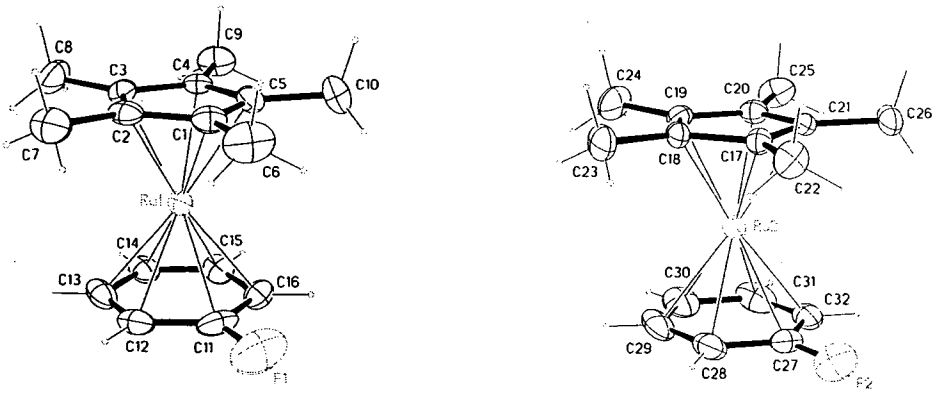
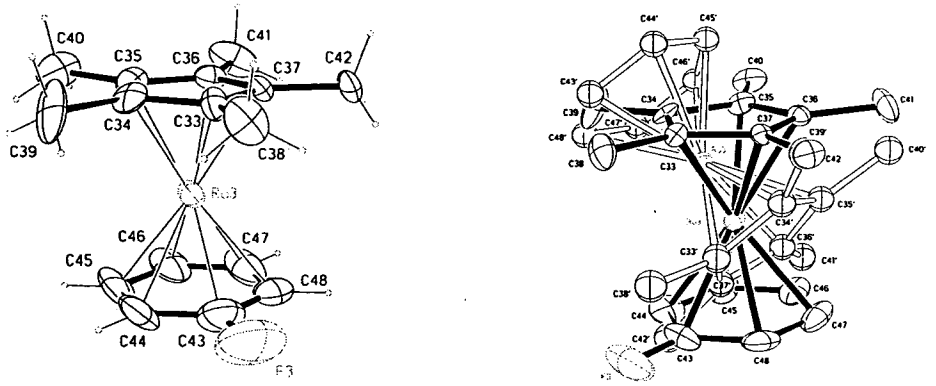
Fig. S5. Thermal ellipsoid plots (20% ellipsoids) of $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ (**4**).

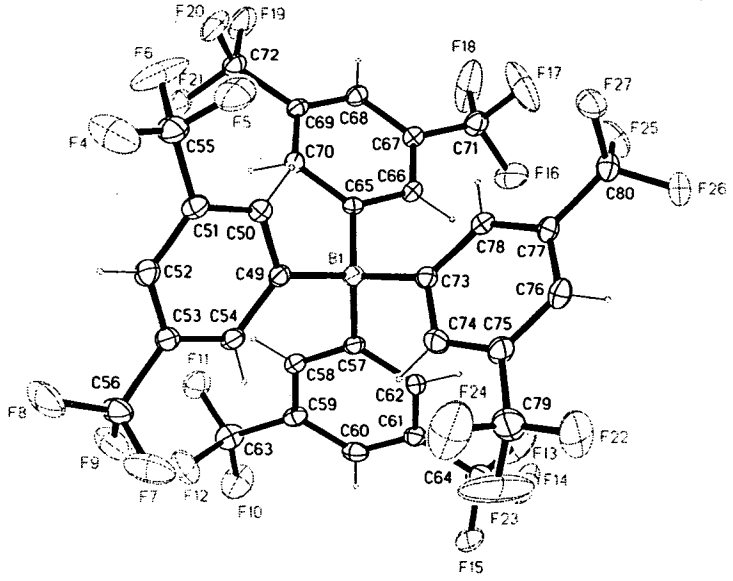
(a) $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ cations 1 and 2



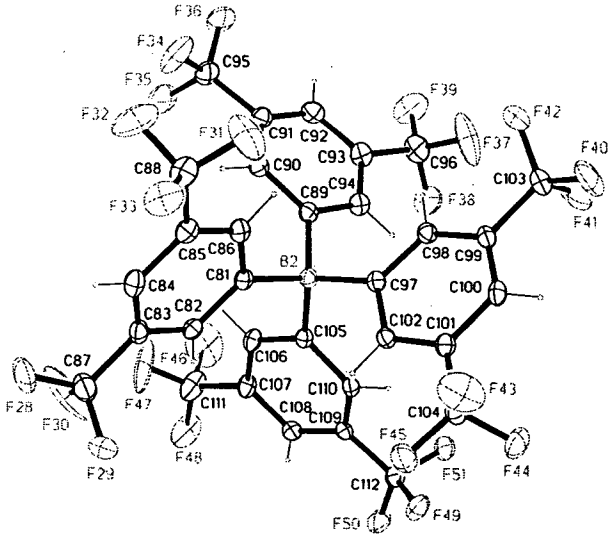
(b) $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ cation 3 with predominant (left) and with both orientations (right)



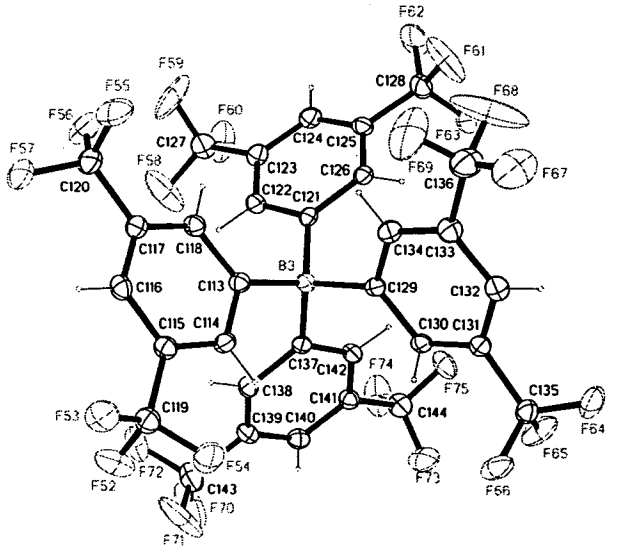
(c) $[BAr'_4]$ anion no. 1 (subordinate F positions omitted)



(d) [BAr'$_4$] anion no. 2 (subordinate F positions omitted)



(e) [BAr'$_4$] anion no. 3 (subordinate F positions omitted)



(f) Packing diagram of [Cp*Ru(η^6-C_6H_5F)][BAr'$_4$] (**4**). H and F omitted.

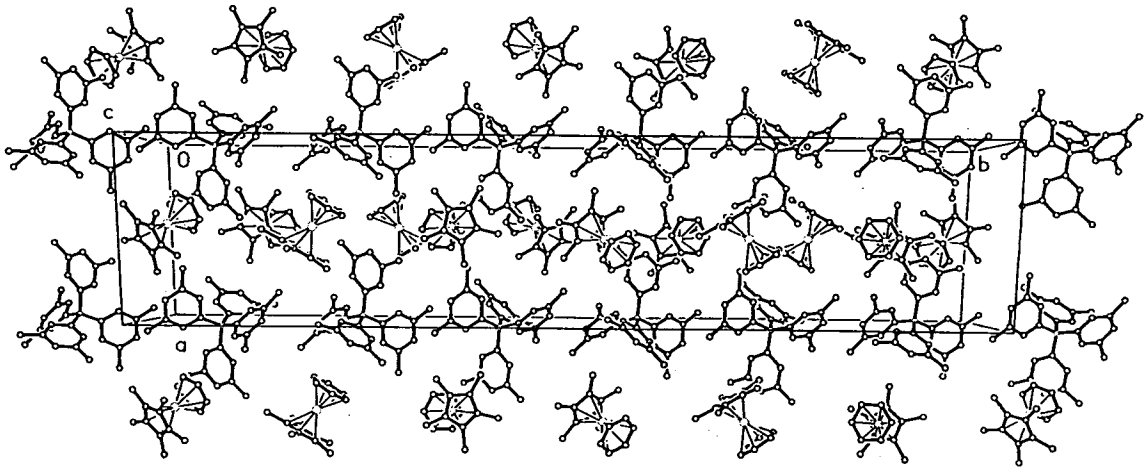


Table S16. Crystal data and structure refinement for $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ **(4)**.

Identification code	608mancf j3fr
Empirical formula	C48 H32 B F25 Ru
Formula weight	1195.62
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c (no. 14)
Unit cell dimensions	a = 12.830(12) Å α = 90 deg.
	b = 58.17(6) Å β = 104.71(2) deg.
	c = 20.348(19) Å γ = 90 deg.
Volume	14688(25) $Å^3$
Z, Calculated density	12, 1.622 Mg/m^3
Absorption coefficient	0.450 mm^{-1}
F(000)	7128
Crystal size	0.80 x 0.40 x 0.30 mm, colorless prism
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochromomator, detector distance 60 mm, 512x512 pixel mode.
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 20 sec. per frame full sphere data collection, 5 x 606 frames
Theta range for data collection	2.03 to 24.00 deg.
Index ranges	-14<=h<=14, -66<=k<=65, -22<=l<=23
Reflections collected / unique	135060 / 22779 [R(int) = 0.0378]
Completeness to theta = 24.00	98.7%
Absorption correction	Semi-empirical from equivalents (prg. SADABS)
Max. and min. rel. transmission	1.00 and 0.87
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	22779 / 0 / 2055
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0643, wR2 = 0.1433 (19241 data)
R indices (all data)	R1 = 0.0756, wR2 = 0.1496 (22779 data)
Extinction coefficient	0.000118(18)
Largest diff. peak and hole	0.961 and -0.528 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S17. Atomic coordinates (x 10^5 for Ru; x 10^4 for C, B, F) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ (**4**). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 1				
Ru(1)	146796(3)	4074(1)	75630(2)	44(1)
C(1)	15802(5)	392(1)	8560(3)	61(2)
C(2)	16216(4)	257(1)	8104(3)	62(2)
C(3)	15453(5)	78(1)	7847(3)	58(1)
C(4)	14582(4)	102(1)	8164(3)	49(1)
C(5)	14802(5)	293(1)	8599(3)	56(1)
C(6)	16350(7)	595(1)	8965(4)	105(3)
C(7)	17282(5)	289(2)	7929(4)	106(3)
C(8)	15579(7)	-110(1)	7370(4)	104(3)
C(9)	13636(5)	-54(1)	8082(4)	84(2)
C(10)	14124(7)	377(1)	9057(3)	97(2)
C(11)	14411(7)	767(1)	7280(4)	86(2)
C(12)	15004(5)	670(1)	6864(4)	75(2)
C(13)	14595(5)	479(1)	6481(3)	76(2)
C(14)	13600(5)	386(1)	6509(3)	72(2)
C(15)	13035(5)	483(1)	6944(3)	73(2)
C(16)	13417(5)	674(1)	7336(4)	76(2)
F(1)	14770(6)	947(1)	7647(4)	178(3)
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 2				
Ru(2)	46844(3)	13444(1)	28255(2)	45(1)
C(17)	4883(4)	1400(1)	3901(2)	44(1)
C(18)	5499(4)	1204(1)	3809(2)	47(1)
C(19)	4766(5)	1038(1)	3443(3)	52(1)
C(20)	3707(4)	1129(1)	3310(3)	54(1)
C(21)	3767(4)	1352(1)	3603(2)	44(1)
C(22)	5335(5)	1613(1)	4280(3)	71(2)
C(23)	6694(4)	1173(1)	4086(3)	75(2)
C(24)	5059(7)	799(1)	3260(4)	95(2)
C(25)	2672(5)	1008(1)	2975(4)	87(2)
C(26)	2848(5)	1507(1)	3623(3)	76(2)
C(27)	4828(6)	1680(1)	2346(4)	75(2)
C(28)	5802(5)	1572(1)	2451(3)	78(2)
C(29)	5835(6)	1354(2)	2201(3)	90(2)
C(30)	4922(8)	1243(2)	1827(3)	94(2)
C(31)	3905(6)	1363(2)	1734(3)	98(3)
C(32)	3891(6)	1582(2)	2002(3)	81(2)
F(2)	4933(9)	1887(2)	2654(6)	152(5)
F(2A)	3102(9)	1236(2)	1407(5)	117(6)
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 predominant orientation				
Ru(3)	47379(5)	20693(1)	76048(3)	59(1)
C(33)	6303(6)	2037(1)	7386(4)	58(2)
C(34)	5735(8)	1830(2)	7176(5)	72(3)
C(35)	5479(7)	1732(2)	7778(6)	73(3)
C(36)	5933(6)	1879(2)	8338(4)	60(2)
C(37)	6443(6)	2063(1)	8093(4)	53(2)
C(38)	6726(9)	2190(2)	6914(6)	103(4)

C(39)	5390(13)	1736(3)	6482(7)	144(6)
C(40)	4880(10)	1496(2)	7767(8)	120(5)
C(41)	5931(10)	1836(3)	9070(6)	126(5)
C(42)	7025(8)	2255(2)	8527(5)	83(3)
C(43)	3929(9)	2370(2)	7048(7)	130(5)
C(44)	3329(8)	2177(2)	6789(5)	143(7)
C(45)	2957(6)	2032(2)	7220(7)	126(5)
C(46)	3186(7)	2079(2)	7909(6)	124(5)
C(47)	3786(8)	2272(2)	8167(5)	146(8)
C(48)	4158(8)	2417(2)	7737(8)	134(6)
F(3)	4244(11)	2507(2)	6696(7)	236(6)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 subordinate orientation

Ru(3')	52007(11)	19177(2)	73978(7)	52(1)
C(33')	5143(6)	2286(1)	7531(4)	88(2)
C(34')	5736(6)	2186(1)	8146(4)	88(2)
C(35')	5038(6)	2038(1)	8384(3)	88(2)
C(36')	4015(6)	2046(1)	7916(4)	88(2)
C(37')	4080(6)	2199(1)	7389(4)	88(2)
C(38')	5569(10)	2454(2)	7103(6)	105(2)
C(39')	6901(8)	2229(2)	8487(6)	105(2)
C(40')	5333(10)	1896(2)	9022(5)	105(2)
C(41')	3032(8)	1915(2)	7969(6)	105(2)
C(42')	3178(9)	2260(2)	6784(6)	105(2)
C(43')	6152(6)	1843(1)	6627(4)	88(2)
C(44')	6689(6)	1750(1)	7246(4)	88(2)
C(45')	6159(6)	1601(1)	7581(4)	88(2)
C(46')	5091(6)	1545(1)	7296(4)	88(2)
C(47')	4554(6)	1638(1)	6678(4)	88(2)
C(48')	5084(7)	1787(1)	6343(3)	88(2)

*** $BAr'_4]$ no. 1

B(1)	10317(4)	855(1)	5080(3)	38(1)
C(49)	10178(3)	1063(1)	5596(2)	37(1)
C(50)	10822(4)	1069(1)	6263(2)	44(1)
C(51)	10712(4)	1237(1)	6729(2)	49(1)
C(52)	9937(4)	1405(1)	6548(3)	53(1)
C(53)	9278(4)	1403(1)	5901(3)	50(1)
C(54)	9395(4)	1233(1)	5437(2)	44(1)
C(55)	11462(5)	1242(1)	7422(3)	66(2)
C(56)	8421(5)	1583(1)	5686(3)	76(2)
C(57)	9651(3)	904(1)	4287(2)	39(1)
C(58)	9712(3)	1115(1)	3981(2)	40(1)
C(59)	9187(4)	1164(1)	3312(2)	45(1)
C(60)	8596(4)	992(1)	2907(2)	51(1)
C(61)	8529(4)	777(1)	3189(3)	52(1)
C(62)	9034(4)	735(1)	3867(2)	46(1)
C(63)	9184(5)	1407(1)	3063(3)	61(2)
C(64)	7879(5)	593(1)	2756(4)	76(2)
C(65)	11580(3)	827(1)	5041(2)	34(1)
C(66)	11899(3)	635(1)	4717(2)	37(1)
C(67)	12945(4)	604(1)	4672(2)	39(1)
C(68)	13735(4)	767(1)	4932(2)	41(1)
C(69)	13439(4)	960(1)	5231(2)	40(1)
C(70)	12381(4)	989(1)	5289(2)	39(1)
C(71)	13241(4)	389(1)	4362(3)	57(1)
C(72)	14241(4)	1141(1)	5518(3)	51(1)
C(73)	9848(3)	623(1)	5362(2)	38(1)

C(74)	8771(4)	622(1)	5390(3)	53(1)
C(75)	8297(4)	437(1)	5618(3)	57(1)
C(76)	8876(4)	237(1)	5827(3)	51(1)
C(77)	9947(4)	234(1)	5815(2)	38(1)
C(78)	10412(3)	424(1)	5594(2)	37(1)
C(79)	7144(6)	452(1)	5641(5)	93(2)
C(80)	10610(4)	26(1)	6069(2)	48(1)
F(4)	11195(7)	1381(1)	7832(3)	201(5)
F(5)	11554(4)	1038(1)	7730(2)	103(2)
F(6)	12465(5)	1271(1)	7412(3)	148(3)
F(7)	7448(4)	1498(1)	5682(3)	130(2)
F(8)	8553(5)	1759(1)	6081(3)	186(3)
F(9)	8285(4)	1651(1)	5059(2)	105(1)
F(10)	8714(4)	1431(1)	2418(2)	106(2)
F(11)	10159(3)	1498(1)	3197(2)	74(1)
F(12)	8627(3)	1547(1)	3377(2)	88(1)
F(13)	8406(4)	450(1)	2515(4)	155(3)
F(14)	7415(5)	445(1)	3165(3)	125(2)
F(15)	7018(4)	665(1)	2345(2)	93(2)
F(16)	12506(4)	301(1)	3880(3)	110(3)
F(17)	13380(8)	213(1)	4815(3)	168(4)
F(18)	14142(5)	391(1)	4214(5)	167(4)
F(19)	15202(3)	1106(1)	5393(2)	100(1)
F(20)	14421(3)	1159(1)	6189(2)	85(1)
F(21)	13946(3)	1351(1)	5281(2)	73(1)
F(22)	6734(4)	271(1)	5821(4)	148(3)
F(23)	6509(4)	524(2)	5099(5)	219(5)
F(24)	6989(5)	612(1)	6066(6)	207(5)
F(25)	11336(3)	-19(1)	5721(2)	80(1)
F(26)	10043(3)	-165(1)	6045(2)	79(1)
F(27)	11179(3)	48(1)	6713(2)	74(1)
F(4')	12236	1111	7517	62(2)
F(5')	11849	1452	7531	62(2)
F(6')	11005	1206	7895	62(2)
F(13')	6948	571	2790	62(2)
F(14')	8133	648	2018	62(2)
F(15')	8230	429	2866	62(2)
F(16')	14125	313	4639	62(2)
F(17')	13306	451	3715	62(2)
F(18')	12698	226	4418	62(2)
F(22')	6671	616	5378	62(2)
F(23')	7094	415	6307	62(2)
F(24')	6619	272	5021	62(2)

