Supporting Information

Pentamethylcyclopentadienyl Ruthenium Complexes with Sulfur and Selenium Donor Ligands

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X-ray Crystallographic Data for

(1) $[Cp^*Ru(NO)(SC_6F_4H)_2]$ (**1**)

(2) $[Cp^*Ru(PMe_3)_2(SC_6F_4H)_2]$ (**6**)

(3) $[Cp^*Ru\{\eta^2\text{-}Se_2P(i\text{-}Pr)_2\}\{\eta^2\text{-}SeP(i\text{-}Pr)_2\}][PF_6]$ (**7**)

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Table 1. Crystal data and structure refinement for wy0390wm.

Identification code	wy0390wm
Empirical formula	$C_{22}H_{34}F_4P_2RuS$
Formula weight	569.56
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 9.0410(6) Å alpha = 90° b = 15.8143(10) Å beta = 90° c = 35.550(2) Å gamma = 90°
Volume, Z	5082.8(6) $Å^3$, 8
Density (calculated)	1.489 Mg/m^3
Absorption coefficient	0.861 mm^{-1}
F(000)	2336
Crystal size	0.42 x 0.30 x 0.14 mm
θ range for data collection	1.41 to 27.50°
Limiting indices	$-11 \le h \le 11$, $-20 \le k \le 20$, $-46 \le l \le 37$
Reflections collected	29632
Independent reflections	11286 (R_{int} = 0.0244)
Completeness to θ = 27.50°	98.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11286 / 0 / 542
Goodness-of-fit on F^2	0.777
Final R indices [I>2σ(I)]	R1 = 0.0292, wR2 = 0.0785
R indices (all data)	R1 = 0.0362, wR2 = 0.0826
Absolute structure parameter	0.01(2)
Extinction coefficient	0.00000(8)
Largest diff. peak and hole	0.405 and -0.402 $eÅ^{-3}$

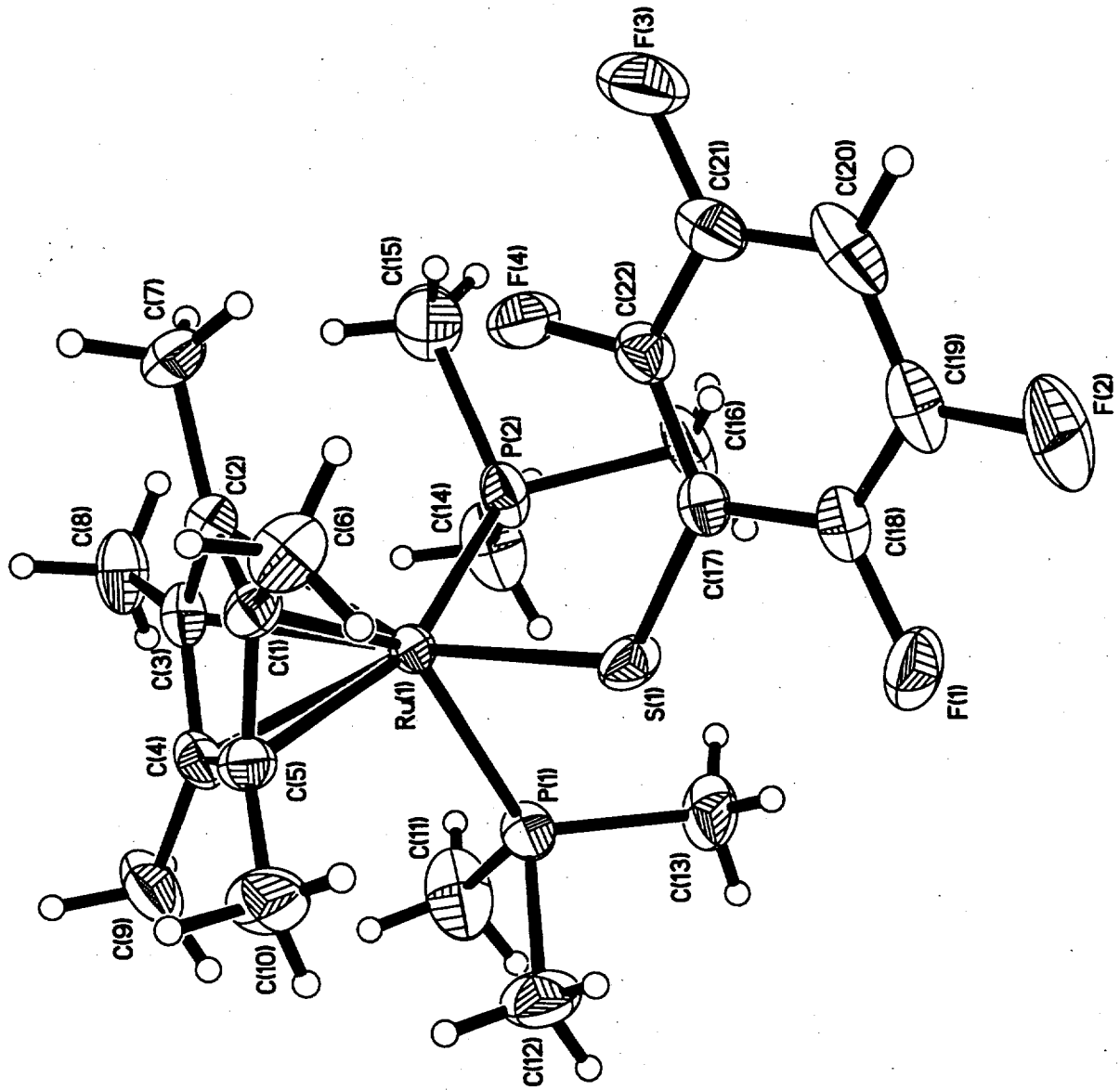
F(3)
C(21)
C(20)
C(15)
F(4)
C(22)
C(7)
C(19)
F(2)
C(16)
P(2)
C(2)
C(14)
C(8)
C(6)
C(18)
C(17)
C(3)
C(1)
Ru(1)
S(1)
F(1)
C(4)
C(5)
P(1)
C(11)
C(13)
C(9)
C(10)
C(12)

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for wy0390wm. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	4251(4)	1040(2)	7493(1)	51(1)
C(2)	2886(4)	647(2)	7422(1)	50(1)
C(3)	1831(4)	1285(2)	7328(1)	54(1)
C(4)	2584(5)	2063(2)	7322(1)	60(1)
C(5)	4090(5)	1924(2)	7434(1)	56(1)
C(6)	5682(5)	600(3)	7578(1)	78(1)
C(7)	2679(6)	-299(2)	7377(1)	77(1)
C(8)	280(5)	1136(3)	7181(1)	84(1)
C(9)	2002(7)	2882(3)	7158(1)	102(2)
C(10)	5376(6)	2536(3)	7437(2)	94(2)
C(11)	329(7)	3420(4)	8003(2)	116(2)
C(12)	3377(6)	3634(3)	8126(2)	98(2)
C(13)	1595(6)	2905(3)	8683(1)	88(2)
C(14)	-1090(5)	1387(4)	8234(1)	103(2)
C(15)	204(7)	-172(3)	8088(2)	112(2)
C(16)	1017(6)	694(4)	8740(1)	99(2)
C(17)	5092(4)	657(2)	8606(1)	49(1)
C(18)	6139(4)	745(3)	8892(1)	57(1)
C(19)	6863(4)	90(3)	9049(1)	72(1)
C(20)	6602(5)	-741(4)	8935(1)	83(2)
C(21)	5527(5)	-856(3)	8666(1)	66(1)
C(22)	4794(4)	-183(2)	8506(1)	57(1)
C(23)	6266(4)	4531(2)	9024(1)	53(1)
C(24)	6424(4)	5430(2)	8970(1)	50(1)
C(25)	5646(4)	5850(2)	9255(1)	50(1)
C(26)	5018(4)	5225(2)	9502(1)	51(1)
C(27)	5366(4)	4420(2)	9346(1)	54(1)
C(28)	6789(6)	3867(3)	8752(1)	85(2)
C(29)	7110(5)	5816(3)	8633(1)	78(1)
C(30)	5314(6)	6793(3)	9265(1)	78(1)
C(31)	3908(5)	5369(3)	9805(1)	86(1)
C(32)	4623(5)	3599(3)	9460(2)	92(2)
C(33)	8613(5)	2965(2)	9522(1)	73(1)
C(34)	7177(5)	3388(2)	10202(1)	72(1)
C(35)	10112(5)	3881(2)	10066(1)	66(1)
C(36)	7555(6)	5481(2)	10511(1)	70(1)
C(37)	9979(4)	6157(2)	10114(1)	63(1)
C(38)	7183(5)	6924(2)	10085(1)	60(1)
C(39)	10554(4)	5994(2)	9043(1)	45(1)
C(40)	10038(4)	6818(2)	9075(1)	54(1)
C(41)	10643(5)	7495(2)	8874(1)	62(1)
C(42)	11802(5)	7388(3)	8633(1)	73(1)
C(43)	12322(5)	6580(3)	8597(1)	66(1)
C(44)	11753(4)	5911(2)	8792(1)	55(1)
F(1)	6496(3)	1524(2)	9012(1)	82(1)
F(2)	7889(3)	217(2)	9316(1)	115(1)

