Table 1: Details of crystal structure determinations

	1b	1d	$[RcCH_2PPh_3][BF_4]^-\cdot 0.5CH_2Cl_2$
empirical formula	$C_{43}H_{24}BF_{24}Ru$	$C_{12}H_{11}F_3O_3RuS$	$C_{29.5}H_{27}BClF_4PRu$
fw	1108.5	345.34	635.81
crystal grown by	CH_2Cl_2 / pentane layering	CH_2Cl_2 / Et_2O layering	evapn of CH_2Cl_2 / hexane soln
crystal appearance	pale green prism	pale yellow fragment	colourless plate
crystal size	0.2 × 0.2 × 0.8	0.1 × 0.1 × 0.3	0.1 × 0.2 × 0.3
diffractometer	Enraf-Nonius DIP2000 image-plate	Enraf-Nonius Kappa CCD	Enraf-Nonius Kappa CCD
temperature / K	150	150	150
radiation	Mo Kα	Mo Kα	Mo Kα
wavelength / Å	0.71069	0.71069	0.71069
crystal system	monoclinic	monoclinic	monoclinic
space group	*C* 2	*P* $2_1/c$	*C* 2/*c*
a (Å)	15.703(1)	16.2555(3)	33.0591(7)
b (Å)	12.742(1)	13.2704(3)	12.5182(3)
c (Å)	10.787(1)	18.7369(5)	13.7757(3)
α (°)	90	90	90
β (°)	97.974(4)	104.543(2)	101.591(1)
γ (°)	90	90	90
cell volume / $Å^3$	2137.5	3912.4	5584.7
Z	2	12	8
calc density / Mg/m^3	1.72	1.76	1.51
absorpn coefft / mm^{-1}	0.50	1.37	0.76
F_{000}	1094	2328	2568
absorption correction	semi-emprical from equiv refs	semi-empirical from equiv refls	semi-empirical from equiv refs
max θ / °	26.57	27.5	27.48
Index ranges	$-19 \le h \le 19, -15 \le k \le 15, 0 \le l \le 12$	$-21 \le h \le 20, 0 \le k \le 17, 0 \le l \le 24$	$-42 \le h \le 42, -14 \le k \le 16, -17 \le l \le 17$
reflections measured	6875	28639	10107
unique reflections	4149	9253	6308
R_{int}	0.028	0.039	0.047
obs refs (& criterion)	4122 $\{I > 3\sigma(I)\}$	5483 $\{I > 3\sigma(I)\}$	4083 $\{I > 2\sigma(I)\}$
solution method	SIR92	SIR92	SIR92
refinement method	full-matrix least-sq on *F* (obs data)	full-matrix least-sq on *F* (obs data)	full-matrix least-sq on F^2 (all data)
refinement programs	CRYSTALS	CRYSTALS	Shelxs97
parameters refined	339	553	350
weighting scheme	3-term Chebychev polynomial	3-term Chebychev polynomial	unit weights
goodness of fit	1.0545	1.0248	1.054
final *R* indices (obs data)	*R* = 0.0328, *wR* = 0.0398	*R* = 0.0371, *wR* = 0.0494	*R*1 = 0.0632, *wR*2 = 0.1607
final *R* indices (all data)			*R*1 = 0.1121, *wR*2 = 0.1854
biggest hole & peak / $eÅ^{-3}$	-0.70, 1.48	-0.76, 1.23	-1.069, 1.689

Table 2: Atomic coordinates, occupancies and equivalent isotropic thermal parameters (Å^2) of refined atoms of 1b

Atom	x	y	z	U_{equiv}	Occupancy
Ru1	0.5	0.50584(5)	0.0	0.0256	1.0
F1	0.77349(15)	0.1757(2)	0.8269(2)	0.0592	1.0
F2	0.7826(2)	0.3295(3)	0.9045(3)	0.0956	1.0
F3	0.86386(14)	0.2841(2)	0.7741(4)	0.0812	1.0
F4	0.7207(4)	0.6263(3)	0.5828(4)	0.1446	1.0
F5	0.6153(4)	0.6021(3)	0.4474(5)	0.1570	1.0
F6	0.7329(5)	0.5542(5)	0.4110(7)	0.1978	1.0
F7	0.61143(19)	0.1967(3)	0.0093(3)	0.0964	1.0
F8	0.6965(3)	0.0792(3)	0.0688(5)	0.1221	1.0
F9	0.7081(3)	0.2210(5)	0.1588(4)	0.1425	1.0
F10	0.35192(17)	-0.0805(3)	0.2034(4)	0.0957	1.0
F11	0.45002(19)	-0.1499(2)	0.1138(3)	0.0625	1.0
F12	0.4511(2)	-0.1736(2)	0.3072(3)	0.0809	1.0
C1	0.5263(3)	0.4801(3)	0.1933(4)	0.0528	1.0
C2	0.4563(4)	0.4135(3)	0.1475(4)	0.0522	1.0
C3	0.3881(3)	0.4778(3)	0.0966(5)	0.0608	1.0
C4	0.4132(3)	0.5853(3)	0.1138(5)	0.0517	1.0
C5	0.4969(3)	0.5869(4)	0.1756(4)	0.0534	1.0
C6	0.6044(6)	0.4611(7)	0.1671(8)	0.0560	0.5
C7	0.58421(17)	0.2931(2)	0.5541(3)	0.0270	1.0
C8	0.64696(17)	0.2571(2)	0.6502(3)	0.0287	1.0
C9	0.71887(18)	0.3167(2)	0.6954(3)	0.0314	1.0
C10	0.7309(2)	0.4148(3)	0.6489(3)	0.0438	1.0
C11	0.6702(3)	0.4535(3)	0.5549(4)	0.0487	1.0
C12	0.5982(2)	0.3928(3)	0.5092(3)	0.0389	1.0
C13	0.52223(16)	0.1471(2)	0.3839(3)	0.0249	1.0
C14	0.47710(18)	0.0533(2)	0.3525(3)	0.0289	1.0
C15	0.48812(17)	-0.0047(4)	0.2465(3)	0.0317	1.0
C16	0.54630(19)	0.0262(2)	0.1683(3)	0.0334	1.0
C17	0.59202(18)	0.1180(2)	0.1976(3)	0.0316	1.0
C18	0.58029(17)	0.1773(2)	0.3034(3)	0.0270	1.0
C19	0.7828(2)	0.2767(3)	0.8006(4)	0.0403	1.0
C20	0.6806(5)	0.5618(5)	0.5036(6)	0.1023	1.0
C21	0.4355(2)	-0.1019(3)	0.2180(4)	0.0438	1.0
C22	0.6521(2)	0.1560(3)	0.1107(3)	0.0419	1.0
B1	0.5	0.2206(3)	0.5	0.0241	1.0
H11	0.5828(8)	0.4591(7)	0.214(4)	0.070(6)*	1.0
H21	0.459(1)	0.3414(9)	0.138(3)	0.070(6)*	1.0
H31	0.3364(15)	0.4546(7)	0.054(4)	0.070(6)*	1.0
H41	0.3829(12)	0.6426(8)	0.079(3)	0.070(6)*	1.0
H51	0.5310(9)	0.6457(8)	0.189(4)	0.070(6)*	1.0
H61	0.6533(15)	0.516(2)	0.177(6)	0.070(6)*	0.5
H62	0.626(3)	0.3873(18)	0.147(11)	0.070(6)*	0.5

*common refined value of U_{iso}

Table 3: Atomic coordinates and isotropic thermal parameters (Å^2) of geometrically-positioned atoms of 1b