*** BAr'_4]	no. 2			
B(2)	10318(4)	817(1)	9999(3)	37(1)
C(81)	9797(3)	804(1)	9173(2)	36(1)
C(82)	9036(3)	955(1)	8795(2)	39(1)
C(83)	8698(4)	945(1)	8089(2)	45(1)
C(84)	9117(4)	785(1)	7734(2)	49(1)
C(85)	9879(4)	630(1)	8095(2)	44(1)
C(86)	10197(4)	640(1)	8792(2)	40(1)
C(87)	7892(5)	1112(1)	7715(3)	65(2)
C(88)	10341(5)	453(1)	7716(3)	61(2)
C(89)	10037(3)	588(1)	10394(2)	38(1)
C(90)	9334(4)	412(1)	10102(2)	42(1)
C(91)	9080(4)	233(1)	10486(3)	49(1)
C(92)	9552(4)	218(1)	11171(3)	53(1)

C(93)	10270(4)	386(1)	11475(2)	49(1)
C(94)	10482(4)	570(1)	11096(2)	45(1)
C(95)	8268(5)	56(1)	10152(3)	61(2)
C(96)	10861(5)	374(1)	12214(3)	67(2)
C(97)	11614(3)	845(1)	10092(2)	35(1)
C(98)	12402(3)	693(1)	10443(2)	39(1)
C(99)	13497(3)	723(1)	10490(2)	40(1)
C(100)	13849(4)	908(1)	10182(2)	42(1)
C(101)	13095(3)	1061(1)	9822(2)	39(1)
C(102)	12005(3)	1030(1)	9779(2)	38(1)
C(103)	14285(4)	557(1)	10902(3)	57(1)
C(104)	13479(4)	1261(1)	9483(3)	58(1)
C(105)	9804(3)	1028(1)	10335(2)	35(1)
C(106)	8698(4)	1028(1)	10292(2)	44(1)
C(107)	8196(4)	1199(1)	10570(2)	46(1)
C(108)	8785(4)	1382(1)	10922(2)	42(1)
C(109)	9884(3)	1384(1)	10990(2)	36(1)
C(110)	10376(3)	1213(1)	10697(2)	35(1)
C(111)	7004(5)	1192(1)	10482(4)	76(2)
C(112)	10553(4)	1568(1)	11392(2)	45(1)
F(28)	7410(5)	1051(1)	7097(3)	150(3)
F(29)	8273(4)	1311(1)	7657(3)	117(2)
F(30)	7093(5)	1139(2)	8005(4)	198(5)
F(31)	11240(4)	363(1)	8066(2)	127(2)
F(32)	9675(4)	282(1)	7500(3)	118(2)
F(33)	10546(3)	537(1)	7154(2)	84(1)
F(34)	8315(4)	4(1)	9521(2)	116(2)
F(35)	7271(3)	125(1)	10073(3)	126(2)
F(36)	8336(4)	-140(1)	10469(2)	112(2)
F(37)	11897(4)	358(1)	12300(2)	155(3)
F(38)	10749(4)	565(1)	12547(2)	100(1)
F(39)	10526(5)	211(1)	12543(2)	124(2)
F(40)	15242(3)	563(1)	10764(2)	108(2)
F(41)	14475(4)	598(1)	11557(2)	117(2)
F(42)	13981(3)	342(1)	10816(2)	94(1)
F(43)	13967(4)	1189(1)	9008(3)	120(2)
F(44)	14211(3)	1382(1)	9895(2)	106(2)
F(45)	12711(3)	1401(1)	9163(2)	76(1)
F(46)	6783(5)	1049(2)	10980(5)	185(4)
F(47)	6470(3)	1101(1)	9950(3)	157(4)
F(48)	6563(3)	1371(1)	10637(4)	143(3)
F(49)	11261(3)	1661(1)	11079(2)	64(1)
F(50)	9990(3)	1741(1)	11548(2)	75(1)
F(51)	11168(3)	1489(1)	11982(1)	65(1)
F(28')	7652	1293	8087	62(2)
F(29')	6977	1045	7565	62(2)
F(30')	8034	1201	7174	62(2)
F(34')	7671	19	10593	62(2)
F(35')	8729	-102	9981	62(2)
F(36')	7717	134	9628	62(2)
F(46')	6521	1361	9930	62(2)
F(47')	6791	1252	10984	62(2)
F(48')	6631	998	10380	62(2)
*** BAr'_4]	no. 3			
B(3)	9621(4)	2562(1)	5536(3)	38(1)
C(113)	9831(4)	2343(1)	5084(2)	39(1)
C(114)	9301(4)	2332(1)	4391(2)	43(1)

C(115)	9449(4)	2152(1)	3974(2)	46(1)
C(116)	10177(4)	1980(1)	4230(2)	47(1)
C(117)	10720(4)	1985(1)	4903(2)	45(1)
C(118)	10552(4)	2163(1)	5325(2)	41(1)
C(119)	8778(5)	2143(1)	3258(3)	56(1)
C(120)	11529(5)	1803(1)	5191(3)	61(2)
C(121)	10207(3)	2533(1)	6346(2)	35(1)
C(122)	9956(4)	2346(1)	6699(2)	42(1)
C(123)	10368(4)	2319(1)	7392(2)	47(1)
C(124)	11054(4)	2481(1)	7767(2)	49(1)
C(125)	11333(4)	2666(1)	7435(2)	45(1)
C(126)	10920(3)	2694(1)	6738(2)	39(1)
C(127)	10049(6)	2115(1)	7751(3)	69(2)
C(128)	12071(5)	2846(1)	7819(3)	61(2)
C(129)	10118(3)	2785(1)	5214(2)	36(1)
C(130)	9521(4)	2969(1)	4865(2)	37(1)
C(131)	10000(4)	3143(1)	4571(2)	40(1)
C(132)	11097(4)	3144(1)	4632(2)	48(1)
C(133)	11704(4)	2963(1)	4974(3)	48(1)
C(134)	11217(4)	2788(1)	5246(2)	45(1)
C(135)	9304(4)	3328(1)	4167(3)	51(1)
C(136)	12886(5)	2960(1)	5059(4)	80(2)
C(137)	8341(4)	2594(1)	5502(2)	36(1)
C(138)	7538(4)	2439(1)	5199(2)	43(1)
C(139)	6463(4)	2470(1)	5205(2)	49(1)
C(140)	6153(4)	2658(1)	5523(3)	49(1)
C(141)	6936(4)	2810(1)	5844(2)	43(1)
C(142)	7993(4)	2781(1)	5829(2)	40(1)
C(143)	5634(5)	2301(1)	4850(4)	73(2)
C(144)	6597(4)	3012(1)	6200(3)	61(2)
F(52)	7811(3)	2060(1)	3220(2)	94(1)
F(53)	9203(3)	2014(1)	2855(2)	84(1)
F(54)	8624(3)	2350(1)	2961(2)	85(1)
F(55)	12520(3)	1863(1)	5187(3)	113(2)
F(56)	11584(4)	1752(1)	5832(2)	102(1)
F(57)	11348(3)	1605(1)	4855(2)	97(1)
F(58)	9220(7)	2003(1)	7406(3)	185(4)
F(59)	10780(6)	1969(1)	7970(5)	179(4)
F(60)	9758(6)	2172(1)	8305(3)	119(2)
F(61)	12848(5)	2900(1)	7553(3)	148(3)
F(62)	12504(5)	2800(1)	8451(2)	127(3)
F(63)	11559(4)	3044(1)	7846(3)	129(3)
F(64)	9854(4)	3508(1)	4057(3)	108(2)
F(65)	8596(4)	3411(1)	4475(2)	89(2)
F(66)	8728(4)	3253(1)	3579(2)	91(2)
F(67)	13248(4)	3088(1)	4672(4)	144(3)
F(68)	13410(5)	3012(3)	5670(5)	252(7)
F(69)	13264(5)	2763(1)	4979(7)	226(6)
F(70)	4728(4)	2313(1)	5000(5)	189(4)
F(71)	5506(6)	2289(1)	4213(3)	196(4)
F(72)	5937(5)	2084(1)	5032(3)	139(2)
F(73)	5850(4)	3138(1)	5816(3)	109(2)
F(74)	6152(5)	2940(1)	6705(3)	113(2)
F(75)	7380(3)	3147(1)	6516(2)	79(1)
F(58')	10819	2115	8355	62(2)
F(59')	9115	2140	7764	62(2)
F(60')	10210	1951	7427	62(2)
F(61')	11789	2920	8329	62(2)

F(62')	12188	3028	7481	62(2)
F(63')	13002	2765	8001	62(2)
F(64')	8285	3292	4068	62(2)
F(65')	9580	3357	3611	62(2)
F(66')	9392	3495	4396	62(2)
F(67')	13392	2835	5512	62(2)
F(68')	13091	2877	4495	62(2)
F(69')	13274	3175	5293	62(2)
F(73')	7013	2995	6799	62(2)
F(74')	6833	3202	5875	62(2)
F(75')	5666	3014	6187	62(2)
F(70')	5918	2166	4498	62(2)
F(71')	5192	2180	5218	62(2)
F(72')	4828	2430	4467	62(2)

Remarks:

1) Structure contains three independent $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ per asymmetric unit.

2) F atom of $[Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 2 in two alternatively occupied F sites (occupation factors 0.60(1) for F(2), and 0.40(1) for F(2a)). $[Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 disordered and adopting alternatively two orientations with refined occupation factors of 0.684(2) for predominant and 0.316(2) for subordinate orientation (the latter refined with idealized geometry and isotropic temperature factors).

3) A part of the CF_3 groups of the three independent $[BAr'_4]$ anions was refined with split positions for F using anisotropic displacement parameters for the predominately occupied sites (unprimed) and isotropic ones combined with fixed unrefined positions taken from a difference Fourier synthesis for the subordinately occupied primed F atoms. One common isotropic displacement parameter was used for all primed F. Site occupation factors for predominately occupied F atoms were between 0.779(6) and 0.928(5), while for the corresponding primed F atoms they were between 1-0.779(6) and 1-0.928(5).

Table S18. Hydrogen coordinates and (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ (**4**).

	x	y	z	U_{eq}
H(6A)	16811	542	9393	157
H(6B)	15809	699	9054	157
H(6C)	16781	675	8710	157
H(7A)	17837	204	8249	159
H(7B)	17467	451	7953	159
H(7C)	17226	233	7473	159
H(8A)	15954	-239	7629	156
H(8B)	15991	-53	7065	156
H(8C)	14874	-159	7108	156
H(9A)	13810	-177	8415	126
H(9B)	13460	-120	7628	126
H(9C)	13023	32	8147	126
H(10A)	14341	298	9491	146
H(10B)	13371	345	8847	146
H(10C)	14224	541	9127	146
H(12A)	15670	733	6845	90
H(13A)	14986	412	6198	91
H(14A)	13316	259	6237	87
H(15A)	12379	417	6971	87
H(16A)	13034	740	7626	92
H(22A)	5340	1595	4755	107
H(22B)	4893	1744	4090	107
H(22C)	6065	1637	4241	107
H(23A)	6839	1107	4538	112
H(23B)	7050	1321	4107	112
H(23C)	6965	1071	3790	112
H(24A)	5032	694	3626	143
H(24B)	5781	800	3194	143
H(24C)	4551	750	2845	143
H(25A)	2417	923	3314	131
H(25B)	2795	903	2633	131
H(25C)	2135	1121	2762	131
H(26A)	2596	1474	4024	113
H(26B)	2266	1483	3219	113
H(26C)	3086	1666	3640	113
H(27A)	4802	1832	2526	89
H(28A)	6437	1646	2691	93
H(29A)	6501	1277	2287	107
H(30A)	4960	1096	1642	112
H(31A)	3251	1291	1485	117
H(32A)	3236	1661	1946	97
H(38A)	7435	2139	6907	154
H(38B)	6260	2182	6463	154
H(38C)	6762	2346	7073	154
H(39A)	5947	1637	6408	216
H(39B)	4736	1650	6431	216
H(39C)	5272	1859	6156	216
H(40A)	5399	1374	7857	180
H(40B)	4483	1497	8108	180
H(40C)	4393	1473	7328	180
H(41A)	6551	1747	9288	189

H(41B)	5951	1981	9299	189
H(41C)	5289	1755	9089	189
H(42A)	7775	2217	8693	124
H(42B)	6953	2392	8258	124
H(42C)	6716	2279	8904	124
H(44A)	3172	2145	6317	172
H(45A)	2545	1900	7042	151
H(46A)	2931	1980	8204	148
H(47A)	3943	2304	8640	176
H(48A)	4570	2549	7914	161
H(38D)	5465	2607	7245	158
H(38E)	6321	2427	7156	158
H(38F)	5193	2435	6637	158
H(39D)	6958	2355	8797	158
H(39E)	7210	2095	8728	158
H(39F)	7278	2267	8151	158
H(40D)	5196	1983	9390	158
H(40E)	4910	1759	8959	158
H(40F)	6080	1857	9122	158
H(41D)	2634	2004	8216	158
H(41E)	2590	1884	7524	158
H(41F)	3245	1773	8201	158
H(42D)	2789	2388	6892	158
H(42E)	3467	2298	6409	158
H(42F)	2702	2131	6666	158
H(43B)	6511	1943	6401	105
H(44B)	7411	1787	7438	105
H(45B)	6522	1538	7999	105
H(46B)	4732	1444	7523	105
H(47B)	3832	1601	6486	105
H(48B)	4721	1850	5925	105
H(50)	11352	955	6403	52
H(52)	9861	1519	6860	63
H(54)	8924	1234	5000	53
H(58)	10131	1232	4242	48
H(60)	8246	1021	2450	61
H(62)	8961	589	4050	55
H(66)	11379	524	4523	45
H(68)	14449	746	4903	49
H(70)	12208	1122	5503	47
H(74)	8352	754	5246	63
H(76)	8551	109	5973	61
H(78)	11147	417	5601	44
H(82)	8741	1068	9024	47
H(84)	8897	780	7256	59
H(86)	10705	533	9024	48
H(90)	9025	414	9631	51
H(92)	9390	95	11427	64
H(94)	10944	687	11318	53
H(98)	12186	565	10657	46
H(100)	14587	930	10216	51
H(102)	11509	1136	9531	45
H(106)	8278	905	10065	53
H(108)	8446	1499	11107	51
H(110)	11123	1222	10745	42
H(114)	8825	2451	4201	51
H(116)	10299	1861	3947	57
H(118)	10934	2162	5785	49

H(122)	9487	2233	6458	51
H(124)	11323	2464	8239	59
H(126)	11124	2823	6524	46
H(130)	8777	2976	4828	45
H(132)	11423	3263	4445	57
H(134)	11647	2665	5462	53
H(138)	7727	2309	4983	52
H(140)	5427	2681	5521	59
H(142)	8504	2890	6047	48

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S19. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ (**4**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 1						
Ru(1)	36(1)	48(1)	46(1)	5(1)	8(1)	0(1)
C(1)	57(3)	60(3)	54(3)	6(3)	-6(3)	-6(3)
C(2)	41(3)	72(4)	66(4)	29(3)	2(3)	1(3)
C(3)	58(3)	58(3)	56(3)	7(3)	10(3)	15(3)
C(4)	50(3)	41(3)	52(3)	13(2)	5(2)	-5(2)
C(5)	63(3)	59(3)	43(3)	2(2)	13(3)	-3(3)
C(6)	111(6)	77(5)	98(5)	-11(4)	-28(5)	-31(4)
C(7)	38(3)	145(7)	136(7)	61(6)	25(4)	17(4)
C(8)	133(7)	85(5)	92(5)	-13(4)	24(5)	45(5)
C(9)	71(4)	67(4)	107(5)	17(4)	10(4)	-27(3)
C(10)	120(6)	119(6)	64(4)	-8(4)	43(4)	5(5)
C(11)	114(6)	38(3)	90(5)	9(3)	-4(5)	3(4)
C(12)	65(4)	76(5)	82(5)	35(4)	14(4)	-1(3)
C(13)	58(4)	115(6)	52(3)	30(4)	12(3)	12(4)
C(14)	56(4)	98(5)	57(4)	23(3)	5(3)	12(3)
C(15)	38(3)	105(5)	69(4)	20(4)	4(3)	11(3)
C(16)	65(4)	77(5)	87(5)	18(4)	20(4)	30(4)
F(1)	209(7)	102(4)	209(7)	4(4)	25(6)	8(4)
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 2						
Ru(2)	38(1)	57(1)	40(1)	1(1)	11(1)	2(1)
C(17)	44(3)	47(3)	39(3)	1(2)	8(2)	-1(2)
C(18)	41(3)	58(3)	44(3)	6(2)	11(2)	8(2)
C(19)	69(4)	41(3)	50(3)	5(2)	21(3)	5(3)
C(20)	50(3)	62(3)	49(3)	4(3)	10(2)	-11(3)
C(21)	41(3)	54(3)	39(3)	8(2)	14(2)	8(2)
C(22)	82(4)	63(4)	63(4)	-14(3)	8(3)	-4(3)
C(23)	48(3)	101(5)	71(4)	11(4)	7(3)	15(3)
C(24)	147(7)	48(4)	94(5)	-7(3)	37(5)	19(4)
C(25)	70(4)	87(5)	92(5)	11(4)	-5(4)	-36(4)
C(26)	65(4)	106(5)	58(4)	17(3)	21(3)	37(4)
C(27)	80(5)	72(4)	78(4)	27(4)	32(4)	-2(4)
C(28)	65(4)	104(6)	72(4)	19(4)	30(3)	-5(4)
C(29)	76(5)	150(8)	52(4)	12(4)	34(4)	18(5)
C(30)	130(7)	114(6)	48(4)	-8(4)	43(4)	-1(5)
C(31)	71(5)	177(9)	36(3)	5(4)	-2(3)	-30(6)
C(32)	62(4)	121(6)	61(4)	40(4)	20(3)	21(4)
F(2)	186(10)	98(7)	199(11)	32(7)	101(8)	10(6)
F(2A)	80(8)	189(14)	70(7)	-31(7)	-2(5)	-6(7)
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 predominant orientation						
Ru(3)	44(1)	72(1)	55(1)	-15(1)	4(1)	0(1)
C(33)	51(5)	61(5)	64(5)	-12(4)	17(4)	-12(4)
C(34)	62(5)	72(6)	94(7)	-20(5)	45(5)	18(5)
C(35)	56(5)	61(6)	112(8)	-2(6)	38(5)	-8(4)
C(36)	47(5)	66(5)	68(5)	14(4)	17(4)	7(4)
C(37)	40(4)	60(5)	48(4)	-8(4)	-5(3)	-1(4)
C(38)	92(8)	132(10)	90(8)	22(7)	35(6)	-28(7)
C(39)	195(15)	145(13)	115(10)	-98(10)	84(11)	-55(11)
C(40)	92(8)	92(8)	198(15)	24(9)	75(9)	-6(7)

