butadiene produced (*2E,4E*)-methyl hepta-2,4-dienoate in 49%. From the reaction product, *supine,prone*-Ru(η^3:η^3-2,7-octadiene-1,8-diyl)(η^4-1,5-COD), a oxidative coupling product between butadiene molecules and 1,5-COD were observed in 54% and 21% yields, respectively.

Treatment of 2c with butadiene. Similar to **2b**, treatment of **2c** (10.5 mg, 0.029 mmol) with excess butadiene produced (*2E,4E*)-methyl hepta-2,4-dienoate in 56%.

Catalytic cross dimerization between butadiene and methyl acrylate promoted by 1a. As a typical example, the catalysis was carried out as follows. Complex **1a** (60

mg, 0.2 mmol) was placed in a 25 mL Schlenk tube into which benzene (1 mL) and methyl acrylate (960 μL, 10 mmol) were added. The solution was transferred into an autoclave by cannular tube and then butadiene (225 mL, 10 mmol) was added. The autoclave was degassed by three freeze-pump-thaw cycles and then dry nitrogen gas was introduced in it. The reaction was performed at 80 ˚C for 4 h to give a mixture of (*2E,5Z*)-methyl hepta-2,4-dienoate in 32% and (*2E,4E*)-methyl hepta-2,4-dienoate in 11% yield. ^{1}H NMR spectrum of (*2E,5Z*)-methyl hepta-2,4-dienoate: ^{1}H NMR (300 MHz, $CDCl_3$, r.t.): δ 1.60 (d, $J_{H\text{-}H}$ = 6.5 Hz, 3H, 7-*Me*), 2.93 (br.t, $J_{H\text{-}H}$ = 6 Hz, 2H, 4-CH_2), 3.70 (s, 3H, O*Me*), 5.38 (dtq, 14.1, 6.9, 1.5 Hz, 1H, 5-C*H*), 5.61 (dqt, $J_{H\text{-}H}$ = 14.1, 6.5, 1.5 Hz, 1H, 6-C*H*), 5.82 (dt, $J_{H\text{-}H}$ = 15.6, 1.8 Hz, 2-C*H*), 6.94 (dt, $J_{H\text{-}H}$ = 15.6, 6.2 Hz, 3-C*H*). *lit.*[3]: ^{1}H NMR (360 MHz, $CDCl_3$): δ 1.63 (d, *J* = 6.7 Hz, 3H), 2.95 (dd, *J* = 6.6, 6.4 Hz, 2H), 3.73 (s, 3H), 5.35-5.48 (m, 1H), 5.55-5.71 (m, 2H), 5.84 (dt, *J* = 15.7, 1.7 Hz, 1H), 6.96 (dt, *J* = 15.7, 6.3 Hz, 1H).





CHROMATOGRAM 1 MEMORIZED

CHROMATOPAC C-R6A FILE 6
SAMPLE NO 0 METHOD 461
REPORT NO 11036

PKNO	TIME	AREA	MK	IDNO	CONC	NAME
1	1.538	2449			0.1491	
2	1.728	47	V		0.0028	
3	1.835	171	V		0.0104	
4	2.458	129			0.0078	
5	2.908	1624259	SV		98.8754	
6	4.062	66	T		0.004	
7	5.418	61			0.0037	
8	6.992	96			0.0059	
9	14.377	574			0.035	
10	14.703	52			0.0032	
11	16.298	259			0.0158	
12	16.402	51	V		0.0031	
13	16.615	126	V		0.0077	
14	17.032	46	V		0.0028	
15	17.542	6579			0.4005	
16	17.825	53	V		0.0032	
17	18.375	146			0.0089	
18	18.758	52	V		0.0032	
19	19.112	2229			0.1357	
20	22.042	32			0.0019	
21	24.14	121			0.0074	
22	25.578	54			0.0033	
23	26.47	37			0.0023	
24	28.505	61			0.0037	
25	28.78	51			0.0031	
26	35.657	136			0.0083	
27	37.453	41			0.0025	
28	49.125	4756			0.2895	
	TOTAL	1642734			100	

Figure S2. GLC Chart for the catalytic cross dimerization between butadiene and methyl acrylate promoted by 1a.

Table S1. Assignment of GLC signals.

Retention time (min)	area	assignment
1.538	2449	acetone
2.908	1624259	benzene
14.377	574	an isomer of methyl heptadienoate
16.298	259	an isomer of methyl heptadienoate
17.542	6579	(2*E*,5*Z*)-methyl hepta-2,5-dienoate
19.112	2229	(2*E*,4*E*)-methyl hepta-2,4-dienoate
24.14	121	naphthalene
35.657	136	dimethyl 2-hexenoate
49.125	4756	triphenylmethane as an internal standard

conditions: detector: FID. column: TC-WAX (0.25 mmf x 30 m). Injector: 220 ˚C. Detector: 220 ˚C. Initial temp.: 50 ˚C. Initial time: 5 min. Program rate: 5 ˚C/min. Final temp. = 220 ˚C. Final time: 30 min.

X-ray Crystallography of 2b and 2c. The crystallographic data were measured on a Rigaku RASA7R-Mercury II diffractometer using Mo-Kα (λ = 0.71069 Å) radiation with a graphite crystal monochrometer. A single crystal was selected by use of a polarized microscope and mounted onto a glass capillary with Paraton N oil. The data were processed using a CrystalStructure package software.[4] All non-hydrogen atoms were found by using the results of the Direct methods (SHELXL-97[5]). All non-hydrogen atoms were found on difference maps. All hydrogen atoms were located in the calculated positions.

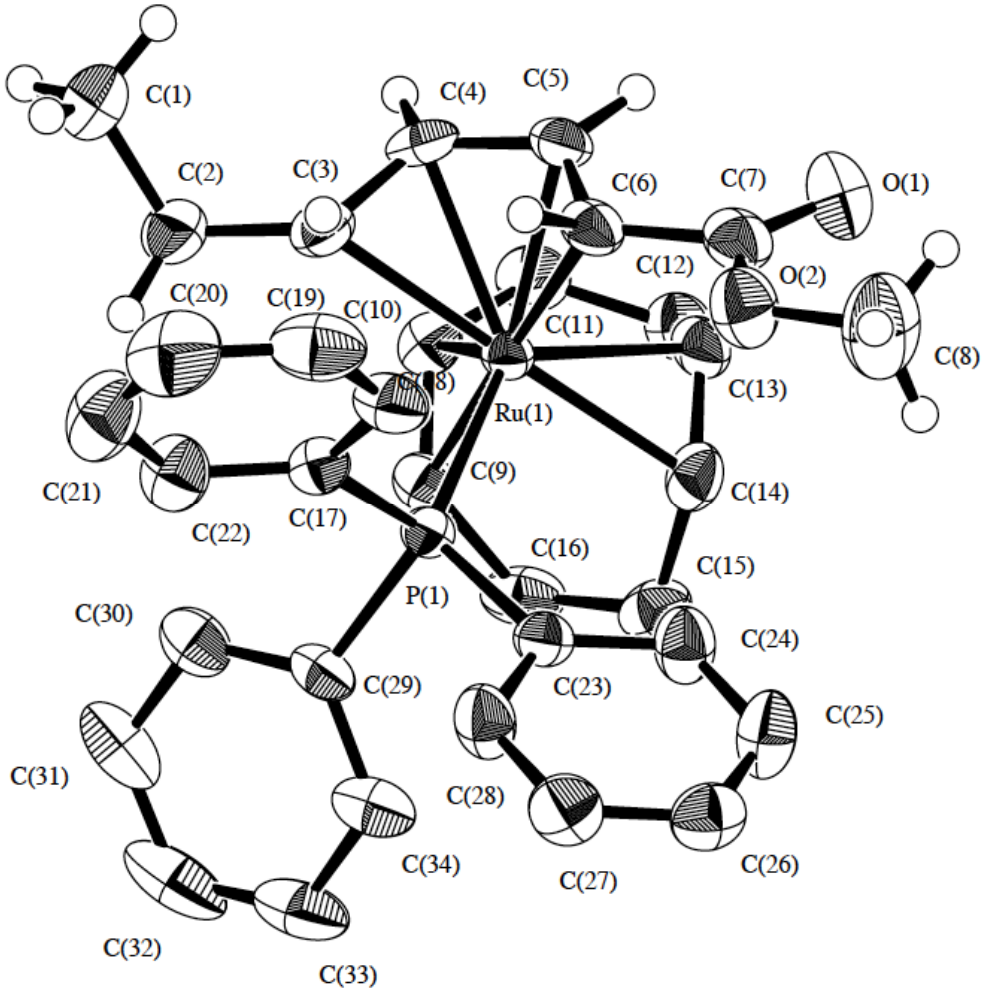


Figure S3. Molecular structure of **2b** with numbering schemes. Hydrogen atoms in the 1,5-COD ligand were omitted for clarity. Ellipsoids represent 50% probability.