F(3)	5184(4)	-1642(2)	8548(1)	103(1)
F(4)	3787(3)	-366(1)	8247(1)	88(1)
F(5)	8912(3)	7009(1)	9308(1)	81(1)
F(6)	10050(3)	8276(2)	8929(1)	96(1)
F(7)	13474(4)	6439(2)	8361(1)	108(1)
F(8)	12354(3)	5142(1)	8742(1)	81(1)
P(1)	1938(1)	2832(1)	8174(1)	60(1)
P(2)	747(1)	885(1)	8235(1)	64(1)
P(3)	8310(1)	3874(1)	9831(1)	44(1)
P(4)	8030(1)	5878(1)	10040(1)	42(1)
Ru(1)	2574(1)	1557(1)	7907(1)	38(1)
Ru(2)	7443(1)	5058(1)	9528(1)	34(1)
S(1)	4360(1)	1574(1)	8410(1)	60(1)
S(2)	9901(1)	5084(1)	9262(1)	55(1)

Table 3. Bond lengths [Å] and angles [°] for wy0390wm.

C(1)-C(2)	1.404(5)	C(1)-C(5)	1.421(5)
C(1)-C(6)	1.500(5)	C(1)-Ru(1)	2.266(3)
C(2)-C(3)	1.429(5)	C(2)-C(7)	1.516(5)
C(2)-Ru(1)	2.262(3)	C(3)-C(4)	1.406(5)
C(3)-C(8)	1.515(6)	C(3)-Ru(1)	2.207(3)
C(4)-C(5)	1.435(6)	C(4)-C(9)	1.515(5)
C(4)-Ru(1)	2.227(3)	C(5)-C(10)	1.513(6)
C(5)-Ru(1)	2.244(4)	C(11)-P(1)	1.830(5)
C(12)-P(1)	1.825(5)	C(13)-P(1)	1.840(4)
C(14)-P(2)	1.841(5)	C(15)-P(2)	1.820(5)
C(16)-P(2)	1.838(4)	C(17)-C(18)	1.396(5)
C(17)-C(22)	1.401(5)	C(17)-S(1)	1.740(3)
C(18)-F(1)	1.344(5)	C(18)-C(19)	1.345(6)
C(19)-F(2)	1.343(5)	C(19)-C(20)	1.395(7)
C(20)-C(21)	1.377(7)	C(21)-F(3)	1.349(5)
C(21)-C(22)	1.376(5)	C(22)-F(4)	1.327(4)
C(23)-C(27)	1.415(5)	C(23)-C(24)	1.442(5)
C(23)-C(28)	1.504(5)	C(23)-Ru(2)	2.245(3)
C(24)-C(25)	1.399(5)	C(24)-C(29)	1.482(5)
C(24)-Ru(2)	2.264(3)	C(25)-C(26)	1.439(5)
C(25)-C(30)	1.522(5)	C(25)-Ru(2)	2.270(3)
C(26)-C(27)	1.424(5)	C(26)-C(31)	1.491(5)
C(26)-Ru(2)	2.211(3)	C(27)-C(32)	1.517(5)
C(27)-Ru(2)	2.228(3)	C(33)-P(3)	1.829(4)
C(34)-P(3)	1.839(4)	C(35)-P(3)	1.831(4)
C(36)-P(4)	1.841(3)	C(37)-P(4)	1.836(4)
C(38)-P(4)	1.830(3)	C(39)-C(40)	1.390(5)
C(39)-C(44)	1.410(5)	C(39)-S(2)	1.738(3)
C(40)-F(5)	1.347(4)	C(40)-C(41)	1.399(5)
C(41)-F(6)	1.361(5)	C(41)-C(42)	1.363(6)
C(42)-C(43)	1.368(6)	C(43)-F(7)	1.357(5)
C(43)-C(44)	1.365(5)	C(44)-F(8)	1.344(4)
P(1)-Ru(1)	2.3019(10)	P(2)-Ru(1)	2.2845(10)
P(3)-Ru(2)	2.2977(8)	P(4)-Ru(2)	2.2958(8)
Ru(1)-S(1)	2.4104(9)	Ru(2)-S(2)	2.4156(9)

C(2)-C(1)-C(5)	108.6(3)	C(2)-C(1)-C(6)	126.1(3)
C(5)-C(1)-C(6)	125.1(4)	C(2)-C(1)-Ru(1)	71.8(2)
C(5)-C(1)-Ru(1)	70.8(2)	C(6)-C(1)-Ru(1)	127.8(3)
C(1)-C(2)-C(3)	108.4(3)	C(1)-C(2)-C(7)	124.3(4)
C(3)-C(2)-C(7)	126.1(4)	C(1)-C(2)-Ru(1)	72.10(19)
C(3)-C(2)-Ru(1)	69.27(19)	C(7)-C(2)-Ru(1)	134.0(3)
C(4)-C(3)-C(2)	107.4(3)	C(4)-C(3)-C(8)	125.4(4)
C(2)-C(3)-C(8)	126.0(4)	C(4)-C(3)-Ru(1)	72.3(2)
C(2)-C(3)-Ru(1)	73.46(19)	C(8)-C(3)-Ru(1)	129.3(3)
C(3)-C(4)-C(5)	108.7(3)	C(3)-C(4)-C(9)	125.8(5)
C(5)-C(4)-C(9)	124.6(4)	C(3)-C(4)-Ru(1)	70.72(18)
C(5)-C(4)-Ru(1)	71.9(2)	C(9)-C(4)-Ru(1)	131.7(3)
C(1)-C(5)-C(4)	106.8(3)	C(1)-C(5)-C(10)	123.3(4)
C(4)-C(5)-C(10)	129.2(4)	C(1)-C(5)-Ru(1)	72.5(2)
C(4)-C(5)-Ru(1)	70.7(2)	C(10)-C(5)-Ru(1)	129.1(3)
C(18)-C(17)-C(22)	114.2(3)	C(18)-C(17)-S(1)	117.8(3)
C(22)-C(17)-S(1)	128.0(3)	F(1)-C(18)-C(19)	117.3(4)
F(1)-C(18)-C(17)	119.0(3)	C(19)-C(18)-C(17)	123.7(4)
F(2)-C(19)-C(18)	120.9(5)	F(2)-C(19)-C(20)	117.5(4)

