Table 1. Crystal data and structure refinement for 2a".

Identification code	sample2a"
Empirical formula	$C_{28}H_{29}F_6O_2PRu$
Formula weight	643.55
Temperature	152(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pca2_1$
Unit cell dimensions	a = 30.83(2) Å α = 90° b = 8.103(5) Å β = 90° c = 10.494(6) Å γ = 90°
Volume, Z	2622(3) Å^3, 4
Density (calculated)	1.631 Mg/m^3
Absorption coefficient	0.727 mm^{-1}
F(000)	1304
Crystal size	0.2 x 0.2 x 0.1 mm
θ range for data collection	1.32 to 28.07°
Limiting indices	$-4 \le h \le 40$, $-1 \le k \le 10$, $-13 \le \ell \le 13$
Reflections collected	3220
Independent reflections	3220 (R_{int} = 0.0000)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3147 / 142 / 347
Goodness-of-fit on F^2	1.083
Final R indices [I>2σ(I)]	R1 = 0.0445, wR2 = 0.1029
R indices (all data)	R1 = 0.0757, wR2 = 0.1233
Absolute structure parameter	0.08(14)
Largest diff. peak and hole	0.692 and -2.242 eÅ^{-3}

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

	x	y	z	U(eq)
Ru	-8937(1)	-5059(1)	-13597(1)	19(1)
O(1)	-9967(2)	-5424(7)	-12374(6)	33(1)
O(2)	-8354(2)	-8013(7)	-14073(8)	44(2)
C(2)	-9411(2)	-3111(9)	-14227(9)	26(2)
C(3)	-9040(3)	-3001(10)	-15043(8)	26(2)
C(4)	-8989(3)	-4566(14)	-15663(8)	26(2)
C(5)	-9334(3)	-5628(11)	-15267(9)	28(2)
C(1)	-9596(2)	-4732(10)	-14357(9)	28(2)
C(7)	-9600(3)	-1705(10)	-13465(11)	38(2)
C(8)	-8781(3)	-1475(11)	-15300(11)	39(2)
C(9)	-8669(3)	-4893(14)	-16745(11)	51(3)
C(10)	-9422(3)	-7313(11)	-15819(10)	44(2)
C(6)	-10000(2)	-5335(11)	-13718(13)	39(2)
C(11)	-9708(3)	-6797(10)	-11928(9)	31(2)
C(12)	-9229(3)	-6436(11)	-11899(8)	28(2)
C(13)	-9069(3)	-4865(10)	-11591(8)	20(2)
C(14)	-8600(2)	-4586(9)	-11726(7)	22(1)
C(15)	-8502(2)	-3200(9)	-12519(8)	23(1)
C(16)	-8284(2)	-5729(10)	-11131(7)	24(2)
C(17)	-8398(3)	-6367(11)	-9935(8)	30(2)
C(18)	-8109(3)	-7344(11)	-9248(10)	39(2)
C(19)	-7694(3)	-7643(11)	-9704(9)	36(2)
C(20)	-7577(3)	-6981(10)	-10885(9)	33(2)
C(21)	-7868(3)	-6054(10)	-11587(9)	29(2)
C(22)	-8063(3)	-2657(9)	-12858(8)	24(2)
C(23)	-7857(3)	-1458(9)	-12089(9)	29(2)
C(24)	-7432(3)	-1050(11)	-12311(10)	42(2)
C(25)	-7201(3)	-1763(11)	-13285(11)	44(3)
C(26)	-7402(3)	-2874(10)	-14076(10)	37(2)
C(27)	-7831(3)	-3312(10)	-13867(8)	33(2)
C(28)	-8563(2)	-6880(9)	-13815(8)	24(2)
P	-9190(1)	-431(3)	-9268(3)	32(1)
F(1)	-9339(2)	1456(7)	-9311(7)	55(2)
F(2)	-9042(3)	-2316(7)	-9220(9)	73(2)
F(3)	-8809(2)	39(8)	-8302(6)	51(2)
F(4)	-9507(2)	-732(8)	-8100(7)	51(2)
F(5)	-9572(2)	-912(10)	-10225(7)	74(2)
F(6)	-8874(2)	-107(8)	-10447(7)	56(2)

Table 3. Bond lengths [Å] and angles [°] for 2a".