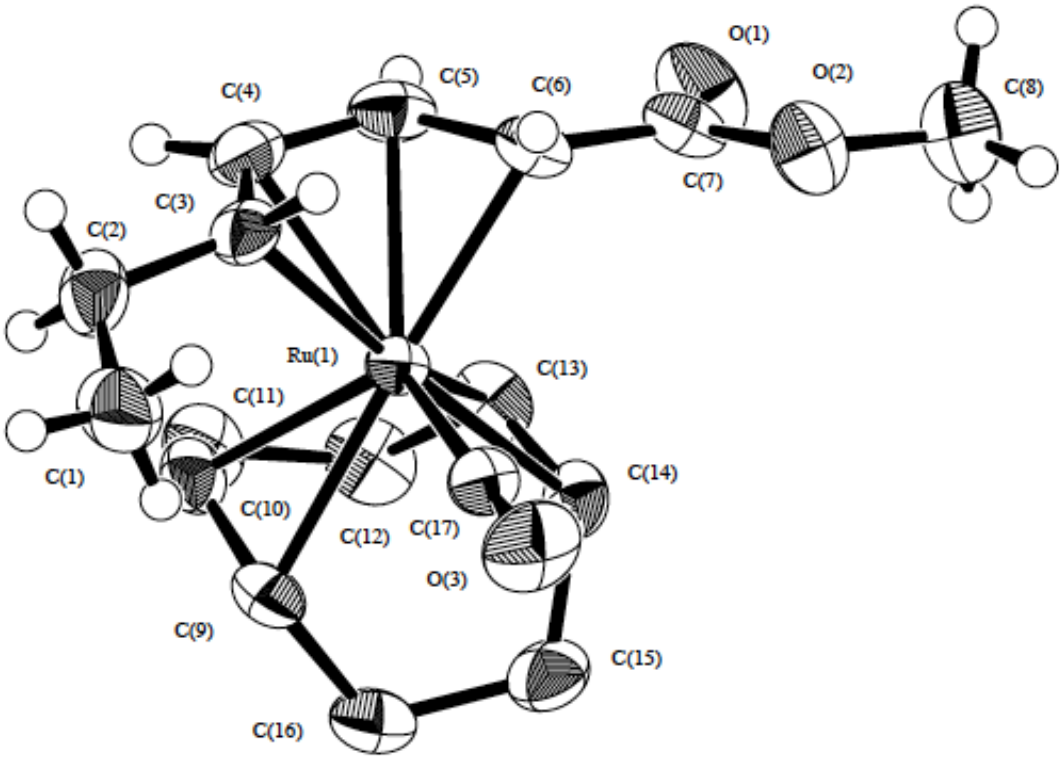


Figure S4. Molecular structure of **2c** with numbering schemes. Hydrogen atoms in the 1,5-COD ligand were omitted for clarity. Ellipsoids represent 50% probability.

Table S2. Crystallographic and physical data for **2b** and **2c**.

	2b	**2c**
formula	$C_{34}H_{40}O_2PRu$	$C_{17}H_{24}O_3Ru$
formula weight	612.73	377.44
crystal system	*orthorhombic*	*triclinic*
space group	*P*bca (No. 61)	*P*-1 (No. 2)
a (Å)	17.433(4)	7.715(4)
b (Å)	10.070(3)	8.091(4)
c (Å)	33.077(8)	14.138(7)
α (deg)		101.756(4)
β (deg)		95.319(4)
γ (deg)		108.580(6)
V (Å^3)	5807(2)	807.1(7)
Z	8	2
temp (K)	200.0	200.0
dimension (mm x mm x mm)	0.28 x 0.13 x 0.07	0.74 x 0.18 x 0.14
F(000)	2552.00	388.00
μ	0.624	0.979
radiation	Mo Kα	Mo Kα
radiation wavelength (Å)	0.71075	0.71075
relns nmber total	6608	3590
reflns threshold expression	$F^2 > 2.0\ \sigma F^2$	$F^2 > 2.0\ \sigma F^2$
R	0.0628	0.0281
wR	0.1825	0.0740
goodness of fit	0.952	1.072

Table S3. Atomic coordinates for **2b**.

atom	*x*	*y*	*z*	U_{ani}
Ru(1)	1.060567(19)	0.27596(5)	0.127393(10)	0.02776(14)
P(1)	0.94374(6)	0.15450(13)	0.11363(4)	0.0284(2)
O(1)	1.2049(2)	0.0278(4)	0.17232(14)	0.0570(11)
O(2)	1.0925(2)	-0.0802(4)	0.17900(14)	0.0544(10)
C(1)	0.9342(4)	0.5593(9)	0.2177(2)	0.080(2)
C(2)	0.9452(3)	0.4974(6)	0.17670(17)	0.0450(13)
C(3)	0.9964(3)	0.3756(5)	0.17814(14)	0.0386(11)
C(4)	1.0761(3)	0.3900(5)	0.18326(14)	0.0396(11)
C(5)	1.1234(2)	0.2756(5)	0.18374(14)	0.0372(10)
C(6)	1.0877(3)	0.1495(5)	0.18015(14)	0.0371(11)
C(7)	1.1361(3)	0.0307(6)	0.17642(15)	0.0453(13)
C(8)	1.1326(5)	-0.2044(7)	0.1762(3)	0.079(2)
C(9)	1.0342(3)	0.4012(5)	0.07454(15)	0.0364(10)
C(10)	1.0814(3)	0.4724(5)	0.10083(15)	0.0373(10)
C(11)	1.1654(3)	0.5013(6)	0.09596(17)	0.0449(12)
C(12)	1.2084(2)	0.3812(6)	0.08147(17)	0.0444(12)
C(13)	1.1758(2)	0.2552(5)	0.09923(15)	0.0381(11)
C(14)	1.1248(3)	0.1714(6)	0.07884(16)	0.0407(11)
C(15)	1.0923(3)	0.2029(6)	0.03735(16)	0.0441(13)
C(16)	1.0602(3)	0.3440(7)	0.03399(16)	0.0483(14)
C(17)	0.8794(2)	0.1392(5)	0.15782(14)	0.0339(10)
C(18)	0.8995(3)	0.0416(6)	0.18622(16)	0.0450(12)
C(19)	0.8557(4)	0.0247(7)	0.22072(18)	0.0600(17)
C(20)	0.7911(4)	0.1019(8)	0.2275(2)	0.072(2)
C(21)	0.7713(4)	0.1974(7)	0.1996(2)	0.0653(19)
C(22)	0.8144(3)	0.2156(6)	0.16457(18)	0.0487(13)
C(23)	0.9404(2)	-0.0223(5)	0.09884(14)	0.0342(10)
C(24)	1.0034(3)	-0.0934(5)	0.08736(19)	0.0465(12)

Table S3. continued

C(25)	0.9974(3)	-0.2232(6)	0.0737(2)	0.0543(15)
C(26)	0.9276(3)	-0.2859(6)	0.07276(18)	0.0476(13)
C(27)	0.8631(3)	-0.2172(6)	0.08540(19)	0.0495(13)
C(28)	0.8698(3)	-0.0866(5)	0.0983(2)	0.0474(13)
C(29)	0.8823(2)	0.2244(5)	0.07340(15)	0.0368(10)
C(30)	0.8511(3)	0.3524(6)	0.07730(18)	0.0439(12)
C(31)	0.8092(3)	0.4092(7)	0.0459(2)	0.0572(17)
C(32)	0.8008(3)	0.3389(9)	0.0098(2)	0.068(2)
C(33)	0.8330(3)	0.2161(8)	0.00531(18)	0.0608(18)
C(34)	0.8733(3)	0.1596(7)	0.03671(16)	0.0490(14)

Table S4. Anisotropic parameters for **2b**.

atom	*U*11	*U*22	*U*33	*U*12	*U*13	*U*23
Ru(1)	0.0227(2)	0.0366(2)	0.0239(2)	-0.00094(14)	0.00034(12)	-0.00176(14)
P(1)	0.0256(5)	0.0329(6)	0.0267(5)	-0.0001(4)	-0.0011(4)	-0.0016(4)
O(1)	0.041(2)	0.060(2)	0.071(2)	0.008(2)	0.0038(19)	0.011(2)
O(2)	0.049(2)	0.046(2)	0.068(2)	0.0039(19)	-0.000(2)	0.005(2)
C(1)	0.071(5)	0.104(7)	0.066(4)	0.034(4)	-0.008(3)	-0.038(4)
C(2)	0.043(3)	0.054(3)	0.038(2)	0.002(2)	0.005(2)	-0.008(2)
C(3)	0.040(2)	0.046(3)	0.030(2)	-0.002(2)	0.004(2)	-0.008(2)
C(4)	0.049(2)	0.044(3)	0.026(2)	-0.009(2)	-0.002(2)	-0.013(2)
C(5)	0.027(2)	0.058(3)	0.027(2)	-0.001(2)	-0.0039(17)	-0.004(2)
C(6)	0.033(2)	0.053(3)	0.025(2)	0.001(2)	-0.0014(18)	0.004(2)
C(7)	0.044(3)	0.059(3)	0.032(2)	0.004(2)	-0.004(2)	0.006(2)
C(8)	0.081(5)	0.042(4)	0.114(6)	0.009(3)	0.006(4)	0.006(4)
C(9)	0.033(2)	0.041(2)	0.036(2)	-0.003(2)	-0.0010(19)	0.004(2)
C(10)	0.038(2)	0.037(2)	0.037(2)	-0.005(2)	0.007(2)	-0.001(2)
C(11)	0.041(2)	0.048(3)	0.045(2)	-0.013(2)	0.003(2)	0.000(2)
C(12)	0.027(2)	0.062(3)	0.044(2)	-0.009(2)	0.008(2)	-0.003(2)
C(13)	0.025(2)	0.056(3)	0.034(2)	0.001(2)	0.0033(18)	0.000(2)
C(14)	0.034(2)	0.047(3)	0.041(2)	0.002(2)	0.013(2)	-0.004(2)
C(15)	0.044(3)	0.054(3)	0.034(2)	-0.009(2)	0.008(2)	-0.010(2)
C(16)	0.050(3)	0.067(4)	0.027(2)	-0.015(2)	-0.001(2)	0.004(2)
C(17)	0.035(2)	0.036(2)	0.032(2)	-0.004(2)	0.0022(18)	-0.0014(19)
C(18)	0.042(2)	0.057(3)	0.036(2)	-0.007(2)	-0.005(2)	0.003(2)
C(19)	0.066(4)	0.075(4)	0.039(2)	-0.023(3)	-0.002(2)	0.007(2)
C(20)	0.066(4)	0.099(6)	0.051(3)	-0.019(4)	0.026(3)	-0.001(3)
C(21)	0.054(3)	0.070(4)	0.072(4)	-0.004(3)	0.027(3)	-0.011(3)
C(22)	0.041(2)	0.053(3)	0.052(3)	-0.005(2)	0.012(2)	0.002(2)
C(23)	0.034(2)	0.038(2)	0.031(2)	-0.0005(19)	-0.0029(18)	-0.0013(19)
C(24)	0.036(2)	0.038(3)	0.065(3)	-0.000(2)	0.006(2)	-0.001(2)

Table S4. continued

atom	*U*11	*U*22	*U*33	*U*12	*U*13	*U*23
C(25)	0.049(3)	0.040(3)	0.074(4)	0.008(2)	0.013(3)	-0.001(3)
C(26)	0.061(3)	0.034(2)	0.049(3)	-0.005(2)	-0.004(2)	0.000(2)
C(27)	0.048(3)	0.036(3)	0.064(3)	-0.009(2)	-0.006(2)	-0.001(2)
C(28)	0.033(2)	0.037(2)	0.072(3)	-0.002(2)	-0.002(2)	-0.005(2)
C(29)	0.026(2)	0.050(3)	0.034(2)	-0.004(2)	-0.0060(18)	0.005(2)
C(30)	0.030(2)	0.052(3)	0.050(2)	-0.009(2)	-0.001(2)	0.008(2)
C(31)	0.034(2)	0.063(4)	0.074(4)	-0.006(2)	-0.009(2)	0.033(3)
C(32)	0.043(3)	0.103(6)	0.057(3)	-0.024(3)	-0.019(2)	0.042(4)
C(33)	0.051(3)	0.095(5)	0.036(2)	-0.019(3)	-0.013(2)	0.011(3)
C(34)	0.043(3)	0.064(3)	0.040(2)	-0.014(2)	-0.009(2)	0.007(2)

Table S5. Bond distances (Å) for **2b**.