C(18)-C(19)-C(20)	121.6(4)	C(21)-C(20)-C(19)	116.4(4)
F(3)-C(21)-C(22)	118.3(4)	F(3)-C(21)-C(20)	120.1(4)
C(22)-C(21)-C(20)	121.7(4)	F(4)-C(22)-C(21)	116.7(4)
F(4)-C(22)-C(17)	121.0(3)	C(21)-C(22)-C(17)	122.3(4)
C(27)-C(23)-C(24)	106.6(3)	C(27)-C(23)-C(28)	127.9(4)
C(24)-C(23)-C(28)	124.9(4)	C(27)-C(23)-Ru(2)	70.93(19)
C(24)-C(23)-Ru(2)	72.07(19)	C(28)-C(23)-Ru(2)	128.6(3)
C(25)-C(24)-C(23)	108.8(3)	C(25)-C(24)-C(29)	126.9(4)
C(23)-C(24)-C(29)	123.6(4)	C(25)-C(24)-Ru(2)	72.25(19)
C(23)-C(24)-Ru(2)	70.64(19)	C(29)-C(24)-Ru(2)	130.3(3)
C(24)-C(25)-C(26)	108.3(3)	C(24)-C(25)-C(30)	125.6(4)
C(26)-C(25)-C(30)	125.5(4)	C(24)-C(25)-Ru(2)	71.8(2)
C(26)-C(25)-Ru(2)	69.06(18)	C(30)-C(25)-Ru(2)	132.2(3)
C(27)-C(26)-C(25)	106.8(3)	C(27)-C(26)-C(31)	124.6(4)
C(25)-C(26)-C(31)	127.0(4)	C(27)-C(26)-Ru(2)	72.0(2)
C(25)-C(26)-Ru(2)	73.5(2)	C(31)-C(26)-Ru(2)	130.9(3)
C(23)-C(27)-C(26)	109.3(3)	C(23)-C(27)-C(32)	125.3(4)
C(26)-C(27)-C(32)	124.2(4)	C(23)-C(27)-Ru(2)	72.2(2)
C(26)-C(27)-Ru(2)	70.62(19)	C(32)-C(27)-Ru(2)	133.0(3)
C(40)-C(39)-C(44)	113.4(3)	C(40)-C(39)-S(2)	128.7(3)
C(44)-C(39)-S(2)	117.9(3)	F(5)-C(40)-C(39)	121.0(3)
F(5)-C(40)-C(41)	116.0(3)	C(39)-C(40)-C(41)	123.0(3)
F(6)-C(41)-C(42)	120.4(4)	F(6)-C(41)-C(40)	117.8(4)
C(42)-C(41)-C(40)	121.8(4)	C(41)-C(42)-C(43)	116.0(4)
F(7)-C(43)-C(44)	118.4(4)	F(7)-C(43)-C(42)	118.4(4)
C(44)-C(43)-C(42)	123.2(4)	F(8)-C(44)-C(43)	118.8(3)
F(8)-C(44)-C(39)	118.6(3)	C(43)-C(44)-C(39)	122.6(4)
C(12)-P(1)-C(11)	100.5(3)	C(12)-P(1)-C(13)	99.8(2)
C(11)-P(1)-C(13)	99.3(2)	C(12)-P(1)-Ru(1)	113.03(16)
C(11)-P(1)-Ru(1)	120.4(2)	C(13)-P(1)-Ru(1)	120.17(16)
C(15)-P(2)-C(16)	99.5(3)	C(15)-P(2)-C(14)	98.8(3)
C(16)-P(2)-C(14)	101.1(2)	C(15)-P(2)-Ru(1)	118.42(19)
C(16)-P(2)-Ru(1)	118.62(17)	C(14)-P(2)-Ru(1)	116.78(18)
C(33)-P(3)-C(35)	98.4(2)	C(33)-P(3)-C(34)	100.8(2)
C(35)-P(3)-C(34)	99.8(2)	C(33)-P(3)-Ru(2)	114.16(14)
C(35)-P(3)-Ru(2)	120.80(12)	C(34)-P(3)-Ru(2)	119.12(14)
C(38)-P(4)-C(37)	99.86(18)	C(38)-P(4)-C(36)	97.48(18)
C(37)-P(4)-C(36)	100.0(2)	C(38)-P(4)-Ru(2)	118.92(12)
C(37)-P(4)-Ru(2)	118.21(13)	C(36)-P(4)-Ru(2)	118.35(13)
C(3)-Ru(1)-C(4)	36.97(14)	C(3)-Ru(1)-C(5)	62.51(14)
C(4)-Ru(1)-C(5)	37.45(16)	C(3)-Ru(1)-C(2)	37.27(12)
C(4)-Ru(1)-C(2)	61.15(12)	C(5)-Ru(1)-C(2)	61.22(13)
C(3)-Ru(1)-C(1)	61.81(13)	C(4)-Ru(1)-C(1)	61.35(14)
C(5)-Ru(1)-C(1)	36.72(13)	C(2)-Ru(1)-C(1)	36.13(13)
C(3)-Ru(1)-P(2)	99.50(11)	C(4)-Ru(1)-P(2)	130.27(13)
C(5)-Ru(1)-P(2)	160.73(10)	C(2)-Ru(1)-P(2)	100.53(9)
C(1)-Ru(1)-P(2)	130.36(10)	C(3)-Ru(1)-P(1)	118.63(10)
C(4)-Ru(1)-P(1)	94.09(9)	C(5)-Ru(1)-P(1)	103.59(9)
C(2)-Ru(1)-P(1)	154.50(9)	C(1)-Ru(1)-P(1)	138.72(9)
P(2)-Ru(1)-P(1)	90.92(4)	C(3)-Ru(1)-S(1)	153.94(10)
C(4)-Ru(1)-S(1)	133.33(13)	C(5)-Ru(1)-S(1)	98.27(11)
C(2)-Ru(1)-S(1)	119.26(9)	C(1)-Ru(1)-S(1)	92.20(10)
P(2)-Ru(1)-S(1)	96.34(4)	P(1)-Ru(1)-S(1)	81.47(4)
C(26)-Ru(2)-C(27)	37.41(13)	C(26)-Ru(2)-C(23)	62.63(14)
C(27)-Ru(2)-C(23)	36.88(14)	C(26)-Ru(2)-C(24)	61.85(13)
C(27)-Ru(2)-C(24)	61.31(12)	C(23)-Ru(2)-C(24)	37.29(13)
C(26)-Ru(2)-C(25)	37.43(13)	C(27)-Ru(2)-C(25)	61.44(13)
C(23)-Ru(2)-C(25)	61.56(13)	C(24)-Ru(2)-C(25)	35.95(13)
C(26)-Ru(2)-P(4)	101.27(10)	C(27)-Ru(2)-P(4)	132.94(11)

C(23)-Ru(2)-P(4)	162.12(10)	C(24)-Ru(2)-P(4)	129.83(9)
C(25)-Ru(2)-P(4)	101.10(9)	C(26)-Ru(2)-P(3)	117.10(10)
C(27)-Ru(2)-P(3)	93.15(9)	C(23)-Ru(2)-P(3)	103.50(10)
C(24)-Ru(2)-P(3)	139.56(9)	C(25)-Ru(2)-P(3)	153.43(10)
P(4)-Ru(2)-P(3)	90.60(3)	C(26)-Ru(2)-S(2)	153.34(10)
C(27)-Ru(2)-S(2)	132.00(11)	C(23)-Ru(2)-S(2)	97.44(11)
C(24)-Ru(2)-S(2)	91.52(10)	C(25)-Ru(2)-S(2)	118.76(10)
P(4)-Ru(2)-S(2)	95.03(3)	P(3)-Ru(2)-S(2)	83.35(3)
C(17)-S(1)-Ru(1)	122.88(12)	C(39)-S(2)-Ru(2)	120.15(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for wy0390wm.

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
C(1)	48(2)	50(2)	55(2)	-11(2)	6(2)	3(2)
C(2)	55(2)	49(2)	47(2)	-3(1)	-3(1)	-2(1)
C(3)	53(2)	72(2)	37(2)	-1(2)	-4(2)	8(2)
C(4)	82(3)	55(2)	42(2)	9(1)	15(2)	17(2)
C(5)	64(2)	49(2)	57(2)	-6(2)	17(2)	-5(2)
C(6)	54(2)	85(3)	96(3)	-21(3)	-1(2)	16(2)
C(7)	106(4)	52(2)	74(2)	-15(2)	-17(3)	-11(2)
C(8)	64(3)	136(4)	52(2)	-2(2)	-20(2)	13(3)
C(9)	155(6)	88(3)	61(3)	29(2)	16(3)	35(3)
C(10)	94(4)	81(3)	106(4)	-9(3)	46(3)	-29(3)
C(11)	129(5)	130(5)	88(4)	2(3)	3(3)	88(4)
C(12)	129(5)	51(2)	112(4)	-17(2)	24(4)	-3(3)
C(13)	116(4)	93(3)	54(2)	-19(2)	11(3)	35(3)
C(14)	46(2)	180(6)	84(3)	23(4)	9(2)	-10(3)
C(15)	122(5)	128(5)	86(4)	5(3)	5(3)	-79(4)
C(16)	97(4)	150(5)	52(3)	46(3)	-6(2)	-32(3)
C(17)	44(2)	61(2)	42(2)	2(2)	-2(2)	5(2)
C(18)	44(2)	88(3)	40(2)	8(2)	-1(2)	-3(2)
C(19)	48(2)	122(4)	46(2)	24(2)	-2(2)	0(2)
C(20)	61(3)	123(4)	65(3)	45(3)	11(2)	29(3)
C(21)	75(3)	57(2)	66(2)	15(2)	14(2)	14(2)
C(22)	59(2)	56(2)	55(2)	8(2)	-6(2)	8(2)
C(23)	62(2)	52(2)	44(2)	-6(2)	-13(2)	-2(2)
C(24)	56(2)	52(2)	41(2)	6(2)	-4(2)	-5(2)
C(25)	49(2)	49(2)	52(2)	-1(2)	-12(2)	5(2)
C(26)	32(2)	73(2)	48(2)	6(2)	-4(1)	0(2)
C(27)	49(2)	54(2)	60(2)	7(2)	-12(2)	-17(2)
C(28)	120(4)	71(3)	63(3)	-25(2)	-13(3)	0(3)
C(29)	88(4)	101(3)	45(2)	18(2)	0(2)	-8(3)
C(30)	90(3)	61(2)	83(3)	8(2)	-30(3)	19(2)
C(31)	49(2)	130(4)	81(3)	2(3)	17(2)	2(3)
C(32)	84(3)	79(3)	113(4)	26(3)	-26(3)	-47(3)
C(33)	94(3)	41(2)	84(3)	-10(2)	-12(2)	13(2)
C(34)	84(3)	52(2)	79(3)	23(2)	5(2)	-15(2)
C(35)	59(2)	47(2)	91(3)	12(2)	-20(2)	4(2)
C(36)	97(3)	71(2)	43(2)	-3(2)	1(3)	5(3)
C(37)	56(2)	50(2)	82(3)	-11(2)	-14(2)	-8(2)
C(38)	72(3)	46(2)	64(2)	-11(2)	-3(2)	14(2)
C(39)	42(2)	49(2)	44(2)	-3(1)	2(1)	-7(1)
C(40)	48(2)	53(2)	59(2)	3(2)	8(2)	-5(2)
C(41)	65(3)	50(2)	71(2)	12(2)	-6(2)	-8(2)
C(42)	65(3)	92(3)	61(2)	26(2)	-2(2)	-31(2)
C(43)	59(2)	93(3)	46(2)	-5(2)	11(2)	-21(2)
C(44)	48(2)	67(2)	50(2)	-8(2)	8(2)	-12(2)
F(1)	80(2)	104(2)	61(1)	-14(1)	-22(1)	-16(2)
F(2)	74(2)	192(3)	80(2)	40(2)	-37(2)	4(2)
F(3)	136(3)	56(1)	116(2)	21(2)	12(2)	18(2)
F(4)	119(2)	46(1)	98(2)	-2(1)	-51(2)	0(1)