Ru-C(28)	1.886(7)	Ru-C(13)	2.150(9)
Ru-C(5)	2.187(8)	Ru-C(1)	2.199(8)
Ru-C(4)	2.211(9)	Ru-C(2)	2.252(7)
Ru-C(14)	2.253(8)	Ru-C(3)	2.277(8)
Ru-C(12)	2.288(9)	Ru-C(15)	2.311(8)
O(1)-C(6)	1.417(13)	O(1)-C(11)	1.446(10)
O(2)-C(28)	1.155(9)	C(2)-C(3)	1.432(12)
C(2)-C(1)	1.438(10)	C(2)-C(7)	1.508(12)
C(3)-C(4)	1.434(13)	C(3)-C(8)	1.497(11)
C(4)-C(5)	1.428(13)	C(4)-C(9)	1.527(14)
C(5)-C(1)	1.446(12)	C(5)-C(10)	1.508(12)
C(1)-C(6)	1.496(12)	C(11)-C(12)	1.507(11)
C(12)-C(13)	1.403(11)	C(13)-C(14)	1.469(12)
C(14)-C(15)	1.430(11)	C(14)-C(16)	1.483(11)
C(15)-C(22)	1.468(10)	C(16)-C(21)	1.393(11)
C(16)-C(17)	1.402(11)	C(17)-C(18)	1.392(12)
C(18)-C(19)	1.387(12)	C(19)-C(20)	1.398(12)
C(20)-C(21)	1.383(12)	C(22)-C(27)	1.383(11)
C(22)-C(23)	1.413(11)	C(23)-C(24)	1.371(12)
C(24)-C(25)	1.375(14)	C(25)-C(26)	1.373(13)
C(26)-C(27)	1.386(11)	P-F(4)	1.588(6)
P-F(2)	1.594(6)	P-F(6)	1.595(7)
P-F(1)	1.598(5)	P-F(3)	1.597(6)
P-F(5)	1.597(7)		

C(28)-Ru-C(13)	107.0(4)	C(28)-Ru-C(5)	94.6(3)
C(13)-Ru-C(5)	133.9(4)	C(28)-Ru-C(1)	127.9(3)
C(13)-Ru-C(1)	99.8(4)	C(5)-Ru-C(1)	38.5(3)
C(28)-Ru-C(4)	93.9(4)	C(13)-Ru-C(4)	158.9(3)
C(5)-Ru-C(4)	37.9(3)	C(1)-Ru-C(4)	63.6(4)
C(28)-Ru-C(2)	155.5(4)	C(13)-Ru-C(2)	96.5(3)
C(5)-Ru-C(2)	63.2(3)	C(1)-Ru-C(2)	37.7(3)
C(4)-Ru-C(2)	62.5(4)	C(28)-Ru-C(14)	87.6(3)
C(13)-Ru-C(14)	38.9(3)	C(5)-Ru-C(14)	172.6(3)
C(1)-Ru-C(14)	136.1(3)	C(4)-Ru-C(14)	149.1(3)
C(2)-Ru-C(14)	115.8(3)	C(28)-Ru-C(3)	125.3(3)
C(13)-Ru-C(3)	124.9(3)	C(5)-Ru-C(3)	62.7(3)
C(1)-Ru-C(3)	62.6(3)	C(4)-Ru-C(3)	37.2(4)
C(2)-Ru-C(3)	36.8(3)	C(14)-Ru-C(3)	121.4(3)
C(28)-Ru-C(12)	87.3(3)	C(13)-Ru-C(12)	36.7(3)
C(5)-Ru-C(12)	107.5(3)	C(1)-Ru-C(12)	88.7(3)
C(4)-Ru-C(12)	145.4(3)	C(2)-Ru-C(12)	108.3(3)
C(14)-Ru-C(12)	65.5(3)	C(3)-Ru-C(12)	145.2(3)
C(28)-Ru-C(15)	102.4(3)	C(13)-Ru-C(15)	65.3(3)
C(5)-Ru-C(15)	148.6(3)	C(1)-Ru-C(15)	129.4(3)
C(4)-Ru-C(15)	113.9(3)	C(2)-Ru-C(15)	93.6(3)
C(14)-Ru-C(15)	36.5(3)	C(3)-Ru-C(15)	86.0(3)
C(12)-Ru-C(15)	99.5(3)	C(6)-O(1)-C(11)	113.6(7)
C(3)-C(2)-C(1)	108.4(7)	C(3)-C(2)-C(7)	125.3(7)
C(1)-C(2)-C(7)	126.0(8)	C(3)-C(2)-Ru	72.5(4)
C(1)-C(2)-Ru	69.2(4)	C(7)-C(2)-Ru	128.7(6)
C(4)-C(3)-C(2)	107.7(7)	C(4)-C(3)-C(8)	126.1(8)
C(2)-C(3)-C(8)	125.9(8)	C(4)-C(3)-Ru	68.9(5)
C(2)-C(3)-Ru	70.6(4)	C(8)-C(3)-Ru	130.6(6)
C(3)-C(4)-C(5)	108.6(8)	C(3)-C(4)-C(9)	124.2(9)
C(5)-C(4)-C(9)	126.3(9)	C(3)-C(4)-Ru	73.9(5)
C(5)-C(4)-Ru	70.1(5)	C(9)-C(4)-Ru	130.6(8)
C(4)-C(5)-C(1)	107.8(8)	C(4)-C(5)-C(10)	124.6(9)