Atom	x	y	z	U_{iso}
H81	0.6397	0.1863	0.6874	0.0345
H101	0.7824	0.4576	0.6823	0.0521
H121	0.5552	0.4226	0.4414	0.0455
H141	0.4357	0.0274	0.4081	0.0342
H161	0.5551	-0.0164	0.0932	0.0391
H181	0.6145	0.2430	0.3218	0.0318

Table 4: Anisotropic thermal parameters (Å^2) for 1b

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.02955(14)	0.01922(12)	0.02865(16)	0.0000	0.00599(9)	0.0000
F1	0.0466(12)	0.0568(13)	0.0663(16)	0.0120(11)	-0.0206(11)	-0.007(1)
F2	0.088(2)	0.121(3)	0.0618(19)	-0.0472(19)	-0.0482(17)	0.060(2)
F3	0.024(1)	0.0767(19)	0.141(3)	0.0252(18)	0.0035(13)	0.007(1)
F4	0.212(5)	0.072(2)	0.114(3)	0.036(2)	-0.104(4)	-0.083(3)
F5	0.209(6)	0.067(2)	0.156(4)	0.066(3)	-0.114(4)	-0.076(3)
F6	0.258(8)	0.161(5)	0.193(7)	0.083(5)	0.096(6)	-0.067(5)
F7	0.0594(17)	0.159(4)	0.072(2)	0.071(2)	0.0147(14)	0.0119(18)
F8	0.137(3)	0.091(2)	0.166(4)	0.046(3)	0.119(3)	0.052(2)
F9	0.139(4)	0.235(6)	0.066(3)	-0.050(3)	0.058(2)	-0.135(4)
F10	0.0388(13)	0.076(2)	0.171(4)	-0.057(2)	0.0091(17)	-0.0198(12)
F11	0.0847(17)	0.0493(13)	0.0524(15)	-0.0241(11)	0.0053(12)	-0.0176(12)
F12	0.139(3)	0.0465(14)	0.0546(17)	-0.0011(11)	0.0042(16)	-0.0385(16)
C1	0.073(2)	0.058(3)	0.0257(19)	0.0024(14)	0.0005(15)	-0.0051(18)
C2	0.079(4)	0.040(2)	0.044(3)	0.0021(17)	0.030(2)	-0.012(2)
C3	0.0460(19)	0.058(3)	0.086(3)	-0.020(2)	0.037(2)	-0.0221(17)
C4	0.046(2)	0.047(2)	0.068(3)	-0.021(2)	0.028(2)	-0.0052(18)
C5	0.071(3)	0.051(3)	0.039(2)	-0.0239(19)	0.013(2)	-0.020(2)
C6	0.068(5)	0.055(4)	0.039(5)	-0.001(3)	-0.011(4)	0.013(4)
C7	0.0296(13)	0.0290(13)	0.0222(14)	-0.004(1)	0.003(1)	-0.003(1)
C8	0.0226(12)	0.0306(13)	0.0331(16)	-0.0069(11)	0.004(1)	0.001(1)
C9	0.0244(13)	0.0404(15)	0.0290(16)	-0.0066(12)	0.0020(11)	0.0009(11)
C10	0.0452(18)	0.057(2)	0.0282(18)	-0.0065(14)	0.0003(13)	-0.0243(15)
C11	0.065(2)	0.044(2)	0.032(2)	0.0047(15)	-0.0110(17)	-0.0274(19)
C12	0.0498(19)	0.0362(16)	0.0276(17)	0.0020(13)	-0.0053(13)	-0.0191(14)
C13	0.0221(11)	0.0241(12)	0.0266(14)	0.0005(9)	-0.003(1)	0.0029(9)
C14	0.0280(13)	0.0277(12)	0.0298(16)	-0.0021(11)	-0.001(1)	0.001(1)
C15	0.0325(11)	0.0271(19)	0.0325(13)	-0.0036(15)	-0.0065(9)	0.0041(14)
C16	0.0366(13)	0.034(2)	0.0267(14)	-0.005(1)	-0.004(1)	0.0087(11)
C17	0.0274(13)	0.0406(15)	0.0259(15)	0.0022(11)	0.000(1)	0.0079(11)
C18	0.0243(12)	0.0295(13)	0.0258(14)	0.002(1)	-0.002(1)	0.004(1)
C19	0.0181(13)	0.0445(17)	0.054(2)	-0.0103(15)	-0.0099(13)	0.0058(12)
C20	0.140(6)	0.093(4)	0.056(3)	0.040(3)	-0.050(4)	-0.083(4)
C21	0.0468(18)	0.0378(16)	0.046(2)	-0.0137(14)	0.0023(15)	-0.0056(14)
C22	0.0401(17)	0.0517(19)	0.0337(18)	0.0019(14)	0.0039(13)	0.0071(14)
B1	0.0241(18)	0.0242(19)	0.023(2)	0.0000	-0.0007(14)	0.0000

Table 5: Bond lengths for 1b / Å

Ru1 . C1	2.094(4)	C3—H31	0.92(1)
Ru1 . C2	2.166(4)	C4—C5	1.388(7)
Ru1 . C3	2.194(4)	C4—H41	0.92(1)
Ru1—C4	2.203(4)	C5—H51	0.92(1)
Ru1—C5	2.164(4)	C6—H61	1.03(1)
Ru1—C6	2.333(8)	C6—H62	1.03(1)
F1—C19	1.330(5)	C7—C8	1.405(4)
F2—C19	1.308(5)	C7—C12	1.388(4)
F3—C19	1.346(4)	C7—B1	1.652(3)
F4—C20	1.286(6)	C8—C9	1.392(4)
F5—C20	1.229(9)	C9—C10	1.369(5)
F6—C20	1.381(12)	C9—C19	1.497(4)
F7—C22	1.296(5)	C10—C11	1.382(6)
F8—C22	1.318(5)	C11—C12	1.401(5)
F9—C22	1.265(5)	C11—C20	1.504(6)
F10—C21	1.328(5)	C13—C14	1.407(4)
F11—C21	1.327(5)	C13—C18	1.397(4)
F12—C21	1.326(5)	C13—B1	1.639(4)

C1—C2	1.421(6)	C14—C15	1.392(5)
C1—C5	1.442(7)	C15—C16	1.384(5)
C1—C6	1.319(11)	C15—C21	1.497(5)
C1—H11	0.92(1)	C16—C17	1.387(4)
C2—C3	1.399(7)	C17—C18	1.401(4)
C2—H21	0.93(1)	C17—C22	1.500(5)
C3—C4	1.430(6)		

