Supporting Information:

Synthesis and Structure of Cationic Triruthenium Complexes Containing an Oxametallacycle; Reversible Carbon-Oxygen Bond Formation and Scission on an Electron-Deficient Triruthenium Plane

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1. **Results of the X-ray diffraction studies of [(Cp*Ru)$_3$(μ-OH)(μ_3-CH)-(μ_3-η^1:η^3:η^1-CHCMeCH)](PF$_6$)$_2$ (6-PF$_6$)**
2. **Results of the X-ray diffraction studies of [(Cp*Ru)$_3$(μ_3-CH)-{μ_3-OC(H)C(Me)CH-}](BPh$_4$) (8-BPh$_4$)**
3. **Results of the X-ray diffraction studies of [(Cp*Ru)$_3$(μ_3-CH)-{μ_3-OC(Me)C(H)CH-}](PF$_6$) (9-PF$_6$)**

1. Results of the X-ray diffraction studies of $[(Cp^*Ru)_3(\mu\text{-}OH)(\mu_3\text{-}CH)(\mu_3\text{-}\eta^1\text{:}\eta^3\text{:}\eta^1\text{-}CHCMeCH)](BF_4)_2$ (6-BF_4)

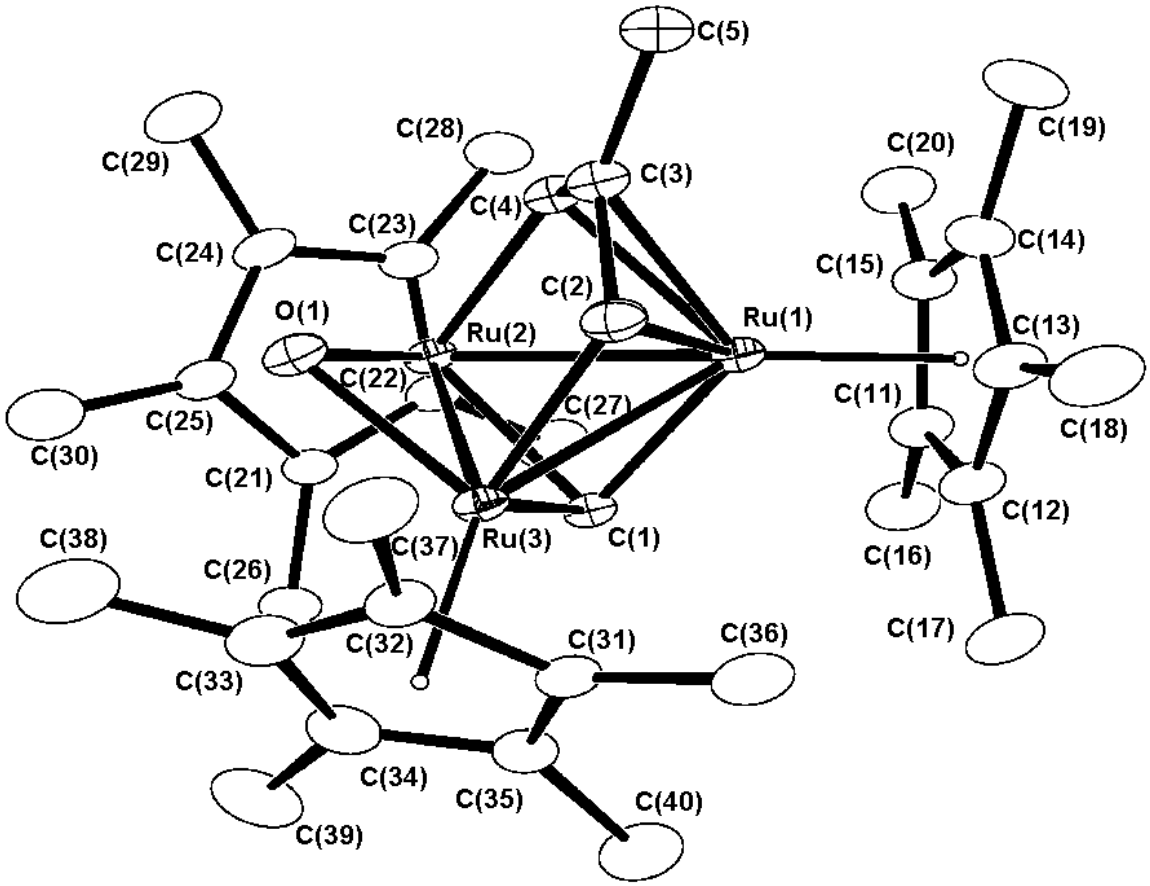

Table S1-1. Crystal data and structure refinement for **6-BF4**.

Identification code, 6
Empirical formula,C35 H58 B2 F8 O4 Ru3
Formula weight, 1019.64
Temperature, 163(2) K
Wavelength, 0.71069 Å
Crystal system, Triclinic
Space group, P-1
Unit cell dimensions,
a = 11.5978(9)Å α = 105.579(3)°
b = 12.3053(9)Å β = 92.274(5)°
c = 16.1981(15)Å γ = 98.537(4)°
Volume, 2194.4(3) $Å^3$
Z, 2
Density (calculated), 1.543 Mg/m^3
Absorption coefficient, 1.086 mm^{-1}
F(000), 1028
Crystal size, 0.500 x 0.200 x 0.100 mm
Theta range for data collection, 2.45 to 30.03 °.
Index ranges,0<=h<=16; -17<=k<=17; -22<=l<=22
Reflections collected, 22998
Independent reflections, 11935 [R(int) = 0.0432]
Reflections observed (>2σ), 9740
Absorption correction, Numerical
Max. and min. transmission, 0.9958 and 0.9852
Refinement method, Full-matrix least-squares on F^2
Data / restraints / parameters, 11910 / 0 / 498
Goodness-of-fit on F^2, 1.098
Final R indices [I>2σ(I)],R_1 = 0.0769 wR_2 = 0.2052
R indices (all data), R_1 = 0.0942 wR_2 = 0.2183
Largest diff. peak and hole, 4.289 and -1.505 $e.Å^{-3}$

Table S1-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **6-BF4**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom, x, y, z, U(eq)

Ru(1),2226(1),2797(1),2672(1),25(1),
Ru(2),2469(1),1583(1),3819(1),25(1),
Ru(3),3530(1),1088(1),2396(1),25(1),
C(1),1816(6),1123(5),2571(4),25(1),
C(2),4061(6),2796(6),2613(5),32(1),
C(3),3970(6),3585(6),3427(4),32(1),
C(4),3100(6),3238(6),3926(4),30(1),
C(5),4654(8),4786(7),3669(5),43(2),
O(1),4162(4),1380(5),3640(3),33(1),
C(11),347(6),2804(7),2215(5),33(1),
C(12),1050(6),2716(7),1507(5),34(1),
C(13),1938(7),3712(7),1691(5),37(2),
C(14),1763(7),4435(7),2525(5),39(2),
C(15),797(7),3876(6),2858(5),35(2),
C(16),-762(7),2031(8),2195(6),45(2),
C(17),795(8),1805(9),672(5),48(2),
C(18),2760(9),4014(10),1082(6),56(2),
C(19),2392(10),5627(7),2916(8),58(2),
C(20),272(8),4382(8),3663(6),49(2),
C(21),1370(6),60(6),4173(4),32(1),
C(22),766(6),1019(6),4313(4),32(1),
C(23),1421(7),1964(7),4953(5),37(2),
C(24),2471(7),1590(7),5185(4),37(2),
C(25),2436(6),430(7),4694(5),34(1),
C(26),883(8),-1108(7),3632(5),45(2),
C(27),-478(7),954(9),3965(6),47(2),
C(28),1025(10),3076(8),5374(6),54(2),
C(29),3421(9),2306(10),5874(6),56(3),
C(30),3359(9),-284(9),4762(7),52(2),
C(31),4043(6),554(6),1056(4),32(1),
C(32),5004(6),563(6),1644(5),33(1),
C(33),4686(8),-275(7),2068(5),43(2),
C(34),3521(8),-815(7),1764(6),45(2),
C(35),3120(6),-296(6),1142(5),37(2),
C(36),4086(8),1247(8),428(5),46(2),
C(37),6210(7),1272(9),1710(6),54(3),
C(40),2009(7),-722(9),570(6),59(3),
C(38),5437(11),-566(11),2729(7),66(3),
C(39),2845(12),-1831(9),1973(9),72(3),
O(2),5385(4),6328(4),1796(3),24(1),
O(3),4250(4),-3603(4),179(3),31(1),
O(4),7455(7),4554(6),2398(6),66(2),
B(1),-1520(10),-1580(10),1596(7),50(2),
F(11),-440(7),-1015(8),1645(5),94(3),
F(12),-1826(6),-1646(7),2395(4),83(2),
F(13),-1686(9),-2623(7),1015(5),104(3),
F(14),-2309(10),-983(11),1265(7),125(4),
B(2),7074(9),3162(10),4476(8),53(3),
F(21),5935(5),2954(6),4669(5),78(2),
F(22),7181(9),2537(10),3699(6),141(5),
F(23),7401(7),4319(6),4630(6),93(3),
F(24),7858(8),2907(8),5019(7),111(3),

Table S1-3. Bond lengths [Å] and angles [°] for **6-BF4**.

Ru(1)-C(1),2.004(7)
Ru(1)-C(4),2.127(7)
Ru(1)-C(2),2.134(7)
Ru(1)-C(13),2.221(7)
Ru(1)-C(14),2.231(7)
Ru(1)-C(15),2.254(7)
Ru(1)-C(12),2.255(7)
Ru(1)-C(3),2.261(7)
Ru(1)-C(11),2.276(7)
Ru(1)-Ru(2),2.7085(8)
Ru(1)-Ru(3),2.7200(7)
Ru(2)-C(4),2.018(7)
Ru(2)-C(1),2.029(6)
Ru(2)-O(1),2.038(5)
Ru(2)-C(24),2.210(7)
Ru(2)-C(23),2.226(7)
Ru(2)-C(22),2.244(7)
Ru(2)-C(25),2.257(7)
Ru(2)-C(21),2.321(7)
Ru(2)-Ru(3),2.6254(7)
Ru(3)-C(1),2.024(6)
Ru(3)-C(2),2.030(7)
Ru(3)-O(1),2.035(5)
Ru(3)-C(32),2.212(7)
Ru(3)-C(31),2.224(6)
Ru(3)-C(35),2.253(7)
Ru(3)-C(33),2.267(8)
Ru(3)-C(34),2.289(8)
C(2)-C(3),1.431(9)
C(3)-C(4),1.405(10)
C(3)-C(5),1.511(10)
C(11)-C(12),1.422(10)
C(11)-C(15),1.454(11)
C(11)-C(16),1.476(11)
C(12)-C(13),1.434(11)
C(12)-C(17),1.492(11)
C(13)-C(14),1.444(11)
C(13)-C(18),1.479(12)
C(14)-C(15),1.427(11)
C(14)-C(19),1.495(12)
C(15)-C(20),1.483(11)
C(21)-C(25),1.412(10)
C(21)-C(22),1.430(10)
C(21)-C(26),1.483(10)
C(22)-C(23),1.425(10)
C(22)-C(27),1.512(11)
C(23)-C(24),1.435(12)
C(23)-C(28),1.503(11)
C(24)-C(25),1.430(11)
C(24)-C(29),1.523(11)
C(25)-C(30),1.499(11)
C(31)-C(35),1.421(10)
C(31)-C(32),1.433(10)
C(31)-C(36),1.491(12)
C(32)-C(33),1.399(12)
C(32)-C(37),1.519(11)
C(33)-C(34),1.419(13)
C(33)-C(38),1.504(13)
C(34)-C(35),1.427(13)
C(34)-C(39),1.500(14)
C(35)-C(40),1.496(11)
B(1)-F(11),1.328(13)
B(1)-F(13),1.355(13)
B(1)-F(12),1.375(12)
B(1)-F(14),1.426(15)
B(2)-F(22),1.308(13)
B(2)-F(24),1.367(15)
B(2)-F(23),1.369(13)
B(2)-F(21),1.373(12)