C(1)-C(5)-Ru	71.2(5)	C(10)-C(5)-Ru	126.8(6)
C(2)-C(1)-C(5)	107.5(7)	C(2)-C(1)-C(6)	125.8(8)
C(5)-C(1)-C(6)	126.7(8)	C(2)-C(1)-Ru	73.2(4)
C(5)-C(1)-Ru	70.3(4)	C(6)-C(1)-Ru	124.6(6)
O(1)-C(6)-C(1)	113.8(7)	O(1)-C(11)-C(12)	113.5(7)
C(13)-C(12)-C(11)	121.7(8)	C(13)-C(12)-Ru	66.3(5)
C(11)-C(12)-Ru	117.7(6)	C(12)-C(13)-C(14)	117.6(8)
C(12)-C(13)-Ru	77.0(5)	C(14)-C(13)-Ru	74.3(5)
C(15)-C(14)-C(13)	112.6(7)	C(15)-C(14)-C(16)	126.6(7)
C(13)-C(14)-C(16)	120.7(7)	C(15)-C(14)-Ru	74.0(4)
C(13)-C(14)-Ru	66.8(4)	C(16)-C(14)-Ru	124.3(5)
C(14)-C(15)-C(22)	124.9(7)	C(14)-C(15)-Ru	69.5(4)
C(22)-C(15)-Ru	127.7(6)	C(21)-C(16)-C(17)	117.9(8)
C(21)-C(16)-C(14)	125.4(7)	C(17)-C(16)-C(14)	116.3(7)
C(18)-C(17)-C(16)	120.9(8)	C(19)-C(18)-C(17)	120.7(9)
C(18)-C(19)-C(20)	118.4(9)	C(21)-C(20)-C(19)	120.9(8)
C(20)-C(21)-C(16)	121.1(8)	C(27)-C(22)-C(23)	118.0(7)
C(27)-C(22)-C(15)	123.2(7)	C(23)-C(22)-C(15)	118.8(7)
C(24)-C(23)-C(22)	119.8(8)	C(23)-C(24)-C(25)	121.4(9)
C(26)-C(25)-C(24)	119.4(9)	C(25)-C(26)-C(27)	120.2(9)
C(22)-C(27)-C(26)	121.1(8)	O(2)-C(28)-Ru	172.8(7)
F(4)-P-F(2)	90.3(4)	F(4)-P-F(6)	179.2(4)
F(2)-P-F(6)	90.5(4)	F(4)-P-F(1)	89.5(4)
F(2)-P-F(1)	179.8(4)	F(6)-P-F(1)	89.8(4)
F(4)-P-F(3)	89.9(4)	F(2)-P-F(3)	89.9(4)
F(6)-P-F(3)	90.3(3)	F(1)-P-F(3)	90.0(4)
F(4)-P-F(5)	89.6(4)	F(2)-P-F(5)	89.9(5)
F(6)-P-F(5)	90.2(4)	F(1)-P-F(5)	90.2(4)
F(3)-P-F(5)	179.5(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2a".

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru	18(1)	21(1)	20(1)	0(1)	0(1)	1(1)
O(1)	27(3)	38(3)	33(3)	0(3)	5(3)	3(2)
O(2)	35(3)	32(3)	63(5)	-12(3)	-6(3)	7(2)
C(2)	26(3)	25(3)	27(4)	4(3)	-6(3)	2(3)
C(3)	39(4)	26(3)	15(3)	5(3)	-6(3)	-1(3)
C(4)	38(5)	37(4)	2(3)	-3(3)	-1(3)	0(4)
C(5)	33(4)	27(3)	25(4)	-2(3)	-15(3)	3(3)
C(1)	27(3)	32(4)	26(3)	3(3)	-5(3)	1(3)
C(7)	42(4)	33(4)	38(6)	3(5)	-5(5)	14(3)
C(8)	49(5)	25(4)	42(5)	9(4)	4(5)	-5(4)
C(9)	55(5)	61(7)	36(5)	-3(5)	12(4)	17(5)
C(10)	55(6)	37(4)	40(5)	-7(4)	-23(5)	2(4)
C(6)	20(3)	54(5)	42(5)	11(6)	-10(4)	-5(3)
C(11)	27(4)	33(4)	34(4)	6(4)	6(4)	-2(3)
C(12)	35(4)	28(4)	20(3)	5(3)	0(3)	-4(3)
C(13)	25(3)	26(4)	9(3)	0(3)	1(3)	5(3)
C(14)	28(3)	22(4)	15(3)	-4(3)	-2(3)	-1(3)
C(15)	24(3)	20(3)	25(4)	-5(3)	0(3)	2(3)
C(16)	29(3)	28(4)	15(3)	-1(3)	-2(3)	-5(3)
C(17)	32(4)	37(5)	21(4)	6(3)	2(3)	-8(3)
C(18)	38(4)	49(5)	29(5)	12(5)	-4(4)	-4(4)
C(19)	38(4)	33(5)	36(5)	7(4)	-5(4)	-4(4)
C(20)	38(5)	31(4)	31(5)	2(4)	0(4)	-3(3)
C(21)	32(4)	26(4)	29(4)	2(3)	4(3)	-2(3)
C(22)	27(3)	19(3)	26(4)	4(3)	-3(3)	1(3)
C(23)	36(4)	21(4)	30(4)	-2(3)	-1(4)	-4(3)
C(24)	48(5)	35(5)	43(5)	-2(4)	-7(5)	-15(4)
C(25)	31(4)	38(5)	63(8)	12(4)	4(4)	-5(3)
C(26)	41(5)	32(4)	39(5)	13(4)	15(4)	0(3)
C(27)	38(4)	24(4)	37(6)	-4(3)	9(3)	-3(3)
C(28)	26(3)	23(3)	23(5)	-3(3)	-4(3)	0(2)
P	31(1)	30(1)	35(1)	5(1)	0(1)	-1(1)
F(1)	73(4)	33(3)	59(4)	15(3)	11(4)	16(3)
F(2)	107(5)	30(3)	81(5)	2(3)	12(5)	16(3)
F(3)	36(2)	66(3)	52(5)	8(3)	-11(2)	-7(3)
F(4)	50(3)	54(3)	49(3)	13(3)	16(3)	-11(3)
F(5)	70(4)	94(5)	58(4)	6(4)	-34(4)	-28(4)
F(6)	63(4)	60(4)	45(3)	1(3)	25(3)	1(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2a".