C(41)	91(8)	209(16)	77(8)	64(9)	22(6)	9(9)
C(42)	57(5)	85(7)	88(7)	-40(6)	-16(5)	-8(5)
C(43)	124(13)	102(11)	151(15)	53(11)	12(11)	25(9)
C(44)	83(10)	179(17)	124(12)	-38(12)	-54(9)	32(10)
C(45)	43(6)	188(16)	128(12)	-35(11)	-11(7)	-12(7)
C(46)	44(6)	187(16)	138(13)	-30(11)	20(7)	23(8)
C(47)	75(9)	220(20)	130(13)	-84(14)	-1(9)	47(11)
C(48)	104(11)	108(11)	161(16)	-31(11)	-17(11)	60(9)
F(3)	236(13)	194(12)	265(15)	115(11)	39(11)	62(10)
*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 subordinate orientation						
Ru(3')	43(1)	51(1)	56(1)	-11(1)	-1(1)	6(1)
*** $BAr'_4]$ no. 1						
B(1)	32(3)	40(3)	38(3)	-5(2)	4(2)	-1(2)
C(49)	33(2)	38(2)	40(2)	-3(2)	7(2)	-5(2)
C(50)	44(3)	42(3)	43(3)	-1(2)	8(2)	0(2)
C(51)	46(3)	56(3)	40(3)	-7(2)	6(2)	-5(2)
C(52)	46(3)	55(3)	56(3)	-20(2)	11(2)	3(2)
C(53)	43(3)	50(3)	53(3)	-13(2)	7(2)	5(2)
C(54)	35(3)	51(3)	43(3)	-10(2)	4(2)	-4(2)
C(55)	64(4)	76(4)	49(3)	-10(3)	-1(3)	9(3)
C(56)	64(4)	88(5)	67(4)	-32(4)	-3(3)	32(3)
C(57)	27(2)	43(3)	43(3)	-8(2)	4(2)	1(2)
C(58)	35(2)	45(3)	38(2)	-5(2)	7(2)	-4(2)
C(59)	37(3)	58(3)	39(3)	-5(2)	10(2)	-2(2)
C(60)	42(3)	66(4)	39(3)	-9(2)	0(2)	14(2)
C(61)	42(3)	50(3)	55(3)	-23(2)	-5(2)	10(2)
C(62)	39(3)	34(2)	57(3)	-10(2)	-1(2)	4(2)
C(63)	60(4)	78(4)	45(3)	13(3)	13(3)	-12(3)
C(64)	56(4)	69(4)	87(5)	-32(4)	-13(3)	13(3)
C(65)	34(2)	36(2)	30(2)	2(2)	3(2)	2(2)
C(66)	36(2)	40(3)	36(2)	-4(2)	8(2)	-8(2)
C(67)	38(3)	43(3)	37(2)	-2(2)	11(2)	-3(2)
C(68)	37(3)	47(3)	39(2)	2(2)	9(2)	-7(2)
C(69)	35(2)	44(3)	38(2)	3(2)	4(2)	-9(2)
C(70)	40(3)	34(2)	39(2)	0(2)	4(2)	-3(2)
C(71)	43(3)	60(3)	72(4)	-11(3)	21(3)	-7(3)
C(72)	44(3)	53(3)	53(3)	3(2)	7(2)	-12(2)
C(73)	35(2)	38(2)	41(2)	-6(2)	7(2)	1(2)
C(74)	41(3)	45(3)	73(4)	2(3)	15(3)	5(2)
C(75)	40(3)	51(3)	84(4)	-6(3)	25(3)	-7(2)
C(76)	54(3)	43(3)	59(3)	-5(2)	23(3)	-15(2)
C(77)	43(3)	36(2)	35(2)	-8(2)	12(2)	-5(2)
C(78)	31(2)	44(3)	34(2)	-6(2)	8(2)	-5(2)
C(79)	55(4)	76(5)	153(8)	10(5)	37(5)	2(4)
C(80)	60(3)	41(3)	44(3)	-4(2)	14(2)	-7(2)
F(4)	257(9)	215(8)	70(3)	-90(4)	-71(5)	166(7)
F(5)	114(4)	114(4)	59(3)	23(3)	-18(3)	-19(3)
F(6)	82(4)	252(9)	83(4)	36(4)	-29(3)	-88(5)
F(7)	63(3)	182(5)	147(4)	16(4)	29(3)	54(3)
F(8)	182(5)	151(5)	158(5)	-104(4)	-79(4)	117(4)
F(9)	108(3)	96(3)	101(3)	11(2)	9(3)	50(3)
F(10)	141(4)	103(3)	55(2)	27(2)	-12(2)	-29(3)
F(11)	64(2)	74(2)	85(2)	6(2)	22(2)	-15(2)
F(12)	94(3)	61(2)	119(3)	24(2)	47(2)	16(2)
F(13)	82(3)	161(6)	223(7)	-163(6)	43(4)	-21(3)
F(14)	155(5)	92(4)	100(4)	-15(3)	-21(4)	-59(4)
F(15)	76(3)	79(3)	88(3)	-7(2)	-44(2)	-9(2)
F(16)	93(4)	115(4)	98(4)	-77(4)	-23(3)	31(3)

F(17)	341(12)	71(4)	90(4)	7(3)	51(6)	87(5)
F(18)	112(5)	100(4)	346(12)	-112(6)	163(7)	-47(4)
F(19)	48(2)	94(3)	159(4)	-40(3)	30(2)	-31(2)
F(20)	112(3)	80(2)	46(2)	2(2)	-9(2)	-48(2)
F(21)	82(2)	49(2)	77(2)	12(2)	0(2)	-25(2)
F(22)	75(3)	78(3)	327(10)	6(4)	116(5)	-12(3)
F(23)	36(3)	411(16)	205(8)	97(10)	23(4)	12(5)
F(24)	114(5)	158(6)	400(14)	-127(8)	157(8)	-30(4)
F(25)	100(3)	66(2)	89(2)	17(2)	52(2)	35(2)
F(26)	87(2)	37(2)	107(3)	3(2)	14(2)	-9(2)
F(27)	91(2)	62(2)	55(2)	-5(2)	-6(2)	13(2)
*** BAr'_4] no. 2						
B(2)	31(3)	40(3)	38(3)	2(2)	7(2)	-3(2)
C(81)	28(2)	44(3)	38(2)	1(2)	11(2)	-5(2)
C(82)	34(2)	40(3)	44(3)	-2(2)	11(2)	-7(2)
C(83)	35(3)	53(3)	43(3)	5(2)	3(2)	-9(2)
C(84)	44(3)	66(3)	36(3)	0(2)	7(2)	-12(2)
C(85)	43(3)	47(3)	43(3)	-4(2)	15(2)	-7(2)
C(86)	35(2)	46(3)	41(3)	2(2)	12(2)	-3(2)
C(87)	56(4)	71(4)	61(4)	12(3)	1(3)	2(3)
C(88)	63(4)	75(4)	49(3)	-14(3)	24(3)	-6(3)
C(89)	30(2)	43(3)	43(3)	1(2)	13(2)	0(2)
C(90)	38(3)	46(3)	44(3)	4(2)	12(2)	0(2)
C(91)	42(3)	46(3)	60(3)	2(2)	15(2)	-3(2)
C(92)	53(3)	50(3)	61(3)	15(3)	23(3)	-2(2)
C(93)	48(3)	61(3)	41(3)	7(2)	19(2)	0(2)
C(94)	42(3)	52(3)	43(3)	3(2)	18(2)	-2(2)
C(95)	63(4)	51(3)	67(4)	8(3)	17(3)	-17(3)
C(96)	77(4)	79(4)	48(3)	12(3)	21(3)	5(3)
C(97)	33(2)	44(3)	29(2)	-2(2)	8(2)	1(2)
C(98)	38(3)	39(3)	39(2)	-1(2)	10(2)	1(2)
C(99)	34(2)	46(3)	35(2)	-3(2)	3(2)	8(2)
C(100)	27(2)	55(3)	43(3)	-6(2)	6(2)	0(2)
C(101)	34(2)	47(3)	37(2)	-2(2)	10(2)	0(2)
C(102)	31(2)	40(3)	40(2)	2(2)	7(2)	4(2)
C(103)	42(3)	66(4)	59(3)	6(3)	3(2)	11(3)
C(104)	37(3)	72(4)	65(3)	16(3)	12(3)	-8(3)
C(105)	32(2)	42(3)	31(2)	1(2)	7(2)	-3(2)
C(106)	32(2)	55(3)	45(3)	-8(2)	11(2)	-8(2)
C(107)	31(2)	60(3)	47(3)	-9(2)	14(2)	-3(2)
C(108)	45(3)	45(3)	38(2)	-3(2)	12(2)	5(2)
C(109)	37(2)	39(3)	31(2)	3(2)	5(2)	2(2)
C(110)	29(2)	39(2)	34(2)	3(2)	5(2)	0(2)
C(111)	49(3)	90(5)	99(5)	-43(4)	38(4)	-13(3)
C(112)	45(3)	50(3)	39(3)	-2(2)	7(2)	0(2)
F(28)	178(6)	105(4)	100(4)	-23(3)	-90(4)	47(4)
F(29)	103(4)	50(3)	159(5)	26(3)	-36(3)	1(3)
F(30)	120(5)	315(11)	184(7)	164(8)	86(5)	148(7)
F(31)	128(4)	183(5)	66(2)	-25(3)	16(2)	96(4)
F(32)	142(4)	86(3)	157(4)	-55(3)	95(4)	-36(3)
F(33)	121(3)	87(3)	62(2)	-13(2)	56(2)	-9(2)
F(34)	153(5)	115(4)	81(3)	-26(3)	30(3)	-84(4)
F(35)	52(3)	94(3)	221(7)	-22(4)	12(3)	-19(2)
F(36)	138(4)	58(3)	116(4)	31(2)	-13(3)	-40(3)
F(37)	76(3)	322(8)	60(2)	36(4)	5(2)	61(4)
F(38)	136(4)	93(3)	59(2)	-9(2)	1(2)	-7(3)
F(39)	209(5)	101(3)	51(2)	24(2)	12(3)	-50(3)
F(40)	49(2)	119(3)	154(4)	53(3)	26(2)	35(2)

F(41)	150(4)	121(4)	54(2)	1(2)	-23(2)	61(3)
F(42)	75(2)	59(2)	128(3)	18(2)	-10(2)	15(2)
F(43)	126(4)	128(4)	143(4)	50(3)	102(3)	19(3)
F(44)	71(2)	93(3)	129(3)	35(3)	-22(2)	-45(2)
F(45)	51(2)	77(2)	97(3)	38(2)	9(2)	-4(2)
F(46)	82(4)	269(10)	230(9)	67(7)	90(5)	-19(5)
F(47)	26(2)	305(10)	134(5)	-133(6)	7(3)	-10(3)
F(48)	37(2)	121(5)	268(9)	-82(5)	31(4)	15(3)
F(49)	66(2)	65(2)	58(2)	-2(2)	13(2)	-28(2)
F(50)	62(2)	54(2)	104(3)	-30(2)	10(2)	0(2)
F(51)	75(2)	69(2)	39(2)	1(1)	-9(1)	-9(2)
*** BAr'_4] no. 3						
B(3)	37(3)	37(3)	38(3)	-3(2)	6(2)	1(2)
C(113)	37(2)	40(3)	38(2)	-1(2)	10(2)	2(2)
C(114)	44(3)	42(3)	40(3)	1(2)	7(2)	9(2)
C(115)	54(3)	46(3)	36(2)	-5(2)	10(2)	0(2)
C(116)	53(3)	43(3)	46(3)	-12(2)	14(2)	-2(2)
C(117)	43(3)	42(3)	48(3)	-5(2)	10(2)	4(2)
C(118)	42(3)	45(3)	36(2)	-4(2)	8(2)	0(2)
C(119)	69(4)	54(3)	43(3)	-6(3)	10(3)	1(3)
C(120)	62(4)	51(3)	63(4)	-13(3)	5(3)	16(3)
C(121)	35(2)	31(2)	39(2)	-3(2)	9(2)	5(2)
C(122)	43(3)	42(3)	40(3)	-5(2)	7(2)	-2(2)
C(123)	58(3)	45(3)	39(3)	2(2)	15(2)	4(2)
C(124)	60(3)	51(3)	32(2)	1(2)	6(2)	6(2)
C(125)	42(3)	49(3)	39(3)	-7(2)	2(2)	1(2)
C(126)	38(2)	36(2)	40(3)	-1(2)	8(2)	5(2)
C(127)	88(5)	70(4)	45(3)	10(3)	11(3)	-11(4)
C(128)	68(4)	56(4)	51(3)	-5(3)	0(3)	-10(3)
C(129)	37(2)	38(2)	31(2)	-4(2)	6(2)	5(2)
C(130)	40(3)	40(3)	29(2)	-4(2)	5(2)	3(2)
C(131)	52(3)	38(3)	28(2)	-6(2)	6(2)	2(2)
C(132)	55(3)	51(3)	39(3)	-1(2)	14(2)	-6(2)
C(133)	42(3)	53(3)	52(3)	2(2)	18(2)	0(2)
C(134)	42(3)	49(3)	43(3)	3(2)	12(2)	6(2)
C(135)	64(3)	40(3)	47(3)	-3(2)	9(3)	2(2)
C(136)	53(4)	90(5)	101(5)	29(4)	24(4)	4(4)
C(137)	41(3)	37(2)	29(2)	0(2)	7(2)	0(2)
C(138)	47(3)	41(3)	40(3)	-4(2)	11(2)	1(2)
C(139)	43(3)	53(3)	47(3)	-3(2)	8(2)	-11(2)
C(140)	39(3)	57(3)	53(3)	1(2)	13(2)	-1(2)
C(141)	41(3)	45(3)	44(3)	-3(2)	10(2)	0(2)
C(142)	36(3)	42(3)	41(3)	-8(2)	9(2)	-3(2)
C(143)	65(4)	67(4)	89(5)	-18(3)	20(4)	-16(3)
C(144)	47(3)	65(4)	74(4)	-17(3)	22(3)	6(3)
F(52)	71(2)	142(4)	58(2)	-1(2)	-4(2)	-24(2)
F(53)	112(3)	91(3)	43(2)	-19(2)	12(2)	22(2)
F(54)	129(3)	70(2)	46(2)	6(2)	3(2)	12(2)
F(55)	54(2)	103(3)	172(5)	14(3)	14(3)	24(2)
F(56)	143(4)	89(3)	68(2)	12(2)	14(2)	59(3)
F(57)	109(3)	63(2)	101(3)	-26(2)	-9(2)	36(2)
F(58)	249(9)	205(7)	73(3)	45(4)	-11(4)	-177(7)
F(59)	176(7)	82(4)	322(11)	123(6)	144(7)	61(4)
F(60)	215(7)	82(3)	90(4)	15(3)	97(4)	-14(4)
F(61)	128(5)	198(7)	131(5)	-80(5)	59(4)	-114(5)
F(62)	169(5)	104(4)	61(3)	7(2)	-55(3)	-49(4)
F(63)	115(4)	58(3)	171(6)	-41(3)	-41(4)	9(3)
F(64)	84(3)	60(3)	166(5)	57(3)	7(3)	-5(2)

F(65)	113(3)	87(3)	73(3)	15(2)	34(2)	61(3)
F(66)	125(4)	68(2)	50(2)	-18(2)	-31(2)	44(2)
F(67)	62(3)	162(6)	229(8)	95(6)	76(4)	8(3)
F(68)	44(3)	550(20)	153(7)	-71(10)	3(4)	-27(7)
F(69)	85(4)	102(5)	530(20)	54(8)	151(8)	38(4)
F(70)	64(3)	156(6)	356(11)	-134(7)	74(5)	-57(3)
F(71)	236(8)	253(8)	64(3)	-12(4)	-23(4)	-184(7)
F(72)	141(5)	73(3)	181(6)	-31(3)	-2(4)	-42(3)
F(73)	94(3)	92(3)	117(4)	-32(3)	-15(3)	55(3)
F(74)	148(5)	95(3)	135(4)	-36(3)	110(4)	-16(3)
F(75)	55(2)	72(3)	113(3)	-52(2)	24(2)	-6(2)

Table S20. Bond lengths [Å] and angles [deg] for $[Cp^*Ru(\eta^6\text{-}C_6H_5F)][BAr'_4]$ **(4)**.

Bond distances

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 1

Ru(1)-C(3)	2.167(6)
Ru(1)-C(1)	2.171(5)
Ru(1)-C(11)	2.174(6)
Ru(1)-C(4)	2.178(5)
Ru(1)-C(5)	2.179(5)
Ru(1)-C(2)	2.181(5)
Ru(1)-C(12)	2.198(6)
Ru(1)-C(16)	2.207(6)
Ru(1)-C(15)	2.210(6)
Ru(1)-C(13)	2.217(6)
Ru(1)-C(14)	2.241(6)
C(1)-C(2)	1.416(8)
C(1)-C(5)	1.427(8)
C(1)-C(6)	1.511(8)
C(2)-C(3)	1.434(8)
C(2)-C(7)	1.510(8)
C(3)-C(4)	1.432(8)
C(3)-C(8)	1.497(8)
C(4)-C(5)	1.402(7)
C(4)-C(9)	1.492(7)
C(5)-C(10)	1.508(8)
C(11)-F(1)	1.301(9)
C(11)-C(12)	1.394(10)
C(11)-C(16)	1.415(10)
C(12)-C(13)	1.380(10)
C(13)-C(14)	1.401(9)
C(14)-C(15)	1.398(9)
C(15)-C(16)	1.385(9)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 2

Ru(2)-C(17)	2.162(5)
Ru(2)-C(18)	2.168(5)
Ru(2)-C(19)	2.169(5)
Ru(2)-C(20)	2.178(5)
Ru(2)-C(29)	2.179(6)
Ru(2)-C(31)	2.195(6)
Ru(2)-C(30)	2.210(6)
Ru(2)-C(21)	2.200(5)
Ru(2)-C(27)	2.212(7)
Ru(2)-C(32)	2.210(6)
Ru(2)-C(28)	2.223(6)
C(17)-C(18)	1.427(7)
C(17)-C(21)	1.433(7)
C(17)-C(22)	1.494(7)
C(18)-C(19)	1.421(7)
C(18)-C(23)	1.505(7)
C(19)-C(20)	1.419(8)
C(19)-C(24)	1.508(8)
C(20)-C(21)	1.424(7)
C(20)-C(25)	1.503(7)
C(21)-C(26)	1.494(7)
C(27)-F(2)	1.350(12)
C(27)-C(32)	1.355(10)
C(27)-C(28)	1.366(9)
C(28)-C(29)	1.371(10)
C(29)-C(30)	1.384(11)
C(30)-C(31)	1.450(11)
C(31)-F(2A)	1.304(13)
C(31)-C(32)	1.386(11)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 predominant orientation