C(1)-Ru(1)-C(4),95.3(3)
C(1)-Ru(1)-C(2),95.2(3)
C(4)-Ru(1)-C(2),68.9(3)
C(1)-Ru(1)-C(13),128.7(3)
C(4)-Ru(1)-C(13),135.8(3)
C(2)-Ru(1)-C(13),99.2(3)
C(1)-Ru(1)-C(14),151.5(3)
C(4)-Ru(1)-C(14),104.7(3)
C(2)-Ru(1)-C(14),110.8(3)
C(13)-Ru(1)-C(14),37.9(3)
C(1)-Ru(1)-C(15),119.0(3)
C(4)-Ru(1)-C(15),102.8(3)
C(2)-Ru(1)-C(15),145.7(3)
C(13)-Ru(1)-C(15),62.8(3)
C(14)-Ru(1)-C(15),37.1(3)
C(1)-Ru(1)-C(12),94.5(3)
C(4)-Ru(1)-C(12),164.7(3)
C(2)-Ru(1)-C(12),121.8(3)
C(13)-Ru(1)-C(12),37.4(3)
C(14)-Ru(1)-C(12),62.2(3)
C(15)-Ru(1)-C(12),62.1(3)
C(1)-Ru(1)-C(3),112.3(3)
C(4)-Ru(1)-C(3),37.2(3)
C(2)-Ru(1)-C(3),37.9(3)
C(13)-Ru(1)-C(3),108.9(3)
C(14)-Ru(1)-C(3),95.7(3)
C(15)-Ru(1)-C(3),117.0(3)
C(12)-Ru(1)-C(3),145.4(3)
C(1)-Ru(1)-C(11),89.5(3)
C(4)-Ru(1)-C(11),131.8(3)
C(2)-Ru(1)-C(11),158.4(3)
C(13)-Ru(1)-C(11),62.2(3)
C(14)-Ru(1)-C(11),62.0(3)
C(15)-Ru(1)-C(11),37.4(3)
C(12)-Ru(1)-C(11),36.6(3)
C(3)-Ru(1)-C(11),154.4(3)
C(1)-Ru(1)-Ru(2),48.19(17)
C(4)-Ru(1)-Ru(2),47.5(2)
C(2)-Ru(1)-Ru(2),83.0(2)
C(13)-Ru(1)-Ru(2),176.6(2)
C(14)-Ru(1)-Ru(2),143.7(2)
C(15)-Ru(1)-Ru(2),116.7(2)
C(12)-Ru(1)-Ru(2),139.2(2)
C(3)-Ru(1)-Ru(2),74.44(19)
C(11)-Ru(1)-Ru(2),115.14(19)
C(1)-Ru(1)-Ru(3),47.84(18)

C(4)-Ru(1)-Ru(3),82.21(19)
C(2)-Ru(1)-Ru(3),47.6(2)
C(13)-Ru(1)-Ru(3),121.9(2)
C(14)-Ru(1)-Ru(3),153.9(2)
C(15)-Ru(1)-Ru(3),166.7(2)
C(12)-Ru(1)-Ru(3),113.02(19)
C(3)-Ru(1)-Ru(3),74.40(19)
C(11)-Ru(1)-Ru(3),131.16(19)
Ru(2)-Ru(1)-Ru(3),57.845(19)
C(4)-Ru(2)-C(1),98.0(3)
C(4)-Ru(2)-O(1),83.3(3)
C(1)-Ru(2)-O(1),99.1(2)
C(4)-Ru(2)-C(24),101.3(3)
C(1)-Ru(2)-C(24),155.2(3)
O(1)-Ru(2)-C(24),98.5(3)
C(4)-Ru(2)-C(23),94.8(3)
C(1)-Ru(2)-C(23),125.4(3)
O(1)-Ru(2)-C(23),135.1(3)
C(24)-Ru(2)-C(23),37.7(3)
C(4)-Ru(2)-C(22),122.9(3)
C(1)-Ru(2)-C(22),94.6(3)
O(1)-Ru(2)-C(22),148.3(3)
C(24)-Ru(2)-C(22),61.8(3)
C(23)-Ru(2)-C(22),37.2(3)
C(4)-Ru(2)-C(25),135.7(3)
C(1)-Ru(2)-C(25),126.3(3)
O(1)-Ru(2)-C(25),88.1(2)
C(24)-Ru(2)-C(25),37.3(3)
C(23)-Ru(2)-C(25),62.4(3)
C(22)-Ru(2)-C(25),61.0(3)
C(4)-Ru(2)-C(21),156.5(3)
C(1)-Ru(2)-C(21),95.7(3)
O(1)-Ru(2)-C(21),113.3(2)
C(24)-Ru(2)-C(21),61.2(3)
C(23)-Ru(2)-C(21),61.7(3)
C(22)-Ru(2)-C(21),36.5(3)
C(25)-Ru(2)-C(21),35.9(2)
C(4)-Ru(2)-Ru(3),86.69(19)
C(1)-Ru(2)-Ru(3),49.56(18)
O(1)-Ru(2)-Ru(3),49.81(14)
C(24)-Ru(2)-Ru(3),146.6(2)
C(23)-Ru(2)-Ru(3),174.9(2)
C(22)-Ru(2)-Ru(3),138.65(19)
C(25)-Ru(2)-Ru(3),119.5(2)
C(21)-Ru(2)-Ru(3),116.67(18)
C(4)-Ru(2)-Ru(1),50.97(19)
C(1)-Ru(2)-Ru(1),47.43(19)
O(1)-Ru(2)-Ru(1),97.25(16)
C(24)-Ru(2)-Ru(1),145.9(2)
C(23)-Ru(2)-Ru(1),116.1(2)
C(22)-Ru(2)-Ru(1),112.88(19)
C(25)-Ru(2)-Ru(1),172.30(19)
C(21)-Ru(2)-Ru(1),136.41(18)
Ru(3)-Ru(2)-Ru(1),61.30(2)
C(1)-Ru(3)-C(2),97.9(3)
C(1)-Ru(3)-O(1),99.3(2)
C(2)-Ru(3)-O(1),84.1(3)
C(1)-Ru(3)-C(32),154.0(2)
C(2)-Ru(3)-C(32),95.8(3)
O(1)-Ru(3)-C(32),104.0(2)
C(1)-Ru(3)-C(31),118.2(3)
C(2)-Ru(3)-C(31),97.3(3)
O(1)-Ru(3)-C(31),141.7(2)
C(32)-Ru(3)-C(31),37.7(3)
C(1)-Ru(3)-C(35),92.6(2)
C(2)-Ru(3)-C(35),129.7(3)
O(1)-Ru(3)-C(35),142.3(3)
C(32)-Ru(3)-C(35),61.8(3)
C(31)-Ru(3)-C(35),37.0(3)
C(1)-Ru(3)-C(33),136.2(3)
C(2)-Ru(3)-C(33),125.9(3)
O(1)-Ru(3)-C(33),86.4(3)
C(32)-Ru(3)-C(33),36.4(3)
C(31)-Ru(3)-C(33),61.7(3)
C(35)-Ru(3)-C(33),61.2(3)
C(1)-Ru(3)-C(34),101.9(3)
C(2)-Ru(3)-C(34),156.1(3)
O(1)-Ru(3)-C(34),105.7(3)
C(32)-Ru(3)-C(34),60.9(3)
C(31)-Ru(3)-C(34),61.4(3)
C(35)-Ru(3)-C(34),36.6(3)
C(33)-Ru(3)-C(34),36.3(3)
C(1)-Ru(3)-Ru(2),49.70(17)
C(2)-Ru(3)-Ru(2),87.2(2)
O(1)-Ru(3)-Ru(2),49.93(14)
C(32)-Ru(3)-Ru(2),153.42(19)
C(31)-Ru(3)-Ru(2),167.78(19)
C(35)-Ru(3)-Ru(2),133.48(19)
C(33)-Ru(3)-Ru(2),124.2(2)
C(34)-Ru(3)-Ru(2),116.0(2)
C(1)-Ru(3)-Ru(1),47.22(19)
C(2)-Ru(3)-Ru(1),50.9(2)
O(1)-Ru(3)-Ru(1),96.98(15)
C(32)-Ru(3)-Ru(1),138.5(2)
C(31)-Ru(3)-Ru(1),113.6(2)
C(35)-Ru(3)-Ru(1),116.8(2)
C(33)-Ru(3)-Ru(1),174.8(2)
C(34)-Ru(3)-Ru(1),144.9(2)
Ru(2)-Ru(3)-Ru(1),60.857(19)
Ru(1)-C(1)-Ru(3),84.9(2)
Ru(1)-C(1)-Ru(2),84.4(2)
Ru(3)-C(1)-Ru(2),80.7(2)
C(3)-C(2)-Ru(3),121.5(5)
C(3)-C(2)-Ru(1),75.9(4)
Ru(3)-C(2)-Ru(1),81.5(3)
C(4)-C(3)-C(2),116.3(6)
C(4)-C(3)-C(5),122.2(6)
C(2)-C(3)-C(5),120.9(6)
C(4)-C(3)-Ru(1),66.2(4)
C(2)-C(3)-Ru(1),66.2(4)
C(5)-C(3)-Ru(1),132.3(6)
C(3)-C(4)-Ru(2),123.3(5)
C(3)-C(4)-Ru(1),76.6(4)
Ru(2)-C(4)-Ru(1),81.5(2)
Ru(3)-O(1)-Ru(2),80.26(17)
C(12)-C(11)-C(15),107.9(7)
C(12)-C(11)-C(16),123.8(7)
C(15)-C(11)-C(16),127.4(7)

C(12)-C(11)-Ru(1),70.9(4)
C(15)-C(11)-Ru(1),70.5(4)
C(16)-C(11)-Ru(1),132.8(5)
C(11)-C(12)-C(13),108.8(7)
C(11)-C(12)-C(17),124.6(7)
C(13)-C(12)-C(17),126.2(7)
C(11)-C(12)-Ru(1),72.5(4)
C(13)-C(12)-Ru(1),70.0(4)
C(17)-C(12)-Ru(1),129.4(6)
C(12)-C(13)-C(14),107.3(7)
C(12)-C(13)-C(18),125.7(8)
C(14)-C(13)-C(18),126.4(8)
C(12)-C(13)-Ru(1),72.6(4)
C(14)-C(13)-Ru(1),71.4(4)
C(18)-C(13)-Ru(1),128.2(6)
C(15)-C(14)-C(13),108.6(7)
C(15)-C(14)-C(19),125.8(8)
C(13)-C(14)-C(19),125.2(8)
C(15)-C(14)-Ru(1),72.3(4)
C(13)-C(14)-Ru(1),70.7(4)
C(19)-C(14)-Ru(1),128.7(6)
C(14)-C(15)-C(11),107.4(6)
C(14)-C(15)-C(20),125.3(8)
C(11)-C(15)-C(20),126.9(8)
C(14)-C(15)-Ru(1),70.6(4)
C(11)-C(15)-Ru(1),72.1(4)
C(20)-C(15)-Ru(1),128.4(6)
C(25)-C(21)-C(22),107.0(6)
C(25)-C(21)-C(26),128.2(7)
C(22)-C(21)-C(26),124.6(7)
C(25)-C(21)-Ru(2),69.6(4)
C(22)-C(21)-Ru(2),68.8(4)
C(26)-C(21)-Ru(2),130.4(5)
C(23)-C(22)-C(21),109.7(7)
C(23)-C(22)-C(27),125.2(7)
C(21)-C(22)-C(27),124.1(7)
C(23)-C(22)-Ru(2),70.7(4)
C(21)-C(22)-Ru(2),74.7(4)
C(27)-C(22)-Ru(2),130.3(5)
C(22)-C(23)-C(24),106.2(7)
C(22)-C(23)-C(28),126.7(8)
C(24)-C(23)-C(28),126.7(8)
C(22)-C(23)-Ru(2),72.1(4)
C(24)-C(23)-Ru(2),70.5(4)
C(28)-C(23)-Ru(2),127.5(6)
C(25)-C(24)-C(23),108.4(6)
C(25)-C(24)-C(29),126.6(8)
C(23)-C(24)-C(29),124.9(8)
C(25)-C(24)-Ru(2),73.1(4)
C(23)-C(24)-Ru(2),71.7(4)
C(29)-C(24)-Ru(2),123.5(6)
C(21)-C(25)-C(24),108.6(7)
C(21)-C(25)-C(30),126.2(8)
C(24)-C(25)-C(30),125.1(7)
C(21)-C(25)-Ru(2),74.5(4)
C(24)-C(25)-Ru(2),69.6(4)
C(30)-C(25)-Ru(2),124.1(6)
C(35)-C(31)-C(32),107.0(7)
C(35)-C(31)-C(36),128.0(7)
C(32)-C(31)-C(36),124.7(7)
C(35)-C(31)-Ru(3),72.6(4)
C(32)-C(31)-Ru(3),70.7(4)
C(36)-C(31)-Ru(3),126.1(5)
C(33)-C(32)-C(31),108.9(7)
C(33)-C(32)-C(37),126.0(8)
C(31)-C(32)-C(37),124.8(8)
C(33)-C(32)-Ru(3),73.9(4)
C(31)-C(32)-Ru(3),71.6(4)
C(37)-C(32)-Ru(3),126.0(5)
C(32)-C(33)-C(34),108.2(8)
C(32)-C(33)-C(38),126.5(9)
C(34)-C(33)-C(38),125.3(9)
C(32)-C(33)-Ru(3),69.7(4)
C(34)-C(33)-Ru(3),72.7(4)
C(38)-C(33)-Ru(3),123.5(6)
C(33)-C(34)-C(35),107.9(7)
C(33)-C(34)-C(39),127.4(10)
C(35)-C(34)-C(39),124.4(9)
C(33)-C(34)-Ru(3),71.0(5)
C(35)-C(34)-Ru(3),70.3(4)
C(39)-C(34)-Ru(3),128.8(6)
C(31)-C(35)-C(34),108.1(7)
C(31)-C(35)-C(40),125.8(9)
C(34)-C(35)-C(40),125.2(8)
C(31)-C(35)-Ru(3),70.4(4)
C(34)-C(35)-Ru(3),73.1(4)
C(40)-C(35)-Ru(3),130.6(5)
F(11)-B(1)-F(13),112.8(10)
F(11)-B(1)-F(12),110.9(9)
F(13)-B(1)-F(12),111.9(10)
F(11)-B(1)-F(14),108.7(11)
F(13)-B(1)-F(14),103.5(10)
F(12)-B(1)-F(14),108.7(9)
F(22)-B(2)-F(24),107.1(11)
F(22)-B(2)-F(23),116.4(12)
F(24)-B(2)-F(23),102.2(9)
F(22)-B(2)-F(21),109.4(9)
F(24)-B(2)-F(21),113.6(11)
F(23)-B(2)-F(21),108.2(9)