	x	y	z	U(eq)
H(7A)	-9848(3)	-2088(10)	-12998(11)	57
H(7B)	-9687(3)	-835(10)	-14032(11)	57
H(7C)	-9386(3)	-1296(10)	-12882(11)	57
H(8A)	-8880(3)	-599(11)	-14759(11)	58
H(8B)	-8816(3)	-1159(11)	-16176(11)	58
H(8C)	-8480(3)	-1689(11)	-15131(11)	58
H(9A)	-8692(3)	-6025(14)	-17008(11)	76
H(9B)	-8380(3)	-4675(14)	-16456(11)	76
H(9C)	-8736(3)	-4185(14)	-17453(11)	76
H(10A)	-9670(3)	-7788(11)	-15406(10)	66
H(10B)	-9174(3)	-8010(11)	-15687(10)	66
H(10C)	-9477(3)	-7215(11)	-16716(10)	66
H(6A)	-10237(2)	-4604(11)	-13939(13)	46
H(6B)	-10069(2)	-6423(11)	-14046(13)	46
H(11A)	-9759(3)	-7739(10)	-12478(9)	37
H(11B)	-9803(3)	-7093(10)	-11076(9)	37
H(12)	-9017(3)	-7278(11)	-11621(8)	0(16)
H(13)	-9285(3)	-3905(10)	-11446(8)	13(19)
H(15)	-8682(2)	-2321(9)	-12466(8)	1(16)
H(17)	-8670(3)	-6135(11)	-9596(8)	36
H(18)	-8195(3)	-7801(11)	-8476(10)	47
H(19)	-7498(3)	-8270(11)	-9234(9)	43
H(20)	-7300(3)	-7165(10)	-11202(9)	40
H(21)	-7785(3)	-5641(10)	-12377(9)	34
H(23)	-8010(3)	-947(9)	-11435(9)	35
H(24)	-7298(3)	-274(11)	-11790(10)	50
H(25)	-6910(3)	-1495(11)	-13408(11)	53
H(26)	-7250(3)	-3335(10)	-14755(10)	45
H(27)	-7965(3)	-4058(10)	-14413(8)	40

Table 6. Crystal data and structure refinement for 7.

Identification code	sample7
Empirical formula	$C_{22}H_{25}F_6O_2PRu$
Formula weight	567.46
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 16.847(4) Å $\alpha = 90^\circ$ b = 14.805(4) Å $\beta = 90^\circ$ c = 18.318(5) Å $\gamma = 90^\circ$
Volume, Z	4569(2) $Å^3$, 8
Density (calculated)	1.650 Mg/m^3
Absorption coefficient	0.822 mm^{-1}
F(000)	2288
Crystal size	0.25 x 0.2 x 0.15 mm
θ range for data collection	2.14 to 27.56°
Limiting indices	$0 \le h \le 21$, $0 \le k \le 17$, $-23 \le \ell \le 0$
Reflections collected	5120
Independent reflections	5120 (R_{int} = 0.0000)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4399 / 0 / 413
Goodness-of-fit on F^2	1.036
Final R indices [I>2σ(I)]	R1 = 0.0722, wR2 = 0.1752
R indices (all data)	R1 = 0.1322, wR2 = 0.1935
Largest diff. peak and hole	4.189 and -0.822 $eÅ^{-3}$