F(5)	79(2)	49(1)	114(2)	10(1)	42(2)	8(1)
F(6)	103(2)	51(1)	134(2)	25(1)	5(2)	-6(1)
F(7)	98(2)	137(3)	90(2)	3(2)	51(2)	-22(2)
F(8)	72(2)	77(1)	95(2)	-20(1)	33(1)	2(1)
P(1)	72(1)	55(1)	52(1)	0(1)	7(1)	24(1)
P(2)	56(1)	95(1)	43(1)	14(1)	-4(1)	-24(1)
P(3)	50(1)	30(1)	52(1)	4(1)	-3(1)	-1(1)
P(4)	46(1)	35(1)	43(1)	-4(1)	-2(1)	1(1)
Ru(1)	37(1)	39(1)	37(1)	3(1)	-2(1)	2(1)
Ru(2)	35(1)	30(1)	37(1)	1(1)	2(1)	-3(1)
S(1)	65(1)	43(1)	73(1)	-8(1)	-31(1)	3(1)
S(2)	49(1)	42(1)	75(1)	7(1)	23(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for wy0390wm.

	x	y	z	U(eq)
H(6A)	6160	445	7347	118
H(6B)	5488	100	7723	118
H(6C)	6313	972	7718	118
H(7A)	2930	-460	7124	116
H(7B)	1667	-443	7426	116
H(7C)	3310	-591	7551	116
H(8A)	318	1029	6915	126
H(8B)	-316	1627	7228	126
H(8C)	-145	656	7307	126
H(9A)	2210	2898	6893	152
H(9B)	2474	3352	7279	152
H(9C)	953	2914	7197	152
H(10A)	5803	2564	7190	141
H(10B)	6109	2345	7613	141
H(10C)	5033	3087	7510	141
H(11A)	222	3932	8145	173
H(11B)	-543	3080	8032	173
H(11C)	465	3556	7742	173
H(12A)	3054	4150	8241	146
H(12B)	3571	3731	7864	146
H(12C)	4265	3441	8247	146
H(13A)	1347	3477	8748	132
H(13B)	2469	2738	8817	132
H(13C)	791	2538	8750	132
H(14A)	-1765	1052	8379	155
H(14B)	-1445	1429	7980	155
H(14C)	-1019	1943	8341	155
H(15A)	-567	-377	8250	168
H(15B)	1042	-544	8103	168
H(15C)	-150	-154	7833	168
H(16A)	167	410	8841	149
H(16B)	1148	1225	8868	149
H(16C)	1879	349	8777	149
H(20A)	7125	-1193	9037	100
H(28A)	6044	3775	8564	127
H(28B)	6972	3349	8884	127
H(28C)	7686	4054	8633	127
H(29A)	6368	5899	8443	117
H(29B)	7866	5447	8538	117
H(29C)	7539	6351	8699	117
H(30A)	4450	6908	9117	117
H(30B)	6141	7100	9165	117
H(30C)	5143	6965	9521	117
H(31A)	2941	5419	9696	130
H(31B)	4146	5880	9938	130
H(31C)	3923	4901	9977	130
H(32A)	3718	3533	9322	138
H(32B)	4411	3612	9725	138
H(32C)	5270	3133	9407	138

H(33A)	8971	2497	9667	110
H(33B)	9328	3110	9333	110
H(33C)	7698	2812	9403	110
H(34A)	7681	2903	10302	107
H(34B)	6242	3218	10099	107
H(34C)	7018	3791	10400	107
H(35A)	10293	3337	10177	99
H(35B)	10117	4306	10258	99
H(35C)	10872	4003	9885	99
H(36A)	7865	5884	10697	105
H(36B)	8048	4952	10554	105
H(36C)	6505	5401	10528	105
H(37A)	10067	6498	10337	94
H(37B)	10338	6469	9901	94
H(37C)	10553	5651	10144	94
H(38A)	7531	7191	10311	91
H(38B)	6127	6866	10096	91
H(38C)	7447	7264	9871	91
H(42A)	12214	7838	8501	87

Table 1. Crystal data and structure refinement for wy0169wc.

Identification code	wy0169wc
Empirical formula	$C_{22}H_{17}F_8NORuS_2$
Formula weight	628.56
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 22.6486(14) Å alpha = 90° b = 11.2357(7) Å beta = 90° c = 9.0880(6) Å gamma = 90°
Volume, Z	2312.6(3) $Å^3$, 4
Density (calculated)	1.805 Mg/m^3
Absorption coefficient	0.939 mm^{-1}
F(000)	1248
Crystal size	0.34 x 0.32 x 0.27 mm
θ range for data collection	2.02 to 27.49°
Limiting indices	$-28 \le h \le 16$, $-14 \le k \le 14$, $-11 \le l \le 11$
Reflections collected	12904
Independent reflections	5156 (R_{int} = 0.0175)
Completeness to θ = 27.49°	98.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5156 / 1 / 322
Goodness-of-fit on F^2	1.003
Final R indices [$I>2\sigma(I)$]	R1 = 0.0186, wR2 = 0.0487
R indices (all data)	R1 = 0.0202, wR2 = 0.0497
Absolute structure parameter	-0.024(18)
Extinction coefficient	0.00119(16)
Largest diff. peak and hole	0.266 and -0.221 $eÅ^{-3}$