Symmetry transformations used to generate equivalent atoms:

Table S1-4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **6-BF4**. The nisotropic displacement factor exponent takes the form: -2 p^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom, U11, U22, U33, U23, U13, U12

Ru(1),24(1),26(1),23(1),2(1),3(1),3(1)
Ru(2),23(1),28(1),21(1),2(1),1(1),1(1)
Ru(3),21(1),27(1),23(1),-1(1),2(1),3(1)
C(1),26(3),26(3),21(3),2(2),2(2),3(2)
C(2),25(3),33(3),33(3),4(3),3(2),1(3)
C(3),30(3),33(4),28(3),3(3),4(2),-3(3)
C(4),27(3),31(3),25(3),1(2),2(2),1(2)
C(5),45(4),34(4),39(4),-1(3),5(3),-8(3)
O(1),26(2),40(3),27(2),2(2),-2(2),1(2)
C(11),24(3),39(4),38(4),12(3),0(3),10(3)
C(12),31(3),41(4),30(3),9(3),1(3),8(3)
C(13),38(4),44(4),35(4),19(3),6(3),12(3)
C(14),43(4),30(4),46(4),15(3),5(3),7(3)
C(15),34(3),35(4),38(4),8(3),7(3),15(3)
C(16),27(3),59(5),53(5),23(4),-1(3),11(3)
C(17),41(4),64(6),33(4),3(4),-7(3),13(4)
C(18),56(6),72(7),47(5),29(5),10(4),6(5)
C(19),61(6),29(4),80(7),12(4),7(5),4(4)
C(20),49(5),55(5),46(5),6(4),14(4),29(4)
C(21),34(3),30(3),29(3),8(3),1(3),-1(3)
C(22),30(3),38(4),30(3),11(3),8(2),4(3)
C(23),41(4),36(4),30(3),6(3),12(3),1(3)
C(24),37(4),50(4),22(3),11(3),0(3),-3(3)
C(25),32(3),43(4),29(3),16(3),0(3),4(3)
C(26),57(5),32(4),37(4),5(3),5(3),-8(3)
C(27),29(4),68(6),51(5),29(4),8(3),3(4)
C(28),73(6),39(4),44(5),2(4),32(4),6(4)
C(29),55(5),71(6),31(4),11(4),-15(4),-18(5)
C(30),51(5),59(6),55(5),27(4),1(4),20(4)
C(31),33(3),31(3),25(3),-4(2),6(2),4(3)
C(32),25(3),37(4),33(3),0(3),4(2),11(3)
C(33),42(4),44(4),41(4),3(3),10(3),18(3)
C(34),46(4),32(4),56(5),5(3),20(4),13(3)
C(35),29(3),32(4),35(3),-12(3),4(3),-2(3)
C(36),54(5),47(5),34(4),5(3),13(3),12(4)
C(37),25(3),69(6),49(5),-15(4),11(3),2(4)
C(40),32(4),66(6),50(5),-25(4),-4(3),-9(4)
C(38),82(8),78(7),52(6),22(5),12(5),47(6)
C(39),82(8),35(5),101(9),15(5),36(7),11(5)
O(2),23(2),27(2),16(2),6(2),2(1),-16(2)
O(3),34(2),35(3),19(2),11(2),2(2),-15(2)
O(4),71(5),47(4),86(5),36(4),1(4),-3(3)
B(1),49(5),56(6),38(5),5(4),2(4),1(5)
F(11),67(4),125(7),67(4),13(4),6(3),-35(4)
F(12),71(4),121(6),51(4),24(4),14(3),-2(4)
F(13),160(9),65(5),65(5),-2(4),12(5),-21(5)
F(14),125(8),176(10),95(7),45(7),11(6),85(8)
B(2),40(5),46(6),58(6),-7(5),1(4),4(4)
F(21),37(3),70(4),97(5),-21(4),11(3),-4(3)
F(22),103(7),170(10),87(6),-62(6),29(5),0(6)
F(23),75(5),52(4),137(7),15(4),3(5),-9(3)
F(24),81(6),110(7),139(8),27(6),-29(5),26(5)

Table S1-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **6-BF4**.

Atom, x, y, z, U(eq)

H(5A),4847,5004,3145,65
H(5B),5376,4817,4015,65
H(5C),4180,5317,4003,65
H(16A),-1153,2322,2715,67
H(16B),-599,1264,2171,67
H(16C),-1270,1993,1687,67
H(17A),1527,1688,405,72
H(17B),268,2038,289,72
H(17C),422,1090,775,72
H(18A),3504,4428,1399,85
H(18B),2425,4501,780,85
H(18C),2896,3315,664,85
H(19A),3219,5668,2804,86
H(19B),2326,5842,3538,86
H(19C),2044,6154,2662,86
H(20A),-194,3771,3849,73
H(20B),-232,4913,3561,73
H(20C),895,4795,4112,73
H(26A),705,-1087,3040,67
H(26B),165,-1394,3859,67
H(26C),1457,-1616,3638,67
H(27A),-597,472,3369,71
H(27B),-623,1725,3984,71
H(27C),-1020,624,4316,71
H(28A),1653,3713,5393,80
H(28B),835,3092,5961,80
H(28C),329,3149,5043,80
H(29A),3413,3120,5940,84
H(29B),4186,2122,5704,84
H(29C),3275,2136,6422,84
H(30A),4130,146,4731,78
H(30B),3212,-990,4288,78
H(30C),3337,-475,5312,78
H(36A),4364,2054,730,68
H(36B),3302,1165,147,68
H(36C),4622,979,-6,68
H(37A),6174,1857,1405,82
H(37B),6761,774,1450,82
H(37C),6473,1643,2316,82
H(40A),1357,-857,917,89
H(40B),2077,-1438,143,89
H(40C),1863,-150,276,89
H(38A),4974,-1134,2960,99
H(38B),5724,126,3197,99
H(38C),6104,-881,2462,99
H(39A),2008,-1790,1937,109
H(39B),3099,-1832,2557,109
H(39C),2987,-2535,1563,109
H(2),4560(60),3130(60),2190(50),19(17)
H(4),2940(80),3720(80),4380(60),40(20)
H(6),4410(90),2240(100),3800(70),60(30)

2. Results of the X-ray diffraction studies of $[(Cp^*Ru)_3(\mu_3\text{-}CH)\text{-}\{\mu_3\text{-}OC(H)C(Me)CH\text{-}\}](BPh_4)$ (8-BPh_4)

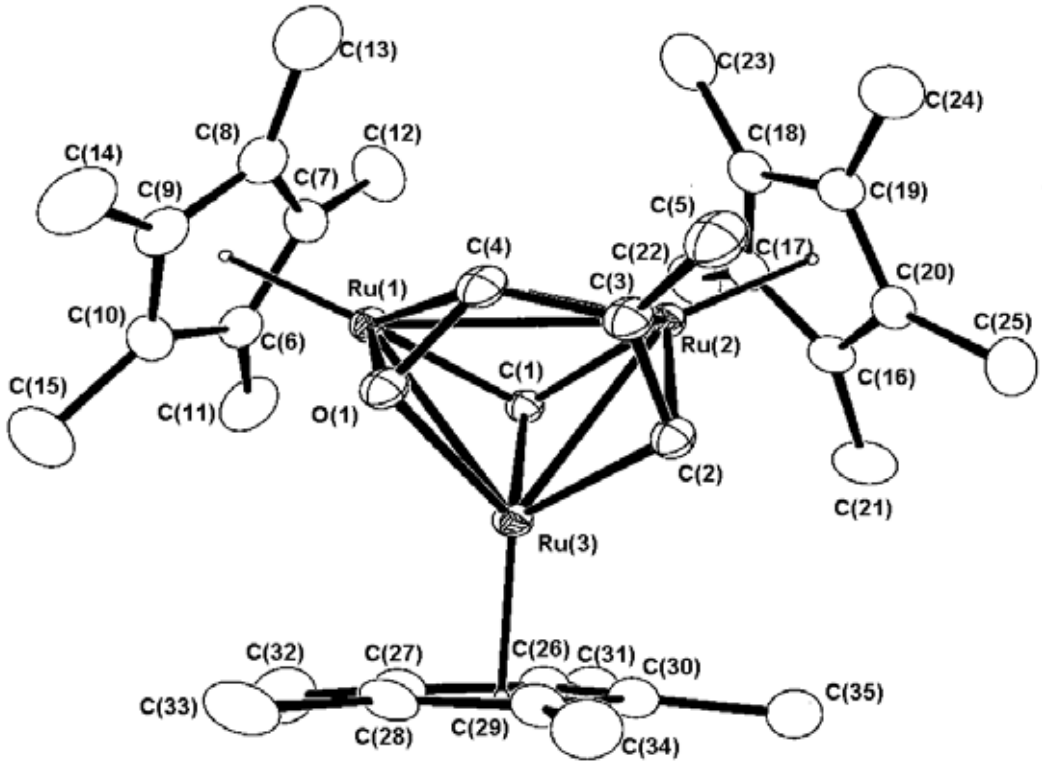

Table S2-1. Crystal data and structure refinement for **8-BPh4**.