Table 7. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 7. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru	5933(1)	7717(1)	-464(1)	41(1)
O(1)	6504(6)	5528(5)	-766(5)	108(3)
O(2)	5995(5)	9697(5)	-29(5)	117(3)
C(1)	5705(5)	6745(5)	-1333(4)	61(2)
C(2)	4991(5)	6836(5)	-931(4)	56(2)
C(3)	4747(4)	7741(5)	-975(4)	51(2)
C(4)	5306(4)	8208(4)	-1447(3)	46(2)
C(5)	5907(4)	7594(5)	-1662(4)	51(2)
C(6)	6165(8)	5878(7)	-1433(6)	100(4)
C(7)	4543(7)	6089(7)	-561(6)	95(4)
C(8)	3990(5)	8109(9)	-676(6)	84(3)
C(9)	5235(6)	9162(6)	-1710(5)	83(3)
C(10)	6570(6)	7774(8)	-2177(4)	82(3)
C(11)	7157(8)	6077(9)	-517(6)	99(4)
C(13)	6910(5)	6887(7)	-83(4)	67(2)
C(14)	6248(5)	6788(7)	429(4)	65(2)
C(15)	5959(5)	7521(6)	814(4)	57(2)
C(12)	7230(6)	7731(9)	-204(6)	79(3)
C(16)	5218(4)	7501(4)	1245(3)	44(2)
C(17)	5011(5)	8269(6)	1627(5)	69(2)
C(18)	4330(6)	8287(6)	2057(5)	76(3)
C(19)	3877(6)	7544(6)	2122(5)	69(2)
C(20)	4073(6)	6784(7)	1759(6)	82(3)
C(21)	4737(6)	6754(6)	1325(5)	73(2)
C(22)	5982(5)	8953(6)	-162(5)	64(2)
P	7550(1)	9897(1)	1757(1)	53(1)
F(1)	7553(45)	10086(36)	908(29)	146(21)
F(2)	7646(17)	9879(15)	2591(7)	58(6)
F(3)	8461(29)	10053(25)	1668(26)	82(14)
F(4)	7383(24)	10893(22)	1815(17)	86(10)
F(5)	6603(18)	9708(43)	1665(30)	111(18)
F(6)	7780(24)	8846(19)	1739(25)	91(13)
F(1')	7509(18)	10273(13)	2601(15)	75(7)
F(2')	7629(26)	9021(23)	2000(19)	94(9)
F(3')	7440(22)	10975(24)	1501(15)	81(8)
F(4')	7597(38)	9667(55)	881(36)	90(13)
F(5')	6732(27)	9769(40)	1842(31)	100(12)
F(6')	8477(22)	10075(40)	1830(26)	112(19)
F(1'')	7632(27)	9493(27)	2615(24)	91(15)
F(2'')	7418(56)	9804(76)	974(35)	134(35)
F(3'')	7848(35)	8792(34)	1515(37)	127(24)
F(4'')	7232(33)	10797(44)	2004(45)	166(39)
F(5'')	6652(34)	9379(40)	1822(34)	116(23)
F(6'')	8423(36)	10312(30)	1759(31)	52(10)

Table 8. Bond lengths [Å] and angles [°] for 7.

Ru-C(22)	1.914(8)	Ru-C(13)	2.169(7)
Ru-C(1)	2.181(7)	Ru-C(5)	2.202(7)
Ru-C(14)	2.202(7)	Ru-C(3)	2.207(6)
Ru-C(4)	2.211(6)	Ru-C(2)	2.227(7)
Ru-C(12)	2.236(9)	Ru-C(15)	2.359(7)
O(1)-C(11)	1.44(2)	O(1)-C(6)	1.445(13)
O(2)-C(22)	1.128(10)	C(1)-C(2)	1.417(11)
C(1)-C(5)	1.435(11)	C(1)-C(6)	1.511(12)
C(2)-C(3)	1.403(11)	C(2)-C(7)	1.500(11)
C(3)-C(4)	1.454(10)	C(3)-C(8)	1.491(11)
C(4)-C(5)	1.416(10)	C(4)-C(9)	1.497(10)
C(5)-C(10)	1.486(11)	C(6)-H(6A)	0.97
C(6)-H(6B)	0.97	C(7)-H(7A)	0.96
C(7)-H(7B)	0.96	C(7)-H(7C)	0.96
C(8)-H(8A)	0.96	C(8)-H(8B)	0.96
C(8)-H(8C)	0.96	C(9)-H(9A)	0.96
C(9)-H(9B)	0.96	C(9)-H(9C)	0.96
C(10)-H(10A)	0.96	C(10)-H(10B)	0.96
C(10)-H(10C)	0.96	C(11)-C(13)	1.498(14)
C(11)-H(11A)	0.97	C(11)-H(11B)	0.97
C(13)-C(12)	1.38(2)	C(13)-C(14)	1.465(12)
C(14)-C(15)	1.383(12)	C(14)-H(14)	1.14(9)
C(15)-C(16)	1.477(10)	C(15)-H(15)	1.10(7)
C(12)-H(12B)	0.91(8)	C(12)-H(12A)	0.98(10)
C(16)-C(21)	1.379(11)	C(16)-C(17)	1.379(11)
C(17)-C(18)	1.392(12)	C(17)-H(17A)	0.93
C(18)-C(19)	1.345(13)	C(18)-H(18A)	0.93
C(19)-C(20)	1.347(13)	C(19)-H(19A)	0.93
C(20)-C(21)	1.374(12)	C(20)-H(20A)	0.93
C(21)-H(21A)	0.93	P-F(2')	1.38(4)
P-F(5')	1.40(4)	P-F(2'')	1.46(6)
P-F(4)	1.51(3)	P-F(4'')	1.51(5)
P-F(2)	1.537(13)	P-F(3)	1.56(5)
P-F(1)	1.58(5)	P-F(6'')	1.59(5)
P-F(6)	1.60(2)	P-F(6')	1.59(4)
P-F(5)	1.63(4)		

