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An Unprecedented Derivative of Benzynechromium Tricarbonyl, $Ru_3(CO)_8[\mu_3\text{-}C_6H_4Cr(CO)_3][\mu_3\text{-}PBu^t]$

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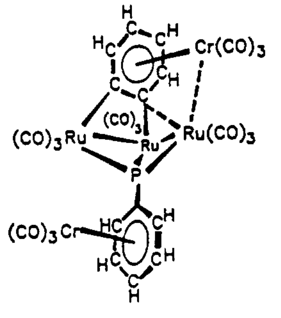
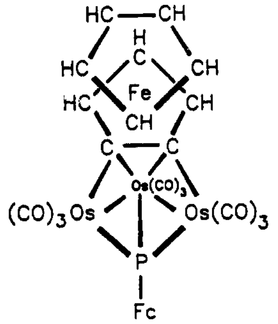
Summary: The reaction of $Ru_3(CO)_{12}$ with $P[C_6H_5Cr(CO)_3]_2Bu^t$ affords the benzynechromium tricarbonyl derivative $Ru_3(CO)_8[\mu_3\text{-}C_6H_4Cr(CO)_3][\mu_3\text{-}PBu^t]$ (**5**). The aryne is bound symmetrically to the closed Ru_3 cluster, and the η^2-bound carbon atoms are four-electron donors. In addition, there is a $Ru\rightarrow Cr$ bond of length 2.920 (1) Å. **5**: monoclinic, $P2_1/a$, a = 13.616 (2) Å, b = 14.229 (1) Å, c = 13.617 (2) Å, β = 94.15 (1)°, Z = 4, R = 0.033 (R_w = 0.036) from 4980 observed reflections.

We have recently described the structure of the benzynechromium tricarbonyl derivative 1, in which the aryne moiety acts as a four-electron donor to the open cluster with two electrons coming from the η^2-carbon atoms and the other two predominantly from the chromium atom.[1] The ferrocyne and ferrodicyne complexes $Os_3(CO)_9(\mu_3\text{-}(C_5H_3)Fe(C_5H_5)][\mu_3\text{-}P(C_6H_4)Fe(C_5H_5)]$ (2) and $Os_3(H)_2(CO)_8(PPr^i{}_2C_5H_2)Fe(C_5H_2PPr^i{}_2)Os_3(H)_2(CO)_8$ (3) are likewise electron precise; however, the iron atoms are not involved in any metal–metal bonding.[2] (Such bonding is possible in clusters as in 4.[3])



1



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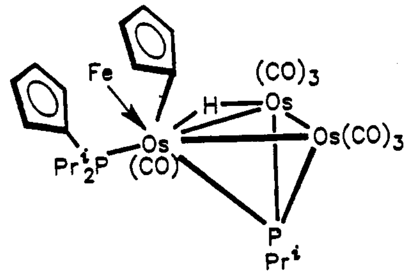

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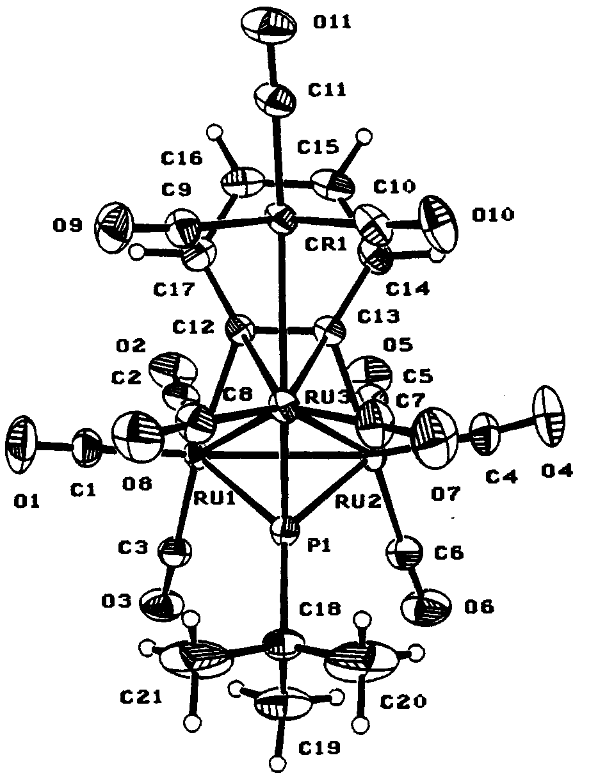

Figure 1. ORTEP diagram of 5.