Identification code, 8
Empirical formula, C59 H71 B O Ru3
Formula weight, 1110.18
Temperature, 223(2) K
Wavelength, 0.71069 Å
Crystal system, Orthorhombic
Space group, Pbca
Unit cell dimensions,
a = 19.5902(2)Å α = 90°
b = 19.8383(2)Å β = 90°
c = 26.3502(3)Å γ = 90°
Volume, 10240.64(19) $Å^3$
Z, 8
Density, 1.440 Mg/m^3
Absorption coefficient, 0.913 mm^{-1}
F(000), 4560
Crystal size, 0.80 x 0.80 x 0.50 mm
Theta range for data collection, 2.19 to 27.48 °.
Index ranges,-25<=h<=25; -25<=k<=25; -34<=l<=34
Reflections collected, 93739
Independent reflections, 12711 [R(int) = 0.0351]
Reflections observed (>2σ), 9581
Absorption correction, Numerical
Max. and min. transmission, 0.7573 and 0.6701
Refinement method, Full-matrix least-squares on F^2
Data / restraints / parameters, 11726 / 0 / 606
Goodness-of-fit on F^2, 0.930
Final R indices [I>2σ(I)],R_1 = 0.0208 wR_2 = 0.0456
R indices (all data), R_1 = 0.0305 wR_2 = 0.0470
Largest diff. peak and hole, 0.362 and -0.465 e.$Å^{-3}$

Table S2-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **8-BPh4**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom, x, y, z, U(eq)

Ru(1),5170(1),7525(1),2043(1),24(1),
Ru(2),3983(1),6768(1),1745(1),24(1),
Ru(3),4133(1),8078(1),1520(1),24(1),
O(1),4406(1),8117(1),2296(1),31(1),
C(1),4753(1),7252(1),1402(1),25(1),
C(2),3331(1),7585(1),1833(1),30(1),
C(3),3455(1),7381(1),2339(1),34(1),
C(4),4124(1),7539(1),2500(1),34(1),
C(5),2922(1),7146(1),2709(1),51(1),
C(6),6243(1),7542(1),1809(1),36(1),
C(7),6118(1),6921(1),2055(1),38(1),
C(8),5919(1),7067(1),2570(1),42(1),
C(9),5948(1),7774(1),2634(1),44(1),
C(10),6139(1),8073(1),2168(1),40(1),
C(11),6521(1),7617(2),1281(1),63(1),
C(12),6296(1),6243(1),1848(1),66(1),
C(13),5750(1),6554(2),2967(1),79(1),
C(14),5780(1),8148(2),3112(1),80(1),
C(15),6295(1),8808(1),2088(1),74(1),
C(16),3698(1),6128(1),1093(1),36(1),
C(17),4311(1),5854(1),1305(1),38(1),
C(18),4177(1),5650(1),1810(1),39(1),
C(19),3478(1),5779(1),1910(1),37(1),
C(20),3179(1),6077(1),1468(1),37(1),
C(21),3611(1),6331(1),550(1),58(1),
C(22),4937(1),5699(1),999(1),63(1),
C(23),4653(1),5274(1),2152(1),66(1),
C(24),3107(1),5550(1),2379(1),61(1),
C(25),2438(1),6234(1),1388(1),58(1),
C(26),4163(1),8423(1),713(1),35(1),
C(27),4564(1),8890(1),999(1),40(1),
C(28),4136(1),9184(1),1371(1),42(1),
C(29),3465(1),8921(1),1314(1),38(1),
C(30),3473(1),8450(1),901(1),34(1),
C(31),4404(1),8059(1),251(1),49(1),
C(32),5286(1),9073(2),882(1),65(1),
C(33),4343(2),9704(1),1756(1),66(1),
C(34),2844(1),9141(1),1612(1),58(1),
C(35),2865(1),8110(1),673(1),44(1),
C(36),7942(1),-161(1),932(1),36(1),
C(37),7740(1),-182(1),1438(1),48(1),
C(38),8105(1),-531(1),1807(1),63(1),
C(39),8684(1),-873(1),1692(1),59(1),
C(40),8908(1),-864(2),1198(1),64(1),
C(41),8544(1),-514(1),829(1),57(1),
C(42),7023(1),-360(1),183(1),37(1),
C(43),6513(1),-153(1),-158(1),47(1),
C(44),6104(1),-609(1),-419(1),55(1),
C(45),6190(1),-1290(1),-348(1),57(1),
C(46),6678(1),-1514(1),-18(1),54(1),
C(47),7086(1),-1052(1),245(1),43(1),
C(48),6993(1),794(1),707(1),37(1),
C(49),7101(1),1483(1),687(1),43(1),
C(50),6640(1),1953(1),886(1),55(1),
C(51),6052(1),1741(2),1115(1),62(1),
C(52),5922(1),1065(2),1149(1),64(1),

C(53),6388(1),604(1),952(1),54(1),
C(54),8058(1),533(1),73(1),36(1),
C(55),8551(1),995(1),240(1),52(1),
C(56),9030(1),1286(2),-78(1),65(1),
C(57),9055(1),1101(1),-586(1),59(1),
C(58),8588(1),643(1),-766(1),48(1),
C(59),8100(1),370(1),-444(1),37(1),
B(1),7505(1),207(1),474(1),35(1),

Table S2-3. Bond lengths [Å] and angles [°] for **8-BPh4**.

Ru(1)-C(1),1.9537(16)	C(29)-C(34),1.513(3)
Ru(1)-O(1),2.0155(12)	C(30)-C(35),1.495(3)
Ru(1)-C(6),2.1917(16)	C(36)-C(37),1.391(3)
Ru(1)-C(7),2.2105(18)	C(36)-C(41),1.398(3)
Ru(1)-C(10),2.2108(17)	C(36)-B(1),1.650(3)
Ru(1)-C(8),2.2139(18)	C(37)-C(38),1.392(3)
Ru(1)-C(9),2.2345(18)	C(38)-C(39),1.356(3)
Ru(1)-C(4),2.3767(17)	C(39)-C(40),1.373(3)
Ru(1)-Ru(3),2.68917(18)	C(40)-C(41),1.390(3)
Ru(1)-Ru(2),2.87712(18)	C(42)-C(47),1.387(3)
Ru(2)-C(1),2.0039(16)	C(42)-C(43),1.405(3)
Ru(2)-C(2),2.0767(17)	C(42)-B(1),1.657(3)
Ru(2)-C(16),2.2080(18)	C(43)-C(44),1.390(3)
Ru(2)-C(20),2.2132(17)	C(44)-C(45),1.375(4)
Ru(2)-C(3),2.2334(17)	C(45)-C(46),1.367(3)
Ru(2)-C(19),2.2411(18)	C(46)-C(47),1.400(3)
Ru(2)-C(17),2.2471(19)	C(48)-C(49),1.384(3)
Ru(2)-C(18),2.2565(19)	C(48)-C(53),1.402(3)
Ru(2)-C(4),2.5254(19)	C(48)-B(1),1.656(3)
Ru(2)-Ru(3),2.6807(2)	C(49)-C(50),1.400(3)
Ru(3)-C(2),2.0261(17)	C(50)-C(51),1.366(4)
Ru(3)-C(1),2.0635(17)	C(51)-C(52),1.367(4)
Ru(3)-O(1),2.1143(11)	C(52)-C(53),1.392(3)
Ru(3)-C(29),2.1914(18)	C(54)-C(55),1.402(3)
Ru(3)-C(30),2.2087(17)	C(54)-C(59),1.402(3)
Ru(3)-C(28),2.2294(19)	C(54)-B(1),1.646(3)
Ru(3)-C(26),2.2343(17)	C(55)-C(56),1.384(3)
Ru(3)-C(27),2.2802(18)	C(56)-C(57),1.388(4)
O(1)-C(4),1.380(2)	C(57)-C(58),1.375(3)
C(2)-C(3),1.413(2)	C(58)-C(59),1.387(3)
C(3)-C(4),1.414(3)	
C(3)-C(5),1.505(2)	C(1)-Ru(1)-O(1),97.86(6)
C(6)-C(7),1.416(3)	C(1)-Ru(1)-C(6),99.29(7)
C(6)-C(10),1.429(3)	O(1)-Ru(1)-C(6),142.82(6)
C(6)-C(11),1.500(3)	C(1)-Ru(1)-C(7),102.32(7)
C(7)-C(8),1.439(3)	O(1)-Ru(1)-C(7),159.23(6)
C(7)-C(12),1.493(3)	C(6)-Ru(1)-C(7),37.51(7)
C(8)-C(9),1.414(3)	C(1)-Ru(1)-C(10),128.54(7)
C(8)-C(13),1.497(3)	O(1)-Ru(1)-C(10),107.61(6)
C(9)-C(10),1.415(3)	C(6)-Ru(1)-C(10),37.88(7)
C(9)-C(14),1.498(3)	C(7)-Ru(1)-C(10),62.83(7)
C(10)-C(15),1.506(3)	C(1)-Ru(1)-C(8),134.84(8)
C(16)-C(20),1.421(3)	O(1)-Ru(1)-C(8),121.62(7)
C(16)-C(17),1.431(3)	C(6)-Ru(1)-C(8),63.09(7)
C(16)-C(21),1.496(3)	C(7)-Ru(1)-C(8),37.97(8)
C(17)-C(18),1.414(3)	C(10)-Ru(1)-C(8),62.63(8)
C(17)-C(22),1.500(3)	C(1)-Ru(1)-C(9),161.69(7)
C(18)-C(19),1.419(3)	O(1)-Ru(1)-C(9),98.51(6)
C(18)-C(23),1.496(3)	C(6)-Ru(1)-C(9),62.52(7)
C(19)-C(20),1.432(3)	C(7)-Ru(1)-C(9),62.39(7)
C(19)-C(24),1.503(3)	C(10)-Ru(1)-C(9),37.12(8)
C(20)-C(25),1.498(2)	C(8)-Ru(1)-C(9),37.07(8)
C(26)-C(27),1.429(3)	C(1)-Ru(1)-C(4),94.68(6)
C(26)-C(30),1.439(3)	O(1)-Ru(1)-C(4),35.43(6)
C(26)-C(31),1.492(3)	C(6)-Ru(1)-C(4),165.83(7)
C(27)-C(28),1.415(3)	C(7)-Ru(1)-C(4),136.31(7)
C(27)-C(32),1.493(3)	C(10)-Ru(1)-C(4),131.21(7)
C(28)-C(29),1.424(3)	C(8)-Ru(1)-C(4),104.98(7)
C(28)-C(33),1.503(3)	C(9)-Ru(1)-C(4),103.42(7)
C(29)-C(30),1.433(3)	C(1)-Ru(1)-Ru(3),49.74(5)
	O(1)-Ru(1)-Ru(3),50.99(3)
	C(6)-Ru(1)-Ru(3),125.03(5)
	C(7)-Ru(1)-Ru(3),149.70(5)