C(22)-Ru-C(13)	114.6(4)	C(22)-Ru-C(1)	148.2(3)
C(13)-Ru-C(1)	89.7(3)	C(22)-Ru-C(5)	111.6(3)
C(13)-Ru-C(5)	106.8(3)	C(1)-Ru-C(5)	38.2(3)
C(22)-Ru-C(14)	111.9(4)	C(13)-Ru-C(14)	39.2(3)
C(1)-Ru-C(14)	99.9(4)	C(5)-Ru-C(14)	133.9(3)
C(22)-Ru-C(3)	98.4(3)	C(13)-Ru-C(3)	146.3(4)
C(1)-Ru-C(3)	62.7(3)	C(5)-Ru-C(3)	63.9(3)
C(14)-Ru-C(3)	122.9(3)	C(22)-Ru-C(4)	86.7(3)
C(13)-Ru-C(4)	144.1(3)	C(1)-Ru-C(4)	62.4(3)
C(5)-Ru-C(4)	37.4(3)	C(14)-Ru-C(4)	157.7(3)
C(3)-Ru-C(4)	38.4(3)	C(22)-Ru-C(2)	134.6(3)
C(13)-Ru-C(2)	109.4(4)	C(1)-Ru-C(2)	37.5(3)
C(5)-Ru-C(2)	63.5(3)	C(14)-Ru-C(2)	95.2(4)
C(3)-Ru-C(2)	36.9(3)	C(4)-Ru-C(2)	62.5(3)
C(22)-Ru-C(12)	83.6(4)	C(13)-Ru-C(12)	36.4(4)
C(1)-Ru-C(12)	109.5(4)	C(5)-Ru-C(12)	103.4(3)
C(14)-Ru-C(12)	67.2(4)	C(3)-Ru-C(12)	167.1(3)
C(4)-Ru-C(12)	129.6(3)	C(2)-Ru-C(12)	141.6(4)
C(22)-Ru-C(15)	80.2(3)	C(13)-Ru-C(15)	66.3(3)
C(1)-Ru-C(15)	130.3(3)	C(5)-Ru-C(15)	168.2(3)
C(14)-Ru-C(15)	35.1(3)	C(3)-Ru-C(15)	116.0(3)
C(4)-Ru-C(15)	140.9(3)	C(2)-Ru-C(15)	166.4(3)