Ru(3)-C(36)	2.153(8)
Ru(3)-C(37)	2.161(7)
Ru(3)-C(35)	2.168(10)
Ru(3)-C(33)	2.173(8)
Ru(3)-C(48)	2.195(8)
Ru(3)-C(43)	2.194(9)
Ru(3)-C(34)	2.213(10)
Ru(3)-C(44)	2.212(8)
Ru(3)-C(47)	2.214(8)
Ru(3)-C(45)	2.230(7)
Ru(3)-C(46)	2.231(8)
C(33)-C(37)	1.412(11)
C(33)-C(34)	1.417(12)
C(33)-C(38)	1.507(12)
C(34)-C(35)	1.462(14)
C(34)-C(39)	1.475(14)
C(35)-C(36)	1.423(13)
C(35)-C(40)	1.573(14)
C(36)-C(37)	1.409(11)
C(36)-C(41)	1.512(13)
C(37)-C(42)	1.499(11)
C(43)-F(3)	1.208(15)
C(43)-C(44)	1.385(5)
C(43)-C(48)	1.386(5)
C(44)-C(45)	1.385(5)
C(45)-C(46)	1.385(5)
C(46)-C(47)	1.385(5)
C(47)-C(48)	1.385(5)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3 subordinate orientation

Ru(3')-C(33')	2.161(6)
Ru(3')-C(34')	2.166(6)
Ru(3')-C(37')	2.176(6)
Ru(3')-C(46')	2.180(7)
Ru(3')-C(35')	2.183(6)
Ru(3')-C(36')	2.190(6)
Ru(3')-C(45')	2.195(6)
Ru(3')-C(47')	2.204(6)
Ru(3')-C(44')	2.235(7)
Ru(3')-C(48')	2.245(7)
Ru(3')-C(43')	2.260(7)
C(33')-C(34')	1.413(4)
C(33')-C(37')	1.413(4)
C(33')-C(38')	1.502(4)

C(34')-C(35')	1.413(4)
C(34')-C(39')	1.502(5)
C(35')-C(36')	1.413(4)
C(35')-C(40')	1.502(4)
C(36')-C(37')	1.413(4)
C(36')-C(41')	1.502(4)
C(37')-C(42')	1.502(4)
C(43')-C(44')	1.383(4)
C(43')-C(48')	1.383(4)
C(44')-C(45')	1.383(4)
C(45')-C(46')	1.383(4)
C(46')-C(47')	1.383(4)
C(47')-C(48')	1.383(4)

*** BAr'_4] no. 1

B(1)-C(73)	1.640(7)
B(1)-C(49)	1.641(7)
B(1)-C(57)	1.647(7)
B(1)-C(65)	1.651(7)
C(49)-C(54)	1.388(6)
C(49)-C(50)	1.400(6)
C(50)-C(51)	1.391(7)
C(51)-C(52)	1.378(7)
C(51)-C(55)	1.493(7)
C(52)-C(53)	1.372(7)
C(53)-C(54)	1.400(7)
C(53)-C(56)	1.501(8)
C(55)-F(4')	1.227(6)
C(55)-F(6')	1.264(7)
C(55)-F(4)	1.267(8)
C(55)-F(6)	1.303(8)
C(55)-F(5')	1.315(7)
C(55)-F(5)	1.336(8)
C(56)-F(8)	1.285(7)
C(56)-F(9)	1.305(8)
C(56)-F(7)	1.341(9)
C(57)-C(58)	1.387(7)
C(57)-C(62)	1.409(6)
C(58)-C(59)	1.387(6)
C(59)-C(60)	1.389(7)
C(59)-C(63)	1.504(8)
C(60)-C(61)	1.386(8)
C(61)-C(62)	1.389(7)
C(61)-C(64)	1.500(7)
C(63)-F(10)	1.305(6)
C(63)-F(11)	1.321(6)
C(63)-F(12)	1.346(7)
C(64)-F(15')	1.054(7)
C(64)-F(13')	1.221(7)
C(64)-F(13)	1.249(7)
C(64)-F(15)	1.276(7)
C(64)-F(14)	1.430(9)
C(64)-F(14')	1.646(8)
C(65)-C(70)	1.392(6)
C(65)-C(66)	1.407(6)
C(66)-C(67)	1.380(6)
C(67)-C(68)	1.392(6)
C(67)-C(71)	1.490(7)
C(68)-C(69)	1.376(7)
C(69)-C(70)	1.402(6)
C(69)-C(72)	1.486(7)
C(71)-F(18')	1.201(5)
C(71)-F(16')	1.215(6)
C(71)-F(18)	1.267(7)
C(71)-F(16)	1.282(7)
C(71)-F(17)	1.359(8)
C(71)-F(17')	1.387(6)
C(72)-F(19)	1.336(6)
C(72)-F(20)	1.329(6)
C(72)-F(21)	1.330(6)
C(73)-C(78)	1.385(6)
C(73)-C(74)	1.397(7)
C(74)-C(75)	1.374(7)
C(75)-C(76)	1.386(7)
C(75)-C(79)	1.495(8)
C(76)-C(77)	1.381(7)
C(77)-C(78)	1.382(6)
C(77)-C(80)	1.493(7)
C(79)-F(22')	1.184(8)
C(79)-F(23)	1.265(10)
C(79)-F(22)	1.268(8)
C(79)-F(24)	1.322(10)
C(79)-F(23')	1.389(10)
C(79)-F(24')	1.645(10)
C(80)-F(26)	1.320(6)
C(80)-F(25)	1.331(6)
C(80)-F(27)	1.334(6)

*** BAr'_4] no. 2

B(2)-C(105)	1.623(7)
B(2)-C(97)	1.633(7)
B(2)-C(89)	1.641(7)
B(2)-C(81)	1.645(7)
C(81)-C(82)	1.392(6)
C(81)-C(86)	1.405(6)
C(82)-C(83)	1.393(6)
C(83)-C(84)	1.367(7)
C(83)-C(87)	1.483(7)
C(84)-C(85)	1.394(7)
C(85)-C(86)	1.373(6)
C(85)-C(88)	1.498(7)
C(87)-F(29')	1.201(6)
C(87)-F(30')	1.269(6)
C(87)-F(29)	1.271(7)
C(87)-F(28)	1.302(7)
C(87)-F(30)	1.317(8)
C(87)-F(28')	1.376(7)
C(88)-F(31)	1.302(7)
C(88)-F(32)	1.314(7)
C(88)-F(33)	1.329(6)
C(89)-C(90)	1.398(6)
C(89)-C(94)	1.401(6)
C(90)-C(91)	1.387(7)
C(91)-C(92)	1.375(7)
C(91)-C(95)	1.498(7)
C(92)-C(93)	1.379(7)
C(93)-C(94)	1.383(7)
C(93)-C(96)	1.505(8)
C(95)-F(35')	1.193(6)
C(95)-F(36')	1.208(6)
C(95)-F(36)	1.303(7)
C(95)-F(35)	1.310(7)

C(95)-F(34)	1.336(7)
C(95)-F(34')	1.337(6)
C(96)-F(39)	1.295(7)
C(96)-F(37)	1.300(7)
C(96)-F(38)	1.329(7)
C(97)-C(98)	1.394(6)
C(97)-C(102)	1.405(6)
C(98)-C(99)	1.395(6)
C(99)-C(100)	1.380(7)
C(99)-C(103)	1.491(7)
C(100)-C(101)	1.380(6)
C(101)-C(102)	1.391(6)
C(101)-C(104)	1.495(7)
C(103)-F(42)	1.308(7)
C(103)-F(41)	1.315(7)
C(103)-F(40)	1.326(6)
C(104)-F(44)	1.299(7)
C(104)-F(45)	1.318(6)
C(104)-F(43)	1.342(7)
C(105)-C(106)	1.399(6)
C(105)-C(110)	1.404(6)
C(106)-C(107)	1.383(7)
C(107)-C(108)	1.392(7)
C(107)-C(111)	1.495(7)
C(108)-C(109)	1.381(6)
C(109)-C(110)	1.391(6)
C(109)-C(112)	1.482(6)
C(111)-F(47')	1.176(6)
C(111)-F(48')	1.224(7)
C(111)-F(47)	1.244(7)
C(111)-F(48)	1.262(8)
C(111)-F(46)	1.398(10)
C(111)-F(46')	1.502(8)
C(112)-F(50)	1.322(6)
C(112)-F(51)	1.340(5)
C(112)-F(49)	1.349(6)

*** BAr'_4] no. 3

B(3)-C(113)	1.633(7)
B(3)-C(137)	1.635(7)
B(3)-C(121)	1.636(7)
B(3)-C(129)	1.651(7)
C(113)-C(114)	1.402(6)
C(113)-C(118)	1.402(6)
C(114)-C(115)	1.390(7)
C(115)-C(116)	1.379(7)
C(115)-C(119)	1.493(7)
C(116)-C(117)	1.370(7)
C(117)-C(118)	1.395(6)
C(117)-C(120)	1.496(7)
C(119)-F(52)	1.315(7)
C(119)-F(53)	1.326(6)
C(119)-F(54)	1.342(6)
C(120)-F(56)	1.321(7)
C(120)-F(55)	1.321(7)
C(120)-F(57)	1.329(6)
C(121)-C(122)	1.388(6)
C(121)-C(126)	1.404(6)
C(122)-C(123)	1.385(7)
C(123)-C(124)	1.381(7)
C(123)-C(127)	1.502(8)
C(124)-C(125)	1.368(7)
C(125)-C(126)	1.391(6)
C(125)-C(128)	1.494(7)
C(127)-F(60')	1.207(7)
C(127)-F(59')	1.213(7)
C(127)-F(59)	1.260(8)
C(127)-F(58)	1.293(8)
C(127)-F(60)	1.316(7)
C(127)-F(58')	1.367(6)
C(128)-F(63')	1.251(6)
C(128)-F(61')	1.258(6)
C(128)-F(61)	1.288(8)
C(128)-F(62')	1.290(6)
C(128)-F(62)	1.294(7)
C(128)-F(63)	1.330(7)
C(129)-C(134)	1.396(6)
C(129)-C(130)	1.402(6)
C(130)-C(131)	1.395(6)
C(131)-C(132)	1.382(7)
C(131)-C(135)	1.502(7)
C(132)-C(133)	1.384(7)
C(133)-C(134)	1.383(7)
C(133)-C(136)	1.482(8)
C(135)-F(66')	1.073(5)
C(135)-F(65')	1.279(5)
C(135)-F(64')	1.287(6)
C(135)-F(66)	1.309(6)
C(135)-F(64)	1.313(6)
C(135)-F(65)	1.320(6)
C(136)-F(67')	1.224(7)
C(136)-F(67)	1.256(8)
C(136)-F(69)	1.274(10)
C(136)-F(68)	1.290(10)
C(136)-F(68')	1.331(8)
C(136)-F(69')	1.385(8)
C(137)-C(138)	1.391(6)
C(137)-C(142)	1.404(6)
C(138)-C(139)	1.394(7)
C(139)-C(140)	1.378(7)
C(139)-C(143)	1.494(8)
C(140)-C(141)	1.374(7)
C(141)-C(142)	1.375(6)
C(141)-C(144)	1.502(7)
C(143)-F(70')	1.181(7)
C(143)-F(71')	1.262(7)
C(143)-F(71)	1.266(8)
C(143)-F(70)	1.277(8)
C(143)-F(72)	1.343(8)
C(143)-F(72')	1.353(7)
C(144)-F(75')	1.188(5)
C(144)-F(73')	1.204(6)
C(144)-F(73)	1.298(7)
C(144)-F(75)	1.309(7)
C(144)-F(74)	1.361(7)
C(144)-F(74')	1.362(6)

Bond angles

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 1

C(3)-Ru(1)-C(1)	64.1(2)

C(3)-Ru(1)-C(11)	162.2(3)
C(1)-Ru(1)-C(11)	108.1(2)
C(3)-Ru(1)-C(4)	38.5(2)
C(1)-Ru(1)-C(4)	63.9(2)
C(11)-Ru(1)-C(4)	154.9(3)
C(3)-Ru(1)-C(5)	63.6(2)
C(1)-Ru(1)-C(5)	38.3(2)
C(11)-Ru(1)-C(5)	121.2(3)
C(4)-Ru(1)-C(5)	37.6(2)
C(3)-Ru(1)-C(2)	38.5(2)
C(1)-Ru(1)-C(2)	38.0(2)
C(11)-Ru(1)-C(2)	125.5(3)
C(4)-Ru(1)-C(2)	64.1(2)
C(5)-Ru(1)-C(2)	63.6(2)
C(3)-Ru(1)-C(12)	129.6(3)
C(1)-Ru(1)-C(12)	116.4(2)
C(11)-Ru(1)-C(12)	37.2(3)
C(4)-Ru(1)-C(12)	167.8(3)
C(5)-Ru(1)-C(12)	149.3(3)
C(2)-Ru(1)-C(12)	108.1(2)
C(3)-Ru(1)-C(16)	160.1(3)
C(1)-Ru(1)-C(16)	120.2(3)
C(11)-Ru(1)-C(16)	37.7(3)
C(4)-Ru(1)-C(16)	123.2(2)
C(5)-Ru(1)-C(16)	106.7(2)
C(2)-Ru(1)-C(16)	155.3(3)
C(12)-Ru(1)-C(16)	68.0(3)
C(3)-Ru(1)-C(15)	129.4(3)
C(1)-Ru(1)-C(15)	148.4(2)
C(11)-Ru(1)-C(15)	66.0(3)
C(4)-Ru(1)-C(15)	107.4(2)
C(5)-Ru(1)-C(15)	115.9(2)
C(2)-Ru(1)-C(15)	167.7(3)
C(12)-Ru(1)-C(15)	78.6(2)
C(16)-Ru(1)-C(15)	36.6(2)
C(3)-Ru(1)-C(13)	109.6(2)
C(1)-Ru(1)-C(13)	142.2(2)
C(11)-Ru(1)-C(13)	65.8(3)
C(4)-Ru(1)-C(13)	135.8(3)
C(5)-Ru(1)-C(13)	172.9(3)
C(2)-Ru(1)-C(13)	112.8(2)
C(12)-Ru(1)-C(13)	36.4(3)
C(16)-Ru(1)-C(13)	79.1(3)
C(15)-Ru(1)-C(13)	66.2(2)
C(3)-Ru(1)-C(14)	109.6(2)
C(1)-Ru(1)-C(14)	173.5(2)
C(11)-Ru(1)-C(14)	77.4(3)
C(4)-Ru(1)-C(14)	112.5(2)
C(5)-Ru(1)-C(14)	141.6(2)
C(2)-Ru(1)-C(14)	136.1(2)
C(12)-Ru(1)-C(14)	65.9(3)
C(16)-Ru(1)-C(14)	66.2(3)
C(15)-Ru(1)-C(14)	36.6(2)
C(13)-Ru(1)-C(14)	36.6(2)
C(2)-C(1)-C(5)	107.8(5)
C(2)-C(1)-C(6)	126.2(6)
C(5)-C(1)-C(6)	125.9(6)
C(2)-C(1)-Ru(1)	71.4(3)
C(5)-C(1)-Ru(1)	71.1(3)
C(6)-C(1)-Ru(1)	125.7(4)
C(1)-C(2)-C(3)	107.8(5)
C(1)-C(2)-C(7)	126.8(6)
C(3)-C(2)-C(7)	125.4(7)
C(1)-C(2)-Ru(1)	70.6(3)
C(3)-C(2)-Ru(1)	70.2(3)
C(7)-C(2)-Ru(1)	126.0(4)
C(4)-C(3)-C(2)	107.7(5)
C(4)-C(3)-C(8)	126.0(6)
C(2)-C(3)-C(8)	126.2(6)
C(4)-C(3)-Ru(1)	71.2(3)
C(2)-C(3)-Ru(1)	71.3(3)
C(8)-C(3)-Ru(1)	126.2(4)
C(5)-C(4)-C(3)	107.8(5)
C(5)-C(4)-C(9)	125.5(5)
C(3)-C(4)-C(9)	126.6(5)
C(5)-C(4)-Ru(1)	71.3(3)
C(3)-C(4)-Ru(1)	70.3(3)
C(9)-C(4)-Ru(1)	126.6(4)
C(4)-C(5)-C(1)	108.9(5)
C(4)-C(5)-C(10)	126.2(6)
C(1)-C(5)-C(10)	124.9(6)
C(4)-C(5)-Ru(1)	71.2(3)
C(1)-C(5)-Ru(1)	70.6(3)
C(10)-C(5)-Ru(1)	126.0(4)
F(1)-C(11)-C(12)	120.4(8)
F(1)-C(11)-C(16)	117.1(8)
C(12)-C(11)-C(16)	122.4(7)
F(1)-C(11)-Ru(1)	128.0(5)
C(12)-C(11)-Ru(1)	72.3(4)
C(16)-C(11)-Ru(1)	72.4(4)
C(13)-C(12)-C(11)	118.7(6)
C(13)-C(12)-Ru(1)	72.5(4)
C(11)-C(12)-Ru(1)	70.5(4)
C(12)-C(13)-C(14)	120.5(7)
C(12)-C(13)-Ru(1)	71.0(4)
C(14)-C(13)-Ru(1)	72.6(3)
C(13)-C(14)-C(15)	119.6(7)
C(13)-C(14)-Ru(1)	70.7(3)
C(15)-C(14)-Ru(1)	70.5(3)
C(16)-C(15)-C(14)	121.6(6)
C(16)-C(15)-Ru(1)	71.6(3)
C(14)-C(15)-Ru(1)	72.9(3)
C(15)-C(16)-C(11)	117.0(6)
C(15)-C(16)-Ru(1)	71.8(4)
C(11)-C(16)-Ru(1)	69.9(4)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 2

C(17)-Ru(2)-C(18)	38.48(18)
C(17)-Ru(2)-C(19)	63.99(19)
C(18)-Ru(2)-C(19)	38.25(19)
C(17)-Ru(2)-C(20)	64.02(19)
C(18)-Ru(2)-C(20)	64.1(2)
C(19)-Ru(2)-C(20)	38.1(2)
C(17)-Ru(2)-C(29)	131.5(3)
C(18)-Ru(2)-C(29)	108.0(2)
C(19)-Ru(2)-C(29)	114.7(3)
C(20)-Ru(2)-C(29)	146.2(3)
C(17)-Ru(2)-C(31)	157.4(3)
C(18)-Ru(2)-C(31)	160.3(3)
C(19)-Ru(2)-C(31)	124.7(3)
C(20)-Ru(2)-C(31)	108.6(3)
C(29)-Ru(2)-C(31)	67.1(3)