C(10)-Ru(1)-Ru(3),121.61(6)
C(8)-Ru(1)-Ru(3),171.56(5)
C(9)-Ru(1)-Ru(3),141.51(6)
C(4)-Ru(1)-Ru(3),66.64(4)
C(1)-Ru(1)-Ru(2),44.06(5)
O(1)-Ru(1)-Ru(2),78.09(3)
C(6)-Ru(1)-Ru(2),134.95(5)
C(7)-Ru(1)-Ru(2),113.57(5)
C(10)-Ru(1)-Ru(2),172.09(6)
C(8)-Ru(1)-Ru(2),119.49(5)
C(9)-Ru(1)-Ru(2),148.97(6)
C(4)-Ru(1)-Ru(2),56.50(5)
Ru(3)-Ru(1)-Ru(2),57.460(5)
C(1)-Ru(2)-C(2),98.06(7)
C(1)-Ru(2)-C(16),96.60(7)
C(2)-Ru(2)-C(16),112.35(7)
C(1)-Ru(2)-C(20),133.15(7)
C(2)-Ru(2)-C(20),94.73(7)
C(16)-Ru(2)-C(20),37.49(7)
C(1)-Ru(2)-C(3),113.82(7)
C(2)-Ru(2)-C(3),38.05(7)
C(16)-Ru(2)-C(3),137.76(7)
C(20)-Ru(2)-C(3),103.82(7)
C(1)-Ru(2)-C(19),147.11(7)
C(2)-Ru(2)-C(19),112.94(7)
C(16)-Ru(2)-C(19),62.31(7)
C(20)-Ru(2)-C(19),37.50(7)
C(3)-Ru(2)-C(19),97.82(7)
C(1)-Ru(2)-C(17),86.48(7)
C(2)-Ru(2)-C(17),149.72(7)
C(16)-Ru(2)-C(17),37.46(7)
C(20)-Ru(2)-C(17),62.13(7)
C(3)-Ru(2)-C(17),158.86(7)
C(19)-Ru(2)-C(17),61.26(7)
C(1)-Ru(2)-C(18),112.20(7)
C(2)-Ru(2)-C(18),149.56(7)
C(16)-Ru(2)-C(18),62.33(7)
C(20)-Ru(2)-C(18),62.33(7)
C(3)-Ru(2)-C(18),124.05(7)
C(19)-Ru(2)-C(18),36.78(7)
C(17)-Ru(2)-C(18),36.60(7)
C(1)-Ru(2)-C(4),89.04(6)
C(2)-Ru(2)-C(4),60.44(6)
C(16)-Ru(2)-C(4),171.58(6)
C(20)-Ru(2)-C(4),135.53(7)
C(3)-Ru(2)-C(4),33.86(6)
C(19)-Ru(2)-C(4),115.21(7)
C(17)-Ru(2)-C(4),149.83(7)
C(18)-Ru(2)-C(4),121.16(7)
C(1)-Ru(2)-Ru(3),49.74(5)
C(2)-Ru(2)-Ru(3),48.39(5)
C(16)-Ru(2)-Ru(3),114.42(5)
C(20)-Ru(2)-Ru(3),127.27(5)
C(3)-Ru(2)-Ru(3),71.23(5)
C(19)-Ru(2)-Ru(3),160.06(5)
C(17)-Ru(2)-Ru(3),129.58(5)
C(18)-Ru(2)-Ru(3),161.93(5)
C(4)-Ru(2)-Ru(3),64.86(4)
C(1)-Ru(2)-Ru(1),42.68(5)
C(2)-Ru(2)-Ru(1),93.43(5)
C(16)-Ru(2)-Ru(1),135.81(5)
C(20)-Ru(2)-Ru(1),171.46(5)
C(3)-Ru(2)-Ru(1),84.21(5)
C(19)-Ru(2)-Ru(1),139.55(5)
C(17)-Ru(2)-Ru(1),109.35(4)
C(18)-Ru(2)-Ru(1),110.85(5)
C(4)-Ru(2)-Ru(1),51.70(4)
Ru(3)-Ru(2)-Ru(1),57.745(5)
C(2)-Ru(3)-C(1),97.78(7)
C(2)-Ru(3)-O(1),79.64(6)
C(1)-Ru(3)-O(1),91.49(6)
C(2)-Ru(3)-C(29),90.37(7)
C(1)-Ru(3)-C(29),156.86(7)
O(1)-Ru(3)-C(29),111.32(6)
C(2)-Ru(3)-C(30),90.49(7)
C(1)-Ru(3)-C(30),119.88(7)
O(1)-Ru(3)-C(30),148.24(6)
C(29)-Ru(3)-C(30),38.01(7)
C(2)-Ru(3)-C(28),123.33(8)
C(1)-Ru(3)-C(28),138.82(7)
O(1)-Ru(3)-C(28),97.72(6)
C(29)-Ru(3)-C(28),37.56(7)
C(30)-Ru(3)-C(28),62.76(7)
C(2)-Ru(3)-C(26),123.76(7)
C(1)-Ru(3)-C(26),94.81(7)
O(1)-Ru(3)-C(26),154.44(6)
C(29)-Ru(3)-C(26),62.97(7)
C(30)-Ru(3)-C(26),37.80(7)
C(28)-Ru(3)-C(26),61.98(7)
C(2)-Ru(3)-C(27),150.90(7)
C(1)-Ru(3)-C(27),104.57(7)
O(1)-Ru(3)-C(27),117.59(6)
C(29)-Ru(3)-C(27),62.11(8)
C(30)-Ru(3)-C(27),62.31(7)
C(28)-Ru(3)-C(27),36.54(7)
C(26)-Ru(3)-C(27),36.90(7)
C(2)-Ru(3)-Ru(2),50.03(5)
C(1)-Ru(3)-Ru(2),47.82(4)
O(1)-Ru(3)-Ru(2),81.32(4)
C(29)-Ru(3)-Ru(2),136.80(6)
C(30)-Ru(3)-Ru(2),115.05(5)
C(28)-Ru(3)-Ru(2),173.36(6)
C(26)-Ru(3)-Ru(2),120.68(5)
C(27)-Ru(3)-Ru(2),149.17(5)
C(2)-Ru(3)-Ru(1),100.41(5)
C(1)-Ru(3)-Ru(1),46.26(4)
O(1)-Ru(3)-Ru(1),47.79(3)
C(29)-Ru(3)-Ru(1),152.81(5)
C(30)-Ru(3)-Ru(1),163.15(5)
C(28)-Ru(3)-Ru(1),119.30(5)
C(26)-Ru(3)-Ru(1),126.35(5)
C(27)-Ru(3)-Ru(1),108.48(5)
Ru(2)-Ru(3)-Ru(1),64.795(5)
C(4)-O(1)-Ru(1),86.72(10)
C(4)-O(1)-Ru(3),104.25(10)
Ru(1)-O(1)-Ru(3),81.22(4)
Ru(1)-C(1)-Ru(2),93.26(7)
Ru(1)-C(1)-Ru(3),84.00(7)
Ru(2)-C(1)-Ru(3),82.44(6)
C(3)-C(2)-Ru(3),112.82(12)
C(3)-C(2)-Ru(2),76.99(11)
Ru(3)-C(2)-Ru(2),81.58(6)
C(2)-C(3)-C(4),112.40(15)
C(2)-C(3)-C(5),125.44(17)
C(4)-C(3)-C(5),121.14(17)
C(2)-C(3)-Ru(2),64.96(10)
C(4)-C(3)-Ru(2),84.47(11)
C(5)-C(3)-Ru(2),127.43(15)
O(1)-C(4)-C(3),115.92(16)
O(1)-C(4)-Ru(1),57.85(8)
C(3)-C(4)-Ru(1),130.03(13)
O(1)-C(4)-Ru(2),103.80(10)
C(3)-C(4)-Ru(2),61.67(10)
Ru(1)-C(4)-Ru(2),71.80(5)
C(7)-C(6)-C(10),108.21(17)
C(7)-C(6)-C(11),125.08(19)
C(10)-C(6)-C(11),126.3(2)
C(7)-C(6)-Ru(1),71.96(10)
C(10)-C(6)-Ru(1),71.78(10)
C(11)-C(6)-Ru(1),127.64(14)
C(6)-C(7)-C(8),107.68(17)
C(6)-C(7)-C(12),125.2(2)
C(8)-C(7)-C(12),126.1(2)
C(6)-C(7)-Ru(1),70.52(10)
C(8)-C(7)-Ru(1),71.15(10)
C(12)-C(7)-Ru(1),132.80(13)
C(9)-C(8)-C(7),107.60(18)
C(9)-C(8)-C(13),126.8(2)
C(7)-C(8)-C(13),125.6(2)
C(9)-C(8)-Ru(1),72.26(11)
C(7)-C(8)-Ru(1),70.89(10)
C(13)-C(8)-Ru(1),124.79(13)
C(8)-C(9)-C(10),108.74(18)
C(8)-C(9)-C(14),125.7(2)
C(10)-C(9)-C(14),125.5(2)
C(8)-C(9)-Ru(1),70.68(10)
C(10)-C(9)-Ru(1),70.53(10)
C(14)-C(9)-Ru(1),123.05(14)
C(9)-C(10)-C(6),107.73(18)
C(9)-C(10)-C(15),125.5(2)
C(6)-C(10)-C(15),126.3(2)
C(9)-C(10)-Ru(1),72.35(10)
C(6)-C(10)-Ru(1),70.33(10)
C(15)-C(10)-Ru(1),129.07(15)
C(20)-C(16)-C(17),107.64(17)
C(20)-C(16)-C(21),127.01(19)
C(17)-C(16)-C(21),124.77(19)
C(20)-C(16)-Ru(2),71.46(10)
C(17)-C(16)-Ru(2),72.75(11)
C(21)-C(16)-Ru(2),128.14(14)
C(18)-C(17)-C(16),108.64(16)
C(18)-C(17)-C(22),126.8(2)
C(16)-C(17)-C(22),123.7(2)
C(18)-C(17)-Ru(2),72.07(11)
C(16)-C(17)-Ru(2),69.79(10)
C(22)-C(17)-Ru(2),132.58(14)
C(17)-C(18)-C(19),107.65(16)
C(17)-C(18)-C(23),126.4(2)
C(19)-C(18)-C(23),125.4(2)
C(17)-C(18)-Ru(2),71.34(11)
C(19)-C(18)-Ru(2),71.02(11)
C(23)-C(18)-Ru(2),129.83(15)
C(18)-C(19)-C(20),108.47(17)
C(18)-C(19)-C(24),124.48(19)
C(20)-C(19)-C(24),126.57(18)
C(18)-C(19)-Ru(2),72.20(10)
C(20)-C(19)-Ru(2),70.19(10)
C(24)-C(19)-Ru(2),129.63(15)
C(16)-C(20)-C(19),107.58(16)

C(16)-C(20)-C(25),125.47(19)
C(19)-C(20)-C(25),126.60(18)
C(16)-C(20)-Ru(2),71.06(10)
C(19)-C(20)-Ru(2),72.30(10)
C(25)-C(20)-Ru(2),127.34(15)
C(27)-C(26)-C(30),108.14(17)
C(27)-C(26)-C(31),124.68(19)
C(30)-C(26)-C(31),126.52(18)
C(27)-C(26)-Ru(3),73.30(10)
C(30)-C(26)-Ru(3),70.13(9)
C(31)-C(26)-Ru(3),129.54(14)
C(28)-C(27)-C(26),107.81(18)
C(28)-C(27)-C(32),127.1(2)
C(26)-C(27)-C(32),124.8(2)
C(28)-C(27)-Ru(3),69.77(10)
C(26)-C(27)-Ru(3),69.80(10)
C(32)-C(27)-Ru(3),130.33(15)
C(27)-C(28)-C(29),108.82(17)
C(27)-C(28)-C(33),126.2(2)
C(29)-C(28)-C(33),124.9(2)
C(27)-C(28)-Ru(3),73.68(11)
C(29)-C(28)-Ru(3),69.77(11)
C(33)-C(28)-Ru(3),123.87(15)
C(28)-C(29)-C(30),108.01(17)
C(28)-C(29)-C(34),125.61(19)
C(30)-C(29)-C(34),126.24(19)
C(28)-C(29)-Ru(3),72.67(11)
C(30)-C(29)-Ru(3),71.65(10)
C(34)-C(29)-Ru(3),124.84(14)
C(29)-C(30)-C(26),107.17(17)
C(29)-C(30)-C(35),126.17(18)
C(26)-C(30)-C(35),126.36(17)
C(29)-C(30)-Ru(3),70.34(10)
C(26)-C(30)-Ru(3),72.07(10)
C(35)-C(30)-Ru(3),127.71(13)
C(37)-C(36)-C(41),114.34(19)
C(37)-C(36)-B(1),124.42(18)
C(41)-C(36)-B(1),121.16(17)
C(36)-C(37)-C(38),122.5(2)
C(39)-C(38)-C(37),121.5(2)
C(38)-C(39)-C(40),118.3(2)
C(39)-C(40)-C(41),120.3(2)
C(40)-C(41)-C(36),123.1(2)
C(47)-C(42)-C(43),115.30(19)
C(47)-C(42)-B(1),124.52(18)
C(43)-C(42)-B(1),120.17(19)
C(44)-C(43)-C(42),122.4(2)
C(45)-C(44)-C(43),120.1(2)
C(46)-C(45)-C(44),119.4(2)
C(45)-C(46)-C(47),120.1(2)
C(42)-C(47)-C(46),122.6(2)
C(49)-C(48)-C(53),114.4(2)
C(49)-C(48)-B(1),126.03(18)
C(53)-C(48)-B(1),119.53(19)
C(48)-C(49)-C(50),123.0(2)
C(51)-C(50)-C(49),120.3(2)
C(50)-C(51)-C(52),119.1(2)
C(51)-C(52)-C(53),119.9(2)
C(52)-C(53)-C(48),123.2(2)
C(55)-C(54)-C(59),114.53(18)
C(55)-C(54)-B(1),120.51(17)
C(59)-C(54)-B(1),124.93(17)
C(56)-C(55)-C(54),123.4(2)
C(55)-C(56)-C(57),119.8(2)
C(58)-C(57)-C(56),118.9(2)
C(57)-C(58)-C(59),120.4(2)
C(58)-C(59)-C(54),123.0(2)
C(54)-B(1)-C(36),107.61(15)
C(54)-B(1)-C(48),111.12(17)
C(36)-B(1)-C(48),110.78(15)
C(54)-B(1)-C(42),110.13(15)
C(36)-B(1)-C(42),109.49(16)
C(48)-B(1)-C(42),107.71(15)

Symmetry transformations used to generate equivalent atoms:

Table S2-4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **8-BPh4**. The anisotropic displacement factor exponent takes the form: -2 p^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom, U11, U22, U33, U23, U13, U12