Ru(1) - P(1)	2.4189(11)	Ru(1) - C(3)	2.253(5)
Ru(1) - C(4)	2.192(5)	Ru(1) - C(5)	2.162(4)
Ru(1) - C(6)	2.212(5)	Ru(1) - C(9)	2.204(5)
Ru(1) - C(10)	2.195(5)	Ru(1) - C(13)	2.225(4)
Ru(1) - C(14)	2.223(5)	P(1) - C(17)	1.849(4)
P(1) - C(23)	1.847(5)	P(1) - C(29)	1.848(5)
O(1) - C(7)	1.208(7)	O(2) - C(7)	1.353(7)
O(2) - C(8)	1.437(8)	C(1) - C(2)	1.506(9)
C(2) - C(3)	1.518(8)	C(3) - C(4)	1.408(7)
C(4) - C(5)	1.417(8)	C(5) - C(6)	1.419(8)
C(6) - C(7)	1.469(8)	C(9) - C(10)	1.396(7)
C(9) - C(16)	1.529(7)	C(10) - C(11)	1.501(7)
C(11) - C(12)	1.502(8)	C(12) - C(13)	1.509(8)
C(13) - C(14)	1.400(7)	C(14) - C(15)	1.518(7)
C(15) - C(16)	1.531(9)	C(17) - C(18)	1.404(7)
C(17) - C(22)	1.388(7)	C(18) - C(19)	1.384(8)
C(19) - C(20)	1.387(11)	C(20) - C(21)	1.378(10)
C(21) - C(22)	1.392(9)	C(23) - C(24)	1.364(7)
C(23) - C(28)	1.391(7)	C(24) - C(25)	1.387(8)
C(25) - C(26)	1.372(8)	C(26) - C(27)	1.385(8)
C(27) - C(28)	1.387(8)	C(29) - C(30)	1.405(8)
C(29) - C(34)	1.386(7)	C(30) - C(31)	1.392(8)
C(31) - C(32)	1.396(10)	C(32) - C(33)	1.367(12)
C(33) - C(34)	1.376(8)		

Table S6. Bond angles (deg) for **2b**.

P(1) - Ru(1) - C(3)	86.96(13)	P(1) - Ru(1) - C(4)	121.84(15)
P(1) - Ru(1) - C(5)	126.01(14)	P(1) - Ru(1) - C(6)	92.13(14)
P(1) - Ru(1) - C(9)	87.95(14)	P(1) - Ru(1) - C(10)	121.32(13)
P(1) - Ru(1) - C(13)	129.36(14)	P(1) - Ru(1) - C(14)	92.77(14)
C(3) - Ru(1) - C(4)	36.90(19)	C(3) - Ru(1) - C(5)	67.07(18)
C(3) - Ru(1) - C(6)	76.99(19)	C(3) - Ru(1) - C(9)	103.45(19)
C(3) - Ru(1) - C(10)	88.81(19)	C(3) - Ru(1) - C(13)	143.37(19)
C(3) - Ru(1) - C(14)	177.9(2)	C(4) - Ru(1) - C(5)	38.0(2)
C(4) - Ru(1) - C(6)	67.1(2)	C(4) - Ru(1) - C(9)	113.3(2)
C(4) - Ru(1) - C(10)	81.07(19)	C(4) - Ru(1) - C(13)	106.9(2)
C(4) - Ru(1) - C(14)	142.6(2)	C(5) - Ru(1) - C(6)	37.9(2)
C(5) - Ru(1) - C(9)	142.2(2)	C(5) - Ru(1) - C(10)	105.2(2)
C(5) - Ru(1) - C(13)	84.44(18)	C(5) - Ru(1) - C(14)	111.52(19)
C(6) - Ru(1) - C(9)	179.56(19)	C(6) - Ru(1) - C(10)	143.09(19)
C(6) - Ru(1) - C(13)	94.77(19)	C(6) - Ru(1) - C(14)	100.9(2)
C(9) - Ru(1) - C(10)	37.01(19)	C(9) - Ru(1) - C(13)	84.84(19)
C(9) - Ru(1) - C(14)	78.64(19)	C(10) - Ru(1) - C(13)	76.6(2)
C(10) - Ru(1) - C(14)	93.1(2)	C(13) - Ru(1) - C(14)	36.70(19)
Ru(1) - P(1) - C(17)	113.83(16)	Ru(1) - P(1) - C(23)	124.29(15)
Ru(1) - P(1) - C(29)	115.55(17)	C(17) - P(1) - C(23)	96.3(2)
C(17) - P(1) - C(29)	104.4(2)	C(23) - P(1) - C(29)	99.1(2)
C(7) - O(2) - C(8)	116.2(5)	C(1) - C(2) - C(3)	112.4(5)
Ru(1) - C(3) - C(2)	128.9(3)	Ru(1) - C(3) - C(4)	69.2(2)
C(2) - C(3) - C(4)	120.1(5)	Ru(1) - C(4) - C(3)	73.9(2)
Ru(1) - C(4) - C(5)	69.8(2)	C(3) - C(4) - C(5)	119.5(5)
Ru(1) - C(5) - C(4)	72.2(2)	Ru(1) - C(5) - C(6)	73.0(2)
C(4) - C(5) - C(6)	118.1(4)	Ru(1) - C(6) - C(5)	69.2(2)
Ru(1) - C(6) - C(7)	121.7(3)	C(5) - C(6) - C(7)	118.9(4)
O(1) - C(7) - O(2)	123.0(5)	O(1) - C(7) - C(6)	126.9(5)

Table S6. continued

O(2) - C(7) - C(6)	110.1(4)	Ru(1) - C(9) - C(10)	71.2(3)
Ru(1) - C(9) - C(16)	114.7(3)	C(10) - C(9) - C(16)	124.4(4)
Ru(1) - C(10) - C(9)	71.8(3)	Ru(1) - C(10) - C(11)	112.3(3)
C(9) - C(10) - C(11)	127.4(4)	C(10) - C(11) - C(12)	111.4(4)
C(11) - C(12) - C(13)	111.4(4)	Ru(1) - C(13) - C(12)	115.1(3)
Ru(1) - C(13) - C(14)	71.6(2)	C(12) - C(13) - C(14)	124.0(4)
Ru(1) - C(14) - C(13)	71.7(3)	Ru(1) - C(14) - C(15)	111.5(3)
C(13) - C(14) - C(15)	123.1(5)	C(14) - C(15) - C(16)	113.3(4)
C(9) - C(16) - C(15)	113.2(4)	P(1) - C(17) - C(18)	115.9(3)
P(1) - C(17) - C(22)	125.2(4)	C(18) - C(17) - C(22)	118.9(4)
C(17) - C(18) - C(19)	120.0(5)	C(18) - C(19) - C(20)	120.9(6)
C(19) - C(20) - C(21)	119.0(6)	C(20) - C(21) - C(22)	121.0(6)
C(17) - C(22) - C(21)	120.1(5)	P(1) - C(23) - C(24)	123.7(4)
P(1) - C(23) - C(28)	118.7(3)	C(24) - C(23) - C(28)	117.6(5)
C(23) - C(24) - C(25)	121.7(5)	C(24) - C(25) - C(26)	120.5(5)
C(25) - C(26) - C(27)	118.9(5)	C(26) - C(27) - C(28)	119.9(5)
C(23) - C(28) - C(27)	121.3(5)	P(1) - C(29) - C(30)	120.5(4)
P(1) - C(29) - C(34)	121.1(4)	C(30) - C(29) - C(34)	117.9(5)
C(29) - C(30) - C(31)	120.8(5)	C(30) - C(31) - C(32)	119.0(6)
C(31) - C(32) - C(33)	120.5(6)	C(32) - C(33) - C(34)	120.1(6)
C(29) - C(34) - C(33)	121.6(6)		

Table S7. Torsion angles (deg) for **2b**.