C(12)-Ru-C(15)	76.8(3)	C(11)-O(1)-C(6)	111.5(9)
C(2)-C(1)-C(5)	109.7(7)	C(2)-C(1)-C(6)	125.4(8)
C(5)-C(1)-C(6)	124.9(8)	C(2)-C(1)-Ru	73.0(4)
C(5)-C(1)-Ru	71.7(4)	C(6)-C(1)-Ru	123.9(7)
C(3)-C(2)-C(1)	108.0(6)	C(3)-C(2)-C(7)	125.6(8)
C(1)-C(2)-C(7)	126.3(9)	C(3)-C(2)-Ru	70.8(4)
C(1)-C(2)-Ru	69.5(4)	C(7)-C(2)-Ru	128.1(6)
C(2)-C(3)-C(4)	107.4(6)	C(2)-C(3)-C(8)	125.3(8)
C(4)-C(3)-C(8)	126.8(8)	C(2)-C(3)-Ru	72.3(4)
C(4)-C(3)-Ru	70.9(4)	C(8)-C(3)-Ru	128.7(6)
C(5)-C(4)-C(3)	108.9(6)	C(5)-C(4)-C(9)	125.0(7)
C(3)-C(4)-C(9)	126.0(7)	C(5)-C(4)-Ru	71.0(4)
C(3)-C(4)-Ru	70.7(3)	C(9)-C(4)-Ru	127.6(5)
C(4)-C(5)-C(1)	106.0(6)	C(4)-C(5)-C(10)	126.8(8)
C(1)-C(5)-C(10)	127.0(8)	C(4)-C(5)-Ru	71.6(4)
C(1)-C(5)-Ru	70.1(4)	C(10)-C(5)-Ru	127.1(5)
O(1)-C(6)-C(1)	114.0(8)	O(1)-C(6)-H(6A)	108.8(6)
C(1)-C(6)-H(6A)	108.8(6)	O(1)-C(6)-H(6B)	108.8(6)
C(1)-C(6)-H(6B)	108.8(6)	H(6A)-C(6)-H(6B)	107.7
C(2)-C(7)-H(7A)	109.5(6)	C(2)-C(7)-H(7B)	109.5(5)
H(7A)-C(7)-H(7B)	109.5	C(2)-C(7)-H(7C)	109.5(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(6)	C(3)-C(8)-H(8B)	109.5(5)
H(8A)-C(8)-H(8B)	109.5	C(3)-C(8)-H(8C)	109.5(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(5)	C(4)-C(9)-H(9B)	109.5(4)
H(9A)-C(9)-H(9B)	109.5	C(4)-C(9)-H(9C)	109.5(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(5)	C(5)-C(10)-H(10B)	109.5(5)
H(10A)-C(10)-H(10B)	109.5	C(5)-C(10)-H(10C)	109.5(5)
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
O(1)-C(11)-C(13)	114.1(9)	O(1)-C(11)-H(11A)	108.7(5)
C(13)-C(11)-H(11A)	108.7(6)	O(1)-C(11)-H(11B)	108.7(5)
C(13)-C(11)-H(11B)	108.7(5)	H(11A)-C(11)-H(11B)	107.6
C(12)-C(13)-C(14)	119.4(9)	C(12)-C(13)-C(11)	122.2(9)
C(14)-C(13)-C(11)	118.1(10)	C(12)-C(13)-Ru	74.4(5)
C(14)-C(13)-Ru	71.6(4)	C(11)-C(13)-Ru	119.6(7)
C(15)-C(14)-C(13)	121.1(10)	C(15)-C(14)-Ru	78.7(5)
C(13)-C(14)-Ru	69.2(4)	C(15)-C(14)-H(14)	117(4)
C(13)-C(14)-H(14)	121(4)	Ru-C(14)-H(14)	116(4)
C(14)-C(15)-C(16)	123.7(8)	C(14)-C(15)-Ru	66.3(4)
C(16)-C(15)-Ru	121.2(5)	C(14)-C(15)-H(15)	120(3)
C(16)-C(15)-H(15)	115(3)	Ru-C(15)-H(15)	93(3)
C(13)-C(12)-Ru	69.1(5)	C(13)-C(12)-H(12B)	122(5)
Ru-C(12)-H(12B)	123(5)	C(13)-C(12)-H(12A)	124(5)
Ru-C(12)-H(12A)	112(5)	H(12B)-C(12)-H(12A)	104(7)
C(21)-C(16)-C(17)	117.3(7)	C(21)-C(16)-C(15)	124.7(7)
C(17)-C(16)-C(15)	117.9(7)	C(16)-C(17)-C(18)	120.8(8)
C(16)-C(17)-H(17A)	119.6(5)	C(18)-C(17)-H(17A)	119.6(6)
C(19)-C(18)-C(17)	120.2(8)	C(19)-C(18)-H(18A)	119.9(6)
C(17)-C(18)-H(18A)	119.9(6)	C(18)-C(19)-C(20)	120.0(9)
C(18)-C(19)-H(19A)	120.0(6)	C(20)-C(19)-H(19A)	120.0(6)
C(19)-C(20)-C(21)	120.8(9)	C(19)-C(20)-H(20A)	119.6(6)
C(21)-C(20)-H(20A)	119.6(6)	C(20)-C(21)-C(16)	120.9(8)
C(20)-C(21)-H(21A)	119.5(6)	C(16)-C(21)-H(21A)	119.5(4)
O(2)-C(22)-Ru	175.4(8)	F(2')-P-F(5')	86(3)
F(2'')-P-F(4'')	109(6)	F(4)-P-F(2)	88.0(14)
F(4)-P-F(3)	93(2)	F(2)-P-F(3)	90(2)
F(4)-P-F(1)	84(3)	F(2)-P-F(1)	169(2)
F(3)-P-F(1)	82(3)	F(2'')-P-F(6'')	100(4)
F(4'')-P-F(6'')	89(3)	F(4)-P-F(6)	176(2)
F(2)-P-F(6)	89(2)	F(3)-P-F(6)	85(2)
F(1)-P-F(6)	99(3)	F(2')-P-F(6')	92(3)

F(5')-P-F(6')	169(3)	F(4)-P-F(5)	90(3)
F(2)-P-F(5)	102(2)	F(3)-P-F(5)	168(3)
F(1)-P-F(5)	86(3)	F(6)-P-F(5)	94(3)