Table 6: Bond angles for 1b / °

C1—Ru1—C1*	162.0(2)	Ru1—C1—C6	82.9(4)
C1—Ru1—C2	38.93(18)	C2—C1—C6	120.9(5)
C1—Ru1—C2*	127.40(17)	C5—C1—C6	115.8(5)
C2—Ru1—C2*	114.2(2)	Ru1—C1—H11	109.7(25)
C1—Ru1—C3	63.99(19)	C2—C1—H11	125.6(5)
C2—Ru1—C3	37.4(2)	C5—C1—H11	125.7(5)
C1—Ru1—C3*	112.79(18)	C6—C1—H11	26.9(25)
C2—Ru1—C3*	128.10(18)	Ru1—C2—C1	67.8(2)
C3—Ru1—C3*	161.2(2)	Ru1—C2—C3	72.4(3)
C1—Ru1—C4	64.46(18)	C1—C2—C3	107.5(3)
C2—Ru1—C4	63.68(17)	Ru1—C2—H21	115.7(23)
C3—Ru1—C4	37.98(18)	C1—C2—H21	125.7(4)
C1—Ru1—C4*	125.12(18)	C3—C2—H21	125.7(4)
C2—Ru1—C4*	160.51(16)	Ru1—C3—C2	70.2(2)
C3—Ru1—C4*	159.73(15)	Ru1—C3—C4	71.4(2)
C1—Ru1—C5	39.5(2)	C2—C3—C4	109.1(3)
C2—Ru1—C5	64.43(16)	Ru1—C3—H31	121.7(34)
C3—Ru1—C5	62.93(16)	C2—C3—H31	125.4(4)
C1—Ru1—C5*	157.07(17)	C4—C3—H31	125.4(4)
C2—Ru1—C5*	161.87(17)	Ru1—C4—C3	70.7(2)
C3—Ru1—C5*	127.64(19)	Ru1—C4—C5	70.0(2)
C1—Ru1—C6	34.1(3)	C3—C4—C5	107.6(4)
C1*—Ru1—C6	138.7(3)	Ru1—C4—H41	117.4(24)
C2—Ru1—C6	63.9(3)	C3—C4—H41	126.0(4)
C2*—Ru1—C6	100.0(3)	C5—C4—H41	125.7(4)
C3—Ru1—C6	96.7(3)	Ru1—C5—C1	67.6(2)
C4—Ru1—C4*	125.3(2)	Ru1—C5—C4	73.0(2)
C4—Ru1—C5	37.06(18)	C1—C5—C4	108.2(4)
C4—Ru1—C5*	111.06(17)	Ru1—C5—H51	116.3(25)
C5—Ru1—C5*	123.0(3)	C1—C5—H51	125.4(4)
C3*—Ru1—C6	78.7(3)	C4—C5—H51	125.4(4)
C4—Ru1—C6	96.0(3)	Ru1—C6—C1	63.0(4)
C4*—Ru1—C6	96.9(3)	Ru1—C6—H61	110.5(36)
C5—Ru1—C6	62.6(3)	C1—C6—H61	123.6(5)
C5*—Ru1—C6	134.0(3)	Ru1—C6—H62	106.2(60)
Ru1—C1—C2	73.2(3)	C1—C6—H62	123.7(5)
Ru1—C1—C5	72.8(2)	H11—C6—H62	110.5(45)
C2—C1—C5	107.5(4)	H61—C6—H62	112.1(13)
C8—C7—C12	115.3(3)	F1—C19—C9	114.2(3)
C8—C7—B1	121.6(2)	F2—C19—C9	113.1(3)
C12—C7—B1	123.1(3)	F3—C19—C9	111.7(4)
C7—C8—C9	122.1(3)	F4—C20—F5	111.0(8)
C8—C9—C10	121.1(3)	F4—C20—F6	103.8(6)
C8—C9—C19	120.4(3)	F5—C20—F6	102.2(6)
C10—C9—C19	118.5(3)	F4—C20—C11	114.2(4)
C9—C10—C11	118.5(3)	F5—C20—C11	116.1(5)
C10—C11—C12	120.1(3)	F6—C20—C11	107.9(7)
C10—C11—C20	119.9(4)	F10—C21—F11	106.1(3)
C12—C11—C20	120.0(4)	F10—C21—F12	108.0(4)

C7—C12—C11	122.8(3)	F11—C21—F12	105.1(3)
C14—C13—C18	115.7(3)	F10—C21—C15	111.3(3)
C14—C13—B1	121.1(2)	F11—C21—C15	113.6(3)
C18—C13—B1	123.0(2)	F12—C21—C15	112.3(3)
C13—C14—C15	122.2(3)	F7—C22—F8	103.3(4)
C14—C15—C16	121.2(3)	F7—C22—F9	108.5(4)
C14—C15—C21	118.7(3)	F8—C22—F9	104.8(5)
C16—C15—C21	120.1(3)	F7—C22—C17	112.2(3)
C15—C16—C17	117.7(3)	F8—C22—C17	112.5(3)
C16—C17—C18	121.2(3)	F9—C22—C17	114.6(3)
C16—C17—C22	118.7(3)	C7—B1—C7**	112.0(3)
C18—C17—C22	120.0(3)	C7—B1—C13	110.14(13)
C13—C18—C17	121.9(3)	C7—B1—C13**	107.11(13)
F1—C19—F2	107.6(4)	C13—B1—C13**	110.4(3)
F1—C19—F3	104.4(3)	C1—H11—C6	112.8(41)
F2—C19—F3	105.1(3)		

*related to asymmetric unit by twofold rotation axis at 0.5, y, 0
**related to asymmetric unit by twofold rotation axis at 0.5, y, 0.5
Note – geometrically-positioned H atoms have been excluded

Table 7: Atomic coordinates, equivalent isotropic thermal parameters (Å^2) and site occupancies of refined atoms for 1d

Atom	*x*	*y*	*z*	U_{equiv}	Occ.
Ru(1)	0.341991(19)	0.00731(2)	0.326789(16)	0.0181	1.0
C(1)	0.4741(3)	0.0029(3)	0.3580(2)	0.0261	1.0
C(2)	0.4500(3)	0.1069(3)	0.3676(3)	0.0304	1.0
C(3)	0.4043(3)	0.1058(3)	0.4225(2)	0.0335	1.0
C(4)	0.3999(3)	0.0051(3)	0.4483(2)	0.0312	1.0
C(5)	0.4447(3)	-0.0590(3)	0.4111(2)	0.0270	1.0
C(6)	0.4577(3)	-0.0329(4)	0.2853(3)	0.0354	1.0
C(7)	0.2067(3)	0.0463(4)	0.3040(3)	0.0383	1.0
C(8)	0.2160(3)	-0.0595(4)	0.3098(3)	0.0439	1.0
C(9)	0.2528(3)	-0.0936(3)	0.2535(3)	0.0360	1.0
C(10)	0.2669(3)	-0.0079(4)	0.2123(2)	0.0332	1.0
C(11)	0.2372(3)	0.0784(3)	0.2432(3)	0.0307	1.0
Ru(2)	0.32475(2)	0.50497(2)	0.327575(17)	0.0211	1.0
C(12)	0.2581(5)	0.5817(5)	0.2343(3)	0.0653	1.0
C(13)	0.3375(3)	0.6351(4)	0.2618(3)	0.0443	1.0
C(14)	0.3324(4)	0.6721(4)	0.3335(4)	0.0643	1.0
C(15)	0.2567(5)	0.6449(4)	0.3481(4)	0.0612	1.0
C(16)	0.2087(3)	0.5888(4)	0.2844(4)	0.0490	1.0
C(17)	0.2590(7)	0.4956(6)	0.2049(4)	0.0955	1.0
C(18)	0.3900(6)	0.4464(6)	0.4342(3)	0.0778	1.0
C(19)	0.3139(5)	0.3814(7)	0.4008(5)	0.0854	1.0
C(20)	0.3266(4)	0.3418(5)	0.3389(5)	0.0771	1.0
C(21)	0.4008(4)	0.3693(4)	0.3288(3)	0.0534	1.0
C(22)	0.4431(3)	0.4325(4)	0.3848(3)	0.0410	1.0
Ru(3)	0.0	0.0	0.0	0.0281	1.0
C(23)	0.1340(3)	-0.0130(6)	0.0206(4)	0.0624	1.0
C(24)	0.1134(4)	0.0927(5)	0.0279(4)	0.0575	1.0
C(25)	0.0773(4)	0.0968(4)	0.0862(3)	0.0452	1.0
C(26)	0.0714(4)	-0.0003(4)	0.1169(3)	0.0454	1.0
C(27)	0.1091(4)	-0.0691(4)	0.0776(3)	0.0495	1.0
C(28)	0.1174(7)	-0.038(1)	-0.0514(6)	0.0507	0.5
Ru(4)	0.0	0.5	0.0	0.0208	1.0
C(29)	-0.0550(6)	0.5715(6)	0.0775(6)	0.0916	1.0
C(30)	-0.1164(4)	0.5748(6)	0.0055(6)	0.0976	1.0
C(31)	-0.0786(5)	0.6320(5)	-0.0391(6)	0.0906	1.0