C(17)-Ru(2)-C(30)	164.2(3)
C(18)-Ru(2)-C(30)	126.9(3)
C(19)-Ru(2)-C(30)	108.3(3)
C(20)-Ru(2)-C(30)	119.4(3)
C(29)-Ru(2)-C(30)	36.8(3)
C(31)-Ru(2)-C(30)	38.4(3)
C(17)-Ru(2)-C(21)	38.35(18)
C(18)-Ru(2)-C(21)	64.16(18)
C(19)-Ru(2)-C(21)	63.64(19)
C(20)-Ru(2)-C(21)	37.9(2)
C(29)-Ru(2)-C(21)	169.9(3)
C(31)-Ru(2)-C(21)	122.5(3)
C(30)-Ru(2)-C(21)	153.0(3)
C(17)-Ru(2)-C(27)	108.2(2)
C(18)-Ru(2)-C(27)	131.7(2)
C(19)-Ru(2)-C(27)	169.9(3)
C(20)-Ru(2)-C(27)	146.1(2)
C(29)-Ru(2)-C(27)	64.9(3)
C(31)-Ru(2)-C(27)	65.0(3)
C(30)-Ru(2)-C(27)	77.5(3)
C(21)-Ru(2)-C(27)	114.8(2)
C(17)-Ru(2)-C(32)	125.9(3)
C(18)-Ru(2)-C(32)	163.0(3)
C(19)-Ru(2)-C(32)	153.9(3)
C(20)-Ru(2)-C(32)	119.7(2)
C(29)-Ru(2)-C(32)	78.0(3)
C(31)-Ru(2)-C(32)	36.7(3)
C(30)-Ru(2)-C(32)	67.3(3)
C(21)-Ru(2)-C(32)	107.8(2)
C(27)-Ru(2)-C(32)	35.7(3)
C(17)-Ru(2)-C(28)	109.7(2)
C(18)-Ru(2)-C(28)	109.8(2)
C(19)-Ru(2)-C(28)	138.4(2)
C(20)-Ru(2)-C(28)	173.4(2)
C(29)-Ru(2)-C(28)	36.3(3)
C(31)-Ru(2)-C(28)	78.0(3)
C(30)-Ru(2)-C(28)	66.0(3)
C(21)-Ru(2)-C(28)	138.1(3)
C(27)-Ru(2)-C(28)	35.9(2)
C(32)-Ru(2)-C(28)	65.2(3)
C(18)-C(17)-C(21)	108.4(4)
C(18)-C(17)-C(22)	125.0(5)
C(21)-C(17)-C(22)	126.5(5)
C(18)-C(17)-Ru(2)	71.0(3)
C(21)-C(17)-Ru(2)	72.2(3)
C(22)-C(17)-Ru(2)	125.3(4)
C(19)-C(18)-C(17)	107.4(4)
C(19)-C(18)-C(23)	126.2(5)
C(17)-C(18)-C(23)	126.4(5)
C(19)-C(18)-Ru(2)	70.9(3)
C(17)-C(18)-Ru(2)	70.5(3)
C(23)-C(18)-Ru(2)	126.7(4)
C(20)-C(19)-C(18)	108.7(4)
C(20)-C(19)-C(24)	125.6(6)
C(18)-C(19)-C(24)	125.7(6)
C(20)-C(19)-Ru(2)	71.3(3)
C(18)-C(19)-Ru(2)	70.8(3)
C(24)-C(19)-Ru(2)	126.4(4)
C(19)-C(20)-C(21)	108.3(4)
C(19)-C(20)-C(25)	127.3(6)
C(21)-C(20)-C(25)	124.2(5)
C(19)-C(20)-Ru(2)	70.6(3)
C(21)-C(20)-Ru(2)	71.8(3)
C(25)-C(20)-Ru(2)	127.4(4)
C(20)-C(21)-C(17)	107.3(4)
C(20)-C(21)-C(26)	127.2(5)
C(17)-C(21)-C(26)	125.5(5)
C(20)-C(21)-Ru(2)	70.2(3)
C(17)-C(21)-Ru(2)	69.4(3)
C(26)-C(21)-Ru(2)	127.0(4)
F(2)-C(27)-C(32)	126.0(9)
F(2)-C(27)-C(28)	111.1(8)
C(32)-C(27)-C(28)	122.9(8)
F(2)-C(27)-Ru(2)	126.3(6)
C(32)-C(27)-Ru(2)	72.1(4)
C(28)-C(27)-Ru(2)	72.5(4)
C(27)-C(28)-C(29)	118.8(7)
C(27)-C(28)-Ru(2)	71.6(4)
C(29)-C(28)-Ru(2)	70.1(4)
C(28)-C(29)-C(30)	122.3(7)
C(28)-C(29)-Ru(2)	73.6(4)
C(30)-C(29)-Ru(2)	72.8(4)
C(29)-C(30)-C(31)	117.0(8)
C(29)-C(30)-Ru(2)	70.4(4)
C(31)-C(30)-Ru(2)	70.2(4)
F(2A)-C(31)-C(32)	129.3(10)
F(2A)-C(31)-C(30)	111.2(11)
C(32)-C(31)-C(30)	119.5(7)
F(2A)-C(31)-Ru(2)	125.9(8)
C(32)-C(31)-Ru(2)	72.2(4)
C(30)-C(31)-Ru(2)	71.3(4)
C(27)-C(32)-C(31)	119.5(7)
C(27)-C(32)-Ru(2)	72.2(4)
C(31)-C(32)-Ru(2)	71.1(4)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3
predominant orientation

C(36)-Ru(3)-C(37)	38.1(3)
C(36)-Ru(3)-C(35)	38.5(3)
C(37)-Ru(3)-C(35)	63.8(3)
C(36)-Ru(3)-C(33)	64.2(3)
C(37)-Ru(3)-C(33)	38.0(3)
C(35)-Ru(3)-C(33)	64.3(3)
C(36)-Ru(3)-C(48)	126.3(4)
C(37)-Ru(3)-C(48)	107.1(3)
C(35)-Ru(3)-C(48)	164.0(5)
C(33)-Ru(3)-C(48)	117.6(4)
C(36)-Ru(3)-C(43)	157.9(4)
C(37)-Ru(3)-C(43)	122.8(4)
C(35)-Ru(3)-C(43)	159.1(5)
C(33)-Ru(3)-C(43)	107.6(4)
C(48)-Ru(3)-C(43)	36.80(16)
C(36)-Ru(3)-C(34)	64.5(4)
C(37)-Ru(3)-C(34)	63.4(3)
C(35)-Ru(3)-C(34)	39.0(4)
C(33)-Ru(3)-C(34)	37.7(3)
C(48)-Ru(3)-C(34)	151.0(5)
C(43)-Ru(3)-C(34)	122.8(5)
C(36)-Ru(3)-C(44)	165.4(4)
C(37)-Ru(3)-C(44)	152.7(4)
C(35)-Ru(3)-C(44)	128.3(4)
C(33)-Ru(3)-C(44)	119.5(4)

C(48)-Ru(3)-C(44)	66.0(3)
C(43)-Ru(3)-C(44)	36.65(16)
C(34)-Ru(3)-C(44)	109.1(4)
C(36)-Ru(3)-C(47)	107.7(4)
C(37)-Ru(3)-C(47)	113.4(3)
C(35)-Ru(3)-C(47)	132.4(5)
C(33)-Ru(3)-C(47)	144.2(4)
C(48)-Ru(3)-C(47)	36.63(14)
C(43)-Ru(3)-C(47)	66.0(3)
C(34)-Ru(3)-C(47)	171.2(5)
C(44)-Ru(3)-C(47)	77.5(3)
C(36)-Ru(3)-C(45)	132.8(4)
C(37)-Ru(3)-C(45)	170.8(4)
C(35)-Ru(3)-C(45)	109.7(4)
C(33)-Ru(3)-C(45)	146.9(4)
C(48)-Ru(3)-C(45)	77.5(3)
C(43)-Ru(3)-C(45)	65.7(3)
C(34)-Ru(3)-C(45)	116.4(4)
C(44)-Ru(3)-C(45)	36.33(16)
C(47)-Ru(3)-C(45)	65.4(3)
C(36)-Ru(3)-C(46)	110.5(4)
C(37)-Ru(3)-C(46)	138.0(4)
C(35)-Ru(3)-C(46)	111.4(4)
C(33)-Ru(3)-C(46)	174.7(4)
C(48)-Ru(3)-C(46)	65.7(2)
C(43)-Ru(3)-C(46)	77.5(3)
C(34)-Ru(3)-C(46)	140.5(4)
C(44)-Ru(3)-C(46)	65.4(3)
C(47)-Ru(3)-C(46)	36.32(15)
C(45)-Ru(3)-C(46)	36.18(16)
C(37)-C(33)-C(34)	108.6(8)
C(37)-C(33)-C(38)	127.9(8)
C(34)-C(33)-C(38)	123.3(9)
C(37)-C(33)-Ru(3)	70.5(4)
C(34)-C(33)-Ru(3)	72.7(5)
C(38)-C(33)-Ru(3)	125.6(7)
C(33)-C(34)-C(35)	106.7(8)
C(33)-C(34)-C(39)	127.7(10)
C(35)-C(34)-C(39)	125.6(10)
C(33)-C(34)-Ru(3)	69.6(5)
C(35)-C(34)-Ru(3)	68.9(5)
C(39)-C(34)-Ru(3)	123.3(9)
C(36)-C(35)-C(34)	107.7(8)
C(36)-C(35)-C(40)	129.4(10)
C(34)-C(35)-C(40)	122.7(10)
C(36)-C(35)-Ru(3)	70.2(5)
C(34)-C(35)-Ru(3)	72.2(6)
C(40)-C(35)-Ru(3)	126.5(7)
C(37)-C(36)-C(35)	107.8(7)
C(37)-C(36)-C(41)	126.2(9)
C(35)-C(36)-C(41)	125.9(10)
C(37)-C(36)-Ru(3)	71.2(4)
C(35)-C(36)-Ru(3)	71.3(5)
C(41)-C(36)-Ru(3)	126.0(7)
C(36)-C(37)-C(33)	109.2(7)
C(36)-C(37)-C(42)	124.3(8)
C(33)-C(37)-C(42)	126.4(8)
C(36)-C(37)-Ru(3)	70.6(4)
C(33)-C(37)-Ru(3)	71.4(4)
C(42)-C(37)-Ru(3)	123.6(6)
F(3)-C(43)-C(44)	123.1(14)
F(3)-C(43)-C(48)	116.9(14)
C(44)-C(43)-C(48)	120.0
F(3)-C(43)-Ru(3)	130.3(10)
C(44)-C(43)-Ru(3)	72.4(3)
C(48)-C(43)-Ru(3)	71.6(3)
C(45)-C(44)-C(43)	120.0
C(45)-C(44)-Ru(3)	72.6(3)
C(43)-C(44)-Ru(3)	71.0(3)
C(44)-C(45)-C(46)	120.0
C(44)-C(45)-Ru(3)	71.1(3)
C(46)-C(45)-Ru(3)	71.9(3)
C(45)-C(46)-C(47)	120.0
C(45)-C(46)-Ru(3)	71.9(3)
C(47)-C(46)-Ru(3)	71.2(2)
C(48)-C(47)-C(46)	120.0
C(48)-C(47)-Ru(3)	71.0(3)
C(46)-C(47)-Ru(3)	72.5(3)
C(47)-C(48)-C(43)	120.0
C(47)-C(48)-Ru(3)	72.4(3)
C(43)-C(48)-Ru(3)	71.6(3)

*** $Cp^*Ru(\eta^6\text{-}C_6H_5F)]^+$ no. 3

subordinate orientation

C(33')-Ru(3')-C(34')	38.1
C(33')-Ru(3')-C(37')	38.0
C(34')-Ru(3')-C(37')	63.6
C(33')-Ru(3')-C(46')	173.7
C(34')-Ru(3')-C(46')	141.7
C(37')-Ru(3')-C(46')	136.2
C(33')-Ru(3')-C(35')	63.5
C(34')-Ru(3')-C(35')	37.9
C(37')-Ru(3')-C(35')	63.3
C(46')-Ru(3')-C(35')	112.7
C(33')-Ru(3')-C(36')	63.4
C(34')-Ru(3')-C(36')	63.3
C(37')-Ru(3')-C(36')	37.8
C(46')-Ru(3')-C(36')	110.4
C(35')-Ru(3')-C(36')	37.7
C(33')-Ru(3')-C(45')	147.8
C(34')-Ru(3')-C(45')	115.0
C(37')-Ru(3')-C(45')	166.9
C(46')-Ru(3')-C(45')	36.9
C(35')-Ru(3')-C(45')	107.0
C(36')-Ru(3')-C(45')	129.2
C(33')-Ru(3')-C(47')	142.6
C(34')-Ru(3')-C(47')	175.4
C(37')-Ru(3')-C(47')	114.4
C(46')-Ru(3')-C(47')	36.8
C(35')-Ru(3')-C(47')	137.6
C(36')-Ru(3')-C(47')	112.4
C(45')-Ru(3')-C(47')	66.0
C(33')-Ru(3')-C(44')	120.5
C(34')-Ru(3')-C(44')	106.4
C(37')-Ru(3')-C(44')	156.0
C(46')-Ru(3')-C(44')	65.7
C(35')-Ru(3')-C(44')	123.4
C(36')-Ru(3')-C(44')	159.7
C(45')-Ru(3')-C(44')	36.4
C(47')-Ru(3')-C(44')	77.1
C(33')-Ru(3')-C(48')	117.3
C(34')-Ru(3')-C(48')	148.0

C(37')-Ru(3')-C(48')	111.3
C(46')-Ru(3')-C(48')	65.5
C(35')-Ru(3')-C(48')	171.0
C(36')-Ru(3')-C(48')	133.6
C(45')-Ru(3')-C(48')	77.1
C(47')-Ru(3')-C(48')	36.2
C(44')-Ru(3')-C(48')	64.6
C(33')-Ru(3')-C(43')	108.6
C(34')-Ru(3')-C(43')	119.7
C(37')-Ru(3')-C(43')	127.7
C(46')-Ru(3')-C(43')	77.0
C(35')-Ru(3')-C(43')	153.3
C(36')-Ru(3')-C(43')	164.3
C(45')-Ru(3')-C(43')	65.0
C(47')-Ru(3')-C(43')	64.9
C(44')-Ru(3')-C(43')	35.8
C(48')-Ru(3')-C(43')	35.8
C(34')-C(33')-C(37')	108.0
C(34')-C(33')-C(38')	126.0
C(37')-C(33')-C(38')	126.0
C(34')-C(33')-Ru(3')	71.1
C(37')-C(33')-Ru(3')	71.6
C(38')-C(33')-Ru(3')	123.0
C(33')-C(34')-C(35')	108.0
C(33')-C(34')-C(39')	126.0
C(35')-C(34')-C(39')	126.0
C(33')-C(34')-Ru(3')	70.8
C(35')-C(34')-Ru(3')	71.7
C(39')-C(34')-Ru(3')	123.2
C(36')-C(35')-C(34')	108.0
C(36')-C(35')-C(40')	126.0
C(34')-C(35')-C(40')	126.0
C(36')-C(35')-Ru(3')	71.4
C(34')-C(35')-Ru(3')	70.4
C(40')-C(35')-Ru(3')	123.9
C(35')-C(36')-C(37')	108.0
C(35')-C(36')-C(41')	126.0
C(37')-C(36')-C(41')	126.0
C(35')-C(36')-Ru(3')	70.9
C(37')-C(36')-Ru(3')	70.6
C(41')-C(36')-Ru(3')	124.1
C(36')-C(37')-C(33')	108.0
C(36')-C(37')-C(42')	126.0
C(33')-C(37')-C(42')	126.0
C(36')-C(37')-Ru(3')	71.6
C(33')-C(37')-Ru(3')	70.4
C(42')-C(37')-Ru(3')	123.6
C(44')-C(43')-C(48')	120.0
C(44')-C(43')-Ru(3')	71.1
C(48')-C(43')-Ru(3')	71.5
C(43')-C(44')-C(45')	120.0
C(43')-C(44')-Ru(3')	73.1
C(45')-C(44')-Ru(3')	70.2
C(44')-C(45')-C(46')	120.0
C(44')-C(45')-Ru(3')	73.4
C(46')-C(45')-Ru(3')	71.0
C(45')-C(46')-C(47')	120.0
C(45')-C(46')-Ru(3')	72.2
C(47')-C(46')-Ru(3')	72.6
C(48')-C(47')-C(46')	120.0
C(48')-C(47')-Ru(3')	73.5
C(46')-C(47')-Ru(3')	70.6
C(47')-C(48')-C(43')	120.0
C(47')-C(48')-Ru(3')	70.3
C(43')-C(48')-Ru(3')	72.7

*** $BAr'_4]$ no. 1

C(73)-B(1)-C(49)	105.8(4)
C(73)-B(1)-C(57)	110.0(4)
C(49)-B(1)-C(57)	112.6(4)
C(73)-B(1)-C(65)	112.8(4)
C(49)-B(1)-C(65)	111.8(4)
C(57)-B(1)-C(65)	104.0(4)
C(54)-C(49)-C(50)	114.9(4)
C(54)-C(49)-B(1)	124.5(4)
C(50)-C(49)-B(1)	120.4(4)
C(51)-C(50)-C(49)	122.8(5)
C(52)-C(51)-C(50)	120.5(4)
C(52)-C(51)-C(55)	119.1(5)
C(50)-C(51)-C(55)	120.3(5)
C(53)-C(52)-C(51)	118.4(5)
C(52)-C(53)-C(54)	120.6(5)
C(52)-C(53)-C(56)	120.0(5)
C(54)-C(53)-C(56)	119.5(5)
C(49)-C(54)-C(53)	122.8(4)
F(4)-C(55)-C(51)	114.7(5)
F(5)-C(55)-C(51)	112.6(5)
F(6)-C(55)-C(51)	112.9(5)
F(4')-C(55)-C(51)	115.9(5)
F(6')-C(55)-C(51)	113.8(5)
F(5')-C(55)-C(51)	107.6(5)
F(4)-C(55)-F(5)	105.3(7)
F(4)-C(55)-F(6)	111.3(7)
F(6)-C(55)-F(5)	98.7(6)
F(4')-C(55)-F(6')	106.9(5)
F(4')-C(55)-F(5')	107.1(5)
F(6')-C(55)-F(5')	104.7(4)
F(8)-C(56)-C(53)	113.7(5)
F(9)-C(56)-C(53)	113.7(5)
F(7)-C(56)-C(53)	110.9(6)
F(8)-C(56)-F(9)	109.4(7)
F(8)-C(56)-F(7)	105.9(6)
F(9)-C(56)-F(7)	102.3(5)
C(58)-C(57)-C(62)	115.6(4)
C(58)-C(57)-B(1)	121.3(4)
C(62)-C(57)-B(1)	123.0(4)
C(57)-C(58)-C(59)	123.5(4)
C(58)-C(59)-C(60)	119.4(5)
C(58)-C(59)-C(63)	118.7(4)
C(60)-C(59)-C(63)	121.5(5)
C(61)-C(60)-C(59)	119.0(5)
C(60)-C(61)-C(62)	120.5(4)
C(60)-C(61)-C(64)	119.0(5)
C(62)-C(61)-C(64)	120.4(5)
C(61)-C(62)-C(57)	121.9(5)
F(10)-C(63)-C(59)	113.5(5)
F(11)-C(63)-C(59)	112.6(5)
F(12)-C(63)-C(59)	111.4(4)
F(10)-C(63)-F(11)	109.7(5)
F(10)-C(63)-F(12)	104.4(5)
F(11)-C(63)-F(12)	104.5(5)
F(13)-C(64)-C(61)	115.7(6)