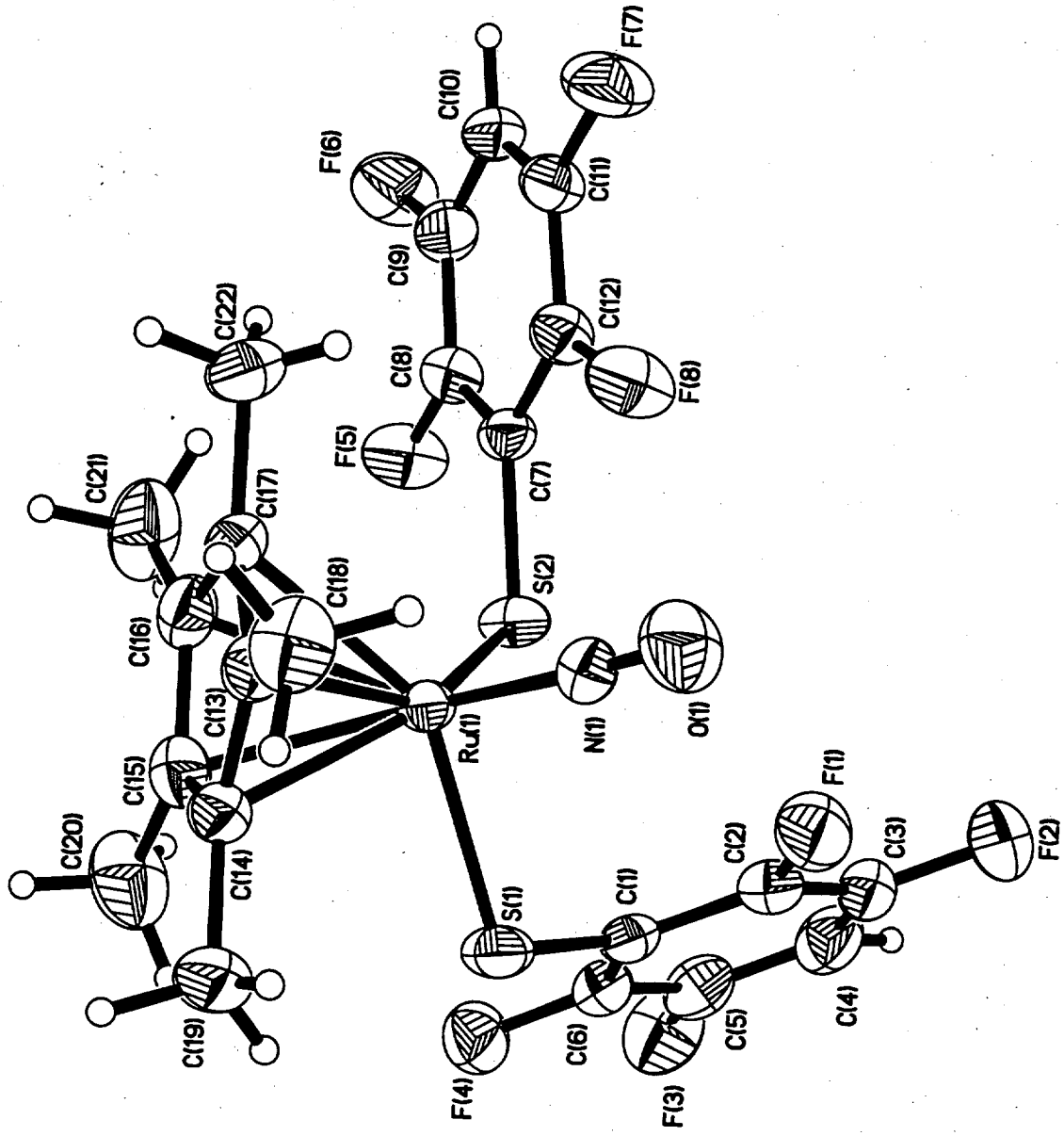

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for wy0169wc. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	5579(1)	3492(2)	9362(2)	40(1)
C(2)	5737(1)	4692(2)	9240(3)	47(1)
C(3)	5726(1)	5442(2)	10436(3)	53(1)
C(4)	5567(1)	5051(2)	11787(4)	60(1)
C(5)	5411(1)	3879(2)	11940(3)	55(1)
C(6)	5419(1)	3127(2)	10753(3)	46(1)
C(7)	7672(1)	2857(2)	8794(2)	37(1)
C(8)	8036(1)	2328(2)	9843(3)	44(1)
C(9)	8644(1)	2382(2)	9761(3)	52(1)
C(10)	8921(1)	2956(2)	8634(3)	52(1)
C(11)	8573(1)	3491(2)	7596(3)	48(1)
C(12)	7967(1)	3465(2)	7685(2)	42(1)
C(13)	6560(1)	1197(2)	4608(2)	42(1)
C(14)	6073(1)	746(2)	5416(2)	40(1)
C(15)	6302(1)	246(2)	6757(3)	46(1)
C(16)	6924(1)	388(2)	6755(3)	48(1)
C(17)	7085(1)	1006(2)	5445(3)	44(1)
C(18)	6541(1)	1707(3)	3089(3)	61(1)
C(19)	5445(1)	689(2)	4905(3)	60(1)
C(20)	5942(2)	-414(2)	7881(4)	81(1)
C(21)	7347(2)	-96(2)	7857(4)	80(1)
C(22)	7705(1)	1247(3)	4933(4)	70(1)
F(1)	5900(1)	5118(1)	7936(2)	66(1)
F(2)	5878(1)	6592(1)	10226(2)	77(1)
F(3)	5256(1)	3452(2)	13275(2)	83(1)
F(4)	5258(1)	1977(1)	10984(2)	64(1)
F(5)	7795(1)	1743(2)	10981(2)	67(1)
F(6)	8964(1)	1846(2)	10809(2)	82(1)
F(7)	8827(1)	4078(1)	6473(2)	73(1)
F(8)	7660(1)	4050(1)	6649(2)	64(1)
N(1)	6496(1)	3593(2)	5726(2)	42(1)
O(1)	6509(1)	4363(2)	4904(2)	71(1)
Ru(1)	6470(1)	2236(1)	6683(1)	33(1)
S(1)	5534(1)	2535(1)	7842(1)	50(1)
S(2)	6900(1)	2777(1)	8987(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for wy0169wc.

C(1)-C(6)	1.378(3)	C(1)-C(2)	1.399(3)
C(1)-S(1)	1.754(2)	C(2)-F(1)	1.329(3)
C(2)-C(3)	1.376(3)	C(3)-F(2)	1.350(3)
C(3)-C(4)	1.353(4)	C(4)-C(5)	1.370(3)
C(5)-F(3)	1.351(3)	C(5)-C(6)	1.370(3)
C(6)-F(4)	1.360(3)	C(7)-C(12)	1.388(3)
C(7)-C(8)	1.392(3)	C(7)-S(2)	1.761(2)
C(8)-F(5)	1.341(3)	C(8)-C(9)	1.382(3)
C(9)-F(6)	1.339(3)	C(9)-C(10)	1.363(4)
C(10)-C(11)	1.368(4)	C(11)-F(7)	1.344(3)
C(11)-C(12)	1.376(3)	C(12)-F(8)	1.342(3)
C(13)-C(14)	1.418(3)	C(13)-C(17)	1.428(3)
C(13)-C(18)	1.495(3)	C(13)-Ru(1)	2.227(2)
C(14)-C(15)	1.439(3)	C(14)-C(19)	1.498(3)
C(14)-Ru(1)	2.2225(19)	C(15)-C(16)	1.418(3)
C(15)-C(20)	1.504(4)	C(15)-Ru(1)	2.2684(18)
C(16)-C(17)	1.425(4)	C(16)-C(21)	1.488(3)
C(16)-Ru(1)	2.3189(18)	C(17)-C(22)	1.504(3)
C(17)-Ru(1)	2.2617(19)	N(1)-O(1)	1.144(3)
N(1)-Ru(1)	1.7558(18)	Ru(1)-S(2)	2.3880(6)
Ru(1)-S(1)	2.3899(6)		

C(6)-C(1)-C(2)	115.3(2)	C(6)-C(1)-S(1)	121.62(17)
C(2)-C(1)-S(1)	122.91(18)	F(1)-C(2)-C(3)	119.27(19)
F(1)-C(2)-C(1)	119.2(2)	C(3)-C(2)-C(1)	121.5(2)
F(2)-C(3)-C(4)	120.5(2)	F(2)-C(3)-C(2)	118.0(2)
C(4)-C(3)-C(2)	121.5(2)	C(3)-C(4)-C(5)	118.2(3)
F(3)-C(5)-C(6)	119.5(2)	F(3)-C(5)-C(4)	119.9(2)
C(6)-C(5)-C(4)	120.6(2)	F(4)-C(6)-C(5)	117.4(2)
F(4)-C(6)-C(1)	119.7(2)	C(5)-C(6)-C(1)	122.8(2)
C(12)-C(7)-C(8)	115.08(19)	C(12)-C(7)-S(2)	125.05(16)
C(8)-C(7)-S(2)	119.80(17)	F(5)-C(8)-C(9)	118.0(2)
F(5)-C(8)-C(7)	119.8(2)	C(9)-C(8)-C(7)	122.2(2)
F(6)-C(9)-C(10)	119.9(2)	F(6)-C(9)-C(8)	118.7(3)
C(10)-C(9)-C(8)	121.3(2)	C(9)-C(10)-C(11)	117.5(2)
F(7)-C(11)-C(10)	119.5(2)	F(7)-C(11)-C(12)	118.9(2)
C(10)-C(11)-C(12)	121.6(2)	F(8)-C(12)-C(11)	117.6(2)
F(8)-C(12)-C(7)	120.17(18)	C(11)-C(12)-C(7)	122.2(2)
C(14)-C(13)-C(17)	108.52(19)	C(14)-C(13)-C(18)	126.4(2)
C(17)-C(13)-C(18)	124.9(2)	C(14)-C(13)-Ru(1)	71.24(12)
C(17)-C(13)-Ru(1)	72.77(12)	C(18)-C(13)-Ru(1)	125.33(16)
C(13)-C(14)-C(15)	107.29(17)	C(13)-C(14)-C(19)	126.3(2)
C(15)-C(14)-C(19)	126.1(2)	C(13)-C(14)-Ru(1)	71.59(11)
C(15)-C(14)-Ru(1)	73.06(11)	C(19)-C(14)-Ru(1)	125.23(15)
C(16)-C(15)-C(14)	108.3(2)	C(16)-C(15)-C(20)	126.6(3)
C(14)-C(15)-C(20)	124.8(2)	C(16)-C(15)-Ru(1)	73.95(10)
C(14)-C(15)-Ru(1)	69.59(11)	C(20)-C(15)-Ru(1)	126.65(18)
C(15)-C(16)-C(17)	108.0(2)	C(15)-C(16)-C(21)	126.7(3)
C(17)-C(16)-C(21)	125.2(2)	C(15)-C(16)-Ru(1)	70.07(10)
C(17)-C(16)-Ru(1)	69.70(11)	C(21)-C(16)-Ru(1)	129.16(18)
C(16)-C(17)-C(13)	107.80(18)	C(16)-C(17)-C(22)	125.8(2)
C(13)-C(17)-C(22)	125.9(2)	C(16)-C(17)-Ru(1)	74.07(11)
C(13)-C(17)-Ru(1)	70.13(11)	C(22)-C(17)-Ru(1)	128.23(16)
O(1)-N(1)-Ru(1)	168.9(2)	N(1)-Ru(1)-C(14)	114.28(8)
N(1)-Ru(1)-C(13)	91.86(8)	C(14)-Ru(1)-C(13)	37.17(7)