Ru(1),21(1),27(1),25(1),-2(1),-1(1),0(1)
Ru(2),22(1),25(1),26(1),3(1),-2(1),-2(1)
Ru(3),27(1),23(1),21(1),1(1),-1(1),1(1)
O(1),31(1),37(1),26(1),-5(1),-1(1),3(1)
C(1),24(1),25(1),25(1),-1(1),1(1),-2(1)
C(2),24(1),34(1),30(1),0(1),1(1),3(1)
C(3),35(1),40(1),28(1),1(1),8(1),3(1)
C(4),35(1),44(1),22(1),3(1),4(1),7(1)
C(5),42(1),70(2),41(1),5(1),16(1),-3(1)
C(6),21(1),46(1),40(1),-5(1),1(1),0(1)
C(7),23(1),39(1),53(1),-6(1),-10(1),3(1)
C(8),24(1),56(1),47(1),13(1),-14(1),-3(1)
C(9),27(1),66(2),38(1),-16(1),-9(1),-1(1)
C(10),26(1),37(1),56(1),-10(1),-6(1),-6(1)
C(11),39(1),98(2),52(1),1(1),15(1),4(1)
C(12),40(1),48(1),111(2),-22(1),-19(1),12(1)
C(13),47(1),113(3),77(2),53(2),-21(1),-10(1)
C(14),58(2),126(3),55(2),-48(2),-10(1),2(2)
C(15),66(2),42(2),115(2),-6(2),-17(2),-18(1)
C(16),45(1),25(1),38(1),-4(1),-2(1),-9(1)
C(17),35(1),23(1),56(1),-7(1),4(1),-6(1)
C(18),34(1),25(1),58(1),8(1),-10(1),-5(1)
C(19),37(1),31(1),44(1),7(1),-1(1),-11(1)
C(20),29(1),31(1),50(1),0(1),-8(1),-8(1)
C(21),93(2),44(1),37(1),-4(1),-9(1),-18(1)
C(22),56(1),39(1),94(2),-20(1),30(1),-3(1)
C(23),54(1),43(1),102(2),28(1),-27(1),-4(1)
C(24),71(2),51(2),62(2),16(1),14(1),-18(1)
C(25),31(1),56(2),86(2),-2(1),-17(1),-7(1)
C(26),49(1),31(1),24(1),8(1),0(1),0(1)
C(27),53(1),33(1),33(1),12(1),-2(1),-9(1)
C(28),68(1),22(1),35(1),4(1),-8(1),0(1)
C(29),52(1),29(1),33(1),4(1),-5(1),13(1)
C(30),45(1),29(1),27(1),5(1),-8(1),7(1)
C(31),68(1),52(1),26(1),4(1),8(1),1(1)
C(32),69(2),73(2),54(1),20(1),2(1),-30(1)
C(33),110(2),35(1),53(1),-9(1),-17(1),-14(1)
C(34),69(2),57(2),47(1),-5(1),-2(1),35(1)
C(35),47(1),46(1),40(1),4(1),-14(1),6(1)
C(36),38(1),41(1),30(1),3(1),-2(1),-5(1)
C(37),52(1),57(1),33(1),7(1),2(1),3(1)
C(38),76(2),78(2),34(1),18(1),-1(1),2(1)
C(39),68(2),59(2),51(1),21(1),-16(1),-2(1)
C(40),57(1),77(2),58(2),9(1),-7(1),20(1)
C(41),52(1),80(2),38(1),6(1),0(1),16(1)
C(42),35(1),46(1),31(1),2(1),5(1),-3(1)
C(43),46(1),54(1),40(1),3(1),-5(1),-5(1)
C(44),48(1),77(2),41(1),0(1),-5(1),-13(1)
C(45),56(1),72(2),45(1),-14(1),9(1),-26(1)
C(46),64(1),46(1),53(1),-6(1),19(1),-12(1)
C(47),43(1),46(1),39(1),1(1),10(1),-4(1)
C(48),35(1),45(1),30(1),1(1),-4(1),-1(1)
C(49),45(1),51(1),34(1),-1(1),-8(1),-4(1)
C(50),72(2),49(2),43(1),-11(1),-16(1),5(1)
C(51),62(2),78(2),44(1),-20(1),-8(1),21(1)
C(52),47(1),90(2),55(2),-13(1),12(1),1(1)
C(53),45(1),60(2),57(1),-4(1),10(1),-6(1)
C(54),31(1),43(1),33(1),9(1),-1(1),3(1)
C(55),45(1),76(2),37(1),9(1),-6(1),-17(1)
C(56),44(1),91(2),59(2),21(1),-9(1),-26(1)
C(57),37(1),84(2),54(1),30(1),8(1),0(1)
C(58),49(1),58(2),35(1),12(1),11(1),18(1)
C(59),40(1),35(1),36(1),6(1),4(1),9(1)
B(1),36(1),41(1),28(1),5(1),1(1),-3(1)

Table S2-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **8-BPh4**.

Atom, x, y, z, U(eq)

H(5A),3116,6807,2932,77
H(5B),2539,6954,2525,77
H(5C),2765,7526,2910,77
H(11A),6505,8088,1182,94
H(11B),6248,7352,1048,94
H(11C),6990,7460,1272,94
H(12A),6092,5896,2058,99
H(12B),6788,6189,1846,99
H(12C),6123,6203,1504,99
H(13A),6159,6307,3058,118
H(13B),5411,6243,2835,118
H(13C),5569,6780,3265,118
H(14A),5986,7919,3399,119
H(14B),5289,8162,3156,119
H(14C),5957,8603,3090,119
H(15A),6395,8888,1732,111
H(15B),6688,8934,2291,111
H(15C),5904,9077,2188,111
H(21A),4014,6572,438,87
H(21B),3214,6620,518,87
H(21C),3549,5932,343,87
H(22A),5084,6102,821,95
H(22B),4833,5348,755,95
H(22C),5298,5547,1223,95
H(23A),4537,5368,2503,99
H(23B),5119,5417,2086,99
H(23C),4612,4794,2088,99
H(24A),2663,5766,2394,92
H(24B),3370,5671,2677,92
H(24C),3048,5065,2368,92
H(25A),2236,6374,1707,87
H(25B),2205,5835,1264,87
H(25C),2395,6594,1141,87
H(31A),4077,7712,161,73
H(31B),4843,7854,319,73
H(31C),4448,8375,-28,73
H(32A),5532,8675,772,98
H(32B),5501,9255,1184,98
H(32C),5295,9409,615,98
H(33A),4129,9603,2079,100
H(33B),4199,10147,1642,100
H(33C),4835,9699,1796,100
H(34A),2483,8810,1572,86
H(34B),2687,9574,1487,86
H(34C),2962,9180,1968,86
H(35A),3011,7709,492,67
H(35B),2641,8415,439,67
H(35C),2549,7983,940,67
H(37),7341,50,1534,57
H(38),7946,-530,2144,76
H(39),8925,-1109,1943,71
H(40),9309,-1096,1109,77
H(41),8711,-515,495,68
H(43),6447,311,-212,56
H(44),5768,-450,-644,66
H(45),5915,-1599,-525,69
H(46),6740,-1979,32,65
H(47),7416,-1217,472,52
H(49),7501,1643,531,52
H(50),6736,2416,863,66
H(51),5741,2056,1248,74
H(52),5519,913,1304,77
H(53),6291,142,985,65
H(55),8555,1113,585,63
H(56),9337,1607,50,78
H(57),9387,1286,-803,70
H(58),8598,514,-1109,57
H(59),7784,61,-578,44
H(4),4268(10),7433(11),2843(8),45(6)
H(1),4948(9),7129(10),1079(7),33(5)
H(2),2842(10),7579(10),1718(7),38(5)

3. Results of the X-ray diffraction studies of [(Cp*Ru)$_3$(μ_3-CH)-{μ_3-OC(Me)C(H)CH-}](PF$_6$) (9-PF$_6$)

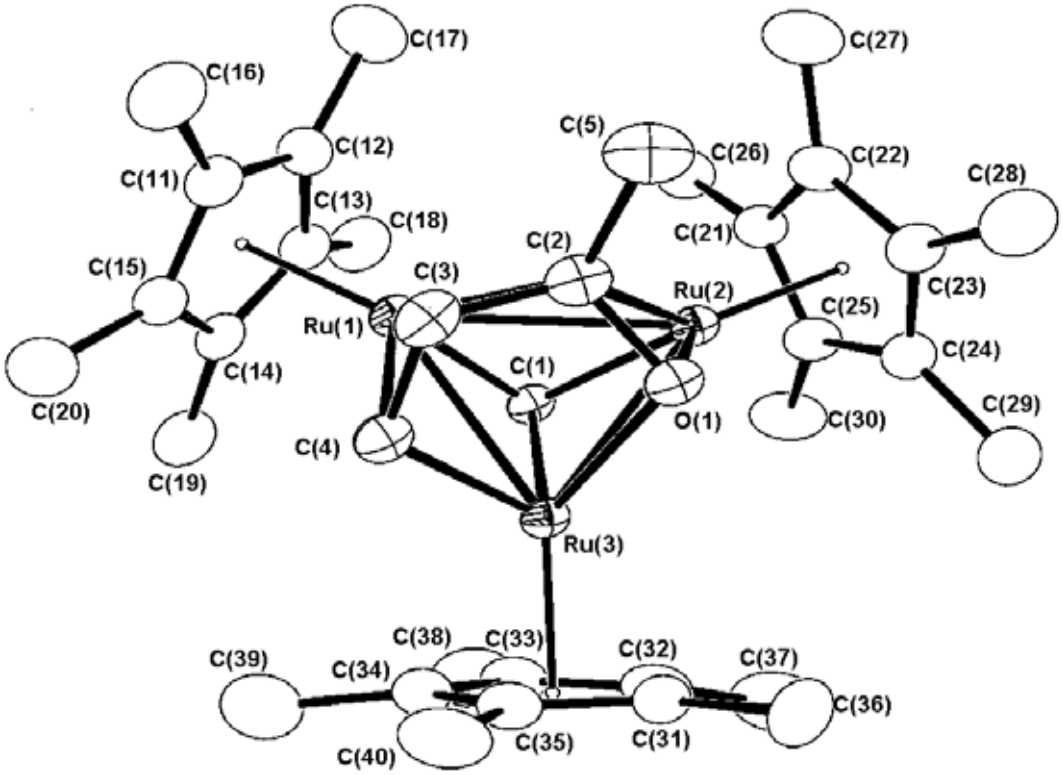

Table S3-1. Crystal data and structure refinement for **9-PF6**.

Identification code,9
Empirical formula,C35 H51 F6 O P Ru3
Formula weight,935.94
Temperature,253(2) K
Wavelength,0.71069 Å
Crystal system, Triclinic
Space group, P-1(#2)
Unit cell dimensions,
a = 11.2603(6)Å α = 92.738(3)°,
b = 13.3116(7)Å β = 102.493(2)°,
c = 14.2274(6)Å γ = 102.0860(17)°
Volume, 2026.24(17) $Å^3$
Z, 2
Density (calculated), 1.534 Mg/m^3
Absorption coefficient, 1.195 mm^{-1}
F(000), 940
Crystal size, 0.25 x 0.25 x 0.05 mm
Theta range for data collection, 2.66 to 30.02 °.
Index ranges,-15<=h<=15; -18<=k<=18; -20<=l<=20
Reflections collected, 17784
Independent reflections, 11233 [R(int) = 0.0255]
Reflections observed (>2σ), 9747
Max. and min. transmission, 0.9427 and 0.7544
Refinement method, Full-matrix least-squares on F^2
Data / restraints / parameters, 11233 / 0 / 444
Goodness-of-fit on F^2, 1.101
Final R indices [I>2σ(I)],R_1 = 0.0531 wR_2 = 0.1462
R indices (all data), R_1 = 0.0611 wR_2 = 0.1531
Largest diff. peak and hole, 2.415 and -1.172 e.$Å^{-3}$

Table S3-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **9-PF6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom, x, y, z, U(eq)

Ru(1),9374(1),7303(1),6779(1),31(1)
Ru(2),7265(1),8031(1),7178(1),30(1)
Ru(3),7331(1),6019(1),7064(1),30(1)
C(1),8512(3),7326(3),7871(3),31(1)
C(2),7395(5),7333(4),5532(3),46(1)
C(3),8157(4),6650(4),5364(3),48(1)
C(4),8293(4),5912(4),6030(3),41(1)
C(5),7114(7),8125(5),4851(4),64(2)
O(1),6507(3),6935(2),6036(2),38(1)
C(11),11029(4),7774(4),6132(3),44(1)
C(12),11028(4),8602(4),6811(4),47(1)
C(13),11150(4),8217(4),7747(3),44(1)
C(14),11212(4),7156(4),7637(3),41(1)
C(15),11142(4),6885(4),6646(4),42(1)
C(16),11016(6),7840(6),5080(4),67(2)
C(17),11040(7),9686(5),6563(6),75(2)
C(18),11403(6),8852(6),8692(5),67(2)
C(19),11487(5),6516(5),8461(4),61(1)
C(20),11302(5),5886(5),6211(5),63(2)
C(21),7752(4),9550(3),8035(3),41(1)
C(22),7085(5),9672(4),7095(4),46(1)
C(23),5855(4),9037(4),6932(4),46(1)
C(24),5758(4),8505(4),7764(4),45(1)
C(25),6937(4),8815(4),8451(3),41(1)
C(26),8983(6),10207(5),8565(5),62(1)
C(27),7542(7),10448(5),6445(5),66(2)
C(28),4812(7),8950(6),6063(5),75(2)
C(29),4560(6),7888(5),7924(6),69(2)
C(30),7222(7),8538(5),9471(4),61(2)
C(31),5620(4),4806(4),7102(4),46(1)
C(32),6173(5),5230(4),8082(4),50(1)
C(33),7416(5),5078(4),8312(3),48(1)
C(34),7607(4),4515(4),7513(4),46(1)
C(35),6504(5),4340(4),6768(4),46(1)
C(36),4338(5),4772(6),6533(6),77(2)
C(37),5478(9),5605(6),8750(6),88(3)
C(38),8268(8),5341(6),9303(5),90(3)
C(39),8707(7),4061(6),7499(8),91(3)
C(40),6300(8),3677(5),5831(5),73(2)
P(1),8316(2),7176(1),2062(1),54(1)
F(1),8203(5),8258(4),1668(4),98(2)
F(2),9612(6),7709(5),2756(5),135(2)
F(3),9071(6),6981(7),1297(5),142(3)
F(4),7080(6),6689(5),1267(6),148(3)
F(5),7540(9),7377(7),2803(5),159(3)
F(6),8485(7),6149(5),2470(8),189(5)

Table S3-3. Bond lengths [Å] and angles [°] for **9-PF6**.