C(32)	0.0024(4)	0.6658(4)	0.0018(4)	0.0564	1.0
C(33)	0.0173(4)	0.6297(4)	0.0746(3)	0.0430	1.0
C(34)	-0.0599(9)	0.495(1)	0.0960(6)	0.0597	0.5
O(1)	0.1294(2)	0.2955(3)	0.2223(2)	0.0405	1.0
O(2)	0.0507(2)	0.4243(2)	0.2675(2)	0.0430	1.0
O(3)	0.1141(2)	0.2866(3)	0.3475(2)	0.0560	1.0
S(1)	0.08049(7)	0.32272(8)	0.27340(6)	0.0285	1.0
C(35)	-0.0167(3)	0.2494(3)	0.2411(3)	0.0321	1.0
F(1)	-0.07269(18)	0.2686(2)	0.28033(17)	0.0412	1.0
F(2)	-0.0007(2)	0.1514(2)	0.24516(19)	0.0483	1.0
F(3)	-0.0552(2)	0.2711(2)	0.17047(16)	0.0460	1.0
O(4)	0.2082(2)	0.7203(3)	0.10040(19)	0.0349	1.0
O(5)	0.2072(3)	0.7163(3)	-0.02891(19)	0.0503	1.0
O(6)	0.2879(3)	0.5927(3)	0.0550(2)	0.0546	1.0
S(2)	0.25126(7)	0.69102(8)	0.04572(6)	0.0276	1.0
C(36)	0.3434(3)	0.7738(4)	0.0639(3)	0.0311	1.0
F(4)	0.3945(2)	0.7544(2)	0.0200(2)	0.0530	1.0
F(5)	0.3901(2)	0.7668(3)	0.13307(18)	0.0585	1.0
F(6)	0.3200(2)	0.8702(2)	0.05312(19)	0.0492	1.0
O(7)	0.4691(2)	0.2142(2)	0.06876(18)	0.0328	1.0
O(8)	0.4591(2)	0.2215(3)	0.19629(18)	0.0397	1.0
O(9)	0.3852(2)	0.0904(2)	0.1152(2)	0.0374	1.0
S(3)	0.42068(7)	0.19006(7)	0.12138(6)	0.0235	1.0
C(37)	0.3288(3)	0.2717(4)	0.0936(2)	0.0264	1.0
F(7)	0.2766(2)	0.2652(2)	0.13809(18)	0.0479	1.0
F(8)	0.2822(2)	0.2502(2)	0.02564(17)	0.0486	1.0
F(9)	0.3514(2)	0.3680(2)	0.09273(17)	0.0427	1.0

Table 8: Atomic coordinates, isotropic thermal parameters (Å^2) and site occupancies (where not unity) of geometrically-positioned atoms for 1d

Atom	*x*	*y*	*z*	U_{equiv}	Occ.
H(21)	0.4633	0.1673	0.3405	0.0343	1.0
H(31)	0.3790	0.1663	0.4407	0.0387	1.0
H(41)	0.3701	-0.0165	0.4864	0.0364	1.0
H(51)	0.4544	-0.1330	0.4195	0.0298	1.0
H(61)	0.4499	-0.1067	0.2751	0.0435	1.0
H(62)	0.4538	0.0155	0.2436	0.0435	1.0
H(71)	0.1828	0.0907	0.3369	0.0454	1.0
H(81)	0.1994	-0.1030	0.3475	0.0507	1.0
H(91)	0.2665	-0.1651	0.2441	0.0392	1.0
H(101)	0.2930	-0.0084	0.1693	0.0382	1.0
H(111)	0.2377	0.1492	0.2251	0.0340	1.0
H(131)	0.3849	0.6444	0.2371	0.0513	1.0
H(141)	0.3779	0.7120	0.3676	0.0735	1.0
H(151)	0.2382	0.6606	0.3939	0.0763	1.0
H(161)	0.1503	0.5604	0.2779	0.0560	1.0
H(171)	0.3072	0.4763	0.1835	0.1097	1.0
H(172)	0.2114	0.4471	0.2032	0.1097	1.0
H(181)	0.4006	0.4887	0.4798	0.0914	1.0
H(191)	0.2634	0.3701	0.4211	0.1083	1.0
H(201)	0.2852	0.2970	0.3047	0.0878	1.0
H(211)	0.4234	0.3474	0.2863	0.0613	1.0
H(221)	0.5005	0.4630	0.3898	0.0454	1.0
H(231)	0.1608	-0.0417	-0.0174	0.0738	0.5
H(241)	0.1236	0.1502	-0.0033	0.0661	1.0
H(251)	0.0574	0.1604	0.1051	0.0484	1.0
H(261)	0.0454	-0.0165	0.1585	0.0512	1.0
H(271)	0.1171	-0.1430	0.0873	0.0527	1.0

H(281)	0.1147	0.0161	-0.0893	0.0643	0.5
H(282)	0.1079	-0.1097	-0.0669	0.0643	0.5
H(291)	-0.0627	0.5341	0.1217	0.1255	0.5
H(301)	-0.1737	0.5424	-0.0085	0.1184	1.0
H(311)	-0.1044	0.6473	-0.0923	0.0984	1.0
H(321)	0.0424	0.7084	-0.0178	0.0631	1.0
H(331)	0.0685	0.6425	0.1160	0.0525	1.0
H(341)	-0.0122	0.4644	0.1344	0.0787	0.5
H(342)	-0.1122	0.4541	0.0746	0.0787	0.5