Compound 1 is a product of the reaction of $Ru_3(CO)_{12}$ with $P[C_6H_5Cr(CO)_3]_2Ph$. We now report that the reaction of $Ru_3(CO)_{12}$ with $P[C_6H_5Cr(CO)_3]_2Bu^t$ follows a similar course[4] in that a derivative of benzynechromium tricarbonyl $Ru_3(CO)_8[\mu_3\text{-}C_6H_4Cr(CO)_3][\mu_3\text{-}PBu^t]$ (5) is obtained. However, the structure of 5 reveals an unprecedented bonding mode for the aryne moiety.

The structure of 5 is seen in Figures 1 and 2. The aryne is bound essentially symmetrically in a manner closer to that seen in 2 and 1, although in both 2 and 1 the cluster is open. In 5 the Ru_3 triangle is closed; the longest metal–metal bond, Ru(1)–Ru(3), has a length of 2.9272 (5) Å. The phosphinidene is bound almost symmetrically (Ru(1)–P(1) = 2.324 (1), Ru(2)–P(1) = 2.313 (1), Ru(3)–P(1) = 2.199 (1) Å). The η^2-carbon atoms of the aryne moiety act as four-electron donors, (Ru(1)–C(12) = 2.228 (4), C(12)–Ru(3) = 2.331 (4) Å). The Cr(1)–Ru(3) bond of length 2.920 (1) Å is considerably shorter than that found in 1, 3.098 (3) Å. As in 1, the $Cr(CO)_3$ moiety of the aryne fragment of 5 opens up to accommodate this Cr–Ru interaction (C(9)–Cr(1)–C(10) = 98.4 (2)°).

The slight folding of the aryne ring in 5 along the C(17)···C(14) axis seen in Figure 2 seems to be real. The dihedral angle between the planes C(17)C(12)C(13)C(14) and C(17)C(16)C(15)C(14) is 8.03°. The chromium atom is further away from C(12) and C(13) (Cr(1)–C(12) = 2.350 (4), Cr(1)–C(13) = 2.370 (4) Å) than from the other atoms of the ring (e.g., Cr(1)–C(14) = 2.212 (5) Å). The chromium atom is 1.748 (2) Å from the ring centroid, again showing

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(1) Cullen, W. R.; Rettig, S. J.; Zhang, H. *Organometallics* **1991**, *10*, 2965.

(2) Cullen, W. R.; Rettig, S. J.; Zheng, T. *Organometallics*, in press.

(3) Cullen, W. R.; Rettig, S. J.; Zheng, T. *Organometallics*, in press.

(4) The formation of aryne complexes from arylphosphines is usually initiated by coordination and ortho-metalation reactions followed by P–C (aryl) bond cleavage and capture of the resulting dehydroarene (aryne) moiety.[5]

(5) (a) Deeming, A. J.; Kabir, S. E.; Powell, N. I.; Bates, P. A.; Hursthouse, M. B. *J. Chem. Soc., Dalton Trans.* **1987**, 1529. (b) Bruce, M. I.; Humphrey, P. A.; Shawkatalay, O. b.; Snow, M. R.; Tiekink, E. R. T.; Cullen, W. R. *Organometallics* **1990**, *9*, 2910.