N(1)-Ru(1)-C(17)	105.26(8)	C(14)-Ru(1)-C(17)	62.02(7)
C(13)-Ru(1)-C(17)	37.10(8)	N(1)-Ru(1)-C(15)	151.14(10)
C(14)-Ru(1)-C(15)	37.35(9)	C(13)-Ru(1)-C(15)	61.56(9)
C(17)-Ru(1)-C(15)	61.02(8)	N(1)-Ru(1)-C(16)	140.93(9)
C(14)-Ru(1)-C(16)	61.26(8)	C(13)-Ru(1)-C(16)	60.92(9)
C(17)-Ru(1)-C(16)	36.23(9)	C(15)-Ru(1)-C(16)	35.98(7)
N(1)-Ru(1)-S(2)	101.51(7)	C(14)-Ru(1)-S(2)	144.20(6)
C(13)-Ru(1)-S(2)	147.00(6)	C(17)-Ru(1)-S(2)	109.91(6)
C(15)-Ru(1)-S(2)	107.04(8)	C(16)-Ru(1)-S(2)	91.27(7)
N(1)-Ru(1)-S(1)	97.27(6)	C(14)-Ru(1)-S(1)	88.59(5)
C(13)-Ru(1)-S(1)	121.84(6)	C(17)-Ru(1)-S(1)	148.31(6)
C(15)-Ru(1)-S(1)	88.68(6)	C(16)-Ru(1)-S(1)	120.46(6)
S(2)-Ru(1)-S(1)	86.52(2)	C(1)-S(1)-Ru(1)	112.43(7)
C(7)-S(2)-Ru(1)	109.32(7)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for wy0169wc.

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
C(1)	26(1)	44(1)	51(1)	-6(1)	2(1)	4(1)
C(2)	33(1)	50(1)	57(1)	1(1)	6(1)	1(1)
C(3)	44(1)	41(1)	74(2)	-10(1)	-4(1)	3(1)
C(4)	56(1)	60(1)	64(2)	-17(2)	0(2)	13(1)
C(5)	53(1)	67(1)	44(2)	-3(1)	6(1)	14(1)
C(6)	38(1)	45(1)	55(1)	1(1)	3(1)	5(1)
C(7)	30(1)	42(1)	41(1)	-7(1)	-1(1)	0(1)
C(8)	40(1)	48(1)	45(1)	0(1)	0(1)	-5(1)
C(9)	38(1)	50(1)	68(2)	-2(1)	-14(1)	3(1)
C(10)	31(1)	50(1)	75(2)	-9(1)	0(1)	-1(1)
C(11)	42(1)	48(1)	55(1)	-4(1)	8(1)	-8(1)
C(12)	39(1)	45(1)	44(1)	1(1)	-3(1)	-4(1)
C(13)	42(1)	39(1)	43(1)	-4(1)	1(1)	3(1)
C(14)	36(1)	41(1)	44(1)	-6(1)	0(1)	-1(1)
C(15)	56(1)	38(1)	46(1)	1(1)	3(2)	-1(1)
C(16)	53(1)	39(1)	52(1)	-5(1)	-10(2)	10(1)
C(17)	36(1)	42(1)	53(1)	-9(1)	1(1)	6(1)
C(18)	79(2)	64(2)	40(1)	1(1)	5(1)	6(1)
C(19)	39(1)	62(1)	78(2)	-16(1)	-8(1)	-4(1)
C(20)	114(3)	60(1)	69(2)	13(2)	24(2)	-16(2)
C(21)	101(2)	57(1)	81(2)	1(2)	-43(2)	23(2)
C(22)	38(1)	71(2)	100(2)	-26(2)	14(1)	1(1)
F(1)	70(1)	60(1)	68(1)	8(1)	18(1)	-2(1)
F(2)	76(1)	48(1)	108(1)	-14(1)	0(1)	-7(1)
F(3)	103(1)	93(1)	53(1)	4(1)	20(1)	20(1)
F(4)	69(1)	52(1)	72(1)	8(1)	11(1)	-3(1)
F(5)	56(1)	91(1)	54(1)	23(1)	-5(1)	-7(1)
F(6)	53(1)	90(1)	102(1)	30(1)	-30(1)	-3(1)
F(7)	56(1)	86(1)	78(1)	16(1)	22(1)	-15(1)
F(8)	50(1)	77(1)	66(1)	28(1)	-10(1)	-11(1)
N(1)	41(1)	37(1)	47(1)	2(1)	0(1)	4(1)
O(1)	79(1)	60(1)	74(1)	22(1)	1(1)	-4(1)
Ru(1)	28(1)	36(1)	35(1)	-1(1)	1(1)	0(1)
S(1)	28(1)	62(1)	58(1)	-19(1)	5(1)	-3(1)
S(2)	30(1)	62(1)	39(1)	-6(1)	1(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for wy0169wc.

	x	y	z	U(eq)
H(4)	5564	5563	12590	72
H(10)	9330	2983	8572	62
H(18A)	6832	1320	2488	91
H(18B)	6624	2545	3132	91
H(18C)	6157	1585	2673	91
H(19A)	5391	1224	4093	90
H(19B)	5187	914	5696	90
H(19C)	5354	-108	4598	90
H(20A)	5952	-1250	7669	121
H(20B)	5541	-137	7849	121
H(20C)	6102	-275	8844	121
H(21A)	7164	-104	8810	120
H(21B)	7693	397	7885	120
H(21C)	7457	-892	7586	120
H(22A)	7966	1250	5764	104
H(22B)	7719	2008	4452	104
H(22C)	7824	638	4255	104

Table 1. Crystal data and structure refinement for C22 H43 F6 P3 Ru Se3.

Identification code	leung23
Empirical formula	C22 H43 F6 P3 Ru Se3
Formula weight	852.42
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 15.373(4) A alpha = 90 deg. b = 16.117(5) A beta = 101.02(2) deg. c = 13.214(3) A gamma = 90 deg.
Volume, Z	3214(2) A^3, 4
Density (calculated)	1.762 Mg/m^3
Absorption coefficient	4.081 mm^-1
F(000)	1680
Crystal size	0.4 x 0.3 x 0.25 mm
Theta range for data collection	1.35 to 25.00 deg.
Limiting indices	-18<=h<=17, -19<=k<=0, 0<=l<=15
Reflections collected	5764
Independent reflections	5508 [R(int) = 0.0707]
Absorption correction	Semi-empirical
Max. and min. transmission	0.76 and 0.52
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5409 / 0 / 316
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0780, wR2 = 0.1523
R indices (all data)	R1 = 0.1830, wR2 = 0.2275
Largest diff. peak and hole	1.334 and -0.699 e.A^-3

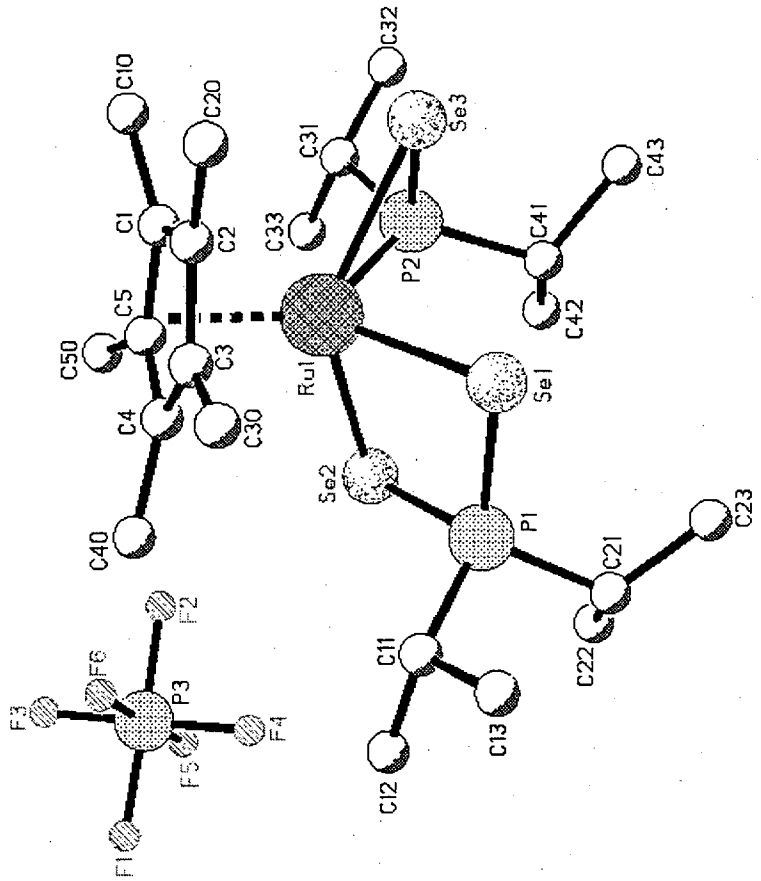
C10
C20
C1
C2
C5
C50
C3
C4
C30
C40
C32
Se3
C31
C33
P2
C41
C43
C42
Ru1
Se1
Se2
P1
C21
C23
C22
C11
C13
C12
F2
F6
F3
P3
F4
F5
F1