Table 9: Anisotropic thermal parameters (Å^2) for 1d

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.01723(17)	0.01772(17)	0.01871(17)	0.00360(11)	0.00321(12)	0.00097(12)
C(1)	0.0143(19)	0.029(2)	0.032(2)	0.0022(17)	0.0008(15)	-0.0008(16)
C(2)	0.017(2)	0.029(2)	0.040(3)	0.0077(18)	-0.0028(18)	-0.0073(16)
C(3)	0.041(3)	0.029(2)	0.027(2)	-0.0064(17)	0.002(2)	-0.0000(19)
C(4)	0.039(3)	0.036(2)	0.0161(19)	0.0027(17)	0.0020(16)	0.003(2)
C(5)	0.025(2)	0.027(2)	0.022(2)	0.0008(16)	-0.0060(16)	-0.0006(17)
C(6)	0.027(2)	0.044(3)	0.039(3)	0.000(2)	0.0128(19)	0.0086(19)
C(7)	0.016(2)	0.053(3)	0.044(3)	0.007(2)	0.0049(19)	0.009(2)
C(8)	0.025(3)	0.052(3)	0.050(3)	0.020(2)	0.000(2)	-0.014(2)
C(9)	0.032(3)	0.023(2)	0.044(3)	-0.0010(18)	-0.010(2)	-0.0060(18)
C(10)	0.029(2)	0.049(3)	0.0179(19)	0.0032(19)	-0.0023(16)	0.004(2)
C(11)	0.025(2)	0.027(2)	0.033(2)	0.0066(17)	-0.0058(18)	-0.0008(17)
Ru(2)	0.02162(18)	0.01786(18)	0.02339(18)	0.00537(12)	0.00509(12)	0.00190(12)
C(12)	0.101(6)	0.050(4)	0.030(3)	0.014(3)	-0.010(3)	0.007(3)
C(13)	0.037(3)	0.035(3)	0.056(3)	0.030(2)	0.003(2)	-0.007(2)
C(14)	0.068(5)	0.017(3)	0.099(6)	-0.002(3)	0.004(4)	0.011(2)
C(15)	0.080(5)	0.038(3)	0.073(4)	-0.001(3)	0.033(4)	0.015(3)
C(16)	0.029(3)	0.039(3)	0.072(4)	0.034(3)	-0.001(3)	0.009(2)
C(17)	0.17(1)	0.074(5)	0.029(3)	0.006(3)	0.002(4)	-0.006(5)
C(18)	0.110(5)	0.098(5)	0.021(3)	0.021(3)	0.007(3)	0.052(4)
C(19)	0.047(4)	0.109(6)	0.115(6)	0.100(5)	0.047(3)	0.044(3)
C(20)	0.048(4)	0.029(3)	0.142(8)	0.033(4)	0.002(5)	-0.001(3)
C(21)	0.056(4)	0.035(3)	0.062(4)	0.003(2)	0.002(3)	0.021(3)
C(22)	0.026(3)	0.032(2)	0.056(3)	0.021(2)	-0.0075(19)	0.0017(19)
Ru(3)	0.0260(3)	0.0193(2)	0.0306(3)	-0.0003(2)	-0.00866(19)	0.0027(2)
C(23)	0.016(2)	0.114(6)	0.055(3)	-0.007(4)	0.004(2)	0.013(3)
C(24)	0.021(3)	0.061(4)	0.084(5)	0.010(3)	-0.001(3)	-0.006(2)
C(25)	0.043(3)	0.027(2)	0.051(3)	-0.007(2)	-0.015(3)	-0.003(2)
C(26)	0.048(3)	0.051(3)	0.029(3)	0.006(2)	-0.006(2)	0.009(2)
C(27)	0.038(3)	0.042(3)	0.052(3)	-0.006(2)	-0.020(2)	0.015(2)
C(28)	0.045(7)	0.067(7)	0.049(7)	0.002(5)	0.028(5)	0.007(5)
Ru(4)	0.0254(3)	0.0175(2)	0.0213(2)	-0.00185(18)	0.00944(18)	0.00030(18)
C(29)	0.098(6)	0.054(4)	0.161(8)	-0.067(5)	0.105(7)	-0.038(4)
C(30)	0.029(4)	0.075(5)	0.19(1)	-0.100(6)	0.034(5)	-0.012(3)
C(31)	0.046(4)	0.043(4)	0.157(8)	-0.034(4)	-0.023(5)	0.020(3)
C(32)	0.054(4)	0.018(3)	0.086(5)	-0.009(2)	-0.004(3)	0.009(2)
C(33)	0.042(3)	0.034(3)	0.055(3)	-0.024(2)	0.017(2)	-0.001(2)
C(34)	0.09(1)	0.063(8)	0.045(6)	0.002(6)	0.049(7)	0.023(7)
O(1)	0.0280(18)	0.0415(19)	0.055(2)	0.0005(16)	0.0166(16)	0.0007(14)
O(2)	0.041(2)	0.0275(17)	0.063(2)	-0.0066(15)	0.0178(18)	-0.0053(14)
O(3)	0.042(2)	0.076(3)	0.038(2)	0.0179(19)	-0.0126(17)	-0.018(2)
S(1)	0.0263(6)	0.0262(5)	0.0322(6)	0.0025(4)	0.0058(4)	-0.0057(4)
C(35)	0.026(3)	0.027(3)	0.042(3)	0.0026(17)	0.008(2)	-0.0000(16)
F(1)	0.0284(16)	0.0485(16)	0.0496(18)	0.0049(13)	0.0151(13)	-0.0039(13)
F(2)	0.0443(19)	0.0257(14)	0.072(2)	-0.0004(13)	0.0095(16)	-0.0059(12)
F(3)	0.0377(17)	0.0617(18)	0.0312(16)	0.0047(13)	-0.0053(12)	-0.0038(15)

O(4)	0.0326(18)	0.0326(16)	0.0443(19)	0.0064(14)	0.0186(15)	0.0067(14)
O(5)	0.053(2)	0.061(2)	0.0314(19)	0.0070(17)	0.0011(16)	-0.022(2)
O(6)	0.075(3)	0.0237(18)	0.082(3)	0.0073(17)	0.050(2)	0.0110(17)
S(2)	0.0318(6)	0.0245(5)	0.0286(5)	0.0042(4)	0.0117(4)	-0.0001(4)
C(36)	0.029(3)	0.034(2)	0.033(3)	0.012(2)	0.012(2)	0.002(2)
F(4)	0.043(2)	0.069(2)	0.058(2)	0.0054(15)	0.0329(17)	-0.0020(14)
F(5)	0.0400(19)	0.091(3)	0.0377(18)	0.0172(16)	-0.0034(14)	-0.0104(17)
F(6)	0.0461(19)	0.0299(16)	0.071(2)	0.0007(14)	0.0125(16)	-0.0079(13)
O(7)	0.0306(17)	0.0333(17)	0.0397(18)	-0.0035(13)	0.0184(14)	-0.0029(14)
O(8)	0.050(2)	0.0408(18)	0.0259(17)	-0.0053(14)	0.0042(15)	0.0064(17)
O(9)	0.042(2)	0.0210(15)	0.054(2)	-0.0001(13)	0.0203(16)	-0.0021(13)
S(3)	0.0260(5)	0.0203(4)	0.0255(5)	-0.0010(4)	0.0091(4)	0.0005(4)
C(37)	0.030(2)	0.0257(19)	0.025(2)	-0.0022(17)	0.0106(18)	-0.0026(18)
F(7)	0.0423(18)	0.0547(18)	0.058(2)	0.0090(14)	0.0343(16)	0.0125(14)
F(8)	0.0355(19)	0.068(2)	0.0368(17)	-0.0109(13)	-0.0021(14)	0.0121(13)
F(9)	0.0491(19)	0.0240(14)	0.0569(19)	0.0044(12)	0.0168(14)	0.0081(12)