Ru(1)-C(1),2.005(4)
Ru(1)-C(4),2.086(4)
Ru(1)-C(3),2.196(4)
Ru(1)-C(14),2.215(4)
Ru(1)-C(15),2.219(4)
Ru(1)-C(13),2.238(4)
Ru(1)-C(11),2.240(4)
Ru(1)-C(12),2.251(4)
Ru(1)-C(2),2.540(5)
Ru(1)-Ru(3),2.6829(4)
Ru(1)-Ru(2),2.8985(4)
Ru(2)-C(1),1.967(4)
Ru(2)-O(1),2.036(3)
Ru(2)-C(25),2.186(4)
Ru(2)-C(21),2.211(4)
Ru(2)-C(24),2.232(4)
Ru(2)-C(22),2.241(5)
Ru(2)-C(23),2.265(5)
Ru(2)-C(2),2.522(5)
Ru(2)-Ru(3),2.6931(5)
Ru(3)-C(4),2.022(4)
Ru(3)-C(1),2.071(4)
Ru(3)-O(1),2.132(3)
Ru(3)-C(34),2.193(5)
Ru(3)-C(35),2.217(5)
Ru(3)-C(33),2.219(4)
Ru(3)-C(31),2.253(4)
Ru(3)-C(32),2.301(4)
C(2)-O(1),1.384(5)
C(2)-C(3),1.419(8)
C(2)-C(5),1.502(7)
C(3)-C(4),1.406(7)
C(11)-C(12),1.430(7)
C(11)-C(15),1.434(7)
C(11)-C(16),1.500(7)
C(12)-C(13),1.439(7)
C(12)-C(17),1.501(8)
C(13)-C(14),1.430(7)
C(13)-C(18),1.493(7)
C(14)-C(15),1.419(7)
C(14)-C(19),1.499(7)
C(15)-C(20),1.501(7)
C(21)-C(22),1.420(7)
C(21)-C(25),1.437(7)
C(21)-C(26),1.494(7)
C(22)-C(23),1.428(7)
C(22)-C(27),1.504(7)
C(23)-C(24),1.420(7)
C(23)-C(28),1.491(7)
C(24)-C(25),1.435(7)
C(24)-C(29),1.495(7)
C(25)-C(30),1.498(7)
C(31)-C(35),1.427(7)
C(31)-C(32),1.433(8)
C(31)-C(36),1.485(7)
C(32)-C(33),1.426(8)
C(32)-C(37),1.485(8)
C(33)-C(34),1.412(8)
C(33)-C(38),1.502(8)
C(34)-C(35),1.416(7)
C(34)-C(39),1.490(8)
C(35)-C(40),1.509(8)
P(1)-F(6),1.543(5)
P(1)-F(5),1.555(5)
P(1)-F(3),1.562(5)
P(1)-F(2),1.576(5)
P(1)-F(4),1.584(6)
P(1)-F(1),1.590(5)

C(1)-Ru(1)-C(4),97.89(16)
C(1)-Ru(1)-C(3),115.36(17)
C(4)-Ru(1)-C(3),38.2(2)
C(1)-Ru(1)-C(14),97.75(16)
C(4)-Ru(1)-C(14),113.08(19)
C(3)-Ru(1)-C(14),136.14(19)
C(1)-Ru(1)-C(15),133.07(17)
C(4)-Ru(1)-C(15),92.49(17)
C(3)-Ru(1)-C(15),100.81(19)
C(14)-Ru(1)-C(15),37.34(17)
C(1)-Ru(1)-C(13),90.06(16)
C(4)-Ru(1)-C(13),150.51(19)
C(3)-Ru(1)-C(13),153.64(18)
C(14)-Ru(1)-C(13),37.47(18)
C(15)-Ru(1)-C(13),62.32(17)
C(1)-Ru(1)-C(11),152.08(17)
C(4)-Ru(1)-C(11),107.84(18)
C(3)-Ru(1)-C(11),91.94(18)
C(14)-Ru(1)-C(11),62.54(17)
C(15)-Ru(1)-C(11),37.52(18)
C(13)-Ru(1)-C(11),62.18(18)
C(1)-Ru(1)-C(12),117.57(18)
C(4)-Ru(1)-C(12),144.48(19)
C(3)-Ru(1)-C(12),117.95(19)
C(14)-Ru(1)-C(12),62.71(18)
C(15)-Ru(1)-C(12),62.49(18)
C(13)-Ru(1)-C(12),37.40(19)
C(11)-Ru(1)-C(12),37.13(19)
C(1)-Ru(1)-C(2),92.13(15)
C(4)-Ru(1)-C(2),61.35(18)
C(3)-Ru(1)-C(2),33.91(19)
C(14)-Ru(1)-C(2),169.37(17)
C(15)-Ru(1)-C(2),132.07(17)
C(13)-Ru(1)-C(2),147.05(18)
C(11)-Ru(1)-C(2),109.43(16)
C(12)-Ru(1)-C(2),115.80(17)
C(1)-Ru(1)-Ru(3),49.92(11)
C(4)-Ru(1)-Ru(3),48.21(12)
C(3)-Ru(1)-Ru(3),71.38(13)
C(14)-Ru(1)-Ru(3),117.64(12)
C(15)-Ru(1)-Ru(3),126.44(12)
C(13)-Ru(1)-Ru(3),134.66(13)
C(11)-Ru(1)-Ru(3),155.55(14)
C(12)-Ru(1)-Ru(3),167.24(14)
C(2)-Ru(1)-Ru(3),66.39(10)
C(1)-Ru(1)-Ru(2),42.61(11)
C(4)-Ru(1)-Ru(2),94.54(12)
C(3)-Ru(1)-Ru(2),86.68(14)
C(14)-Ru(1)-Ru(2),135.84(12)
C(15)-Ru(1)-Ru(2),172.30(12)
C(13)-Ru(1)-Ru(2),110.05(12)
C(11)-Ru(1)-Ru(2),141.47(13)
C(12)-Ru(1)-Ru(2),112.45(14)
C(2)-Ru(1)-Ru(2),54.78(11)
Ru(3)-Ru(1)-Ru(2),57.545(11)
C(1)-Ru(2)-O(1),97.14(14)
C(1)-Ru(2)-C(25),97.05(17)
O(1)-Ru(2)-C(25),145.41(16)
C(1)-Ru(2)-C(21),102.46(17)
O(1)-Ru(2)-C(21),159.28(15)
C(25)-Ru(2)-C(21),38.15(17)
C(1)-Ru(2)-C(24),125.58(17)
O(1)-Ru(2)-C(24),110.18(16)
C(25)-Ru(2)-C(24),37.90(18)
C(21)-Ru(2)-C(24),63.02(17)
C(1)-Ru(2)-C(22),135.82(18)
O(1)-Ru(2)-C(22),122.12(16)
C(25)-Ru(2)-C(22),62.80(18)
C(21)-Ru(2)-C(22),37.19(18)
C(24)-Ru(2)-C(22),62.18(18)
C(1)-Ru(2)-C(23),159.41(17)
O(1)-Ru(2)-C(23),100.26(16)
C(25)-Ru(2)-C(23),62.37(18)
C(21)-Ru(2)-C(23),62.07(18)
C(24)-Ru(2)-C(23),36.81(18)
C(22)-Ru(2)-C(23),36.94(19)
C(1)-Ru(2)-C(2),93.58(17)
O(1)-Ru(2)-C(2),33.24(13)
C(25)-Ru(2)-C(2),169.25(17)
C(21)-Ru(2)-C(2),137.20(16)
C(24)-Ru(2)-C(2),134.06(18)
C(22)-Ru(2)-C(2),108.06(17)
C(23)-Ru(2)-C(2),107.00(18)
C(1)-Ru(2)-Ru(3),49.85(11)
O(1)-Ru(2)-Ru(3),51.32(9)
C(25)-Ru(2)-Ru(3),122.22(12)
C(21)-Ru(2)-Ru(3),149.37(13)
C(24)-Ru(2)-Ru(3),118.56(13)
C(22)-Ru(2)-Ru(3),173.44(13)
C(23)-Ru(2)-Ru(3),139.60(13)
C(2)-Ru(2)-Ru(3),66.46(11)
C(1)-Ru(2)-Ru(1),43.65(11)
O(1)-Ru(2)-Ru(1),75.51(9)
C(25)-Ru(2)-Ru(1),133.65(13)
C(21)-Ru(2)-Ru(1),114.84(12)
C(24)-Ru(2)-Ru(1),169.18(13)
C(22)-Ru(2)-Ru(1),123.34(13)
C(23)-Ru(2)-Ru(1),153.13(13)
C(2)-Ru(2)-Ru(1),55.35(12)
Ru(3)-Ru(2)-Ru(1),57.204(11)
C(4)-Ru(3)-C(1),97.81(16)
C(4)-Ru(3)-O(1),79.43(17)
C(1)-Ru(3)-O(1),91.14(13)
C(4)-Ru(3)-C(34),90.5(2)
C(1)-Ru(3)-C(34),117.49(17)
O(1)-Ru(3)-C(34),150.82(16)
C(4)-Ru(3)-C(35),89.34(19)
C(1)-Ru(3)-C(35),154.36(17)
O(1)-Ru(3)-C(35),114.42(16)
C(34)-Ru(3)-C(35),37.46(19)
C(4)-Ru(3)-C(33),123.9(2)
C(1)-Ru(3)-C(33),93.92(17)
O(1)-Ru(3)-C(33),154.97(18)
C(34)-Ru(3)-C(33),37.3(2)
C(35)-Ru(3)-C(33),62.16(18)
C(4)-Ru(3)-C(31),121.27(19)
C(1)-Ru(3)-C(31),140.68(18)