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for C22 H43 F6 P3 Ru Se3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	2812(1)	71(1)	1795(1)	43(1)
Se(1)	1220(1)	332(1)	898(1)	70(1)
Se(2)	2190(1)	556(1)	3340(1)	56(1)
Se(3)	3167(1)	888(1)	235(1)	62(1)
P(1)	856(3)	389(3)	2412(3)	68(1)
P(2)	3313(2)	1426(2)	1760(3)	50(1)
C(1)	4039(9)	-666(8)	1773(11)	51(4)
C(2)	3328(10)	-1043(9)	1043(11)	60(4)
C(3)	2690(10)	-1362(9)	1612(12)	61(4)
C(4)	2978(11)	-1194(9)	2661(12)	62(4)
C(5)	3795(10)	-747(8)	2776(10)	51(4)
C(10)	4907(9)	-421(10)	1527(13)	70(5)
C(20)	3323(13)	-1218(13)	-71(13)	105(7)
C(30)	1854(12)	-1836(10)	1104(16)	107(7)
C(40)	2590(11)	-1537(12)	3547(14)	96(6)
C(50)	4391(12)	-553(11)	3791(12)	98(7)
C(11)	364(11)	-587(12)	2730(13)	86(6)
C(12)	238(12)	-629(13)	3852(13)	100(7)
C(13)	-488(12)	-794(14)	1929(15)	120(8)
C(21)	57(14)	1206(16)	2594(17)	118(8)
C(22)	315(17)	1662(15)	3631(19)	142(9)
C(23)	-171(16)	1781(15)	1670(17)	150(11)
C(31)	4473(10)	1702(10)	2303(11)	65(4)
C(32)	4844(12)	2402(11)	1805(15)	96(6)
C(33)	4620(11)	1785(11)	3498(14)	89(6)
C(41)	2555(10)	2317(10)	1740(12)	70(5)
C(42)	2698(12)	2800(10)	2756(13)	84(5)
C(43)	2550(15)	2905(12)	830(13)	118(8)
P(3)	2691(3)	-642(4)	6770(4)	89(2)
F(1)	2087(9)	-1167(10)	7370(11)	167(6)
F(2)	3325(10)	-144(11)	6200(12)	187(7)
F(3)	3505(8)	-1031(11)	7483(12)	175(7)
F(4)	1895(11)	-263(22)	6128(16)	317(17)
F(5)	2735(14)	33(11)	7587(13)	208(8)
F(6)	2654(19)	-1279(13)	5958(12)	262(13)

Table 3. Bond lengths [A] and angles [deg] for C22 H43 F6 P3 Ru Se3.

Ru(1)-P(2)	2.320(4)
Ru(1)-Se(1)	2.543(2)
Ru(1)-Se(2)	2.538(2)
Ru(1)-Se(3)	2.590(2)
Ru(1)-C(1)	2.234(13)
Ru(1)-C(2)	2.266(13)
Ru(1)-C(3)	2.325(14)
Ru(1)-C(4)	2.328(14)
Ru(1)-C(5)	2.226(13)
Se(1)-P(1)	2.179(5)
Se(2)-P(1)	2.194(4)
Se(3)-P(2)	2.166(4)
P(1)-C(11)	1.83(2)
P(1)-C(21)	1.85(2)
P(2)-C(41)	1.85(2)
P(2)-C(31)	1.85(2)
C(1)-C(5)	1.45(2)
C(1)-C(2)	1.45(2)
C(1)-C(10)	1.49(2)
C(2)-C(3)	1.44(2)
C(2)-C(20)	1.50(2)
C(3)-C(4)	1.40(2)
C(3)-C(30)	1.54(2)
C(4)-C(5)	1.43(2)
C(4)-C(40)	1.52(2)
C(5)-C(50)	1.51(2)
C(11)-C(12)	1.53(2)
C(11)-C(13)	1.56(2)
C(21)-C(23)	1.52(3)
C(21)-C(22)	1.54(3)
C(31)-C(32)	1.47(2)
C(31)-C(33)	1.56(2)
C(41)-C(42)	1.53(2)
C(41)-C(43)	1.53(2)
P(3)-F(1)	1.578(13)
P(3)-F(2)	1.562(14)
P(3)-F(3)	1.548(12)
P(3)-F(4)	1.48(2)
P(3)-F(5)	1.53(2)
P(3)-F(6)	1.48(2)
C(5)-Ru(1)-C(1)	37.9(5)
C(5)-Ru(1)-C(2)	62.0(5)
C(1)-Ru(1)-C(2)	37.5(5)
C(5)-Ru(1)-P(2)	112.2(4)
C(1)-Ru(1)-P(2)	102.5(4)
C(2)-Ru(1)-P(2)	126.3(4)
C(5)-Ru(1)-C(3)	60.3(5)
C(1)-Ru(1)-C(3)	61.5(5)
C(2)-Ru(1)-C(3)	36.5(5)
P(2)-Ru(1)-C(3)	162.5(4)
C(5)-Ru(1)-C(4)	36.5(5)
C(1)-Ru(1)-C(4)	61.8(5)
C(2)-Ru(1)-C(4)	60.5(5)
P(2)-Ru(1)-C(4)	146.0(4)
C(3)-Ru(1)-C(4)	35.0(5)

C(5)-Ru(1)-Se(2)	91.8(4)
C(1)-Ru(1)-Se(2)	128.5(4)
C(2)-Ru(1)-Se(2)	144.5(4)
P(2)-Ru(1)-Se(2)	84.46(10)
C(3)-Ru(1)-Se(2)	110.7(4)
C(4)-Ru(1)-Se(2)	84.1(4)
C(5)-Ru(1)-Se(1)	148.9(4)
C(1)-Ru(1)-Se(1)	145.3(4)
C(2)-Ru(1)-Se(1)	108.3(4)
P(2)-Ru(1)-Se(1)	97.37(11)
C(3)-Ru(1)-Se(1)	93.7(4)
C(4)-Ru(1)-Se(1)	112.3(4)
Se(2)-Ru(1)-Se(1)	81.17(6)
C(5)-Ru(1)-Se(3)	122.8(4)
C(1)-Ru(1)-Se(3)	87.3(4)
C(2)-Ru(1)-Se(3)	84.8(4)
P(2)-Ru(1)-Se(3)	51.98(10)
C(3)-Ru(1)-Se(3)	116.6(4)
C(4)-Ru(1)-Se(3)	144.8(4)
Se(2)-Ru(1)-Se(3)	130.74(7)
Se(1)-Ru(1)-Se(3)	82.85(6)
P(1)-Se(1)-Ru(1)	88.38(12)
P(1)-Se(2)-Ru(1)	88.17(13)
P(2)-Se(3)-Ru(1)	57.56(11)
C(11)-P(1)-C(21)	105.6(10)
C(11)-P(1)-Se(1)	111.4(6)
C(21)-P(1)-Se(1)	116.3(7)
C(11)-P(1)-Se(2)	111.1(6)
C(21)-P(1)-Se(2)	114.4(8)
Se(1)-P(1)-Se(2)	98.2(2)
C(41)-P(2)-C(31)	112.3(8)
C(41)-P(2)-Se(3)	110.2(5)
C(31)-P(2)-Se(3)	112.2(5)
C(41)-P(2)-Ru(1)	121.4(6)
C(31)-P(2)-Ru(1)	121.3(5)
Se(3)-P(2)-Ru(1)	70.46(12)
C(5)-C(1)-C(2)	106.1(12)
C(5)-C(1)-C(10)	128.6(13)
C(2)-C(1)-C(10)	124.1(14)
C(5)-C(1)-Ru(1)	70.7(8)
C(2)-C(1)-Ru(1)	72.5(8)
C(10)-C(1)-Ru(1)	131.1(10)
C(3)-C(2)-C(1)	107.8(12)
C(3)-C(2)-C(20)	124.7(14)
C(1)-C(2)-C(20)	127(2)
C(3)-C(2)-Ru(1)	73.9(8)
C(1)-C(2)-Ru(1)	70.0(7)
C(20)-C(2)-Ru(1)	130.1(12)
C(4)-C(3)-C(2)	109.3(13)
C(4)-C(3)-C(30)	128(2)
C(2)-C(3)-C(30)	123(2)
C(4)-C(3)-Ru(1)	72.6(8)
C(2)-C(3)-Ru(1)	69.5(8)
C(30)-C(3)-Ru(1)	125.8(11)
C(3)-C(4)-C(5)	107.9(13)
C(3)-C(4)-C(40)	127(2)
C(5)-C(4)-C(40)	124.7(14)
C(3)-C(4)-Ru(1)	72.4(8)
C(5)-C(4)-Ru(1)	67.9(8)
C(40)-C(4)-Ru(1)	132.6(11)
C(4)-C(5)-C(1)	108.9(12)