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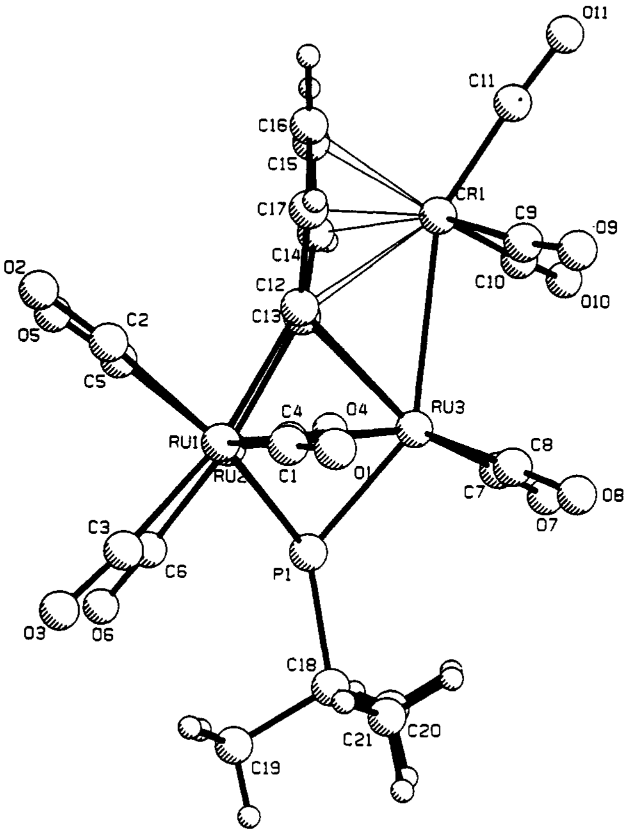

Figure 2. PLUTO plot of 5.

the movement of the metal atom away from the hydrocarbon on aryne formation.[1]

The least-squares plane of the aryne ring ($\chi^2 = 402$) is at an angle of 81.7° to the Ru_3 plane. In 1, the aryne plane is not bent ($\chi^2 = 4.2$) and it is at an angle of 76.4° to the Ru_3 plane.

The aryne moiety of 5 can be regarded as donating four electrons to the Ru_3 P fragment which as a consequence is electron-precise.[6] However, the slippage of the chromium atom appears to result in a loss of electron density which is compensated by the establishment of a Ru→Cr bond.

Table I. Crystal Data for 5

formula	$C_{21}H_{13}CrO_{11}PRu_3$
formula weight	827.51
crystal, color, habit	dark, irregular
crystal dimensions (mm)	0.18 × 0.30 × 0.40
crystal system	monoclinic
space group	$P2_1/a$ (No. 14)
a, Å	13.616 (2)
b, Å	14.229 (1)
c, Å	13.617 (2)
β, deg	94.15 (1)
V, Å^3	2631.2 (6)
Z	4
D_{calc}, g/cm^3	2.089
F_{000}	1592
μ(Mo Kα), cm^{-1}	21.64
scan type	ω–2θ
scan rate, deg/min	32.0
scan width, deg in ω	1.21 + 0.35 tan θ
$2\theta_{max}$, deg	60.0
total no. of reflcns	8237
no. of unique reflcns	7937
reflcns with $I > 3.00\sigma(I)$	4980
no. of variables	335
residuals: R; R_w	0.33; 0.036
goodness of fit indicator	2.42
max shift/error in final cycle	0.11
max peak in final diff map	1.04 e/Å^3
min peak in final diff map	−0.61 e/Å^3

Experimental Section

All manipulations were performed under Ar by using standard Schlenk and vacuum line techniques. Solvents were freshly distilled from the appropriate drying agents prior to use. ^{31}P chemical shifts are reported relative to 85% H_3PO_4.