Table 10: Bond lengths for 1d / Å

Ru(1)—C(1)	2.080(4)	Ru(3)—C(23)	2.121(5)
Ru(1)—C(2)	2.177(4)	Ru(3)—C(24)	2.168(6)
Ru(1)—C(3)	2.245(4)	Ru(3)—C(25)	2.195(5)
Ru(1)—C(4)	2.235(4)	Ru(3)—C(26)	2.206(5)
Ru(1)—C(5)	2.175(4)	Ru(3)—C(27)	2.192(5)
Ru(1)—C(6)	2.272(4)	Ru(3)—C(28)	2.40(1)
Ru(1)—C(7)	2.194(5)	C(23)—C(24)	1.456(9)
Ru(1)—C(8)	2.180(5)	C(23)—C(27)	1.439(9)
Ru(1)—C(9)	2.187(4)	C(23)—C(28)	1.348(13)
Ru(1)—C(10)	2.195(4)	C(24)—C(25)	1.365(9)
Ru(1)—C(11)	2.215(4)	C(25)—C(26)	1.423(7)
C(1)—C(2)	1.458(6)	C(26)—C(27)	1.407(8)
C(1)—C(5)	1.459(6)	Ru(4)—C(29)	2.111(6)
C(1)—C(6)	1.405(6)	Ru(4)—C(30)	2.162(6)
C(2)—C(3)	1.413(7)	Ru(4)—C(31)	2.183(6)
C(3)—C(4)	1.429(6)	Ru(4)—C(32)	2.201(5)
C(4)—C(5)	1.412(6)	Ru(4)—C(33)	2.190(4)
C(7)—C(8)	1.414(8)	Ru(4)—C(34)	2.251(9)
C(7)—C(11)	1.417(7)	C(29)—C(30)	1.463(14)
C(8)—C(9)	1.411(8)	C(29)—C(33)	1.417(8)
C(9)—C(10)	1.425(7)	C(29)—C(34)	1.087(14)
C(10)—C(11)	1.421(7)	C(30)—C(31)	1.382(14)
Ru(2)—C(12)	2.077(5)	C(31)—C(32)	1.420(9)
Ru(2)—C(13)	2.162(4)	C(32)—C(33)	1.408(9)
Ru(2)—C(14)	2.222(5)	O(1)—S(1)	1.436(4)
Ru(2)—C(15)	2.243(6)	O(2)—S(1)	1.428(4)
Ru(2)—C(16)	2.165(5)	O(3)—S(1)	1.441(4)
Ru(2)—C(17)	2.282(7)	S(1)—C(35)	1.825(5)
Ru(2)—C(18)	2.158(5)	C(35)—F(1)	1.329(6)
Ru(2)—C(19)	2.173(5)	C(35)—F(2)	1.325(5)
Ru(2)—C(20)	2.176(6)	C(35)—F(3)	1.346(6)
Ru(2)—C(21)	2.181(5)	O(4)—S(2)	1.432(3)
Ru(2)—C(22)	2.177(5)	O(5)—S(2)	1.441(4)
C(12)—C(13)	1.450(9)	O(6)—S(2)	1.426(4)
C(12)—C(16)	1.38(1)	S(2)—C(36)	1.819(5)
C(12)—C(17)	1.27(1)	C(36)—F(4)	1.332(6)
C(13)—C(14)	1.451(9)	C(36)—F(5)	1.331(6)
C(14)—C(15)	1.375(9)	C(36)—F(6)	1.336(6)
C(15)—C(16)	1.457(9)	O(7)—S(3)	1.443(3)
C(18)—C(19)	1.509(13)	O(8)—S(3)	1.447(3)

C(18)—C(22)	1.428(9)	O(9)—S(3)	1.436(3)
C(19)—C(20)	1.335(12)	S(3)—C(37)	1.813(5)
C(20)—C(21)	1.32(1)	C(37)—F(7)	1.333(5)
C(21)—C(22)	1.385(8)	C(37)—F(8)	1.339(5)
		C(37)—F(9)	1.331(5)

Note – geometrically-positioned H atoms have been excluded

Table 11: Bond angles for 1d / °

C(1)—Ru(1)—C(2)	39.97(16)	C(19)—Ru(2)—C(22)	63.7(2)
C(1)—Ru(1)—C(3)	64.19(17)	C(20)—Ru(2)—C(22)	61.6(2)
C(2)—Ru(1)—C(3)	37.22(18)	C(21)—Ru(2)—C(22)	37.1(2)
C(1)—Ru(1)—C(4)	64.65(17)	Ru(2)—C(12)—C(13)	73.2(3)
C(2)—Ru(1)—C(4)	63.52(17)	Ru(2)—C(12)—C(16)	74.5(3)
C(3)—Ru(1)—C(4)	37.20(16)	C(13)—C(12)—C(16)	110.1(6)
C(1)—Ru(1)—C(5)	40.04(16)	Ru(2)—C(12)—C(17)	82.1(4)
C(2)—Ru(1)—C(5)	65.57(16)	C(13)—C(12)—C(17)	119.2(9)
C(3)—Ru(1)—C(5)	62.95(16)	C(16)—C(12)—C(17)	115.3(8)
C(4)—Ru(1)—C(5)	37.32(17)	Ru(2)—C(13)—C(12)	66.9(3)
C(1)—Ru(1)—C(6)	37.33(17)	Ru(2)—C(13)—C(14)	72.9(3)
C(2)—Ru(1)—C(6)	66.34(18)	C(12)—C(13)—C(14)	103.9(5)
C(3)—Ru(1)—C(6)	99.43(18)	Ru(2)—C(14)—C(13)	68.5(3)
C(4)—Ru(1)—C(6)	99.95(18)	Ru(2)—C(14)—C(15)	72.9(3)
C(5)—Ru(1)—C(6)	66.64(17)	C(13)—C(14)—C(15)	111.0(6)
C(1)—Ru(1)—C(7)	167.13(19)	Ru(2)—C(15)—C(14)	71.2(3)
C(2)—Ru(1)—C(7)	127.28(19)	Ru(2)—C(15)—C(16)	67.8(3)
C(3)—Ru(1)—C(7)	104.33(19)	C(14)—C(15)—C(16)	107.0(6)
C(4)—Ru(1)—C(7)	110.29(19)	Ru(2)—C(16)—C(12)	67.6(3)
C(5)—Ru(1)—C(7)	141.79(19)	Ru(2)—C(16)—C(15)	73.6(3)
C(1)—Ru(1)—C(8)	153.50(19)	C(12)—C(16)—C(15)	107.9(5)
C(2)—Ru(1)—C(8)	160.6(2)	Ru(2)—C(17)—C(12)	64.4(4)
C(3)—Ru(1)—C(8)	124.9(2)	Ru(2)—C(18)—C(19)	70.1(3)
C(4)—Ru(1)—C(8)	106.44(19)	Ru(2)—C(18)—C(22)	71.5(3)
C(5)—Ru(1)—C(8)	117.55(18)	C(19)—C(18)—C(22)	102.9(6)
C(1)—Ru(1)—C(9)	129.37(18)	Ru(2)—C(19)—C(18)	69.1(3)
C(2)—Ru(1)—C(9)	160.3(2)	Ru(2)—C(19)—C(20)	72.2(3)
C(3)—Ru(1)—C(9)	162.5(2)	C(18)—C(19)—C(20)	107.3(5)
C(4)—Ru(1)—C(9)	132.46(18)	Ru(2)—C(20)—C(19)	72.0(4)
C(5)—Ru(1)—C(9)	118.38(16)	Ru(2)—C(20)—C(21)	72.6(3)
C(1)—Ru(1)—C(10)	123.64(17)	C(19)—C(20)—C(21)	111.2(7)
C(2)—Ru(1)—C(10)	126.91(18)	Ru(2)—C(21)—C(20)	72.2(4)
C(3)—Ru(1)—C(10)	149.68(18)	Ru(2)—C(21)—C(22)	71.3(3)
C(4)—Ru(1)—C(10)	169.45(17)	C(20)—C(21)—C(22)	110.9(7)
C(5)—Ru(1)—C(10)	144.04(17)	Ru(2)—C(22)—C(18)	70.1(3)
C(1)—Ru(1)—C(11)	140.13(17)	Ru(2)—C(22)—C(21)	71.6(3)
C(2)—Ru(1)—C(11)	113.54(16)	C(18)—C(22)—C(21)	107.7(6)
C(3)—Ru(1)—C(11)	115.48(17)	C(23)—Ru(3)—C(24)	39.7(3)
C(4)—Ru(1)—C(11)	141.15(18)	C(23)—Ru(3)—C(25)	62.7(2)
C(5)—Ru(1)—C(11)	178.37(16)	C(24)—Ru(3)—C(25)	36.4(2)
C(6)—Ru(1)—C(7)	149.77(19)	C(23)—Ru(3)—C(26)	63.8(2)
C(6)—Ru(1)—C(8)	133.0(2)	C(24)—Ru(3)—C(26)	63.8(2)
C(7)—Ru(1)—C(8)	37.7(2)	C(25)—Ru(3)—C(26)	37.7(2)
C(6)—Ru(1)—C(9)	96.7(2)	C(23)—Ru(3)—C(27)	38.9(3)
C(7)—Ru(1)—C(9)	63.1(2)	C(24)—Ru(3)—C(27)	65.2(2)
C(8)—Ru(1)—C(9)	37.7(2)	C(25)—Ru(3)—C(27)	62.50(19)
C(6)—Ru(1)—C(10)	87.05(18)	C(23)—Ru(3)—C(28)	34.0(3)
C(7)—Ru(1)—C(10)	63.08(19)	C(24)—Ru(3)—C(28)	60.0(4)
C(8)—Ru(1)—C(10)	63.17(19)	C(25)—Ru(3)—C(28)	92.9(4)
C(9)—Ru(1)—C(10)	37.95(18)	C(26)—Ru(3)—C(28)	97.2(3)