O(1)-Ru(3)-C(31),99.55(15)
C(34)-Ru(3)-C(31),62.46(18)
C(35)-Ru(3)-C(31),37.23(19)
C(33)-Ru(3)-C(31),62.04(19)
C(4)-Ru(3)-C(32),149.58(19)
C(1)-Ru(3)-C(32),105.65(18)
O(1)-Ru(3)-C(32),118.50(17)
C(34)-Ru(3)-C(32),61.63(19)
C(35)-Ru(3)-C(32),61.35(18)
C(33)-Ru(3)-C(32),36.7(2)
C(31)-Ru(3)-C(32),36.7(2)
C(4)-Ru(3)-Ru(1),50.26(12)
C(1)-Ru(3)-Ru(1),47.78(11)
O(1)-Ru(3)-Ru(1),79.17(8)
C(34)-Ru(3)-Ru(1),115.06(13)
C(35)-Ru(3)-Ru(1),135.79(13)
C(33)-Ru(3)-Ru(1),121.58(14)
C(31)-Ru(3)-Ru(1),171.52(14)
C(32)-Ru(3)-Ru(1),150.72(15)
C(4)-Ru(3)-Ru(2),102.55(14)
C(1)-Ru(3)-Ru(2),46.53(11)
O(1)-Ru(3)-Ru(2),48.22(8)
C(34)-Ru(3)-Ru(2),160.15(15)
C(35)-Ru(3)-Ru(2),154.83(14)
C(33)-Ru(3)-Ru(2),124.00(14)
C(31)-Ru(3)-Ru(2),120.12(13)
C(32)-Ru(3)-Ru(2),107.61(13)
Ru(1)-Ru(3)-Ru(2),65.252(12)
Ru(2)-C(1)-Ru(1),93.74(16)
Ru(2)-C(1)-Ru(3),83.62(14)
Ru(1)-C(1)-Ru(3),82.30(14)
O(1)-C(2)-C(3),114.2(4)
O(1)-C(2)-C(5),117.9(5)
C(3)-C(2)-C(5),121.5(5)
O(1)-C(2)-Ru(2),53.7(2)
C(3)-C(2)-Ru(2),125.0(3)
C(5)-C(2)-Ru(2),106.8(4)
O(1)-C(2)-Ru(1),100.0(3)
C(3)-C(2)-Ru(1),59.7(2)
C(5)-C(2)-Ru(1),130.2(4)
Ru(2)-C(2)-Ru(1),69.87(11)
C(4)-C(3)-C(2),115.7(4)
C(4)-C(3)-Ru(1),66.6(2)
C(2)-C(3)-Ru(1),86.4(3)
C(3)-C(4)-Ru(3),112.7(3)
C(3)-C(4)-Ru(1),75.2(3)
Ru(3)-C(4)-Ru(1),81.53(16)
C(2)-O(1)-Ru(2),93.0(2)
C(2)-O(1)-Ru(3),107.0(3)
Ru(2)-O(1)-Ru(3),80.46(10)
C(12)-C(11)-C(15),108.1(4)
C(12)-C(11)-C(16),126.2(5)
C(15)-C(11)-C(16),125.5(5)
C(12)-C(11)-Ru(1),71.9(3)
C(15)-C(11)-Ru(1),70.4(2)
C(16)-C(11)-Ru(1),127.0(4)
C(11)-C(12)-C(13),107.4(4)
C(11)-C(12)-C(17),123.9(5)
C(13)-C(12)-C(17),128.4(5)
C(11)-C(12)-Ru(1),71.0(3)
C(13)-C(12)-Ru(1),70.8(2)
C(17)-C(12)-Ru(1),128.6(4)
C(14)-C(13)-C(12),108.2(4)
C(14)-C(13)-C(18),125.1(5)
C(12)-C(13)-C(18),125.9(5)
C(14)-C(13)-Ru(1),70.4(2)
C(12)-C(13)-Ru(1),71.8(3)
C(18)-C(13)-Ru(1),131.7(4)
C(15)-C(14)-C(13),108.0(4)
C(15)-C(14)-C(19),127.1(5)
C(13)-C(14)-C(19),124.4(5)
C(15)-C(14)-Ru(1),71.5(2)
C(13)-C(14)-Ru(1),72.1(2)
C(19)-C(14)-Ru(1),128.6(3)
C(14)-C(15)-C(11),108.3(4)
C(14)-C(15)-C(20),126.7(5)
C(11)-C(15)-C(20),124.6(5)
C(14)-C(15)-Ru(1),71.2(2)
C(11)-C(15)-Ru(1),72.1(3)
C(20)-C(15)-Ru(1),127.7(3)
C(22)-C(21)-C(25),107.7(4)
C(22)-C(21)-C(26),125.9(5)
C(25)-C(21)-C(26),125.5(5)
C(22)-C(21)-Ru(2),72.6(3)
C(25)-C(21)-Ru(2),70.0(2)
C(26)-C(21)-Ru(2),131.4(4)
C(21)-C(22)-C(23),108.3(4)
C(21)-C(22)-C(27),125.3(5)
C(23)-C(22)-C(27),125.9(5)
C(21)-C(22)-Ru(2),70.2(3)
C(23)-C(22)-Ru(2),72.4(3)
C(27)-C(22)-Ru(2),129.5(4)
C(24)-C(23)-C(22),108.4(4)
C(24)-C(23)-C(28),124.3(5)
C(22)-C(23)-C(28),127.3(5)
C(24)-C(23)-Ru(2),70.3(3)
C(22)-C(23)-Ru(2),70.6(3)
C(28)-C(23)-Ru(2),126.2(4)
C(23)-C(24)-C(25),107.7(4)
C(23)-C(24)-C(29),123.9(5)
C(25)-C(24)-C(29),127.6(5)
C(23)-C(24)-Ru(2),72.9(3)
C(25)-C(24)-Ru(2),69.3(2)
C(29)-C(24)-Ru(2),131.3(4)
C(24)-C(25)-C(21),107.9(4)
C(24)-C(25)-C(30),126.3(5)
C(21)-C(25)-C(30),125.4(5)
C(24)-C(25)-Ru(2),72.8(3)
C(21)-C(25)-Ru(2),71.9(2)
C(30)-C(25)-Ru(2),127.2(3)
C(35)-C(31)-C(32),107.4(4)
C(35)-C(31)-C(36),124.5(6)
C(32)-C(31)-C(36),127.9(6)
C(35)-C(31)-Ru(3),70.0(2)
C(32)-C(31)-Ru(3),73.5(3)
C(36)-C(31)-Ru(3),125.0(4)
C(33)-C(32)-C(31),107.4(4)
C(33)-C(32)-C(37),127.7(6)
C(31)-C(32)-C(37),124.2(6)
C(33)-C(32)-Ru(3),68.5(2)
C(31)-C(32)-Ru(3),69.9(2)
C(37)-C(32)-Ru(3),133.8(4)
C(34)-C(33)-C(32),108.5(4)
C(34)-C(33)-C(38),127.2(6)
C(32)-C(33)-C(38),123.6(6)
C(34)-C(33)-Ru(3),70.3(3)
C(32)-C(33)-Ru(3),74.8(3)
C(38)-C(33)-Ru(3),128.1(4)
C(33)-C(34)-C(35),108.1(4)
C(33)-C(34)-C(39),125.9(6)
C(35)-C(34)-C(39),125.5(6)
C(33)-C(34)-Ru(3),72.3(3)
C(35)-C(34)-Ru(3),72.2(3)
C(39)-C(34)-Ru(3),127.5(4)
C(34)-C(35)-C(31),108.4(4)
C(34)-C(35)-C(40),123.9(5)
C(31)-C(35)-C(40),127.5(5)
C(34)-C(35)-Ru(3),70.4(3)
C(31)-C(35)-Ru(3),72.8(3)
C(40)-C(35)-Ru(3),127.1(4)
F(6)-P(1)-F(5),91.3(4)
F(6)-P(1)-F(3),89.7(5)
F(5)-P(1)-F(3),178.6(4)
F(6)-P(1)-F(2),87.8(4)
F(5)-P(1)-F(2),94.4(5)
F(3)-P(1)-F(2),86.6(4)
F(6)-P(1)-F(4),95.7(5)
F(5)-P(1)-F(4),90.9(5)
F(3)-P(1)-F(4),88.0(4)
F(2)-P(1)-F(4),173.5(4)
F(6)-P(1)-F(1),177.4(4)
F(5)-P(1)-F(1),89.2(3)
F(3)-P(1)-F(1),89.9(4)
F(2)-P(1)-F(1),89.6(3)
F(4)-P(1)-F(1),86.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S3-4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **9-PF6**. The anisotropic displacement factor exponent takes the form: $-2\ p^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom, U11, U22, U33, U23, U13, U12

Ru(1),25(1),36(1),29(1),3(1),5(1),2(1)
Ru(2),28(1),34(1),27(1),4(1),5(1),5(1)
Ru(3),27(1),32(1),30(1),3(1),6(1),1(1)
C(1),27(2),36(2),28(2),3(1),3(1),5(1)
C(2),47(2),51(2),29(2),5(2),3(2),-5(2)
C(3),38(2),67(3),31(2),-2(2),6(2),-2(2)
C(4),33(2),47(2),37(2),-7(2),9(2),1(2)
C(5),86(4),67(3),38(2),14(2),14(3),16(3)
O(1),35(1),44(2),30(1),3(1),1(1),3(1)
C(11),32(2),57(3),43(2),11(2),14(2),4(2)
C(12),34(2),42(2),61(3),8(2),9(2),-3(2)
C(13),29(2),51(2),44(2),-8(2),3(2),-1(2)
C(14),22(2),54(2),43(2),6(2),3(2),3(2)
C(15),28(2),47(2),50(2),3(2),11(2),5(2)
C(16),52(3),99(5),54(3),21(3),24(3),10(3)
C(17),74(4),45(3),104(6),17(3),26(4),5(3)
C(18),48(3),82(4),56(3),-26(3),-3(2),8(3)
C(19),41(2),79(4),56(3),23(3),0(2),8(2)
C(20),48(3),61(3),82(4),-13(3),17(3),18(2)
C(21),41(2),39(2),44(2),0(2),11(2),8(2)
C(22),52(3),39(2),49(2),11(2),16(2),13(2)
C(23),41(2),51(3),47(2),7(2),5(2),17(2)
C(24),37(2),45(2),56(3),5(2),15(2),14(2)
C(25),47(2),45(2),36(2),2(2),14(2),16(2)
C(26),52(3),51(3),70(4),-12(3),4(3),-2(2)
C(27),90(5),51(3),66(4),24(3),28(3),16(3)
C(28),64(4),90(5),68(4),3(3),-10(3),37(4)
C(29),48(3),61(3),106(5),10(3),36(3),9(3)
C(30),95(5),60(3),32(2),5(2),19(2),26(3)
C(31),34(2),40(2),61(3),14(2),11(2),-1(2)
C(32),65(3),39(2),55(3),13(2),36(2),9(2)
C(33),58(3),42(2),36(2),16(2),3(2),-3(2)
C(34),39(2),39(2),60(3),12(2),9(2),8(2)
C(35),46(2),37(2),47(2),3(2),11(2),-4(2)
C(36),34(2),78(4),108(6),33(4),1(3),-4(3)
C(37),126(7),68(4),96(5),17(4),85(5),15(4)
C(38),108(6),82(5),47(3),28(3),-15(3),-18(4)
C(39),68(4),67(4),158(8),45(5),42(5),38(4)
C(40),91(5),51(3),60(3),-12(3),17(3),-12(3)
P(1),57(1),50(1),56(1),7(1),14(1),14(1)
F(1),102(3),84(3),107(4),38(3),11(3),29(3)
F(2),119(5),132(5),105(4),17(4),-46(4),-5(4)
F(3),111(4),222(8),107(4),-31(5),43(4),63(5)
F(4),89(4),118(5),194(7),-48(5),-23(4),-4(3)
F(5),228(8),210(7),128(5),89(5),128(6),142(7)
F(6),146(6),103(4),369(13),139(7),105(7),65(4)

Table S3-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **9-PF6**.

Atom, x, y, z, U(eq)

H(5A),6532,8472,5053,96
H(5B),6758,7790,4209,96
H(5C),7871,8618,4855,96
H(16A),10834,7157,4758,100
H(16B),11818,8212,5016,100
H(16C),10388,8194,4794,100
H(17A),10755,10047,7040,112
H(17B),10498,9672,5938,112
H(17C),11874,10033,6552,112
H(18A),11064,9454,8596,100
H(18B),12287,9059,8954,100
H(18C),11019,8452,9135,100
H(19A),11050,6662,8942,91
H(19B),12368,6677,8741,91
H(19C),11218,5797,8228,91
H(20A),11073,5344,6603,95
H(20B),12159,5951,6182,95
H(20C),10778,5725,5570,95
H(26A),9378,9834,9056,93
H(26B),8856,10827,8862,93
H(26C),9506,10382,8120,93
H(27A),6999,10298,5810,100
H(27B),8374,10414,6406,100
H(27C),7545,11128,6703,100
H(28A),5141,9211,5532,113
H(28B),4237,9343,6202,113
H(28C),4388,8238,5895,113
H(29A),4704,7649,8556,104
H(29B),4245,7307,7443,104
H(29C),3961,8313,7875,104
H(30A),8108,8626,9700,91
H(30B),6817,7832,9493,91
H(30C),6922,8979,9875,91
H(36A),4080,5381,6718,116
H(36B),3774,4172,6657,116
H(36C),4331,4742,5856,116
H(37A),6058,5970,9321,132
H(37B),4930,5028,8927,132
H(37C),4996,6061,8435,132
H(38A),8142,5962,9597,135
H(38B),9120,5442,9250,135
H(38C),8087,4786,9694,135
H(39A),8434,3326,7359,136
H(39B),9283,4221,8120,136
H(39C),9111,4344,7011,136
H(40A),6961,3927,5515,109
H(40B),5514,3707,5419,109
H(40C),6296,2976,5964,109
H(1),8860(40),7400(30),8500(30),20(9)
H(2),8740(50),5280(40),5970(40),38(13)
H(3),8570(50),6590(40),4740(40),34(12)