Preparation of Bis(η^6-phenyltricarbonylchromium)-*tert*-butylphosphine. $(C_6H_6)Cr(CO)_3$ (1.62 g, 7.55 mmol) was added to 25 mL of tetrahydrofuran at −78 °C. To the cold, stirred solution was slowly added 4.8 mL of 1.6 M (7.7 mmol) *n*-butyllithium in hexane by using a syringe. The resulting solution was stirred at −78 °C for 50 min. *tert*-Butyldichlorophosphine (0.65 g, 4 mmol) was dissolved in 10 mL of THF and then added dropwise to the solution by means of a syringe. The reaction mixture was stirred at −78 °C for an additional 1 h and allowed to warm to room temperature. The solvent was removed under vacuum. The residue oil was dissolved in 20 mL of CH_2Cl_2 and then filtered through a frit packed with Celite. Evaporation of the solvent and crystallization of the product from CH_2Cl_2/hexanes afforded 0.71 g (37% yield) of bis(η^6-phenyltricarbonylchromium)-*tert*-butylphosphine: mass spectrum (EI) m/e 514 (P^+); $^{31}P\{H\}$ NMR (121.4 MHz, $CDCl_3$) δ 20.6 ppm; ^1H NMR (200 MHz, $CDCl_3$) δ 5.8–5.0 (10 H, m, η^6-C_6H_5), 1.2 (9 H, t-C_4H_9); IR (Nujol) 1955, 1875 cm^{-1}. Anal. Calcd for $C_{22}H_{21}Cr_2O_3P$: C, 51.37; H, 3.72. Found: C, 51.27; H, 3.71.

Preparation of $Ru_3(CO)_8[\mu_3$-$C_6H_4Cr(CO)_3][\mu_3$-$PBu^t]$ (5). $Ru_3(CO)_{12}$ (150 mg, 0.23 mmol) and $PBu^t[C_6H_5$-$Cr(CO)_3]_2$ (130 mg, 0.25 mmol) were refluxed in heptane solution (30 mL) for 5 h. The solvent was removed in vacuo, and the residue was chromatographed on silica gel (200–400 mesh) with CH_2Cl_2/hexanes (1:1.5) as eluent. The product 5 was isolated as a dark red band that afforded a dark red solid (45% yield) after removal of the solvent. The solid was recrystallized from CH_2Cl_2/hexanes at −30 °C: $^{31}P\{^1H\}$ NMR (121.4 MHz, $CDCl_3$) δ 480.3 ppm; ^1H NMR (200 MHz, $CDCl_3$) δ 5.8 (m, 2 H), 5.2 (m, 2 H), 2.01 (9 H); mass spectrum (FAB) m/e 829 (P^+); IR (Nujol) 2080 (m), 2050 (m), 2000 (s), 1940 (s), 1890, 1880 cm^{-1}. Anal. Calcd for $C_{21}H_{13}CrO_{11}PRu_3$: C, 30.48; H, 1.59. Found: C, 30.35; H, 1.59.

X-ray Crystallographic Analysis. Crystal data for 5 appear in Table I. The final unit cell parameters were obtained by least squares on the setting angles for 25 reflections with 2θ = 42.98–49.51°. The intensities of three standard reflections, measure every 200 reflections throughout the data collection, remained constant. No decay correction was applied. The data were processed[8] and corrected for Lorentz and polarization effects and absorption (empirical, based on azimuthal scans of (four) reflections).

The structure was solved by a combination of Patterson and direct methods. The non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated with C–H = 0.98 Å. Neutral atom scattering factors and anomalous dis-

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[6] The known aryne cluster complexes are electron-precise apart from some unsymmetrical open clusters related to 1 in which the aryne donates between two to four electrons to the cluster that, as a consequence, is electron-defficient.[7]

[7] (a) Brown, S. C.; Evans, J.; Smart, L. E. *J. Chem. Soc., Chem. Commun.* **1980**, 1021. (b) Johnson, B. F. G.; Lewis, J.; Massey, A. D.; Braga, D.; Grepioni, F. *J. Organomet. Chem.* **1989**, *369*, C43.