P(1) - Ru(1) - C(3) - C(2)	-85.7(4)	P(1) - Ru(1) - C(3) - C(4)	161.9(3)
C(3) - Ru(1) - P(1) - C(17)	-24.4(2)	C(3) - Ru(1) - P(1) - C(23)	-141.0(2)
C(3) - Ru(1) - P(1) - C(29)	96.5(2)	P(1) - Ru(1) - C(4) - C(3)	-21.4(3)
P(1) - Ru(1) - C(4) - C(5)	109.2(2)	C(4) - Ru(1) - P(1) - C(17)	-11.7(2)
C(4) - Ru(1) - P(1) - C(23)	-128.3(2)	C(4) - Ru(1) - P(1) - C(29)	109.2(2)
P(1) - Ru(1) - C(5) - C(4)	-97.4(3)	P(1) - Ru(1) - C(5) - C(6)	30.6(3)
C(5) - Ru(1) - P(1) - C(17)	34.2(2)	C(5) - Ru(1) - P(1) - C(23)	-82.3(2)
C(5) - Ru(1) - P(1) - C(29)	155.1(2)	P(1) - Ru(1) - C(6) - C(5)	-155.6(2)
P(1) - Ru(1) - C(6) - C(7)	92.5(4)	C(6) - Ru(1) - P(1) - C(17)	52.4(2)
C(6) - Ru(1) - P(1) - C(23)	-64.1(2)	C(6) - Ru(1) - P(1) - C(29)	173.3(2)
P(1) - Ru(1) - C(9) - C(10)	155.7(2)	P(1) - Ru(1) - C(9) - C(16)	-84.3(3)
C(9) - Ru(1) - P(1) - C(17)	-128.0(2)	C(9) - Ru(1) - P(1) - C(23)	115.5(2)
C(9) - Ru(1) - P(1) - C(29)	-7.1(2)	P(1) - Ru(1) - C(10) - C(9)	-28.7(3)
P(1) - Ru(1) - C(10) - C(11)	-152.6(3)	C(10) - Ru(1) - P(1) - C(17)	-111.2(2)
C(10) - Ru(1) - P(1) - C(23)	132.3(2)	C(10) - Ru(1) - P(1) - C(29)	9.7(2)
P(1) - Ru(1) - C(13) - C(12)	124.8(3)	P(1) - Ru(1) - C(13) - C(14)	5.2(3)
C(13) - Ru(1) - P(1) - C(17)	150.4(2)	C(13) - Ru(1) - P(1) - C(23)	33.8(2)
C(13) - Ru(1) - P(1) - C(29)	-88.7(2)	P(1) - Ru(1) - C(14) - C(13)	-176.0(3)
P(1) - Ru(1) - C(14) - C(15)	64.8(3)	C(14) - Ru(1) - P(1) - C(17)	153.5(2)
C(14) - Ru(1) - P(1) - C(23)	36.9(2)	C(14) - Ru(1) - P(1) - C(29)	-85.6(2)
C(3) - Ru(1) - C(4) - C(5)	130.7(4)	C(4) - Ru(1) - C(3) - C(2)	112.5(6)
C(3) - Ru(1) - C(5) - C(4)	-29.6(3)	C(3) - Ru(1) - C(5) - C(6)	98.4(3)
C(5) - Ru(1) - C(3) - C(2)	142.9(5)	C(5) - Ru(1) - C(3) - C(4)	30.5(3)
C(3) - Ru(1) - C(6) - C(5)	-69.2(3)	C(3) - Ru(1) - C(6) - C(7)	178.9(4)
C(6) - Ru(1) - C(3) - C(2)	-178.5(5)	C(6) - Ru(1) - C(3) - C(4)	69.0(3)
C(3) - Ru(1) - C(9) - C(10)	69.3(3)	C(3) - Ru(1) - C(9) - C(16)	-170.7(3)
C(9) - Ru(1) - C(3) - C(2)	1.5(5)	C(9) - Ru(1) - C(3) - C(4)	-111.0(3)
C(3) - Ru(1) - C(10) - C(9)	-114.5(3)	C(3) - Ru(1) - C(10) - C(11)	121.7(3)
C(10) - Ru(1) - C(3) - C(2)	35.8(4)	C(10) - Ru(1) - C(3) - C(4)	-76.7(3)

Table S7. continued

C(3) - Ru(1) - C(13) - C(12)	-63.9(4)	C(3) - Ru(1) - C(13) - C(14)	176.4(3)
C(13) - Ru(1) - C(3) - C(2)	101.1(5)	C(13) - Ru(1) - C(3) - C(4)	-11.4(4)
C(3) - Ru(1) - C(14) - C(13)	-93(5)	C(3) - Ru(1) - C(14) - C(15)	148(5)
C(14) - Ru(1) - C(3) - C(2)	-168(5)	C(14) - Ru(1) - C(3) - C(4)	79(5)
C(4) - Ru(1) - C(5) - C(6)	128.0(4)	C(5) - Ru(1) - C(4) - C(3)	-130.7(4)
C(4) - Ru(1) - C(6) - C(5)	-31.7(2)	C(4) - Ru(1) - C(6) - C(7)	-143.6(4)
C(6) - Ru(1) - C(4) - C(3)	-99.0(3)	C(6) - Ru(1) - C(4) - C(5)	31.7(2)
C(4) - Ru(1) - C(9) - C(10)	31.7(3)	C(4) - Ru(1) - C(9) - C(16)	151.7(3)
C(9) - Ru(1) - C(4) - C(3)	81.3(3)	C(9) - Ru(1) - C(4) - C(5)	-148.0(2)
C(4) - Ru(1) - C(10) - C(9)	-150.7(3)	C(4) - Ru(1) - C(10) - C(11)	85.4(3)
C(10) - Ru(1) - C(4) - C(3)	100.0(3)	C(10) - Ru(1) - C(4) - C(5)	-129.3(3)
C(4) - Ru(1) - C(13) - C(12)	-71.0(3)	C(4) - Ru(1) - C(13) - C(14)	169.4(3)
C(13) - Ru(1) - C(4) - C(3)	172.9(3)	C(13) - Ru(1) - C(4) - C(5)	-56.4(3)
C(4) - Ru(1) - C(14) - C(13)	-16.9(5)	C(4) - Ru(1) - C(14) - C(15)	-136.2(3)
C(14) - Ru(1) - C(4) - C(3)	-176.6(3)	C(14) - Ru(1) - C(4) - C(5)	-45.9(4)
C(5) - Ru(1) - C(6) - C(7)	-111.9(5)	C(6) - Ru(1) - C(5) - C(4)	-128.0(4)
C(5) - Ru(1) - C(9) - C(10)	-0.4(4)	C(5) - Ru(1) - C(9) - C(16)	119.6(4)
C(9) - Ru(1) - C(5) - C(4)	52.7(4)	C(9) - Ru(1) - C(5) - C(6)	-179.3(3)
C(5) - Ru(1) - C(10) - C(9)	179.7(2)	C(5) - Ru(1) - C(10) - C(11)	55.9(3)
C(10) - Ru(1) - C(5) - C(4)	52.4(3)	C(10) - Ru(1) - C(5) - C(6)	-179.6(2)
C(5) - Ru(1) - C(13) - C(12)	-102.0(3)	C(5) - Ru(1) - C(13) - C(14)	138.4(3)
C(13) - Ru(1) - C(5) - C(4)	126.8(3)	C(13) - Ru(1) - C(5) - C(6)	-105.2(3)
C(5) - Ru(1) - C(14) - C(13)	-45.3(3)	C(5) - Ru(1) - C(14) - C(15)	-164.5(3)
C(14) - Ru(1) - C(5) - C(4)	152.1(3)	C(14) - Ru(1) - C(5) - C(6)	-79.9(3)
C(6) - Ru(1) - C(9) - C(10)	-104(26)	C(6) - Ru(1) - C(9) - C(16)	16(26)
C(9) - Ru(1) - C(6) - C(5)	104(26)	C(9) - Ru(1) - C(6) - C(7)	-8(26)
C(6) - Ru(1) - C(10) - C(9)	179.3(3)	C(6) - Ru(1) - C(10) - C(11)	55.4(5)
C(10) - Ru(1) - C(6) - C(5)	0.7(4)	C(10) - Ru(1) - C(6) - C(7)	-111.2(4)
C(6) - Ru(1) - C(13) - C(12)	-138.5(3)	C(6) - Ru(1) - C(13) - C(14)	101.9(3)

Table S7. continued

C(13) - Ru(1) - C(6) - C(5)	74.6(3)	C(13) - Ru(1) - C(6) - C(7)	-37.3(4)
C(6) - Ru(1) - C(14) - C(13)	-83.3(3)	C(6) - Ru(1) - C(14) - C(15)	157.5(3)
C(14) - Ru(1) - C(6) - C(5)	111.1(3)	C(14) - Ru(1) - C(6) - C(7)	-0.8(4)
C(9) - Ru(1) - C(10) - C(11)	-123.9(5)	C(10) - Ru(1) - C(9) - C(16)	120.0(5)
C(9) - Ru(1) - C(13) - C(12)	41.7(3)	C(9) - Ru(1) - C(13) - C(14)	-77.9(3)
C(13) - Ru(1) - C(9) - C(10)	-74.5(3)	C(13) - Ru(1) - C(9) - C(16)	45.5(3)
C(9) - Ru(1) - C(14) - C(13)	96.7(3)	C(9) - Ru(1) - C(14) - C(15)	-22.6(3)
C(14) - Ru(1) - C(9) - C(10)	-111.0(3)	C(14) - Ru(1) - C(9) - C(16)	9.0(3)
C(10) - Ru(1) - C(13) - C(12)	5.1(3)	C(10) - Ru(1) - C(13) - C(14)	-114.5(3)
C(13) - Ru(1) - C(10) - C(9)	99.4(3)	C(13) - Ru(1) - C(10) - C(11)	-24.4(3)
C(10) - Ru(1) - C(14) - C(13)	62.4(3)	C(10) - Ru(1) - C(14) - C(15)	-56.8(4)
C(14) - Ru(1) - C(10) - C(9)	66.4(3)	C(14) - Ru(1) - C(10) - C(11)	-57.4(3)
C(13) - Ru(1) - C(14) - C(15)	-119.2(5)	C(14) - Ru(1) - C(13) - C(12)	119.6(5)
Ru(1) - P(1) - C(17) - C(18)	-78.9(4)	Ru(1) - P(1) - C(17) - C(22)	101.1(4)
Ru(1) - P(1) - C(23) - C(24)	-12.2(5)	Ru(1) - P(1) - C(23) - C(28)	169.5(3)
Ru(1) - P(1) - C(29) - C(30)	-61.2(4)	Ru(1) - P(1) - C(29) - C(34)	110.8(4)
C(17) - P(1) - C(23) - C(24)	-136.8(4)	C(17) - P(1) - C(23) - C(28)	44.9(4)
C(23) - P(1) - C(17) - C(18)	53.0(4)	C(23) - P(1) - C(17) - C(22)	-126.9(4)
C(17) - P(1) - C(29) - C(30)	64.6(4)	C(17) - P(1) - C(29) - C(34)	-123.3(4)
C(29) - P(1) - C(17) - C(18)	154.2(4)	C(29) - P(1) - C(17) - C(22)	-25.8(5)
C(23) - P(1) - C(29) - C(30)	163.6(4)	C(23) - P(1) - C(29) - C(34)	-24.3(4)
C(29) - P(1) - C(23) - C(24)	117.4(4)	C(29) - P(1) - C(23) - C(28)	-60.9(4)
C(8) - O(2) - C(7) - O(1)	-0.6(8)	C(8) - O(2) - C(7) - C(6)	-179.5(5)
C(1) - C(2) - C(3) - Ru(1)	-160.9(4)	C(1) - C(2) - C(3) - C(4)	-74.3(6)
Ru(1) - C(3) - C(4) - C(5)	-54.9(3)	C(2) - C(3) - C(4) - Ru(1)	-123.9(4)
C(2) - C(3) - C(4) - C(5)	-178.7(4)	Ru(1) - C(4) - C(5) - C(6)	-58.6(3)
C(3) - C(4) - C(5) - Ru(1)	56.8(3)	C(3) - C(4) - C(5) - C(6)	-1.8(6)
Ru(1) - C(5) - C(6) - C(7)	115.6(4)	C(4) - C(5) - C(6) - Ru(1)	58.2(3)