F(15)-C(64)-C(61)	114.2(5)
F(14)-C(64)-C(61)	110.0(6)
C(61)-C(64)-F(14')	100.8(5)
F(15')-C(64)-C(61)	112.2(5)
F(13')-C(64)-C(61)	116.5(5)
F(13)-C(64)-F(14)	99.9(7)
F(15)-C(64)-F(14)	99.2(6)
F(13)-C(64)-F(15)	115.3(6)
F(15')-C(64)-F(13')	105.3(6)
F(15')-C(64)-F(14')	101.4(5)
F(13')-C(64)-F(14')	119.7(4)
C(70)-C(65)-C(66)	115.5(4)
C(70)-C(65)-B(1)	123.9(4)
C(66)-C(65)-B(1)	120.5(4)
C(67)-C(66)-C(65)	122.7(4)
C(66)-C(67)-C(68)	120.7(4)
C(66)-C(67)-C(71)	119.7(4)
C(68)-C(67)-C(71)	119.5(4)
C(69)-C(68)-C(67)	117.9(4)
C(68)-C(69)-C(70)	121.2(4)
C(68)-C(69)-C(72)	120.7(4)
C(70)-C(69)-C(72)	118.1(4)
C(65)-C(70)-C(69)	122.0(4)
F(18)-C(71)-C(67)	116.1(5)
F(16)-C(71)-C(67)	116.2(5)
F(17)-C(71)-C(67)	110.3(5)
F(16')-C(71)-C(67)	114.7(4)
F(17')-C(71)-C(67)	105.6(4)
F(18')-C(71)-C(67)	113.9(4)
F(16)-C(71)-F(17)	99.3(6)
F(18)-C(71)-F(16)	111.1(6)
F(18)-C(71)-F(17)	101.4(7)
F(18')-C(71)-F(16')	99.4(4)
F(18')-C(71)-F(17')	118.1(4)
F(16')-C(71)-F(17')	105.1(4)
F(19)-C(72)-C(69)	113.5(5)
F(20)-C(72)-C(69)	112.4(4)
F(21)-C(72)-C(69)	113.7(4)
F(19)-C(72)-F(20)	106.3(4)
F(19)-C(72)-F(21)	105.2(4)
F(20)-C(72)-F(21)	105.0(4)
C(78)-C(73)-C(74)	114.9(4)
C(78)-C(73)-B(1)	127.0(4)
C(74)-C(73)-B(1)	118.1(4)
C(75)-C(74)-C(73)	122.8(5)
C(74)-C(75)-C(76)	120.8(5)
C(74)-C(75)-C(79)	119.5(5)
C(76)-C(75)-C(79)	119.7(5)
C(77)-C(76)-C(75)	117.7(4)
C(78)-C(77)-C(76)	120.6(4)
C(78)-C(77)-C(80)	120.2(4)
C(76)-C(77)-C(80)	119.2(4)
C(77)-C(78)-C(73)	123.2(4)
C(75)-C(79)-F(24')	98.9(5)
F(22)-C(79)-C(75)	116.6(6)
F(23)-C(79)-C(75)	114.5(7)
F(24)-C(79)-C(75)	112.0(7)
F(23)-C(79)-F(22)	107.7(8)
F(23)-C(79)-F(24)	99.5(8)
F(22)-C(79)-F(24)	104.7(8)
F(22')-C(79)-F(23')	114.8(6)
F(22')-C(79)-F(24')	95.9(6)
F(23')-C(79)-F(24')	122.6(5)
F(26)-C(80)-C(77)	114.0(4)
F(25)-C(80)-C(77)	112.8(4)
F(27)-C(80)-C(77)	112.6(4)
F(26)-C(80)-F(25)	105.6(4)
F(26)-C(80)-F(27)	106.0(4)
F(25)-C(80)-F(27)	105.0(4)
*** BAr'_4] no. 2	
C(105)-B(2)-C(97)	112.8(4)
C(105)-B(2)-C(89)	104.0(4)
C(97)-B(2)-C(89)	111.5(4)
C(105)-B(2)-C(81)	111.3(4)
C(97)-B(2)-C(81)	105.1(3)
C(89)-B(2)-C(81)	112.3(4)
C(82)-C(81)-C(86)	115.3(4)
C(82)-C(81)-B(2)	125.5(4)
C(86)-C(81)-B(2)	119.0(4)
C(83)-C(82)-C(81)	122.2(4)
C(84)-C(83)-C(82)	120.9(5)
C(84)-C(83)-C(87)	119.4(5)
C(82)-C(83)-C(87)	119.7(5)
C(83)-C(84)-C(85)	118.5(4)
C(86)-C(85)-C(84)	120.2(4)
C(86)-C(85)-C(88)	120.5(5)
C(84)-C(85)-C(88)	119.3(5)
C(85)-C(86)-C(81)	122.9(4)
F(28)-C(87)-C(83)	114.4(6)
F(29)-C(87)-C(83)	114.3(5)
F(30)-C(87)-C(83)	111.6(5)
F(28')-C(87)-C(83)	116.4(4)
F(29')-C(87)-C(83)	115.1(5)
F(30')-C(87)-C(83)	118.5(5)
F(29)-C(87)-F(30)	107.1(7)
F(28)-C(87)-F(30)	103.5(7)
F(29)-C(87)-F(28)	105.2(6)
F(29')-C(87)-F(30')	105.0(4)
F(29')-C(87)-F(28')	92.7(4)
F(30')-C(87)-F(28')	105.6(4)
F(31)-C(88)-C(85)	114.0(5)
F(32)-C(88)-C(85)	112.6(5)
F(33)-C(88)-C(85)	112.3(5)
F(31)-C(88)-F(32)	106.8(6)
F(31)-C(88)-F(33)	106.1(5)
F(32)-C(88)-F(33)	104.3(5)
C(90)-C(89)-C(94)	115.4(4)
C(90)-C(89)-B(2)	125.9(4)
C(94)-C(89)-B(2)	118.7(4)
C(91)-C(90)-C(89)	122.0(5)
C(92)-C(91)-C(90)	120.9(5)
C(92)-C(91)-C(95)	119.4(5)
C(90)-C(91)-C(95)	119.6(5)
C(91)-C(92)-C(93)	118.7(5)
C(92)-C(93)-C(94)	120.1(5)
C(92)-C(93)-C(96)	121.6(5)
C(94)-C(93)-C(96)	118.3(5)
C(93)-C(94)-C(89)	122.8(5)
F(34)-C(95)-C(91)	113.3(5)
F(35)-C(95)-C(91)	113.1(5)
F(36)-C(95)-C(91)	115.2(5)

F(34')-C(95)-C(91)	105.0(4)
F(35')-C(95)-C(91)	108.8(5)
F(36')-C(95)-C(91)	109.1(4)
F(35)-C(95)-F(34)	103.4(6)
F(36)-C(95)-F(35)	105.5(5)
F(36)-C(95)-F(34)	105.2(5)
F(35')-C(95)-F(34')	118.8(4)
F(35')-C(95)-F(36')	104.6(5)
F(36')-C(95)-F(34')	110.3(5)
F(39)-C(96)-C(93)	113.7(6)
F(37)-C(96)-C(93)	112.1(5)
F(38)-C(96)-C(93)	112.2(5)
F(39)-C(96)-F(37)	109.9(6)
F(39)-C(96)-F(38)	104.9(5)
F(37)-C(96)-F(38)	103.4(6)
C(98)-C(97)-C(102)	114.9(4)
C(98)-C(97)-B(2)	125.5(4)
C(102)-C(97)-B(2)	119.5(4)
C(97)-C(98)-C(99)	122.9(4)
C(100)-C(99)-C(98)	120.4(4)
C(100)-C(99)-C(103)	120.5(4)
C(98)-C(99)-C(103)	119.0(4)
C(99)-C(100)-C(101)	118.7(4)
C(100)-C(101)-C(102)	120.4(4)
C(100)-C(101)-C(104)	118.4(4)
C(102)-C(101)-C(104)	121.2(4)
C(101)-C(102)-C(97)	122.8(4)
F(42)-C(103)-C(99)	113.9(4)
F(41)-C(103)-C(99)	112.2(5)
F(40)-C(103)-C(99)	113.4(5)
F(42)-C(103)-F(41)	106.2(5)
F(42)-C(103)-F(40)	104.8(5)
F(41)-C(103)-F(40)	105.5(5)
F(44)-C(104)-C(101)	113.2(5)
F(45)-C(104)-C(101)	114.6(4)
F(43)-C(104)-C(101)	111.1(5)
F(44)-C(104)-F(45)	107.9(5)
F(44)-C(104)-F(43)	103.9(5)
F(45)-C(104)-F(43)	105.3(5)
C(106)-C(105)-C(110)	114.8(4)
C(106)-C(105)-B(2)	119.2(4)
C(110)-C(105)-B(2)	125.9(4)
C(107)-C(106)-C(105)	123.0(4)
C(106)-C(107)-C(108)	120.8(4)
C(106)-C(107)-C(111)	120.0(5)
C(108)-C(107)-C(111)	119.2(4)
C(109)-C(108)-C(107)	117.8(4)
C(108)-C(109)-C(110)	120.8(4)
C(108)-C(109)-C(112)	119.7(4)
C(110)-C(109)-C(112)	119.4(4)
C(109)-C(110)-C(105)	122.7(4)
F(46)-C(111)-C(107)	108.6(6)
F(47)-C(111)-C(107)	115.8(5)
F(48)-C(111)-C(107)	117.3(5)
C(107)-C(111)-F(46')	106.7(5)
F(47')-C(111)-C(107)	110.2(5)
F(48')-C(111)-C(107)	112.9(5)
F(47)-C(111)-F(48)	112.9(7)
F(47)-C(111)-F(46)	101.9(7)
F(48)-C(111)-F(46)	97.1(7)
F(47')-C(111)-F(48')	104.7(5)
F(47')-C(111)-F(46')	108.3(5)
F(48')-C(111)-F(46')	114.1(5)
F(47)-C(111)-F(46')	66.4(6)
F(48)-C(111)-F(46')	61.5(5)
F(46)-C(111)-F(46')	144.3(5)
F(50)-C(112)-C(109)	114.0(4)
F(51)-C(112)-C(109)	111.9(4)
F(49)-C(112)-C(109)	113.2(4)
F(50)-C(112)-F(51)	106.3(4)
F(50)-C(112)-F(49)	106.5(4)
F(51)-C(112)-F(49)	104.2(4)

*** $BAr'_4]$ no. 3

C(113)-B(3)-C(137)	111.9(4)
C(113)-B(3)-C(121)	112.9(4)
C(137)-B(3)-C(121)	104.8(4)
C(113)-B(3)-C(129)	104.5(4)
C(137)-B(3)-C(129)	112.1(4)
C(121)-B(3)-C(129)	110.7(4)
C(114)-C(113)-C(118)	115.2(4)
C(114)-C(113)-B(3)	119.7(4)
C(118)-C(113)-B(3)	125.0(4)
C(115)-C(114)-C(113)	122.8(4)
C(116)-C(115)-C(114)	120.0(4)
C(116)-C(115)-C(119)	120.7(4)
C(114)-C(115)-C(119)	119.3(4)
C(117)-C(116)-C(115)	119.1(4)
C(116)-C(117)-C(118)	120.9(4)
C(116)-C(117)-C(120)	120.1(4)
C(118)-C(117)-C(120)	119.0(4)
C(117)-C(118)-C(113)	122.0(4)
F(52)-C(119)-C(115)	111.9(5)
F(53)-C(119)-C(115)	113.5(5)
F(54)-C(119)-C(115)	112.9(4)
F(52)-C(119)-F(53)	106.7(5)
F(52)-C(119)-F(54)	105.8(5)
F(53)-C(119)-F(54)	105.4(4)
F(56)-C(120)-C(117)	113.8(5)
F(55)-C(120)-C(117)	112.5(5)
F(57)-C(120)-C(117)	113.5(5)
F(56)-C(120)-F(55)	104.8(5)
F(56)-C(120)-F(57)	105.8(5)
F(55)-C(120)-F(57)	105.7(5)
C(122)-C(121)-C(126)	115.5(4)
C(122)-C(121)-B(3)	119.5(4)
C(126)-C(121)-B(3)	124.9(4)
C(123)-C(122)-C(121)	122.7(4)
C(124)-C(123)-C(122)	120.6(4)
C(124)-C(123)-C(127)	119.0(5)
C(122)-C(123)-C(127)	120.4(5)
C(125)-C(124)-C(123)	118.4(4)
C(124)-C(125)-C(126)	121.0(4)
C(124)-C(125)-C(128)	120.3(4)
C(126)-C(125)-C(128)	118.6(5)
C(125)-C(126)-C(121)	121.8(4)
F(58)-C(127)-C(123)	115.0(5)
F(59)-C(127)-C(123)	115.6(6)
F(60)-C(127)-C(123)	113.0(5)
F(58')-C(127)-C(123)	102.3(5)
F(59')-C(127)-C(123)	107.9(5)
F(60')-C(127)-C(123)	104.5(5)

F(58)-C(127)-F(60)	102.7(7)
F(59)-C(127)-F(58)	106.7(8)
F(59)-C(127)-F(60)	102.3(6)
F(60')-C(127)-F(59')	114.4(5)
F(60')-C(127)-F(58')	107.8(5)
F(59')-C(127)-F(58')	118.3(5)
F(61)-C(128)-C(125)	113.9(5)
F(62)-C(128)-C(125)	115.4(5)
F(63)-C(128)-C(125)	112.0(5)
F(61')-C(128)-C(125)	113.2(5)
F(62')-C(128)-C(125)	116.1(4)
F(63')-C(128)-C(125)	108.6(5)
F(61)-C(128)-F(62)	106.6(6)
F(61)-C(128)-F(63)	104.5(6)
F(62)-C(128)-F(63)	103.3(6)
F(63')-C(128)-F(61')	109.7(4)
F(63')-C(128)-F(62')	103.7(5)
F(61')-C(128)-F(62')	104.9(4)
C(134)-C(129)-C(130)	115.4(4)
C(134)-C(129)-B(3)	118.7(4)
C(130)-C(129)-B(3)	125.8(4)
C(131)-C(130)-C(129)	122.0(4)
C(132)-C(131)-C(130)	120.9(4)
C(132)-C(131)-C(135)	119.9(4)
C(130)-C(131)-C(135)	119.2(4)
C(131)-C(132)-C(133)	118.2(5)
C(134)-C(133)-C(132)	120.5(5)
C(134)-C(133)-C(136)	119.8(5)
C(132)-C(133)-C(136)	119.7(5)
C(133)-C(134)-C(129)	123.0(4)
F(66)-C(135)-C(131)	112.5(4)
F(64)-C(135)-C(131)	113.1(5)
F(65)-C(135)-C(131)	112.8(4)
F(66')-C(135)-C(131)	115.4(4)
F(65')-C(135)-C(131)	108.7(4)
F(64')-C(135)-C(131)	114.2(4)
F(66)-C(135)-F(64)	108.2(5)
F(66)-C(135)-F(65)	105.0(5)
F(64)-C(135)-F(65)	104.5(5)
F(66')-C(135)-F(65')	103.9(4)
F(66')-C(135)-F(64')	101.8(4)
F(65')-C(135)-F(64')	112.4(4)
F(67)-C(136)-C(133)	116.8(6)
F(69)-C(136)-C(133)	114.1(7)
F(68)-C(136)-C(133)	112.1(7)
F(67')-C(136)-C(133)	115.2(5)
F(68')-C(136)-C(133)	109.0(6)
F(69')-C(136)-C(133)	107.3(5)
F(67)-C(136)-F(69)	104.1(8)
F(67)-C(136)-F(68)	106.2(9)
F(69)-C(136)-F(68)	102.1(9)
F(67')-C(136)-F(68')	104.5(5)
F(67')-C(136)-F(69')	101.6(6)
F(68')-C(136)-F(69')	119.5(5)
C(138)-C(137)-C(142)	115.0(4)
C(138)-C(137)-B(3)	124.6(4)
C(142)-C(137)-B(3)	120.3(4)
C(137)-C(138)-C(139)	122.5(4)
C(140)-C(139)-C(138)	120.7(4)
C(140)-C(139)-C(143)	119.6(5)
C(138)-C(139)-C(143)	119.7(5)
C(141)-C(140)-C(139)	118.1(5)
C(140)-C(141)-C(142)	121.1(4)
C(140)-C(141)-C(144)	117.9(5)
C(142)-C(141)-C(144)	121.0(4)
C(141)-C(142)-C(137)	122.7(4)
F(70)-C(143)-C(139)	115.3(6)
F(71)-C(143)-C(139)	114.9(6)
F(72)-C(143)-C(139)	111.3(6)
F(70')-C(143)-C(139)	116.1(5)
F(71')-C(143)-C(139)	116.9(5)
F(72')-C(143)-C(139)	105.0(5)
F(71)-C(143)-F(70)	111.0(8)
F(71)-C(143)-F(72)	100.7(7)
F(70)-C(143)-F(72)	101.8(7)
F(70')-C(143)-F(71')	104.1(5)
F(70')-C(143)-F(72')	109.2(5)
F(71')-C(143)-F(72')	105.0(5)
F(73)-C(144)-C(141)	114.3(5)
F(75)-C(144)-C(141)	115.3(4)
F(74)-C(144)-C(141)	110.7(5)
F(75')-C(144)-C(141)	114.2(5)
F(73')-C(144)-C(141)	108.4(5)
F(74')-C(144)-C(141)	105.9(4)
F(73)-C(144)-F(75)	108.2(5)
F(73)-C(144)-F(74)	103.9(5)
F(75)-C(144)-F(74)	103.4(5)
F(75')-C(144)-F(73')	102.0(4)
F(75')-C(144)-F(74')	109.1(4)
F(73')-C(144)-F(74')	117.5(4)

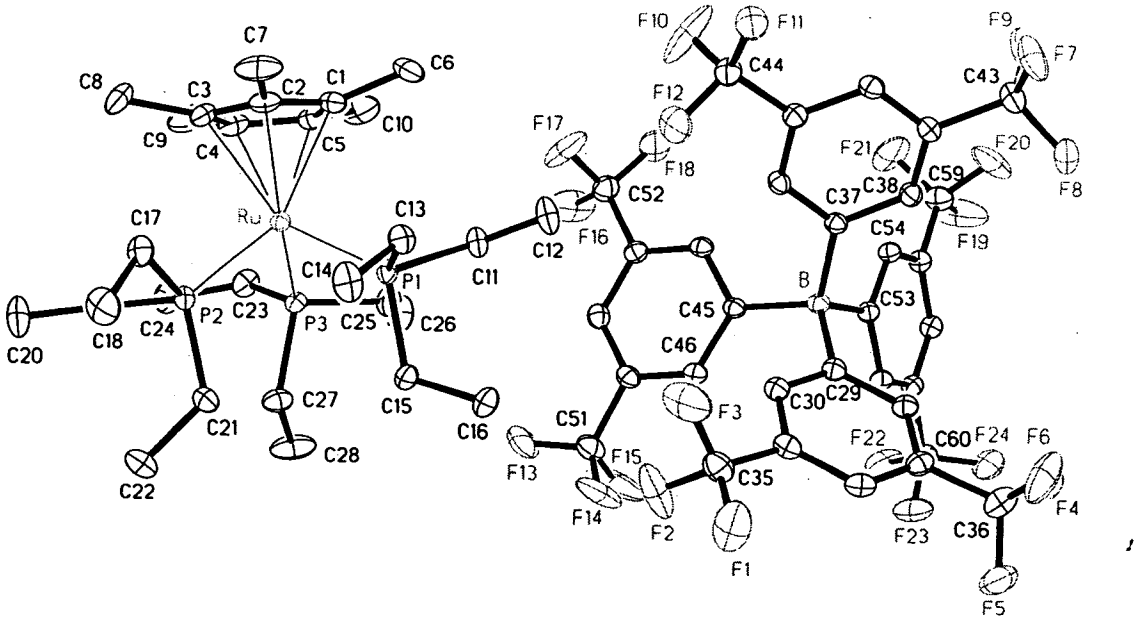
Selected torsion angles

*** BAr'$_4$] no. 1	
C73-B1-C57-C58	164.9(4)
C49-B1-C57-C58	47.1(6)
C65-B1-C57-C58	-74.2(5)
C73-B1-C57-C62	-18.4(6)
C49-B1-C57-C62	-136.2(4)
C65-B1-C57-C62	102.6(5)
C73-B1-C65-C70	-132.5(4)
C49-B1-C65-C70	-13.3(6)
C57-B1-C65-C70	108.4(5)
C73-B1-C65-C66	50.4(5)
C49-B1-C65-C66	169.5(4)
C57-B1-C65-C66	-68.7(5)
C49-B1-C73-C78	-118.6(5)
C57-B1-C73-C78	119.5(5)
C65-B1-C73-C78	3.9(6)
C49-B1-C73-C74	60.2(5)
C57-B1-C73-C74	-61.7(5)
C65-B1-C73-C74	-177.2(4)
*** BAr'$_4$] no. 2	
C105-B2-C81-C82	1.8(6)
C97-B2-C81-C82	-120.6(5)
C89-B2-C81-C82	117.9(5)
C105-B2-C81-C86	176.1(4)
C97-B2-C81-C86	53.7(5)
C89-B2-C81-C86	-67.8(5)
C105-B2-C89-C90	112.9(5)