[8] (a) Cromer, D. T.; Waber, J. T. *International Tables X-Ray Crystallography*; The Kynoch Press: Birmingham, England, 1974; Vol. IV, Table 2.2A. (b) Ibers, J. A.; Hamilton , W. C., *Acta Crystallography*; **1964**, *17*, 781. (c) Cromer, D. T. *International Tables for X-Ray Crystallography*; The Kynoch Press: Birmingham, England, 1974; Vol. IV, Table 2.3.1. (d) TEXSAN-TEXRAY Structure Analysis Package, Molecular Structure Corp., 1985. (e) Motherwell, S.; Clegg, W. PLUTO program for plotting molecular and crystal structures, University of Cambridge, England, 1978. (f) Johnson, C. K. ORTEPII, Report ORNL-5138, Oak Ridge National Laboratory, Oak Ridge, TN, 1976. (g) Calbrese, J. C. PHASE: Patterson Heavy Atom Solution Extractor, University of Wisconsin-Madison, Ph.D. Thesis, 1972. (h) Beurskens, P. T. DIRDIF: Direct Methods for Difference Structures—an automatic procedure for phase extension and refinement of difference structure factors, Technical Report 1984/I, Crystallography Laboratory; Toevnooiveld, 6525 Ed Nijmegan, Netherlands.

Table II. Final Atomic Coordinates (Fractional) and B_{eq} (Å^2)[a]

atom	x	y	z	B_{eq}
Ru(1)	0.26193 (3)	0.60066 (2)	0.14334 (3)	3.17 (1)
Ru(2)	0.29254 (3)	0.59753 (2)	0.35187 (3)	3.43 (2)
Ru(3)	0.21186 (3)	0.43109 (2)	0.25071 (3)	3.38 (1)
Cr(1)	0.00141 (5)	0.46306 (5)	0.26417 (6)	3.72 (3)
P(1)	0.35727 (8)	0.49611 (8)	0.24054 (8)	3.27 (5)
O(1)	0.2147 (4)	0.5014 (4)	−0.0517 (3)	9.2 (3)
O(2)	0.1620 (3)	0.7935 (3)	0.1139 (3)	7.4 (2)
O(3)	0.4477 (3)	0.6971 (3)	0.0819 (3)	6.8 (2)
O(4)	0.2702 (4)	0.5047 (4)	0.5512 (3)	9.5 (3)
O(5)	0.2065 (3)	0.7965 (3)	0.3628 (3)	7.6 (2)
O(6)	0.4963 (3)	0.6770 (4)	0.4061 (4)	8.4 (3)
O(7)	0.2614 (4)	0.2836 (3)	0.4033 (3)	8.7 (3)
O(8)	0.2149 (3)	0.2809 (3)	0.0961 (3)	8.1 (3)
O(9)	−0.0090 (3)	0.3404 (3)	0.0853 (3)	6.7 (2)
O(10)	0.0379 (3)	0.3223 (3)	0.4267 (3)	7.4 (2)
O(11)	−0.2056 (3)	0.3946 (3)	0.2665 (4)	7.9 (3)
C(1)	0.2316 (4)	0.5408 (4)	0.0190 (4)	5.3 (3)
C(2)	0.1941 (3)	0.7215 (4)	0.1248 (4)	4.6 (2)
C(3)	0.3805 (3)	0.6577 (4)	0.1053 (4)	4.6 (2)
C(4)	0.2828 (4)	0.5416 (4)	0.4808 (4)	5.4 (3)
C(5)	0.2347 (4)	0.7224 (4)	0.3598 (4)	4.8 (2)
C(6)	0.4209 (4)	0.6462 (4)	0.3832 (4)	5.0 (3)
C(7)	0.2410 (4)	0.3389 (4)	0.3452 (4)	5.6 (3)
C(8)	0.2121 (4)	0.3387 (4)	0.1548 (4)	5.1 (3)
C(9)	0.0003 (4)	0.3848 (3)	0.1561 (4)	4.7 (2)
C(10)	0.0272 (4)	0.3738 (4)	0.3612 (4)	5.1 (3)
C(11)	−0.1271 (4)	0.4243 (4)	0.2674 (4)	5.0 (3)
C(12)	0.1204 (3)	0.5652 (3)	0.2072 (3)	3.4 (2)
C(13)	0.1372 (3)	0.5616 (3)	0.3107 (3)	3.6 (2)
C(14)	0.0562 (4)	0.5713 (4)	0.3712 (4)	4.7 (2)
C(15)	−0.0350 (4)	0.5981 (3)	0.3287 (5)	5.1 (3)
C(16)	−0.0537 (3)	0.6019 (4)	0.2243 (5)	5.2 (3)
C(17)	0.0240 (4)	0.5806 (3)	0.1650 (4)	4.6 (2)
C(18)	0.4797 (3)	0.4420 (3)	0.2290 (4)	4.7 (2)
C(19)	0.5602 (4)	0.5148 (5)	0.2233 (6)	7.8 (4)
C(20)	0.5015 (6)	0.3780 (7)	0.3132 (8)	14.6 (7)
C(21)	0.4742 (6)	0.3885 (7)	0.1327 (8)	15.0 (7)