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters [$Å^2$ x 10^3] for 7.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru	37(1)	52(1)	33(1)	3(1)	-2(1)	3(1)
O(1)	170(8)	66(5)	88(5)	-3(4)	24(6)	63(5)
O(2)	168(8)	58(4)	124(7)	-24(5)	-43(6)	-7(5)
C(1)	90(6)	48(4)	45(4)	-8(3)	0(4)	6(4)
C(2)	66(5)	49(4)	52(4)	4(3)	-6(3)	-21(4)
C(3)	38(3)	72(5)	42(3)	-1(3)	-8(3)	4(3)
C(4)	58(4)	41(4)	40(3)	5(3)	-7(3)	6(3)
C(5)	56(4)	66(5)	30(3)	-7(3)	0(3)	2(4)
C(6)	157(10)	64(6)	79(7)	-22(5)	6(7)	46(7)
C(7)	117(9)	77(7)	92(7)	15(6)	-14(6)	-51(6)
C(8)	44(4)	111(8)	97(7)	-9(7)	-4(4)	12(5)
C(9)	109(7)	65(6)	73(6)	26(5)	-21(6)	4(5)
C(10)	76(6)	136(9)	34(4)	-1(5)	13(4)	-1(6)
C(11)	118(9)	104(9)	75(6)	15(6)	16(6)	72(8)
C(13)	69(5)	80(6)	51(4)	9(4)	1(4)	39(5)
C(14)	63(4)	96(7)	36(3)	20(4)	3(3)	30(5)
C(15)	62(4)	77(6)	31(3)	8(3)	-8(3)	12(4)
C(12)	48(4)	134(10)	54(5)	1(6)	-7(4)	6(6)
C(16)	61(4)	41(4)	29(3)	3(2)	3(3)	4(3)
C(17)	73(5)	64(5)	69(5)	-8(4)	6(4)	-4(4)
C(18)	82(6)	64(6)	81(6)	-14(5)	18(5)	14(5)
C(19)	59(5)	85(7)	63(5)	6(4)	9(4)	7(4)
C(20)	101(7)	63(6)	82(6)	1(5)	26(6)	-13(5)
C(21)	101(7)	50(5)	69(5)	1(4)	29(5)	13(5)
C(22)	87(6)	46(4)	59(4)	-13(4)	-22(4)	1(4)
P	53(1)	59(1)	46(1)	11(1)	-5(1)	-8(1)
F(1)	207(33)	156(44)	76(22)	61(27)	-60(21)	-70(32)
F(2)	126(16)	28(14)	21(6)	10(9)	0(7)	-22(15)
F(3)	81(18)	54(24)	111(27)	-51(15)	38(16)	-1(17)
F(4)	130(23)	63(15)	63(14)	10(13)	-30(17)	-9(14)
F(5)	18(9)	126(28)	189(48)	-4(25)	-32(15)	-10(12)
F(6)	142(22)	30(12)	102(29)	-18(14)	-16(21)	53(12)
F(1')	129(16)	17(11)	80(12)	7(9)	30(11)	5(12)
F(2')	138(26)	43(16)	101(24)	-19(14)	-3(17)	12(14)
F(3')	98(16)	68(13)	77(18)	41(16)	1(15)	17(10)
F(4')	118(19)	113(33)	40(19)	-24(18)	3(18)	-43(22)
F(5')	80(26)	112(26)	107(19)	32(18)	-29(17)	-61(18)
F(6')	43(15)	152(38)	142(31)	46(22)	-46(17)	-17(16)
F(1'')	107(20)	70(28)	95(25)	57(22)	-9(15)	-18(21)
F(2'')	283(89)	92(44)	28(15)	-6(22)	39(27)	-28(51)
F(3'')	150(33)	86(27)	144(43)	-71(23)	31(25)	-48(26)
F(4'')	119(28)	108(48)	271(93)	-93(56)	71(38)	41(29)
F(5'')	89(30)	166(52)	93(23)	-11(29)	16(21)	-111(35)
F(6'')	67(20)	33(18)	55(16)	-41(16)	37(14)	-18(17)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 7.

	x	y	z	U(eq)
H(6A)	5814(8)	5425(7)	-1639(6)	120
H(6B)	6589(8)	5983(7)	-1781(6)	120
H(7A)	4834(7)	5534(7)	-608(6)	143
H(7B)	4031(7)	6022(7)	-786(6)	143
H(7C)	4477(7)	6231(7)	-53(6)	143
H(8A)	3961(5)	8745(9)	-775(6)	126
H(8B)	3972(5)	8010(9)	-159(6)	126
H(8C)	3549(5)	7808(9)	-903(6)	126
H(9A)	4781(6)	9441(6)	-1488(5)	124
H(9B)	5173(6)	9165(6)	-2231(5)	124
H(9C)	5705(6)	9491(6)	-1581(5)	124
H(10A)	6891(6)	7242(8)	-2224(4)	123
H(10B)	6889(6)	8261(8)	-1993(4)	123
H(10C)	6359(6)	7937(8)	-2645(4)	123
H(11A)	7459(8)	6278(9)	-938(6)	118
H(11B)	7505(8)	5708(9)	-219(6)	118
H(17A)	5329(5)	8780(6)	1596(5)	82
H(18A)	4189(6)	8814(6)	2300(5)	91
H(19A)	3428(6)	7554(6)	2417(5)	83
H(20A)	3754(6)	6274(7)	1803(6)	99
H(21A)	4864(6)	6222(6)	1081(5)	88
H(12B)	7615(48)	7829(48)	-544(41)	49(21)
H(14)	5888(44)	6132(67)	454(43)	66(26)
H(12A)	7356(52)	8160(64)	188(53)	76(27)
H(15)	6333(38)	8122(46)	896(34)	37(16)

Figure 1. 2D ^{1}H EXSY NMR spectrum of the mixture of isomers **2a'** and **2a''** (high field region) in acetone-d_6 at 300K. Initial delay 2 s, τ_m = 1 s, number of scans 256, a matrix 1024×256 was acquired by the TPPI technique and zero-filled to the size 1024×1024.