Table S7. continued

C(4) - C(5) - C(6) - C(7)	173.8(4)	Ru(1) - C(6) - C(7) - O(1)	74.9(6)
Ru(1) - C(6) - C(7) - O(2)	-106.3(4)	C(5) - C(6) - C(7) - O(1)	-7.3(7)
C(5) - C(6) - C(7) - O(2)	171.5(4)	Ru(1) - C(9) - C(10) - C(11)	104.6(5)
Ru(1) - C(9) - C(16) - C(15)	6.2(5)	C(10) - C(9) - C(16) - C(15)	89.5(6)
C(16) - C(9) - C(10) - Ru(1)	-107.6(5)	C(16) - C(9) - C(10) - C(11)	-3.0(9)
Ru(1) - C(10) - C(11) - C(12)	40.6(5)	C(9) - C(10) - C(11) - C(12)	-43.1(7)
C(10) - C(11) - C(12) - C(13)	-35.6(6)	C(11) - C(12) - C(13) - Ru(1)	14.8(5)
C(11) - C(12) - C(13) - C(14)	98.8(6)	Ru(1) - C(13) - C(14) - C(15)	104.2(5)
C(12) - C(13) - C(14) - Ru(1)	-108.3(4)	C(12) - C(13) - C(14) - C(15)	-4.1(8)
Ru(1) - C(14) - C(15) - C(16)	33.0(5)	C(13) - C(14) - C(15) - C(16)	-48.6(7)
C(14) - C(15) - C(16) - C(9)	-25.8(6)	P(1) - C(17) - C(18) - C(19)	178.7(4)
P(1) - C(17) - C(22) - C(21)	-178.4(4)	C(18) - C(17) - C(22) - C(21)	1.7(8)
C(22) - C(17) - C(18) - C(19)	-1.4(8)	C(17) - C(18) - C(19) - C(20)	0.9(10)
C(18) - C(19) - C(20) - C(21)	-0.7(11)	C(19) - C(20) - C(21) - C(22)	1.0(11)
C(20) - C(21) - C(22) - C(17)	-1.5(10)	P(1) - C(23) - C(24) - C(25)	-175.2(4)
P(1) - C(23) - C(28) - C(27)	176.5(4)	C(24) - C(23) - C(28) - C(27)	-1.9(8)
C(28) - C(23) - C(24) - C(25)	3.1(8)	C(23) - C(24) - C(25) - C(26)	-2.5(9)
C(24) - C(25) - C(26) - C(27)	0.5(8)	C(25) - C(26) - C(27) - C(28)	0.7(9)
C(26) - C(27) - C(28) - C(23)	0.0(9)	P(1) - C(29) - C(30) - C(31)	175.5(4)
P(1) - C(29) - C(34) - C(33)	-174.4(4)	C(30) - C(29) - C(34) - C(33)	-2.1(8)
C(34) - C(29) - C(30) - C(31)	3.2(8)	C(29) - C(30) - C(31) - C(32)	-2.2(8)
C(30) - C(31) - C(32) - C(33)	0.2(7)	C(31) - C(32) - C(33) - C(34)	0.9(10)
C(32) - C(33) - C(34) - C(29)	0.2(7)		

Table S8. Geometrical contact (Å) for **2b**.

Ru(1) - C(2)	3.417(6)	Ru(1) - C(7)	3.235(6)
Ru(1) - C(11)	3.093(5)	Ru(1) - C(12)	3.174(5)
Ru(1) - C(15)	3.117(5)	Ru(1) - C(16)	3.164(5)
Ru(1) - C(17)	3.589(4)	P(1) - C(3)	3.217(5)
P(1) - C(6)	3.338(5)	P(1) - C(9)	3.214(5)
P(1) - C(14)	3.363(5)	P(1) - C(18)	2.766(5)
P(1) - C(22)	2.881(5)	P(1) - C(24)	2.841(6)
P(1) - C(28)	2.795(5)	P(1) - C(30)	2.833(6)
P(1) - C(34)	2.825(5)	O(1) - O(2)	2.252(6)
O(1) - C(5)	2.896(7)	O(1) - C(6)	2.397(6)
O(1) - C(8)	2.659(8)	O(1) - C(11)	3.401(7)
O(1) - C(13)	3.369(7)	O(2) - O(1)	2.252(6)
O(2) - C(6)	2.314(7)	O(2) - C(18)	3.590(7)
O(2) - C(24)	3.409(7)	C(1) - C(3)	2.513(10)
C(1) - C(4)	3.214(10)	C(1) - C(6)	3.518(9)
C(2) - Ru(1)	3.417(6)	C(2) - C(4)	2.535(8)
C(2) - C(10)	3.464(7)	C(3) - P(1)	3.217(5)
C(3) - C(1)	2.513(10)	C(3) - C(5)	2.440(7)
C(3) - C(6)	2.779(7)	C(3) - C(9)	3.499(6)
C(3) - C(10)	3.113(7)	C(3) - C(17)	3.205(7)
C(3) - C(22)	3.586(7)	C(4) - C(1)	3.214(10)
C(4) - C(2)	2.535(8)	C(4) - C(6)	2.433(8)
C(4) - C(10)	2.852(6)	C(4) - C(11)	3.466(7)
C(4) - C(13)	3.548(7)	C(5) - O(1)	2.896(7)
C(5) - C(3)	2.440(7)	C(5) - C(7)	2.488(8)
C(5) - C(10)	3.462(7)	C(5) - C(13)	2.948(6)
C(6) - P(1)	3.338(5)	C(6) - O(1)	2.397(6)
C(6) - O(2)	2.314(7)	C(6) - C(1)	3.518(9)
C(6) - C(3)	2.779(7)	C(6) - C(4)	2.433(8)

Table S8. continued

C(6) - C(13)	3.265(7)	C(6) - C(14)	3.420(7)
C(6) - C(18)	3.461(7)	C(7) - Ru(1)	3.235(6)
C(7) - C(5)	2.488(8)	C(7) - C(8)	2.368(9)
C(7) - C(13)	3.480(7)	C(7) - C(14)	3.530(7)
C(8) - O(1)	2.659(8)	C(8) - C(7)	2.368(9)
C(9) - P(1)	3.214(5)	C(9) - C(3)	3.499(6)
C(9) - C(11)	2.598(7)	C(9) - C(12)	3.052(7)
C(9) - C(13)	2.988(7)	C(9) - C(14)	2.805(7)
C(9) - C(15)	2.554(7)	C(9) - C(29)	3.191(7)
C(9) - C(30)	3.231(7)	C(10) - C(2)	3.464(7)
C(10) - C(3)	3.113(7)	C(10) - C(4)	2.852(6)
C(10) - C(5)	3.462(7)	C(10) - C(12)	2.481(7)
C(10) - C(13)	2.738(7)	C(10) - C(14)	3.208(8)
C(10) - C(15)	3.437(7)	C(10) - C(16)	2.588(7)
C(10) - C(25)	3.513(8)	C(11) - Ru(1)	3.093(5)
C(11) - O(1)	3.401(7)	C(11) - C(4)	3.466(7)
C(11) - C(9)	2.598(7)	C(11) - C(13)	2.488(8)
C(11) - C(14)	3.444(8)	C(11) - C(16)	3.174(8)
C(12) - Ru(1)	3.174(5)	C(12) - C(9)	3.052(7)
C(12) - C(10)	2.481(7)	C(12) - C(14)	2.569(8)
C(12) - C(15)	3.074(8)	C(12) - C(16)	3.046(7)
C(13) - O(1)	3.369(7)	C(13) - C(4)	3.548(7)
C(13) - C(5)	2.948(6)	C(13) - C(6)	3.265(7)
C(13) - C(7)	3.480(7)	C(13) - C(9)	2.988(7)
C(13) - C(10)	2.738(7)	C(13) - C(11)	2.488(8)
C(13) - C(15)	2.567(7)	C(13) - C(16)	3.085(7)
C(14) - P(1)	3.363(5)	C(14) -C(6)	3.420(7)
C(14) - C(7)	3.530(7)	C(14) - C(9)	2.805(7)
C(14) - C(10)	3.208(8)	C(14) - C(11)	3.444(8)

Table S8. continued

C(14) - C(12)	2.569(8)	C(14) - C(16)	2.547(8)
C(14) - C(24)	3.416(8)	C(15) - Ru(1)	3.117(5)
C(15) - C(9)	2.554(7)	C(15) - C(10)	3.437(7)
C(15) - C(12)	3.074(8)	C(15) - C(13)	2.567(7)
C(16) - Ru(1)	3.164(5)	C(16) - C(10)	2.588(7)
C(16) - C(11)	3.174(8)	C(16) - C(12)	3.046(7)
C(16) - C(13)	3.085(7)	C(16) - C(14)	2.547(8)
C(16) - C(26)	3.585(8)	C(16) - C(29)	3.574(7)
C(17) - Ru(1)	3.589(4)	C(17) - C(3)	3.205(7)
C(17) - C(19)	2.415(8)	C(17) - C(20)	2.799(8
C(17) - C(21)	2.409(8)	C(17) - C(23)	2.754(6)
C(17) - C(28)	3.013(7)	C(17) - C(29)	2.922(6)
C(17) - C(30)	3.456(7)	C(18) - P(1)	2.766(5
C(18) - O(2)	3.590(7)	C(18) - C(6)	3.461(7)
C(18) - C(20)	2.410(9)	C(18) - C(21)	2.766(9)
C(18) - C(22)	2.405(8)	C(18) - C(23)	3.046(7)
C(18) - C(28)	3.224(8)	C(19) - C(17)	2.415(8)
C(19) - C(21)	2.383(10)	C(19) - C(22)	2.768(9)
C(20) - C(17)	2.799(8)	C(20) - C(18)	2.410(9)
C(20) - C(22)	2.411(9)	C(21) - C(17)	2.409(8)
C(21) - C(18)	2.766(9)	C(21) - C(19)	2.383(10)
C(22) - P(1)	2.881(5)	C(22) - C(3)	3.586(7)
C(22) - C(18)	2.405(8)	C(22) - C(19)	2.768(9
C(22) - C(20)	2.411(9)	C(22) - C(29)	3.241(7)
C(22) - C(30)	3.262(8)	C(23) - C(17)	2.754(6)
C(23) - C(18)	3.046(7)	C(23) - C(25)	2.402(8)
C(23) - C(26)	2.800(8)	C(23) - C(27)	2.421(8)
C(23) - C(29)	2.812(7)	C(23) - C(34)	2.992(7)
C(24) - P(1)	2.841(6)	C(24) - O(2)	3.409(7)