[a] $B_{eq} = {}^{8}/_{3}\pi^2\sum\sum U_{ij}a_ia_j(a_i\cdot a_j)$.

Table III. Bond Lengths (Å) with Estimated Standard Deviations[a]

Ru(1)–Ru(2)	2.8401 (6)	Cr(1)–C(15)	2.185 (5)
Ru(1)–Ru(3)	2.9272 (5)	Cr(1)–C(16)	2.169 (5)
Ru(1)–P(1)	2.324 (1)	Cr(1)–C(17)	2.186 (5)
Ru(1)–C(1)	1.914 (6)	Cr(1)–R	1.748 (2)
Ru(1)–C(2)	1.959 (5)	P(1)–C(18)	1.853 (5)
Ru(1)–C(3)	1.912 (5)	O(1)–C(1)	1.122 (6)
Ru(1)–C(12)	2.228 (4)	O(2)–C(2)	1.120 (6)
Ru(2)–Ru(3)	2.9144 (5)	O(3)–C(3)	1.139 (5)
Ru(2)–P(1)	2.313 (1)	O(4)–C(4)	1.118 (6)
Ru(2)–C(4)	1.941 (6)	O(5)–C(5)	1.124 (6)
Ru(2)–C(5)	1.950 (5)	O(6)–C(6)	1.138 (6)
Ru(2)–C(6)	1.900 (5)	O(7)–C(7)	1.136 (6)
Ru(2)–C(13)	2.208 (4)	O(8)–C(8)	1.150 (6)
Ru(3)–Cr(1)	2.920 (1)	O(9)–C(9)	1.152 (6)
Ru(3)–P(1)	2.199 (1)	O(10)–C(10)	1.156 (6)
Ru(3)–C(7)	1.860 (5)	O(11)–C(11)	1.150 (6)
Ru(3)–C(8)	1.853 (5)	C(12)–C(13)	1.412 (6)
Ru(3)–C(12)	2.331 (4)	C(12)–C(17)	1.412 (6)
Ru(3)–C(13)	2.296 (4)	C(13)–C(14)	1.430 (6)
Cr(1)–C(9)	1.844 (5)	C(14)–C(15)	1.385 (7)
Cr(1)–C(10)	1.848 (6)	C(15)–C(16)	1.427 (8)
Cr(1)–C(11)	1.838 (5)	C(16)–C(17)	1.410 (7)
Cr(1)–C(12)	2.350 (4)	C(18)–C(19)	1.513 (8)
Cr(1)–C(13)	2.370 (4)	C(18)–C(20)	1.477 (9)
Cr(1)–C(14)	2.212 (5)	C(18)–C(21)	1.51 (1)

[a] Here and elsewhere R refers to the unweighted centriod of the C(12–17) aromatic ring.