C(6)—Ru(1)—C(11)	114.42(18)	C(27)—Ru(3)—C(28)	65.5(3)
C(7)—Ru(1)—C(11)	37.49(18)	Ru(3)—C(23)—C(24)	71.9(3)
C(8)—Ru(1)—C(11)	62.79(18)	Ru(3)—C(23)—C(27)	73.2(3)
C(9)—Ru(1)—C(11)	62.95(17)	C(24)—C(23)—C(27)	108.3(5)
C(10)—Ru(1)—C(11)	37.59(18)	Ru(3)—C(23)—C(28)	84.2(5)
Ru(1)—C(1)—C(2)	73.6(2)	C(24)—C(23)—C(28)	109.6(8)
Ru(1)—C(1)—C(5)	73.5(2)	C(27)—C(23)—C(28)	126.4(8)
C(2)—C(1)—C(5)	107.8(4)	Ru(3)—C(24)—C(23)	68.4(3)
Ru(1)—C(1)—C(6)	78.8(3)	Ru(3)—C(24)—C(25)	72.9(3)
C(2)—C(1)—C(6)	116.6(4)	C(23)—C(24)—C(25)	105.6(5)
C(5)—C(1)—C(6)	117.1(4)	Ru(3)—C(25)—C(24)	70.7(3)
Ru(1)—C(2)—C(1)	66.4(2)	Ru(3)—C(25)—C(26)	71.5(3)
Ru(1)—C(2)—C(3)	74.0(3)	C(24)—C(25)—C(26)	111.9(5)
C(1)—C(2)—C(3)	106.6(4)	Ru(3)—C(26)—C(25)	70.7(3)
Ru(1)—C(3)—C(2)	68.8(2)	Ru(3)—C(26)—C(27)	70.8(3)
Ru(1)—C(3)—C(4)	71.0(2)	C(25)—C(26)—C(27)	107.1(5)
C(2)—C(3)—C(4)	109.7(4)	Ru(3)—C(27)—C(23)	67.9(3)
Ru(1)—C(4)—C(3)	71.8(2)	Ru(3)—C(27)—C(26)	71.9(3)
Ru(1)—C(4)—C(5)	69.0(2)	C(23)—C(27)—C(26)	107.0(5)
C(3)—C(4)—C(5)	108.7(4)	Ru(3)—C(28)—C(23)	61.7(4)
Ru(1)—C(5)—C(1)	66.5(2)	C(29)—Ru(4)—C(30)	40.0(4)
Ru(1)—C(5)—C(4)	73.7(3)	C(29)—Ru(4)—C(31)	63.7(4)
C(1)—C(5)—C(4)	107.2(4)	C(30)—Ru(4)—C(31)	37.1(4)
Ru(1)—C(6)—C(1)	63.9(2)	C(29)—Ru(4)—C(32)	63.2(3)
Ru(1)—C(7)—C(8)	70.6(3)	C(30)—Ru(4)—C(32)	63.4(3)
Ru(1)—C(7)—C(11)	72.0(3)	C(31)—Ru(4)—C(32)	37.8(2)
C(8)—C(7)—C(11)	107.9(5)	C(29)—Ru(4)—C(33)	38.4(2)
Ru(1)—C(8)—C(7)	71.7(3)	C(30)—Ru(4)—C(33)	65.3(2)
Ru(1)—C(8)—C(9)	71.4(3)	C(31)—Ru(4)—C(33)	63.5(3)
C(7)—C(8)—C(9)	108.5(4)	C(32)—Ru(4)—C(33)	37.4(2)
Ru(1)—C(9)—C(8)	70.9(3)	C(29)—Ru(4)—C(34)	28.6(4)
Ru(1)—C(9)—C(10)	71.4(3)	C(30)—Ru(4)—C(34)	54.3(5)
C(8)—C(9)—C(10)	107.8(4)	C(31)—Ru(4)—C(34)	87.7(5)
Ru(1)—C(10)—C(9)	70.7(2)	C(32)—Ru(4)—C(34)	91.6(4)
Ru(1)—C(10)—C(11)	72.0(2)	C(33)—Ru(4)—C(34)	61.7(4)
C(9)—C(10)—C(11)	107.7(4)	Ru(4)—C(29)—C(30)	71.8(4)
Ru(1)—C(11)—C(7)	70.5(3)	Ru(4)—C(29)—C(33)	73.8(3)
Ru(1)—C(11)—C(10)	70.5(2)	C(30)—C(29)—C(33)	109.2(8)
C(7)—C(11)—C(10)	108.0(4)	Ru(4)—C(29)—C(34)	82.9(6)
C(12)—Ru(2)—C(13)	39.9(3)	C(30)—C(29)—C(34)	103.5(11)
C(12)—Ru(2)—C(14)	64.1(3)	C(33)—C(29)—C(34)	130.7(12)
C(13)—Ru(2)—C(14)	38.6(2)	Ru(4)—C(30)—C(29)	68.1(4)
C(12)—Ru(2)—C(15)	64.1(3)	Ru(4)—C(30)—C(31)	72.3(4)
C(13)—Ru(2)—C(15)	63.8(2)	C(29)—C(30)—C(31)	105.6(6)
C(14)—Ru(2)—C(15)	35.9(2)	Ru(4)—C(31)—C(30)	70.6(4)
C(12)—Ru(2)—C(16)	38.0(3)	Ru(4)—C(31)—C(32)	71.8(3)
C(13)—Ru(2)—C(16)	64.9(2)	C(30)—C(31)—C(32)	109.8(8)
C(14)—Ru(2)—C(16)	62.5(2)	Ru(4)—C(32)—C(31)	70.4(3)
C(15)—Ru(2)—C(16)	38.5(3)	Ru(4)—C(32)—C(33)	70.9(3)
C(12)—Ru(2)—C(17)	33.5(3)	C(31)—C(32)—C(33)	109.0(7)
C(13)—Ru(2)—C(17)	63.7(3)	Ru(4)—C(33)—C(29)	67.8(3)
C(14)—Ru(2)—C(17)	96.4(3)	Ru(4)—C(33)—C(32)	71.7(3)
C(15)—Ru(2)—C(17)	95.3(3)	C(29)—C(33)—C(32)	106.2(6)
C(16)—Ru(2)—C(17)	60.5(3)	Ru(4)—C(34)—C(29)	68.5(6)
C(12)—Ru(2)—C(18)	170.7(3)	O(1)—S(1)—O(2)	114.8(2)
C(13)—Ru(2)—C(18)	136.1(3)	O(1)—S(1)—O(3)	114.8(3)
C(14)—Ru(2)—C(18)	107.8(3)	O(2)—S(1)—O(3)	115.3(3)