Table S8. continued

C(24) - C(14)	3.416(8)	C(24) - C(26)	2.395(8)
C(24) - C(27)	2.745(8)	C(24) - C(28)	2.357(8)
C(25) - C(10)	3.513(8)	C(25) - C(23)	2.402(8)
C(25) - C(27)	2.374(9)	C(25) - C(28)	2.740(8)
C(26) - C(16)	3.585(8)	C(26) - C(23)	2.800(8)
C(26) - C(24)	2.395(8)	C(26) - C(28)	2.399(8)
C(27) - C(23)	2.421(8)	C(27) - C(24)	2.745(8)
C(27) - C(25)	2.374(9)	C(27) - C(31)	3.515(8)
C(28) - P(1)	2.795(5)	C(28) - C(17)	3.013(7)
C(28) - C(18)	3.224(8)	C(28) - C(24)	2.357(8)
C(28) - C(25)	2.740(8)	C(28) - C(26)	2.399(8)
C(28) - C(29)	3.245(8)	C(28) - C(31)	3.570(8)
C(28) - C(34)	3.209(8)	C(29) - C(9)	3.191(7)
C(29) - C(16)	3.574(7)	C(29) - C(17)	2.922(6)
C(29) - C(22)	3.241(7)	C(29) - C(23)	2.812(7)
C(29) - C(28)	3.245(8)	C(29) - C(31)	2.432(8)
C(29) - C(32)	2.789(8)	C(29) - C(33)	2.412(7)
C(30) - P(1)	2.833(6)	C(30) - C(9)	3.231(7)
C(30) - C(17)	3.456(7)	C(30) - C(22)	3.262(8)
C(30) - C(32)	2.403(9)	C(30) - C(33)	2.766(9)
C(30) - C(34)	2.392(8)	C(31) - C(27)	3.515(8)
C(31) - C(28)	3.570(8)	C(31) - C(29)	2.432(8)
C(31) - C(33)	2.399(10)	C(31) - C(34)	2.767(9)
C(32) - C(29)	2.789(8)	C(32) - C(30)	2.403(9)
C(32) - C(34)	2.378(10)	C(33) - C(29)	2.412(7)
C(33) - C(30)	2.766(9)	C(33) - C(31)	2.399(10)
C(34) - P(1)	2.825(5)	C(34) - C(23)	2.992(7)
C(34) - C(28)	3.209(8)	C(34) - C(30)	2.392(8)
C(34) - C(31)	2.767(9)	C(34) - C(32)	2.378(10)

Table S9. Atomic coordinate for **2c**.

atom	*x*	*y*	*z*	U_{ani}
Ru(1)	0.95787(2)	0.22822(2)	0.753340(12)	0.02786(7)
O(1)	1.1957(3)	0.3752(3)	1.01880(15)	0.0599(6)
O(2)	1.2658(3)	0.1306(2)	0.96080(15)	0.0496(4)
O(3)	1.1024(3)	-0.0361(3)	0.62873(18)	0.0612(5)
C(1)	0.5843(5)	-0.1825(5)	0.5594(2)	0.0597(8)
C(2)	0.5405(3)	-0.0640(4)	0.6439(2)	0.0490(6)
C(3)	0.6887(3)	0.0055(3)	0.7341(2)	0.0372(5)
C(4)	0.6953(3)	0.1512(3)	0.8111(2)	0.0423(5)
C(5)	0.8453(4)	0.2206(4)	0.8896(2)	0.0430(5)
C(6)	0.9837(3)	0.1376(3)	0.88895(18)	0.0359(5)
C(7)	1.1544(4)	0.2291(3)	0.96276(17)	0.0402(5)
C(8)	1.4378(5)	0.2151(5)	1.0295(3)	0.0610(8)
C(9)	0.9452(3)	0.3241(3)	0.61452(18)	0.0373(5)
C(10)	0.8344(3)	0.3858(3)	0.6741(2)	0.0390(5)
C(11)	0.8824(4)	0.5759(4)	0.7359(2)	0.0497(6)
C(12)	1.0795(4)	0.6546(3)	0.7921(2)	0.0500(6)
C(13)	1.1444(3)	0.5136(3)	0.8252(2)	0.0407(5)
C(14)	1.2476(3)	0.4259(3)	0.7733(2)	0.0377(5)
C(15)	1.2985(4)	0.4506(4)	0.6750(2)	0.0477(6)
C(16)	1.1351(4)	0.4422(4)	0.6009(2)	0.0472(6)
C(17)	1.0527(3)	0.0655(3)	0.67509(18)	0.0357(4)

Table S10. Anisotropic parameters for **2c**.

atom	*U*11	*U*22	*U*33	*U*12	*U*13	*U*23
Ru(1)	0.03261(12)	0.02601(11)	0.02802(11)	0.01278(8)	0.00771(7)	0.00793(7)
O(1)	0.0870(16)	0.0526(12)	0.0389(10)	0.0378(12)	-0.0048(10)	-0.0062(9)
O(2)	0.0596(12)	0.0388(9)	0.0507(11)	0.0232(9)	-0.0019(9)	0.0063(8)
O(3)	0.0733(14)	0.0554(12)	0.0672(14)	0.0398(11)	0.0274(12)	0.0063(11)
C(1)	0.0516(17)	0.064(2)	0.0485(17)	0.0038(15)	-0.0022(14)	0.0132(15)
C(2)	0.0335(12)	0.0448(15)	0.0663(19)	0.0064(11)	0.0015(12)	0.0233(13)
C(3)	0.0313(11)	0.0357(12)	0.0466(13)	0.0078(9)	0.0114(9)	0.0187(10)
C(4)	0.0410(12)	0.0470(14)	0.0513(15)	0.0213(11)	0.0222(11)	0.0228(12)
C(5)	0.0582(15)	0.0440(14)	0.0358(12)	0.0242(12)	0.0223(11)	0.0127(11)
C(6)	0.0510(14)	0.0340(12)	0.0276(10)	0.0181(10)	0.0100(9)	0.0117(9)
C(7)	0.0617(15)	0.0380(12)	0.0274(11)	0.0228(11)	0.0108(10)	0.0121(9)
C(8)	0.061(2)	0.056(2)	0.065(2)	0.0251(17)	-0.0036(16)	0.0106(16)
C(9)	0.0464(13)	0.0360(12)	0.0312(11)	0.0129(10)	0.0040(9)	0.0151(9)
C(10)	0.0406(12)	0.0376(12)	0.0441(13)	0.0175(10)	0.0026(10)	0.0176(10)
C(11)	0.0631(17)	0.0384(13)	0.0596(17)	0.0306(13)	0.0101(14)	0.0175(12)
C(12)	0.0678(18)	0.0281(12)	0.0543(16)	0.0188(12)	0.0086(14)	0.0076(11)
C(13)	0.0507(14)	0.0266(11)	0.0372(12)	0.0083(10)	-0.0012(10)	0.0031(9)
C(14)	0.0285(10)	0.0291(11)	0.0465(13)	0.0002(9)	-0.0024(9)	0.0098(10)
C(15)	0.0411(13)	0.0458(15)	0.0585(17)	0.0090(12)	0.0173(12)	0.0234(13)
C(16)	0.0561(16)	0.0490(16)	0.0419(14)	0.0166(13)	0.0161(12)	0.0222(12)
C(17)	0.0388(11)	0.0329(11)	0.0381(12)	0.0142(9)	0.0095(9)	0.0103(9)

Table S11. Bond distances (Å) for **2c**.

Ru(1) - C(3)	2.224(2)	Ru(1) - C(4)	2.207(3)
Ru(1) - C(5)	2.189(3)	Ru(1) - C(6)	2.202(2)
Ru(1) - C(9)	2.258(2)	Ru(1) - C(10)	2.224(3)
Ru(1) - C(13)	2.256(2)	Ru(1) - C(14)	2.248(2)
Ru(1) - C(17)	1.913(2)	O(1) - C(7)	1.208(3)
O(2) - C(7)	1.344(4)	O(2) - C(8)	1.443(4)
O(3) - C(17)	1.132(3)	C(1) - C(2)	1.509(5)
C(2) - C(3)	1.509(3)	C(3) - C(4)	1.416(3)
C(4) - C(5)	1.407(3)	C(5) - C(6)	1.431(4)
C(6) - C(7)	1.477(3)	C(9) - C(10)	1.386(4)
C(9) - C(16)	1.528(4)	C(10) - C(11)	1.516(3)
C(11) - C(12)	1.516(4)	C(12) - C(13)	1.519(4)
C(13) - C(14)	1.390(4)	C(14) - C(15)	1.512(4)
C(15) - C(16)	1.538(4)		

Table S12. Bond angles (deg) for **2c**.