Table IV. Bond Angles (deg) with Estimated Standard Deviations

Ru(2)–Ru(1)–Ru(3)	60.68 (1)	P(1)–Ru(3)–C(7)	101.1 (2)
Ru(2)–Ru(1)–P(1)	52.06 (3)	P(1)–Ru(3)–C(8)	101.9 (2)
Ru(2)–Ru(1)–C(1)	152.2 (2)	P(1)–Ru(3)–C(12)	96.1 (1)
Ru(2)–Ru(1)–C(2)	100.1 (2)	P(1)–Ru(3)–C(13)	96.1 (1)
Ru(2)–Ru(1)–C(3)	102.3 (2)	C(7)–Ru(3)–C(8)	88.6 (3)
Ru(2)–Ru(1)–C(12)	71.0 (1)	C(7)–Ru(3)–C(12)	146.8 (2)
Ru(3)–Ru(1)–P(1)	47.83 (3)	C(7)–Ru(3)–C(13)	113.7 (2)
Ru(3)–Ru(1)–C(1)	91.8 (2)	C(8)–Ru(3)–C(12)	115.4 (2)
Ru(3)–Ru(1)–C(2)	131.5 (1)	C(8)–Ru(3)–C(13)	148.0 (2)
Ru(3)–Ru(1)–C(3)	135.8 (1)	C(12)–Ru(3)–C(13)	35.5 (1)
Ru(3)–Ru(1)–C(12)	51.6 (1)	Ru(3)–Cr(1)–R	81.02 (7)
P(1)–Ru(1)–C(1)	107.1 (2)	Ru(3)–Cr(1)–C(9)	78.9 (2)
P(1)–Ru(1)–C(2)	150.9 (2)	Ru(3)–Cr(1)–C(10)	78.5 (2)
P(1)–Ru(1)–C(3)	88.8 (1)	Ru(3)–Cr(1)–C(11)	153.5 (2)
P(1)–Ru(1)–C(12)	95.5 (1)	C(9)–Cr(1)–R	125.5 (2)
C(1)–Ru(1)–C(2)	102.0 (2)	C(9)–Cr(1)–C(10)	98.4 (2)
C(1)–Ru(1)–C(3)	94.7 (2)	C(9)–Cr(1)–C(11)	83.4 (2)
C(1)–Ru(1)–C(12)	96.1 (2)	C(10)–Cr(1)–R	126.2 (2)
C(2)–Ru(1)–C(3)	89.5 (2)	C(10)–Cr(1)–C(11)	84.8 (2)
C(2)–Ru(1)–C(12)	80.6 (2)	C(11)–Cr(1)–R	125.5 (2)
C(3)–Ru(1)–C(12)	166.6 (2)	Ru(1)–P(1)–Ru(2)	75.54 (4)
Ru(1)–Ru(2)–Ru(3)	61.13 (1)	Ru(1)–P(1)–Ru(3)	80.61 (4)
Ru(1)–Ru(2)–P(1)	52.41 (3)	Ru(1)–P(1)–C(18)	133.3 (2)
Ru(1)–Ru(2)–C(4)	153.7 (2)	Ru(2)–P(1)–Ru(3)	80.43 (4)
Ru(1)–Ru(2)–C(5)	90.6 (2)	Ru(2)–P(1)–C(18)	134.6 (2)
Ru(1)–Ru(2)–C(6)	106.5 (2)	Ru(3)–P(1)–C(18)	130.6 (2)
Ru(1)–Ru(2)–C(13)	71.4 (1)	Ru(1)–C(1)–O(1)	176.5 (6)
Ru(3)–Ru(2)–P(1)	48.07 (3)	Ru(1)–C(2)–O(2)	174.8 (5)
Ru(3)–Ru(2)–C(4)	92.7 (2)	Ru(1)–C(3)–O(3)	175.5 (5)
Ru(3)–Ru(2)–C(5)	128.8 (1)	Ru(2)–C(4)–O(4)	173.6 (6)
Ru(3)–Ru(2)–C(6)	135.3 (2)	Ru(2)–C(5)–O(5)	175.8 (5)
Ru(3)–Ru(2)–C(13)	51.0 (1)	Ru(2)–C(6)–O(6)	176.6 (5)
P(1)–Ru(2)–C(4)	113.0 (2)	Ru(3)–C(7)–O(7)	178.1 (6)
P(1)–Ru(2)–C(5)	141.2 (2)	Ru(3)–C(8)–O(8)	178.1 (5)
P(1)–Ru(2)–C(6)	89.2 (2)	Cr(1)–C(9)–O(9)	173.1 (5)
P(1)–Ru(2)–C(13)	95.3 (1)	Cr(1)–C(10)–O(10)	174.0 (5)