C97-B2-C89-C90	-125.2(5)	C137-B3-C113-C118	-126.6(5)
C81-B2-C89-C90	-7.5(6)	C121-B3-C113-C118	-8.6(6)
C105-B2-C89-C94	-63.3(5)	C129-B3-C113-C118	111.8(5)
C97-B2-C89-C94	58.5(5)	C113-B3-C121-C122	-58.6(5)
C81-B2-C89-C94	176.3(4)	C137-B3-C121-C122	63.5(5)
C105-B2-C97-C98	118.4(5)	C129-B3-C121-C122	-175.4(4)
C89-B2-C97-C98	1.8(6)	C113-B3-C121-C126	125.4(5)
C81-B2-C97-C98	-120.2(4)	C137-B3-C121-C126	-112.5(5)
C105-B2-C97-C102	-64.3(5)	C129-B3-C121-C126	8.6(6)
C89-B2-C97-C102	179.1(4)	C113-B3-C129-C134	-62.4(5)
C81-B2-C97-C102	57.1(5)	C137-B3-C129-C134	176.2(4)
		C121-B3-C129-C134	59.5(5)
*** BAr'_4] no. 3		C113-B3-C129-C130	113.3(5)
C137-B3-C113-C114	56.1(6)	C137-B3-C129-C130	-8.1(6)
C121-B3-C113-C114	174.2(4)	C121-B3-C129-C130	-124.8(4)
C129-B3-C113-C114	-65.4(5)		

Fig. S6. Thermal ellipsoid plots (20% ellipsoids) of $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7).

(a) Asymmetric unit, H atoms and subordinately occupied F sites omitted



(a) Packing diagram, view along b

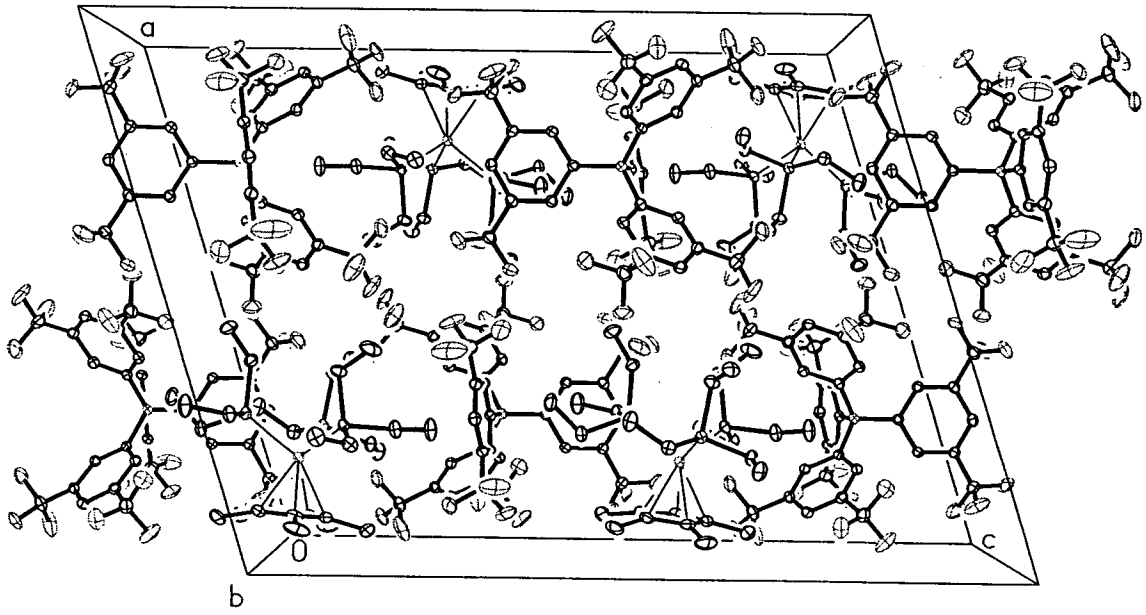


Table S21. Crystal data and structure refinement for $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7).

Identification code	595pvo j3fr
Empirical formula	C60 H72 B F24 P3 Ru
Formula weight	1453.97
Temperature	223(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c (no. 14)
Unit cell dimensions	a = 19.447(5) Å α = 90 deg. b = 13.750(4) Å β = 107.42(2) deg. c = 26.068(6) Å γ = 90 deg.
Volume	6651(3) $Å^3$
Z, Calculated density	4, 1.452 Mg/m^3
Absorption coefficient	0.412 mm^{-1}
F(000)	2968
Crystal size	0.70 x 0.65 x 0.60 mm, yellow oval
Diffractometer	Bruker SMART CCD platform type 3-circle (sealed X-ray tube, Mo Kα radiation, graphite monochr., det.dist. 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 10 sec. per frame 3 x 606 frames
Theta range for data collection	1.69 to 30.00 deg.
Index ranges	-27<=h<=27, -19<=k<=18, -36<=l<=36
Reflections collected / unique	69930 / 19015 [R(int)= 0.031, R(sigma)= 0.030]
Completeness to theta = 30.00	97.9%
Absorption correction	Semi-empirical from equivalents (prg. SADABS)
Max. and min. transmission	1.000 - 0.875
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F^2 (prg SHELXL97)
Data / restraints / parameters	19015 / 231 / 874
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1071 (13862 data)
R indices (all data)	R1 = 0.0677, wR2 = 0.1252 (19015 data)
Extinction coefficient	0.00044(9)
Largest diff. peak and hole	0.575 and -0.621 e $Å^{-3}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma(w(F_o^2)^2)]^{1/2}$

Table S22. Atomic coordinates (x 10^5 for Ru, P; x 10^4 for B, C, F) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	19697(1)	74758(1)	9285(1)	31(1)
P(1)	25042(3)	59919(4)	12878(2)	36(1)
P(2)	27754(4)	78508(5)	4395(2)	38(1)
P(3)	26008(3)	83713(4)	16951(2)	37(1)
C(1)	862(1)	6766(2)	783(1)	52(1)
C(2)	964(1)	6968(2)	277(1)	50(1)
C(3)	1003(1)	7989(2)	231(1)	52(1)
C(4)	954(2)	8417(2)	710(1)	54(1)
C(5)	873(2)	7655(2)	1059(1)	53(1)
C(6)	594(2)	5813(3)	935(2)	89(1)
C(7)	817(2)	6249(3)	-179(2)	88(1)
C(8)	917(2)	8540(4)	-285(2)	94(2)
C(9)	773(2)	9472(3)	752(2)	102(2)
C(10)	650(2)	7796(4)	1558(2)	95(2)
C(11)	2151(2)	5536(2)	1836(1)	51(1)
C(12)	1957(2)	4460(2)	1858(2)	71(1)
C(13)	2344(2)	4962(2)	811(1)	50(1)
C(14)	2798(2)	4961(2)	428(1)	67(1)
C(15)	3477(2)	5849(2)	1632(1)	51(1)
C(16)	3727(2)	4854(2)	1892(1)	65(1)
C(17)	2480(2)	7339(2)	-251(1)	52(1)
C(18)	3040(2)	7089(3)	-533(1)	77(1)
C(19)	2804(2)	9173(2)	318(1)	53(1)
C(20)	2957(3)	9556(3)	-187(2)	83(1)
C(21)	3735(2)	7485(2)	695(1)	49(1)
C(22)	4322(2)	8094(3)	564(2)	83(1)
C(23)	2318(2)	9626(2)	1767(1)	56(1)
C(24)	2477(2)	10390(2)	1408(2)	73(1)
C(25)	2523(2)	7825(2)	2327(1)	59(1)
C(26)	2551(3)	8465(3)	2814(1)	83(1)
C(27)	3581(2)	8548(2)	1848(1)	55(1)
C(28)	3988(2)	9068(3)	2368(2)	97(2)
B	2640(1)	2457(2)	3676(1)	37(1)
C(29)	3333(1)	1902(2)	3580(1)	39(1)
C(30)	3563(1)	2138(2)	3136(1)	43(1)
C(31)	4125(1)	1661(2)	3019(1)	45(1)
C(32)	4474(1)	898(2)	3336(1)	49(1)
C(33)	4245(2)	621(2)	3770(1)	47(1)
C(34)	3689(1)	1116(2)	3891(1)	44(1)
C(35)	4343(2)	1981(3)	2543(2)	62(1)
C(36)	4598(2)	-244(3)	4094(1)	66(1)
C(37)	1948(1)	1876(2)	3276(1)	37(1)
C(38)	1701(1)	995(2)	3429(1)	42(1)
C(39)	1174(1)	440(2)	3072(1)	42(1)
C(40)	868(1)	736(2)	2546(1)	43(1)
C(41)	1103(1)	1602(2)	2384(1)	40(1)
C(42)	1633(1)	2157(2)	2744(1)	39(1)
C(43)	910(2)	-485(2)	3257(1)	58(1)
C(44)	782(2)	1952(2)	1819(1)	54(1)

C(45)		2642(1)	3620(2)	3533(1)	37(1)
C(46)		3278(1)	4144(2)	3589(1)	42(1)
C(47)		3284(1)	5138(2)	3499(1)	46(1)
C(48)		2651(2)	5666(2)	3358(1)	47(1)
C(49)		2015(1)	5174(2)	3315(1)	44(1)
C(50)		2011(1)	4176(2)	3399(1)	40(1)
C(51)		3984(2)	5647(3)	3566(2)	65(1)
C(52)		1325(2)	5730(2)	3174(1)	61(1)
C(53)		2635(1)	2457(2)	4305(1)	37(1)
C(54)		1997(1)	2457(2)	4446(1)	40(1)
C(55)		1991(1)	2587(2)	4973(1)	42(1)
C(56)		2628(2)	2720(2)	5385(1)	44(1)
C(57)		3270(1)	2720(2)	5256(1)	41(1)
C(58)		3271(1)	2589(2)	4728(1)	39(1)
C(59)		1287(2)	2583(3)	5093(1)	60(1)
C(60)		3958(2)	2883(2)	5698(1)	56(1)
F(1)		4883(3)	1515(3)	2472(2)	130(2)
F(2)		4542(3)	2910(2)	2579(2)	132(2)
F(3)		3804(2)	1994(5)	2100(1)	144(2)
F(4)		4395(2)	-394(2)	4541(1)	80(1)
F(5)		5295(1)	-196(3)	4257(2)	104(1)
F(6)		4408(2)	-1077(2)	3823(1)	129(2)
F(7)		698(2)	-1138(2)	2868(1)	96(1)
F(8)		1426(2)	-943(2)	3638(1)	89(1)
F(9)		378(2)	-342(2)	3456(2)	106(1)
F(10)		347(4)	2648(4)	1774(1)	156(3)
F(11)		490(2)	1235(2)	1478(1)	79(1)
F(12)		1303(2)	2301(3)	1617(1)	95(2)
F(13)		3928(2)	6455(4)	3308(4)	200(4)
F(14)		4463(2)	5136(3)	3432(2)	125(2)
F(15)		4311(3)	5837(6)	4066(2)	192(3)
F(16)		1404(2)	6626(2)	3368(2)	145(2)
F(17)		998(2)	5775(4)	2665(1)	134(2)
F(18)		842(2)	5354(3)	3386(2)	106(1)
F(19)		1329(2)	2809(6)	5579(2)	165(3)
F(20)		973(2)	1716(3)	5005(2)	129(2)
F(21)		807(2)	3144(4)	4783(2)	146(2)
F(22)		3999(1)	3757(2)	5903(1)	107(1)
F(23)		4541(1)	2724(2)	5545(1)	88(1)
F(24)		4031(1)	2278(2)	6109(1)	96(1)
F(1A)		3957(8)	2525(10)	2249(5)	65(1)
F(2A)		4350(9)	1225(9)	2199(5)	65(1)
F(3A)		4959(7)	2354(11)	2673(4)	65(1)
F(4A)		5047(9)	-674(10)	3841(6)	65(1)
F(5A)		4301(9)	-695(10)	4254(8)	65(1)
F(6A)		5233(9)	137(9)	4525(6)	65(1)
F(7A)		998(16)	-475(14)	3786(10)	65(1)
F(8A)		210(13)	-602(15)	3037(11)	65(1)
F(9A)		1188(15)	-1183(13)	3204(13)	65(1)
F(10A)	§	778(8)	1381(11)	1467(4)	65(1)
F(11A)		970(8)	2742(10)	1705(4)	65(1)
F(12A)		29(7)	2163(10)	1711(4)	65(1)
F(13A)		4505(5)	5258(8)	3871(6)	65(1)
F(14A)		3985(6)	6505(9)	3739(6)	65(1)
F(15A)		4086(5)	5806(9)	3095(4)	65(1)
F(16A)		810(6)	5277(9)	2847(7)	65(1)
F(17A)		1139(7)	5999(12)	3536(5)	65(1)
F(18A)		1363(6)	6548(10)	2904(7)	65(1)

F(19A)	766(6)	2288(12)	4718(5)	65(1)
F(20A)	1105(6)	3405(9)	5219(7)	65(1)
F(21A)	1285(6)	2043(10)	5490(6)	65(1)

Remarks: §) CF_3 groups orientation disordered with F atoms split into each three predominately and three subordinately (marked by A) occupied sites. Site occupation factors for the major sites between pp = 0.810(4) and 0.932(3); for minor 'A'-sites the factors were pp(A) = 1-pp.

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7).

	x	y	z	U_{eq}
H(6A)	73	5789	792	133
H(6B)	734	5757	1324	133
H(6C)	802	5280	788	133
H(7A)	305	6242	-369	132
H(7B)	969	5606	-37	132
H(7C)	1083	6437	-425	132
H(8A)	409	8615	-476	141
H(8B)	1149	8182	-509	141
H(8C)	1139	9176	-204	141
H(9A)	256	9564	604	153
H(9B)	1019	9865	553	153
H(9C)	925	9668	1127	153
H(10A)	129	7847	1460	143
H(10B)	866	8387	1738	143
H(10C)	810	7245	1796	143
H(11A)	2510	5695	2179	61
H(11B)	1718	5915	1820	61
H(12A)	1783	4350	2166	106
H(12B)	2381	4064	1893	106
H(12C)	1584	4285	1531	106
H(13A)	2435	4355	1018	60
H(13B)	1834	4965	598	60
H(14A)	2677	4397	195	100
H(14B)	3304	4937	632	100
H(14C)	2702	5548	212	100
H(15A)	3738	5981	1371	61
H(15B)	3621	6347	1913	61
H(16A)	4244	4864	2059	97
H(16B)	3605	4352	1618	97
H(16C)	3488	4719	2161	97
H(17A)	2207	6745	-240	62
H(17B)	2143	7804	-480	62
H(18A)	2801	6831	-888	116
H(18B)	3371	6606	-324	116
H(18C)	3306	7671	-566	116
H(19A)	2338	9442	320	63
H(19B)	3169	9452	628	63
H(20A)	2952	10261	-184	125
H(20B)	2591	9320	-503	125
H(20C)	3427	9330	-194	125
H(21A)	3859	7445	1087	59
H(21B)	3770	6824	564	59
H(22A)	4789	7799	729	124
H(22B)	4318	8748	703	124
H(22C)	4230	8122	177	124
H(23A)	1796	9621	1708	68
H(23B)	2545	9827	2140	68
H(24A)	2300	11014	1488	110
H(24B)	2240	10222	1036	110
H(24C)	2993	10428	1469	110
H(25A)	2067	7467	2235	71

H(25B)	2910	7343	2445	71
H(26A)	2503	8060	3107	124
H(26B)	2159	8932	2717	124
H(26C)	3007	8808	2928	124
H(27A)	3801	7906	1852	66
H(27B)	3664	8912	1548	66
H(28A)	4496	9107	2393	145
H(28B)	3932	8709	2673	145
H(28C)	3796	9719	2367	145
H(30)	3326	2642	2908	52
H(32)	4858	574	3260	58
H(34)	3548	918	4190	52
H(38)	1899	775	3784	50
H(40)	511	359	2304	51
H(42)	1782	2742	2623	46
H(46)	3719	3808	3692	51
H(48)	2652	6338	3294	57
H(50)	1570	3864	3364	48
H(54)	1557	2365	4176	48
H(56)	2624	2807	5742	52
H(58)	3714	2590	4652	47

Hydrogen atoms inserted in idealized positions and refined riding with the atoms to which they were bonded. All H atoms had $U_{iso} = U_{eq}$ x 1.2 (x 1.5 for CH_3) of their carrier atoms.