C(3) - Ru(1) - C(4)	37.29(10)	C(3) - Ru(1) - C(5)	66.97(9)
C(3) - Ru(1) - C(6)	77.59(9)	C(3) - Ru(1) - C(9)	104.56(9)
C(3) - Ru(1) - C(10)	93.46(10)	C(3) - Ru(1) - C(13)	149.86(10)
C(3) - Ru(1) - C(14)	172.44(11)	C(3) - Ru(1) - C(17)	89.60(9)
C(4) - Ru(1) - C(5)	37.32(10)	C(4) - Ru(1) - C(6)	67.03(11)
C(4) - Ru(1) - C(9)	115.52(11)	C(4) - Ru(1) - C(10)	85.79(11)
C(4) - Ru(1) - C(13)	112.71(10)	C(4) - Ru(1) - C(14)	147.10(9)
C(4) - Ru(1) - C(17)	125.53(10)	C(5) - Ru(1) - C(6)	38.04(12)
C(5) - Ru(1) - C(9)	144.03(12)	C(5) - Ru(1) - C(10)	108.06(12)
C(5) - Ru(1) - C(13)	88.10(10)	C(5) - Ru(1) - C(14)	114.12(9)
C(5) - Ru(1) - C(17)	131.07(12)	C(6) - Ru(1) - C(9)	177.44(10)
C(6) - Ru(1) - C(10)	145.83(11)	C(6) - Ru(1) - C(13)	93.38(9)
C(6) - Ru(1) - C(14)	98.73(10)	C(6) - Ru(1) - C(17)	97.05(11)
C(9) - Ru(1) - C(10)	36.03(11)	C(9) - Ru(1) - C(13)	85.42(9)
C(9) - Ru(1) - C(14)	78.98(9)	C(9) - Ru(1) - C(17)	81.64(11)
C(10) - Ru(1) - C(13)	77.88(9)	C(10) - Ru(1) - C(14)	93.21(10)
C(10) - Ru(1) - C(17)	116.01(11)	C(13) - Ru(1) - C(14)	35.96(10)
C(13) - Ru(1) - C(17)	120.24(10)	C(14) - Ru(1) - C(17)	84.28(9)
C(7) - O(2) - C(8)	114.5(2)	C(1) - C(2) - C(3)	113.7(2)
Ru(1) - C(3) - C(2)	125.1(2)	Ru(1) - C(3) - C(4)	70.69(14)
C(2) - C(3) - C(4)	121.6(2)	Ru(1) - C(4) - C(3)	72.02(16)
Ru(1) - C(4) - C(5)	70.67(17)	C(3) - C(4) - C(5)	119.2(3)
Ru(1) - C(5) - C(4)	72.00(17)	Ru(1) - C(5) - C(6)	71.45(16)
C(4) - C(5) - C(6)	118.1(2)	Ru(1) - C(6) - C(5)	70.51(17)
Ru(1) - C(6) - C(7)	119.39(18)	C(5) - C(6) - C(7)	117.4(2)
O(1) - C(7) - O(2)	122.0(2)	O(1) - C(7) - C(6)	126.1(3)
O(2) - C(7) - C(6)	111.9(2)	Ru(1) - C(9) - C(10)	70.66(17)
Ru(1) - C(9) - C(16)	112.53(19)	C(10) - C(9) - C(16)	124.0(2)
Ru(1) - C(10) - C(9)	73.31(18)	Ru(1) - C(10) - C(11)	110.6(2)

Table S12. continued

C(9) - C(10) - C(11)	126.0(2)	C(10) - C(11) - C(12)	113.1(3)
C(11) - C(12) - C(13)	112.4(2)	Ru(1) - C(13) - C(12)	113.67(17)
Ru(1) - C(13) - C(14)	71.72(12)	C(12) - C(13) - C(14)	123.4(2)
Ru(1) - C(14) - C(13)	72.32(13)	Ru(1) - C(14) - C(15)	110.34(15)
C(13) - C(14) - C(15)	124.4(2)	C(14) - C(15) - C(16)	113.7(2)
C(9) - C(16) - C(15)	114.5(2)	Ru(1) - C(17) - O(3)	177.3(2)

Table S13. Torsion angles (deg) for **2c**.

C(3) - Ru(1) - C(4) - C(5)	131.1(2)	C(4) - Ru(1) - C(3) - C(2)	115.6(3)
C(3) - Ru(1) - C(5) - C(4)	-29.73(18)	C(3) - Ru(1) - C(5) - C(6)	99.45(16
C(5) - Ru(1) - C(3) - C(2)	145.3(2)	C(5) - Ru(1) - C(3) - C(4)	29.76(19)
C(3) - Ru(1) - C(6) - C(5)	-68.37(14)	C(3) - Ru(1) - C(6) - C(7)	-179.5(2)
C(6) - Ru(1) - C(3) - C(2)	-176.2(2)	C(6) - Ru(1) - C(3) - C(4)	68.25(19)
C(3) - Ru(1) - C(9) - C(10)	75.46(14)	C(3) - Ru(1) - C(9) - C(16)	-164.8(2)
C(9) - Ru(1) - C(3) - C(2)	2.4(2)	C(9) - Ru(1) - C(3) - C(4)	-113.19(19)
C(3) - Ru(1) - C(10) - C(9)	-110.18(14)	C(3) - Ru(1) - C(10) - C(11)	127.0(2)
C(10) - Ru(1) - C(3) - C(2)	37.2(2)	C(10) - Ru(1) - C(3) - C(4)	-78.41(19)
C(3) - Ru(1) - C(13) - C(12)	-69.6(3)	C(3) - Ru(1) - C(13) - C(14)	171.1(2)
C(13) - Ru(1) - C(3) - C(2)	108.8(2)	C(13) - Ru(1) - C(3) - C(4)	-6.8(3)
C(3) - Ru(1) - C(14) - C(13)	-143.9(7)	C(3) - Ru(1) - C(14) - C(15)	95.2(7)
C(14) - Ru(1) - C(3) - C(2)	-114.7(7)	C(14) - Ru(1) - C(3) - C(4)	129.7(7)
C(3) - Ru(1) - C(17) - O(3)	-6(5)	C(17) - Ru(1) - C(3) - C(2)	-78.9(2
C(17) - Ru(1) - C(3) - C(4)	165.6(2)	C(4) - Ru(1) - C(5) - C(6)	129.2(2)
C(5) - Ru(1) - C(4) - C(3)	-131.1(2)	C(4) - Ru(1) - C(6) - C(5)	-30.70(14)
C(4) - Ru(1) - C(6) - C(7)	-141.9(2)	C(6) - Ru(1) - C(4) - C(3)	-99.9(2)
C(6) - Ru(1) - C(4) - C(5)	31.25(18)	C(4) - Ru(1) - C(9) - C(10)	37.36(15)
C(4) - Ru(1) - C(9) - C(16)	157.1(2)	C(9) - Ru(1) - C(4) - C(3)	80.4(2)
C(9) - Ru(1) - C(4) - C(5)	-148.52(18)	C(4) - Ru(1) - C(10) - C(9)	-146.69(14)
C(4) - Ru(1) - C(10) - C(11)	90.4(2)	C(10) - Ru(1) - C(4) - C(3)	101.34(18)
C(10) - Ru(1) - C(4) - C(5)	-127.55(19)	C(4) - Ru(1) - C(13) - C(12)	-74.1(2)
C(4) - Ru(1) - C(13) - C(14)	166.69(17)	C(13) - Ru(1) - C(4) - C(3)	176.33(17)
C(13) - Ru(1) - C(4) - C(5)	-52.6(2)	C(4) - Ru(1) - C(14) - C(13)	-23.0(3)
C(4) - Ru(1) - C(14) - C(15)	-143.9(2)	C(14) - Ru(1) - C(4) - C(3)	-169.27(19)
C(14) - Ru(1) - C(4) - C(5)	-38.2(3)	C(4) - Ru(1) - C(17) - O(3)	5(5)
C(17) - Ru(1) - C(4) - C(3)	-17.9(2)	C(17) - Ru(1) - C(4) - C(5)	113.3(2)
C(5) - Ru(1) - C(6) - C(7)	-111.2(2)	C(6) - Ru(1) - C(5) - C(4)	-129.2(2)
C(5) - Ru(1) - C(9) - C(10)	4.7(2)	C(5) - Ru(1) - C(9) - C(16)	124.5(2)

Table S13. continued

C(9) - Ru(1) - C(5) - C(4)	53.3(2)	C(9) - Ru(1) - C(5) - C(6)	-177.48(13)
C(5) - Ru(1) - C(10) - C(9)	-177.07(13)	C(5) - Ru(1) - C(10) - C(11)	60.1(2)
C(10) - Ru(1) - C(5) - C(4)	56.3(2)	C(10) - Ru(1) - C(5) - C(6)	-174.54(12)
C(5) - Ru(1) - C(13) - C(12)	-102.9(2)	C(5) - Ru(1) - C(13) - C(14)	137.90(19)
C(13) - Ru(1) - C(5) - C(4)	132.9(2)	C(13) - Ru(1) - C(5) - C(6)	-97.94(14)
C(5) - Ru(1) - C(14) - C(13)	-47.2(2)	C(5) - Ru(1) - C(14) - C(15)	-168.2(2)
C(14) - Ru(1) - C(5) - C(4)	158.43(18)	C(14) - Ru(1) - C(5) - C(6)	-72.39(16)
C(5) - Ru(1) - C(17) - O(3)	53(5)	C(17) - Ru(1) - C(5) - C(4)	-97.4(2)
C(17) - Ru(1) - C(5) - C(6)	31.81(18)	C(6) - Ru(1) - C(9) - C(10)	-138(2)
C(6) - Ru(1) - C(9) - C(16)	-18(2)	C(9) - Ru(1) - C(6) - C(5)	145(2)
C(9) - Ru(1) - C(6) - C(7)	33(2)	C(6) - Ru(1) - C(10) - C(9)	176.94(14)
C(6) - Ru(1) - C(10) - C(11)	54.1(2)	C(10) - Ru(1) - C(6) - C(5)	9.3(2)
C(10) - Ru(1) - C(6) - C(7)	-101.9(2)	C(6) - Ru(1) - C(13) - C(12)	-140.5(2)
C(6) - Ru(1) - C(13) - C(14)	100.21(18)	C(13) - Ru(1) - C(6) - C(5)	82.57(15)
C(13) - Ru(1) - C(6) - C(7)	-28.6(2)	C(6) - Ru(1) - C(14) - C(13)	-83.69(18)
C(6) - Ru(1) - C(14) - C(15)	155.4(2)	C(14) - Ru(1) - C(6) - C(5)	118.35(14)
C(14) - Ru(1) - C(6) - C(7)	7.2(2	C(6) - Ru(1) - C(17) - O(3)	72(5)
C(17) - Ru(1) - C(6) - C(5)	-156.40(14)	C(17) - Ru(1) - C(6) - C(7)	92.4(2)
C(9) - Ru(1) - C(10) - C(11)	-122.9(2)	C(10) - Ru(1) - C(9) - C(16)	119.7(2)
C(9) - Ru(1) - C(13) - C(12)	41.7(2)	C(9) - Ru(1) - C(13) - C(14)	-77.52(18)
C(13) - Ru(1) - C(9) - C(10)	-75.65(14)	C(13) - Ru(1) - C(9) - C(16)	44.1(2)
C(9) - Ru(1) - C(14) - C(13)	97.46(18)	C(9) - Ru(1) - C(14) - C(15)	-23.4(2)
C(14) - Ru(1) - C(9) - C(10)	-111.39(14)	C(14) - Ru(1) - C(9) - C(16)	8.4(2)
C(9) - Ru(1) - C(17) - O(3)	-110(5)	C(17)- Ru(1) - C(9) - C(10)	162.86(14)
C(17) - Ru(1) - C(9) - C(16)	-77.4(2)	C(10) - Ru(1) - C(13) - C(12)	6.1(2)
C(10) - Ru(1) - C(13) - C(14)	-113.17(18)	C(13) - Ru(1) - C(10) - C(9)	98.99(14)
C(13) - Ru(1) - C(10) - C(11)	-23.9(2)	C(10) - Ru(1) - C(14) - C(13)	64.19(18)
C(10) - Ru(1) - C(14) - C(15)	-56.7(2)	C(14) - Ru(1) - C(10) - C(9)	66.26(14)
C(14) - Ru(1) - C(10) - C(11)	-56.6(2)	C(10) - Ru(1) - C(17) - O(3)	-99(5)