C(4)–Ru(2)–C(5)	105.6 (2)	Cr(1)–C(11)–O(11)	175.4 (5)
C(4)–Ru(2)–C(6)	93.9 (2)	Ru(1)–C(12)–Ru(3)	79.9 (1)
C(4)–Ru(2)–C(13)	90.5 (2)	Ru(1)–C(12)–C(13)	108.4 (3)
C(5)–Ru(2)–C(6)	91.4 (2)	Ru(1)–C(12)–C(17)	127.6 (3)
C(5)–Ru(2)–C(13)	80.9 (2)	Ru(3)–C(12)–C(13)	70.9 (2)
C(6)–Ru(2)–C(13)	171.9 (2)	Ru(3)–C(12)–C(17)	134.0 (3)
Ru(1)–Ru(3)–Ru(2)	58.18 (1)	C(13)–C(12)–C(17)	119.4 (4)
Ru(1)–Ru(3)–Cr(1)	99.67 (2)	Ru(2)–C(13)–Ru(3)	80.6 (1)
Ru(1)–Ru(3)–P(1)	51.56 (3)	Ru(2)–C(13)–C(12)	109.1 (3)
Ru(1)–Ru(3)–C(7)	151.8 (2)	Ru(2)–C(13)–C(14)	126.6 (3)
Ru(1)–Ru(3)–C(8)	102.7 (2)	Ru(3)–C(13)–C(12)	73.6 (3)
Ru(1)–Ru(3)–C(12)	48.5 (1)	Ru(3)–C(13)–C(14)	131.5 (3)
Ru(1)–Ru(3)–C(13)	68.6 (1)	C(12)–C(13)–C(14)	119.7 (4)
Ru(2)–Ru(3)–Cr(1)	100.47 (2)	C(13)–C(14)–C(15)	119.5 (5)
Ru(2)–Ru(3)–P(1)	51.50 (3)	C(14)–C(15)–C(16)	121.1 (4)
Ru(2)–Ru(3)–C(7)	101.1 (2)	C(15)–C(16)–C(17)	118.4 (5)
Ru(2)–Ru(3)–C(8)	152.8 (2)	C(12)–C(17)–C(16)	121.0 (5)
Ru(2)–Ru(3)–C(12)	68.4 (1)	P(1)–C(18)–C(19)	112.3 (4)
Ru(2)–Ru(3)–C(13)	48.4 (1)	P(1)–C(18)–C(20)	108.7 (4)
Cr(1)–Ru(3)–P(1)	146.15 (4)	P(1)–C(18)–C(21)	107.1 (4)
Cr(1)–Ru(3)–C(7)	103.2 (2)	C(19)–C(18)–C(20)	110.9 (6)
Cr(1)–Ru(3)–C(8)	101.9 (2)	C(19)–C(18)–C(21)	106.9 (6)
Cr(1)–Ru(3)–C(12)	51.7 (1)	C(20)–C(18)–C(21)	110.9 (7)
Cr(1)–Ru(3)–C(13)	52.4 (1)		

persion correction for the non-hydrogen atoms were taken from ref 8a. Final atomic coordinates and equivalent isotropic thermal parameters, bond lengths, and bond angles appear in Tables II–IV. A stereoscopic ORTEP diagram, tables of torsion angles, least-squares planes, and measured and calculated structure factor amplitudes are included as supplementary material.

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Supplementary Material Available: Stereo ORTEP diagram and tables of anisotropic thermal parameters, torsion or conformational angles, and least-squares planes (12 pages); listings of observed and calculated structure factor amplitudes (52 pages). Ordering information is given on any current masthead page.