C(4)-C(5)-C(50)	124.8(14)
C(1)-C(5)-C(50)	125.2(14)
C(4)-C(5)-Ru(1)	75.6(8)
C(1)-C(5)-Ru(1)	71.3(7)
C(50)-C(5)-Ru(1)	128.7(10)
C(12)-C(11)-C(13)	113.7(14)
C(12)-C(11)-P(1)	113.3(14)
C(13)-C(11)-P(1)	111.1(13)
C(23)-C(21)-C(22)	114(2)
C(23)-C(21)-P(1)	113(2)
C(22)-C(21)-P(1)	113(2)
C(32)-C(31)-C(33)	113.1(14)
C(32)-C(31)-P(2)	116.0(12)
C(33)-C(31)-P(2)	110.9(11)
C(42)-C(41)-C(43)	110.5(14)
C(42)-C(41)-P(2)	113.5(11)
C(43)-C(41)-P(2)	113.7(12)
F(6)-P(3)-F(4)	87.6(14)
F(6)-P(3)-F(5)	178.5(11)
F(4)-P(3)-F(5)	92(2)
F(6)-P(3)-F(3)	94.3(14)
F(4)-P(3)-F(3)	177.5(12)
F(5)-P(3)-F(3)	86.3(10)
F(6)-P(3)-F(2)	87.0(10)
F(4)-P(3)-F(2)	92.0(11)
F(5)-P(3)-F(2)	91.6(11)
F(3)-P(3)-F(2)	89.7(8)
F(6)-P(3)-F(1)	92.7(9)
F(4)-P(3)-F(1)	90.4(10)
F(5)-P(3)-F(1)	88.7(10)
F(3)-P(3)-F(1)	87.8(8)
F(2)-P(3)-F(1)	177.5(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for C22 H43 F6 P3 Ru Se3.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	48(1)	44(1)	36(1)	-1(1)	5(1)	0(1)
Se(1)	49(1)	107(1)	48(1)	9(1)	-2(1)	-2(1)
Se(2)	53(1)	70(1)	43(1)	-2(1)	8(1)	3(1)
Se(3)	80(1)	61(1)	45(1)	6(1)	16(1)	-2(1)
P(1)	49(2)	97(3)	57(3)	6(2)	5(2)	-3(2)
P(2)	54(2)	49(2)	45(2)	4(2)	10(2)	3(2)
C(1)	48(8)	35(8)	65(10)	7(7)	0(7)	14(7)
C(2)	83(11)	45(9)	52(9)	-20(7)	15(8)	-2(8)
C(3)	67(10)	41(9)	71(12)	-1(8)	4(9)	-15(8)
C(4)	83(12)	41(9)	65(11)	11(8)	22(9)	11(8)
C(5)	65(10)	43(9)	43(8)	1(7)	6(7)	5(7)
C(10)	65(10)	65(10)	87(12)	4(9)	35(9)	17(9)
C(20)	112(16)	133(19)	68(12)	-46(12)	15(11)	-8(13)
C(30)	109(16)	58(12)	142(19)	-20(12)	-2(13)	-39(11)
C(40)	85(13)	92(14)	109(15)	43(12)	18(11)	-16(11)
C(50)	115(15)	97(14)	61(11)	-12(10)	-35(10)	59(12)
C(11)	66(11)	106(15)	87(13)	11(11)	19(10)	-13(10)
C(12)	92(14)	144(20)	67(12)	8(12)	23(10)	-14(13)
C(13)	75(13)	162(22)	107(16)	17(15)	-21(11)	-49(14)
C(21)	98(15)	172(23)	89(15)	-2(16)	28(12)	48(15)
C(22)	174(24)	132(22)	136(22)	7(17)	69(19)	40(18)
C(23)	154(22)	169(26)	120(20)	48(18)	8(17)	87(19)
C(31)	66(10)	68(11)	62(10)	-21(8)	14(8)	-1(9)
C(32)	95(14)	66(12)	135(18)	-7(12)	42(13)	-25(11)
C(33)	75(12)	79(13)	98(14)	-14(11)	-18(10)	-9(10)
C(41)	61(11)	82(13)	65(11)	9(9)	8(8)	19(9)
C(42)	101(14)	58(11)	91(14)	-3(10)	11(11)	17(10)
C(43)	196(23)	82(14)	75(13)	29(11)	21(14)	78(15)
P(3)	59(3)	131(5)	75(3)	-1(4)	5(3)	-17(3)
F(1)	142(12)	212(17)	151(12)	13(12)	41(10)	-60(11)
F(2)	143(12)	262(20)	161(13)	60(13)	42(10)	-61(13)
F(3)	87(9)	237(18)	197(15)	67(13)	20(9)	51(10)
F(4)	114(13)	632(52)	194(19)	181(26)	3(12)	83(21)
F(5)	302(24)	169(16)	154(14)	-38(12)	48(15)	41(15)
F(6)	456(36)	234(21)	121(13)	-90(14)	117(18)	-180(23)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for C22 H43 F6 P3 Ru Se3.

	x	y	z	U(eq)
H(10A)	4866(9)	-421(10)	793(13)	104
H(10B)	5354(9)	-809(10)	1836(13)	104
H(10C)	5062(9)	124(10)	1793(13)	104
H(20A)	3812(13)	-938(13)	-277(13)	158
H(20B)	2778(13)	-1023(13)	-481(13)	158
H(20C)	3376(13)	-1805(13)	-168(13)	158
H(30A)	1822(12)	-1856(10)	372(16)	160
H(30B)	1339(12)	-1559(10)	1251(16)	160
H(30C)	1877(12)	-2391(10)	1373(16)	160
H(40A)	2915(11)	-1323(12)	4187(14)	143
H(40B)	2630(11)	-2132(12)	3550(14)	143
H(40C)	1980(11)	-1375(12)	3466(14)	143
H(50A)	4898(12)	-249(11)	3670(12)	147
H(50B)	4582(12)	-1060(11)	4145(12)	147
H(50C)	4072(12)	-225(11)	4205(12)	147
H(11A)	794(11)	-1021(12)	2657(13)	103
H(12A)	786(12)	-495(13)	4304(13)	150
H(12B)	59(12)	-1180(13)	4000(13)	150
H(12C)	-210(12)	-241(13)	3954(13)	150
H(13A)	-364(12)	-755(14)	1245(15)	180
H(13B)	-948(12)	-408(14)	2001(15)	180
H(13C)	-678(12)	-1347(14)	2046(15)	180
H(21A)	-495(14)	913(16)	2631(17)	142
H(22A)	451(17)	1263(15)	4178(19)	213
H(22B)	-170(17)	2004(15)	3741(19)	213
H(22C)	825(17)	2003(15)	3621(19)	213
H(23A)	-324(16)	1457(15)	1052(17)	225
H(23B)	331(16)	2124(15)	1628(17)	225
H(23C)	-665(16)	2124(15)	1746(17)	225
H(31A)	4823(10)	1217(10)	2177(11)	78
H(32A)	4736(12)	2317(11)	1073(15)	144
H(32B)	5471(12)	2436(11)	2062(15)	144
H(32C)	4567(12)	2909(11)	1957(15)	144
H(33A)	4367(11)	1313(11)	3779(14)	133
H(33B)	4340(11)	2282(11)	3675(14)	133
H(33C)	5244(11)	1810(11)	3777(14)	133
H(41A)	1956(10)	2083(10)	1649(12)	84
H(42A)	2699(12)	2422(10)	3318(13)	126
H(42B)	2229(12)	3197(10)	2737(13)	126
H(42C)	3257(12)	3085(10)	2851(13)	126
H(43A)	2459(15)	2593(12)	201(13)	177
H(43B)	3107(15)	3191(12)	917(13)	177
H(43C)	2080(15)	3302(12)	803(13)	177