Table S13. continued

C(17) - Ru(1) - C(10) - C(9)	-18.93(15)	C(17) - Ru(1) - C(10) - C(11)	-141.8(2)
C(13) - Ru(1) - C(14) - C(15)	-120.9(3)	C(14) - Ru(1) - C(13) - C(12)	119.2(3)
C(13) - Ru(1) - C(17) - O(3)	170(5)	C(17) - Ru(1) - C(13) - C(12)	119.3(2)
C(17) - Ru(1) - C(13) - C(14)	0.04(17)	C(14) - Ru(1) - C(17) - O(3)	170(5)
C(17) - Ru(1) - C(14) - C(13)	-179.97(15)	C(17) - Ru(1) - C(14) - C(15)	59.1(2)
C(8) - O(2) - C(7) - O(1)	-0.9(4)	C(8) - O(2) - C(7) - C(6)	178.3(2)
C(1) - C(2) - C(3) - Ru(1)	76.7(3)	C(1) - C(2) - C(3) - C(4)	164.2(3)
Ru(1) - C(3) - C(4) - C(5)	-54.5(2)	C(2) - C(3) - C(4) - Ru(1)	-120.0(2)
C(2) - C(3) - C(4) - C(5)	-174.6(2)	Ru(1) - C(4) - C(5) - C(6)	-56.4(2)
C(3) - C(4) - C(5) - Ru(1)	55.2(2)	C(3) - C(4) - C(5) - C(6)	-1.3(4)
Ru(1) - C(5) - C(6) - C(7)	113.8(2)	C(4) - C(5) - C(6) - Ru(1)	56.7(2)
C(4) - C(5) - C(6) - C(7)	170.5(2)	Ru(1) - C(6) - C(7) - O(1)	75.5(3)
Ru(1) - C(6) - C(7) - O(2)	-103.7(2)	C(5) - C(6) - C(7) - O(1)	-6.5(4)
C(5) - C(6) - C(7) - O(2)	174.3(2)	Ru(1) - C(9) - C(10) - C(11)	103.6(3)
Ru(1) - C(9) - C(16) - C(15)	8.2(3)	C(10) - C(9) - C(16) - C(15)	89.4(3)
C(16) - C(9) - C(10) - Ru(1)	-104.7(2)	C(16) - C(9) - C(10) - C(11)	-1.0(5)
Ru(1) - C(10) - C(11) - C(12)	39.2(3)	C(9) - C(10) - C(11) - C(12)	-44.6(4)
C(10) - C(11) - C(12) - C(13)	-34.4(4)	C(11) - C(12) - C(13) - Ru(1)	13.0(3)
C(11) - C(12) - C(13) - C(14)	96.0(3)	Ru(1) - C(13) - C(14) - C(15)	102.9(2)
C(12) - C(13) - C(14) - Ru(1)	-106.8(2)	C(12) - C(13) - C(14) - C(15)	-3.8(3)
Ru(1) - C(14) - C(15) - C(16)	35.4(3)	C(13) - C(14) - C(15) - C(16)	-46.6(3)
C(14) - C(15) - C(16) - C(9)	-29.2(3)		

Table S14. Geometrical contact distance (Å) for **2c**.

Ru(1) - O(3)	3.044(2)	Ru(1) - C(2)	3.330(2)
Ru(1) - C(7)	3.197(2)	Ru(1) - C(11)	3.100(3)
Ru(1) - C(12)	3.186(2)	Ru(1) - C(15)	3.116(3)
Ru(1) - C(16)	3.174(3)	O(1) - O(2)	2.233(3)
O(1) - C(5)	2.865(3)	O(1) - C(5)	3.389(4)
O(1) - C(6)	2.396(2)	O(1) - C(8)	2.599(5)
O(1) - C(11)	3.539(4)	O(1) - C(12)	3.565(4)
O(1) - C(13)	3.199(3	O(2) - O(1)	2.233(3)
O(2) - C(6)	2.338(3)	O(2) - C(6)	3.592(3)
O(3) - Ru(1)	3.044(2)	O(3) - C(2)	3.449(4)
O(3) - C(9)	3.528(4)	C(1) - C(3)	2.527(4)
C(1) - C(17)	3.564(4)	C(2) - Ru(1)	3.330(2)
C(2) - O(3)	3.449(4)	C(2) - C(4)	2.554(3)
C(2) - C(10)	3.535(3)	C(3) - C(1)	2.527(4)
C(3) - C(5)	2.435(3)	C(3) - C(6)	2.773(3)
C(3) - C(9)	3.545(3)	C(3) - C(10)	3.239(4)
C(3) - C(17)	2.924(3)	C(4) - C(2)	2.554(3)
C(4) - C(6)	2.434(4)	C(4) - C(10)	3.016(4)
C(5) - O(1)	2.865(3)	C(5) - O(1)	3.389(4)
C(5) - C(3)	2.435(3)	C(5) - C(7)	2.484(4)
C(5) - C(10)	3.572(4)	C(5) - C(13)	3.091(3)
C(6) - O(1)	2.396(2)	C(6) - O(2)	2.338(3)
C(6) - O(2)	3.592(3)	C(6) - C(3)	2.773(3)
C(6) - C(4)	2.434(4)	C(6) - C(13)	3.244(3)
C(6) - C(14)	3.377(3)	C(6) - C(17)	3.089(3)
C(7) - Ru(1)	3.197(2)	C(7) - C(5)	2.484(4)
C(7) - C(8)	2.345(5)	C(7) - C(13)	3.317(4)
C(7) - C(14)	3.405(4)	C(8) - O(1)	2.599(5)
C(8) - C(7)	2.345(5)	C(8) - C(13)	3.443(4)

Table S14. continued

C(9) - O(3)	3.528(4)	C(9) - C(3)	3.545(3)
C(9) - C(11)	2.586(4)	C(9) - C(12)	3.089(3)
C(9) - C(13)	3.062(3)	C(9) - C(14)	2.866(3)
C(9) - C(15)	2.577(3)	C(9) - C(17)	2.739(4)
C(10) - C(2)	3.535(3)	C(10) - C(3)	3.239(4)
C(10) - C(4)	3.016(4)	C(10) - C(5)	3.572(4)
C(10) - C(12)	2.531(3)	C(10) - C(13)	2.816(3)
C(10) - C(14)	3.250(3)	C(10) - C(15)	3.448(4)
C(10) - C(16)	2.574(4)	C(10) - C(17)	3.513(4)
C(11) - Ru(1)	3.100(3)	C(11) - O(1)	3.539(4)
C(11) - C(9)	2.586(4)	C(11) - C(13)	2.523(4)
C(11) - C(14)	3.443(4)	C(11) - C(16)	3.132(5)
C(12) - Ru(1)	3.186(2)	C(12) - O(1)	3.565(4)
C(12) - C(9)	3.089(3)	C(12) - C(10)	2.531(3)
C(12) - C(14)	2.563(4)	C(12) - C(15)	3.082(5)
C(12) - C(16)	3.039(4)	C(13) - O(1)	3.199(3)
C(13) - C(5)	3.091(3)	C(13) - C(6)	3.244(3)
C(13) - C(7)	3.317(4)	C(13) - C(8)	3.443(4)
C(13) - C(9)	3.062(3)	C(13) - C(10)	2.816(3)
C(13) - C(11)	2.523(4)	C(13) - C(15)	2.568(4)
C(13) - C(16)	3.095(4)	C(14) - C(6)	3.377(3)
C(14) - C(7)	3.405(4)	C(14) - C(9)	2.866(3)
C(14) - C(10)	3.250(3)	C(14) - C(11)	3.443(4)
C(14) - C(12)	2.563(4)	C(14) - C(16)	2.554(4)
C(14) - C(17)	2.803(3)	C(15) - Ru(1)	3.116(3)
C(15) - C(9)	2.577(3)	C(15) - C(10)	3.448(4)
C(15) - C(12)	3.082(5)	C(15) - C(13)	2.568(4)
C(15) - C(17)	3.088(3)	C(16) - Ru(1)	3.174(3)
C(16) - C(10)	2.574(4)	C(16) - C(11)	3.132(5)

Table S14. continued

C(16) - C(12)	3.039(4)	C(16) - C(13)	3.095(4)
C(16) - C(14)	2.554(4)	C(16) - C(17)	3.315(4)
C(17) - C(1)	3.564(4)	C(17) - C(3)	2.924(3)
C(17) - C(6)	3.089(3)	C(17) - C(9)	2.739(4)
C(17) - C(10)	3.513(4)	C(17) - C(14)	2.803(3)
C(17) - C(15)	3.088(3)	C(17) - C(16)	3.315(4)

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