Table S24. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	33(1)	30(1)	28(1)	-1(1)	6(1)	-1(1)
P(1)	42(1)	29(1)	37(1)	1(1)	11(1)	-2(1)
P(2)	46(1)	34(1)	33(1)	2(1)	13(1)	-3(1)
P(3)	41(1)	33(1)	32(1)	-4(1)	6(1)	0(1)
C(1)	32(1)	57(2)	62(2)	3(1)	8(1)	-5(1)
C(2)	35(1)	59(2)	48(2)	-16(1)	0(1)	-3(1)
C(3)	37(1)	68(2)	44(1)	8(1)	0(1)	4(1)
C(4)	38(1)	48(2)	63(2)	-9(1)	-3(1)	8(1)
C(5)	36(1)	75(2)	46(1)	-5(1)	11(1)	6(1)
C(6)	49(2)	78(2)	133(4)	23(2)	16(2)	-20(2)
C(7)	57(2)	116(3)	77(2)	-56(2)	-2(2)	-9(2)
C(8)	67(2)	134(4)	68(2)	51(2)	0(2)	18(2)
C(9)	67(2)	61(2)	143(4)	-22(2)	-23(2)	28(2)
C(10)	59(2)	167(5)	66(2)	-10(3)	29(2)	24(3)
C(11)	72(2)	41(1)	45(1)	5(1)	25(1)	-6(1)
C(12)	106(3)	47(2)	70(2)	9(2)	43(2)	-15(2)
C(13)	60(2)	36(1)	54(2)	-7(1)	18(1)	-4(1)
C(14)	100(3)	45(2)	68(2)	-8(1)	43(2)	0(2)
C(15)	47(2)	42(1)	58(2)	12(1)	7(1)	4(1)
C(16)	64(2)	51(2)	74(2)	19(2)	12(2)	14(1)
C(17)	67(2)	54(2)	37(1)	-5(1)	18(1)	-3(1)
C(18)	93(3)	97(3)	53(2)	-16(2)	39(2)	-5(2)
C(19)	74(2)	39(1)	46(2)	3(1)	18(1)	-7(1)
C(20)	138(4)	57(2)	61(2)	15(2)	41(2)	-14(2)
C(21)	45(1)	54(2)	53(2)	1(1)	20(1)	-5(1)
C(22)	56(2)	102(3)	97(3)	14(2)	33(2)	-17(2)
C(23)	64(2)	42(1)	57(2)	-8(1)	9(1)	6(1)
C(24)	94(3)	45(2)	78(2)	-1(2)	21(2)	6(2)
C(25)	84(2)	55(2)	37(1)	-3(1)	16(1)	-1(2)
C(26)	138(4)	72(2)	43(2)	-10(2)	35(2)	0(2)
C(27)	45(2)	51(2)	59(2)	-17(1)	2(1)	-2(1)
C(28)	56(2)	112(3)	98(3)	-64(3)	-13(2)	0(2)
B	34(1)	45(1)	32(1)	-2(1)	7(1)	-3(1)
C(29)	38(1)	43(1)	35(1)	-5(1)	9(1)	-3(1)
C(30)	43(1)	46(1)	41(1)	-2(1)	12(1)	-2(1)
C(31)	43(1)	50(1)	46(1)	-11(1)	18(1)	-8(1)
C(32)	40(1)	56(2)	51(2)	-15(1)	14(1)	-1(1)
C(33)	44(1)	49(1)	42(1)	-8(1)	4(1)	2(1)
C(34)	42(1)	50(1)	36(1)	-5(1)	8(1)	-2(1)
C(35)	63(2)	64(2)	70(2)	-4(2)	36(2)	-5(2)
C(36)	63(2)	76(2)	53(2)	0(2)	9(2)	19(2)
C(37)	35(1)	42(1)	34(1)	-3(1)	9(1)	-4(1)
C(38)	44(1)	44(1)	36(1)	1(1)	11(1)	-4(1)
C(39)	42(1)	41(1)	46(1)	-1(1)	17(1)	-5(1)
C(40)	40(1)	45(1)	42(1)	-6(1)	10(1)	-8(1)
C(41)	42(1)	43(1)	33(1)	-5(1)	9(1)	-4(1)
C(42)	42(1)	38(1)	36(1)	-3(1)	12(1)	-7(1)
C(43)	66(2)	50(2)	61(2)	0(1)	24(2)	-14(1)
C(44)	69(2)	49(2)	38(1)	-5(1)	6(1)	-8(1)

C(45)	35(1)	44(1)	32(1)	-3(1)	8(1)	-4(1)
C(46)	35(1)	47(1)	43(1)	-4(1)	9(1)	-4(1)
C(47)	46(1)	46(1)	45(1)	-6(1)	14(1)	-10(1)
C(48)	56(2)	43(1)	43(1)	-1(1)	15(1)	-4(1)
C(49)	43(1)	49(1)	39(1)	-2(1)	9(1)	2(1)
C(50)	35(1)	47(1)	35(1)	-4(1)	7(1)	-4(1)
C(51)	57(2)	59(2)	81(2)	-7(2)	21(2)	-16(2)
C(52)	57(2)	59(2)	66(2)	3(2)	19(2)	10(1)
C(53)	36(1)	38(1)	35(1)	-3(1)	9(1)	-1(1)
C(54)	36(1)	45(1)	37(1)	-2(1)	8(1)	0(1)
C(55)	41(1)	46(1)	41(1)	-3(1)	15(1)	1(1)
C(56)	50(1)	45(1)	36(1)	-5(1)	14(1)	1(1)
C(57)	43(1)	39(1)	38(1)	-5(1)	6(1)	-1(1)
C(58)	35(1)	42(1)	39(1)	-4(1)	9(1)	-1(1)
C(59)	50(2)	82(2)	52(2)	-6(2)	23(1)	1(2)
C(60)	51(2)	66(2)	45(2)	-12(1)	4(1)	1(1)
F(1)	152(4)	150(3)	140(3)	59(3)	122(3)	80(3)
F(2)	202(4)	70(2)	178(4)	0(2)	141(4)	-28(3)
F(3)	109(3)	278(6)	48(2)	16(2)	27(2)	-62(3)
F(4)	84(2)	82(2)	74(2)	25(1)	23(1)	19(1)
F(5)	54(1)	148(3)	105(3)	46(2)	17(2)	30(2)
F(6)	192(4)	56(2)	90(2)	-11(1)	-32(2)	38(2)
F(7)	155(3)	58(1)	79(2)	-13(1)	41(2)	-49(2)
F(8)	100(2)	63(1)	94(2)	31(1)	16(2)	-9(1)
F(9)	117(2)	72(2)	175(3)	15(2)	112(3)	-5(1)
F(10)	229(6)	155(4)	54(2)	5(2)	-1(2)	152(4)
F(11)	101(2)	76(2)	40(1)	-10(1)	-8(1)	-32(2)
F(12)	104(3)	132(3)	45(1)	18(2)	16(1)	-35(2)
F(13)	83(2)	117(3)	389(9)	137(5)	51(4)	-21(2)
F(14)	73(2)	97(2)	235(5)	-44(3)	92(3)	-34(2)
F(15)	124(3)	343(8)	119(3)	-107(5)	51(3)	-166(5)
F(16)	84(2)	71(2)	262(6)	-50(3)	23(3)	22(2)
F(17)	94(2)	242(5)	62(2)	44(2)	18(2)	94(3)
F(18)	66(2)	114(3)	155(3)	47(2)	60(2)	37(2)
F(19)	78(2)	357(8)	79(2)	-92(4)	54(2)	-53(3)
F(20)	82(2)	105(3)	231(5)	-28(3)	91(3)	-36(2)
F(21)	78(2)	219(5)	167(4)	96(4)	75(3)	84(3)
F(22)	82(2)	82(2)	119(2)	-53(1)	-26(1)	0(1)
F(23)	44(1)	149(2)	63(1)	-21(1)	2(1)	0(1)
F(24)	87(2)	131(2)	51(1)	18(1)	-8(1)	-3(1)

Table S25. Bond lengths [Å] and angles [deg] for $[Cp^*Ru(PEt_3)_3][BAr'_4]$ (7).

Bond distances	
Ru-C(5)	2.270(3)
Ru-C(2)	2.283(3)
Ru-C(4)	2.286(3)
Ru-C(1)	2.290(3)
Ru-C(3)	2.301(3)
Ru-P(1)	2.3532(8)
Ru-P(2)	2.3542(8)
Ru-P(3)	2.3554(8)
P(1)-C(15)	1.846(3)
P(1)-C(13)	1.848(3)
P(1)-C(11)	1.870(3)
P(2)-C(19)	1.849(3)
P(2)-C(21)	1.853(3)
P(2)-C(17)	1.857(3)
P(3)-C(23)	1.838(3)
P(3)-C(27)	1.843(3)
P(3)-C(25)	1.857(3)
C(1)-C(5)	1.415(4)
C(1)-C(2)	1.417(4)
C(1)-C(6)	1.508(4)
C(2)-C(3)	1.414(4)
C(2)-C(7)	1.506(4)
C(3)-C(4)	1.409(4)
C(3)-C(8)	1.508(4)
C(4)-C(5)	1.426(4)
C(4)-C(9)	1.506(4)
C(5)-C(10)	1.502(5)
C(6)-H(6A)	0.97
C(6)-H(6B)	0.97
C(6)-H(6C)	0.97
C(7)-H(7A)	0.97
C(7)-H(7B)	0.97
C(7)-H(7C)	0.97
C(8)-H(8A)	0.97
C(8)-H(8B)	0.97
C(8)-H(8C)	0.97
C(9)-H(9A)	0.97
C(9)-H(9B)	0.97
C(9)-H(9C)	0.97
C(10)-H(10A)	0.97
C(10)-H(10B)	0.97
C(10)-H(10C)	0.97
C(11)-C(12)	1.532(4)
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(12)-H(12A)	0.97
C(12)-H(12B)	0.97
C(12)-H(12C)	0.97
C(13)-C(14)	1.518(4)
C(13)-H(13A)	0.98
C(13)-H(13B)	0.98
C(14)-H(14A)	0.97
C(14)-H(14B)	0.97
C(14)-H(14C)	0.97
C(15)-C(16)	1.538(4)
C(15)-H(15A)	0.98
C(15)-H(15B)	0.98
C(16)-H(16A)	0.97
C(16)-H(16B)	0.97
C(16)-H(16C)	0.97
C(17)-C(18)	1.523(4)
C(17)-H(17A)	0.98
C(17)-H(17B)	0.98
C(18)-H(18A)	0.97
C(18)-H(18B)	0.97
C(18)-H(18C)	0.97
C(19)-C(20)	1.526(4)
C(19)-H(19A)	0.98
C(19)-H(19B)	0.98
C(20)-H(20A)	0.97
C(20)-H(20B)	0.97
C(20)-H(20C)	0.97
C(21)-C(22)	1.534(4)
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(22)-H(22A)	0.97
C(22)-H(22B)	0.97
C(22)-H(22C)	0.97
C(23)-C(24)	1.498(5)
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(24)-H(24A)	0.97
C(24)-H(24B)	0.97
C(24)-H(24C)	0.97
C(25)-C(26)	1.533(4)
C(25)-H(25A)	0.98
C(25)-H(25B)	0.98
C(26)-H(26A)	0.97
C(26)-H(26B)	0.97
C(26)-H(26C)	0.97
C(27)-C(28)	1.528(4)
C(27)-H(27A)	0.98
C(27)-H(27B)	0.98
C(28)-H(28A)	0.97
C(28)-H(28B)	0.97
C(28)-H(28C)	0.97
B-C(29)	1.633(4)
B-C(53)	1.641(4)
B-C(45)	1.641(4)
B-C(37)	1.643(3)
C(29)-C(30)	1.398(4)
C(29)-C(34)	1.402(4)
C(30)-C(31)	1.384(4)
C(30)-H(30)	0.94
C(31)-C(32)	1.383(4)
C(31)-C(35)	1.492(4)
C(32)-C(33)	1.387(4)

C(32)-H(32)	0.94
C(33)-C(34)	1.391(4)
C(33)-C(36)	1.502(4)
C(34)-H(34)	0.94
C(35)-F(1A)	1.170(14)
C(35)-F(3A)	1.252(12)
C(35)-F(1)	1.289(4)
C(35)-F(3)	1.308(5)
C(35)-F(2)	1.330(5)
C(35)-F(2A)	1.376(13)
C(36)-F(5A)	1.016(16)
C(36)-F(5)	1.296(4)
C(36)-F(6)	1.338(5)
C(36)-F(4)	1.352(5)
C(36)-F(4A)	1.377(15)
C(36)-F(6A)	1.495(16)
C(37)-C(42)	1.393(3)
C(37)-C(38)	1.404(3)
C(38)-C(39)	1.388(3)
C(38)-H(38)	0.94
C(39)-C(40)	1.384(4)
C(39)-C(43)	1.503(4)
C(40)-C(41)	1.385(4)
C(40)-H(40)	0.94
C(41)-C(42)	1.396(3)
C(41)-C(44)	1.497(4)
C(42)-H(42)	0.94
C(43)-F(9A)	1.13(2)
C(43)-F(9)	1.303(4)
C(43)-F(8A)	1.32(2)
C(43)-F(7)	1.326(4)
C(43)-F(7A)	1.34(2)
C(43)-F(8)	1.339(4)
C(44)-F(10A)	1.206(14)
C(44)-F(11A)	1.211(12)
C(44)-F(10)	1.259(4)
C(44)-F(11)	1.334(4)
C(44)-F(12)	1.361(5)
C(44)-F(12A)	1.435(13)
C(45)-C(50)	1.398(3)
C(45)-C(46)	1.402(3)
C(46)-C(47)	1.387(4)
C(46)-H(46)	0.94
C(47)-C(48)	1.380(4)
C(47)-C(51)	1.495(4)
C(48)-C(49)	1.386(4)
C(48)-H(48)	0.94
C(49)-C(50)	1.390(4)
C(49)-C(52)	1.491(4)
C(50)-H(50)	0.94
C(51)-F(13A)	1.209(11)
C(51)-F(14A)	1.263(12)
C(51)-F(13)	1.286(5)
C(51)-F(14)	1.295(5)
C(51)-F(15)	1.296(5)
C(51)-F(15A)	1.317(11)
C(52)-F(17A)	1.168(13)
C(52)-F(16A)	1.268(14)
C(52)-F(17)	1.289(4)
C(52)-F(16)	1.323(5)
C(52)-F(18)	1.328(4)
C(52)-F(18A)	1.340(13)
C(53)-C(54)	1.397(3)
C(53)-C(58)	1.402(3)
C(54)-C(55)	1.389(3)
C(54)-H(54)	0.94
C(55)-C(56)	1.386(4)
C(55)-C(59)	1.493(4)
C(56)-C(57)	1.387(4)
C(56)-H(56)	0.94
C(57)-C(58)	1.390(3)
C(57)-C(60)	1.499(4)
C(58)-H(58)	0.94
C(59)-F(19A)	1.247(12)
C(59)-F(20A)	1.257(12)
C(59)-F(21A)	1.275(12)
C(59)-F(19)	1.282(4)
C(59)-F(21)	1.292(5)
C(59)-F(20)	1.327(5)
C(60)-F(22)	1.309(4)
C(60)-F(23)	1.327(4)
C(60)-F(24)	1.332(4)

Bond angles

C(5)-Ru-C(2)	60.68(11)
C(5)-Ru-C(4)	36.49(11)
C(2)-Ru-C(4)	60.22(10)
C(5)-Ru-C(1)	36.16(11)
C(2)-Ru-C(1)	36.11(11)
C(4)-Ru-C(1)	60.02(11)
C(5)-Ru-C(3)	60.24(11)
C(2)-Ru-C(3)	35.93(11)
C(4)-Ru-C(3)	35.78(11)
C(1)-Ru-C(3)	59.63(11)
C(5)-Ru-P(1)	110.93(9)
C(2)-Ru-P(1)	102.06(8)
C(4)-Ru-P(1)	146.69(9)
C(1)-Ru-P(1)	88.75(8)
C(3)-Ru-P(1)	137.71(8)
C(5)-Ru-P(2)	149.79(8)
C(2)-Ru-P(2)	103.02(8)
C(4)-Ru-P(2)	113.97(9)
C(1)-Ru-P(2)	138.47(8)
C(3)-Ru-P(2)	91.32(8)
P(1)-Ru-P(2)	96.84(3)
C(5)-Ru-P(3)	95.20(8)
C(2)-Ru-P(3)	154.70(7)
C(4)-Ru-P(3)	96.19(8)
C(1)-Ru-P(3)	126.09(8)
C(3)-Ru-P(3)	127.25(9)
P(1)-Ru-P(3)	93.42(3)
P(2)-Ru-P(3)	94.74(3)
C(15)-P(1)-C(13)	100.77(14)
C(15)-P(1)-C(11)	98.68(14)

C(13)-P(1)-C(11)	103.30(13)
C(15)-P(1)-Ru	123.53(9)
C(13)-P(1)-Ru	115.55(10)
C(11)-P(1)-Ru	112.04(10)
C(19)-P(2)-C(21)	104.47(14)
C(19)-P(2)-C(17)	102.86(13)
C(21)-P(2)-C(17)	103.33(14)
C(19)-P(2)-Ru	111.56(10)
C(21)-P(2)-Ru	120.54(9)
C(17)-P(2)-Ru	112.30(10)
C(23)-P(3)-C(27)	100.14(14)
C(23)-P(3)-C(25)	100.56(15)
C(27)-P(3)-C(25)	102.44(16)
C(23)-P(3)-Ru	118.76(10)
C(27)-P(3)-Ru	119.64(10)
C(25)-P(3)-Ru	112.41(11)
C(5)-C(1)-C(2)	108.6(3)
C(5)-C(1)-C(6)	124.8(3)
C(2)-C(1)-C(6)	124.8(3)
C(5)-C(1)-Ru	71.16(16)
C(2)-C(1)-Ru	71.67(15)
C(6)-C(1)-Ru	135.2(2)
C(3)-C(2)-C(1)	107.5(2)
C(3)-C(2)-C(7)	125.9(3)
C(1)-C(2)-C(7)	124.0(3)
C(3)-C(2)-Ru	72.72(15)
C(1)-C(2)-Ru	72.22(15)
C(7)-C(2)-Ru	134.9(2)
C(4)-C(3)-C(2)	108.6(3)
C(4)-C(3)-C(8)	124.2(3)
C(2)-C(3)-C(8)	125.5(3)
C(4)-C(3)-Ru	71.53(15)
C(2)-C(3)-Ru	71.35(15)
C(8)-C(3)-Ru	134.9(2)
C(3)-C(4)-C(5)	108.0(3)
C(3)-C(4)-C(9)	123.2(3)
C(5)-C(4)-C(9)	126.0(4)
C(3)-C(4)-Ru	72.68(16)
C(5)-C(4)-Ru	71.17(15)
C(9)-C(4)-Ru	137.0(2)
C(1)-C(5)-C(4)	107.3(3)
C(1)-C(5)-C(10)	126.0(3)
C(4)-C(5)-C(10)	125.0(3)
C(1)-C(5)-Ru	72.68(16)
C(4)-C(5)-Ru	72.34(16)
C(10)-C(5)-Ru	132.2(2)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-P(1)	120.3(2)
C(12)-C(11)-H(11A)	107.3
P(1)-C(11)-H(11A)	107.3
C(12)-C(11)-H(11B)	107.3
P(1)-C(11)-H(11B)	107.3
H(11A)-C(11)-H(11B)	106.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-P(1)	115.4(2)
C(14)-C(13)-H(13A)	108.4
P(1)-C(13)-H(13A)	108.4
C(14)-C(13)-H(13B)	108.4
P(1)-C(13)-H(13B)	108.4
H(13A)-C(13)-H(13B)	107.5
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-P(1)	116.8(2)
C(16)-C(15)-H(15A)	108.1
P(1)-C(15)-H(15A)	108.1
C(16)-C(15)-H(15B)	108.1
P(1)-C(15)-H(15B)	108.1
H(15A)-C(15)-H(15B)	107.3
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-P(2)	119.6(2)
C(18)-C(17)-H(17A)	107.4
P(2)-C(17)-H(17A)	107.4
C(18)-C(17)-H(17B)	107.4