C(15)—Ru(2)—C(18)	106.7(3)	O(1)—S(1)—C(35)	102.9(2)
C(16)—Ru(2)—C(18)	135.3(3)	O(2)—S(1)—C(35)	103.3(2)
C(12)—Ru(2)—C(19)	142.5(3)	O(3)—S(1)—C(35)	103.3(2)
C(13)—Ru(2)—C(19)	175.8(4)	S(1)—C(35)—F(1)	111.8(3)
C(14)—Ru(2)—C(19)	137.2(4)	S(1)—C(35)—F(2)	111.3(3)
C(15)—Ru(2)—C(19)	113.2(3)	F(1)—C(35)—F(2)	107.9(4)
C(16)—Ru(2)—C(19)	115.0(2)	S(1)—C(35)—F(3)	111.2(3)
C(12)—Ru(2)—C(20)	124.2(3)	F(1)—C(35)—F(3)	106.8(4)
C(13)—Ru(2)—C(20)	148.2(3)	F(2)—C(35)—F(3)	107.6(4)
C(14)—Ru(2)—C(20)	171.6(3)	O(4)—S(2)—O(5)	114.7(2)
C(15)—Ru(2)—C(20)	143.3(3)	O(4)—S(2)—O(6)	115.2(2)
C(16)—Ru(2)—C(20)	122.5(2)	O(5)—S(2)—O(6)	114.9(3)
C(12)—Ru(2)—C(21)	126.0(3)	O(4)—S(2)—C(36)	103.3(2)
C(13)—Ru(2)—C(21)	122.0(2)	O(5)—S(2)—C(36)	103.0(2)
C(14)—Ru(2)—C(21)	143.0(3)	O(6)—S(2)—C(36)	103.3(2)
C(15)—Ru(2)—C(21)	169.8(2)	S(2)—C(36)—F(4)	112.3(4)
C(16)—Ru(2)—C(21)	150.1(2)	S(2)—C(36)—F(5)	112.5(3)
C(12)—Ru(2)—C(22)	147.2(3)	F(4)—C(36)—F(5)	107.2(4)
C(13)—Ru(2)—C(22)	115.73(19)	S(2)—C(36)—F(6)	111.2(3)
C(14)—Ru(2)—C(22)	112.6(2)	F(4)—C(36)—F(6)	106.8(4)
C(15)—Ru(2)—C(22)	133.9(3)	F(5)—C(36)—F(6)	106.5(4)
C(16)—Ru(2)—C(22)	172.1(2)	O(7)—S(3)—O(8)	115.0(2)
C(17)—Ru(2)—C(18)	155.5(3)	O(7)—S(3)—O(9)	115.21(19)
C(17)—Ru(2)—C(19)	120.2(4)	O(8)—S(3)—O(9)	114.2(2)
C(18)—Ru(2)—C(19)	40.8(3)	O(7)—S(3)—C(37)	102.8(2)
C(17)—Ru(2)—C(20)	92.0(3)	O(8)—S(3)—C(37)	103.3(2)
C(18)—Ru(2)—C(20)	63.9(3)	O(9)—S(3)—C(37)	104.0(2)
C(19)—Ru(2)—C(20)	35.8(3)	S(3)—C(37)—F(7)	112.9(3)
C(17)—Ru(2)—C(21)	95.0(3)	S(3)—C(37)—F(8)	112.0(3)
C(18)—Ru(2)—C(21)	63.1(3)	F(7)—C(37)—F(8)	106.5(4)
C(19)—Ru(2)—C(21)	60.4(3)	S(3)—C(37)—F(9)	111.6(3)
C(20)—Ru(2)—C(21)	35.3(3)	F(7)—C(37)—F(9)	106.9(4)
C(17)—Ru(2)—C(22)	127.2(3)	F(8)—C(37)—F(9)	106.6(4)
C(18)—Ru(2)—C(22)	38.4(3)		

Note – geometrically-positioned H atoms have been excluded

Table 12: Atomic coordinates ($\times 10^4$), occupancies and equivalent isotropic thermal parameters (Å $\times 10^3$) for refined atoms of $[RcCH_2PPh_3]^+[BF_4]^-\bullet 0.5CH_2Cl_2$

atom	*x*	*y*	*z*	U_{equiv}	Occupancy
Ru(1)	2597(1)	5958(1)	1479(1)	20(1)	1.0
P(1)	3909(1)	7075(1)	3488(1)	23(1)	1.0
C(1)	2112(2)	5062(5)	544(4)	32(1)	1.0
C(2)	2484(2)	4462(5)	667(4)	30(1)	1.0
C(3)	2772(2)	5086(4)	260(4)	27(1)	1.0
C(4)	2575(2)	6045(4)	-113(4)	29(1)	1.0
C(5)	2162(2)	6032(5)	68(4)	31(1)	1.0
C(6)	2876(2)	7357(5)	2268(4)	26(1)	1.0
C(7)	2474(2)	7197(5)	2486(4)	30(1)	1.0
C(8)	2475(2)	6186(5)	2958(4)	33(2)	1.0
C(9)	2876(2)	5714(5)	3045(4)	28(1)	1.0
C(10)	3119(2)	6442(5)	2599(4)	24(1)	1.0
C(11)	3570(2)	6263(5)	2577(4)	33(1)	1.0
C(12)	4432(2)	6625(5)	3600(4)	26(1)	1.0
C(13)	4514(2)	5531(5)	3618(4)	31(1)	1.0
C(14)	4923(2)	5192(6)	3742(5)	42(2)	1.0
C(15)	5242(2)	5922(6)	3852(5)	41(2)	1.0
C(16)	5160(2)	6997(7)	3843(5)	47(2)	1.0

C(17)	4751(2)	7374(6)	3707(5)	38(2)	1.0
C(18)	3765(2)	6989(4)	4681(4)	23(1)	1.0
C(19)	4022(2)	6524(5)	5470(4)	35(2)	1.0
C(20)	3908(2)	6476(5)	6384(5)	40(2)	1.0
C(21)	3537(2)	6891(5)	6504(4)	38(2)	1.0
C(22)	3280(2)	7389(5)	5714(4)	32(1)	1.0
C(23)	3390(2)	7433(5)	4800(4)	27(1)	1.0
C(24)	3876(2)	8451(5)	3117(5)	37(2)	1.0
C(25)	3814(3)	8716(9)	2135(6)	81(3)	1.0
C(26)	3793(3)	9880(12)	1897(9)	109(5)	1.0
C(27)	3859(4)	10575(12)	2667(15)	129(6)	1.0
C(28)	3927(3)	10293(8)	3586(12)	103(4)	1.0
C(29)	3931(3)	9252(6)	3835(7)	61(2)	1.0
B(1)	3756(2)	3297(6)	4415(5)	31(2)	1.0
F(1)	3395(2)	3042(6)	3873(4)	110(2)	1.0
F(2)	3811(2)	2953(10)	5309(4)	183(5)	1.0
F(3)	3751(2)	4369(6)	4543(9)	179(5)	1.0
F(4)	4090(1)	3102(4)	3995(3)	75(2)	1.0
C(101)	4980(20)	8220(20)	6420(20)	350(50)	0.5
Cl(1)	4910(4)	9424(13)	6038(12)	257(7)	0.5
Cl(2)	5000	7711(9)	7500	298(6)	1.0

Table 13: Atomic coordinates ($\times 10^4$), isotropic displacement parameters ($Å^2 \times 10^3$), and occupancies for hydrogen atoms of $[RcCH_2PPh_3]^+[BF_4]^- \cdot 0.5CH_2Cl_2$.

atom	*x*	*y*	*z*	U_{iso}	occupancy
H(1)	1867	4841	751	38	1.0
H(2)	2532	3777	964	36	1.0
H(3)	3048	4889	244	33	1.0
H(4)	2695	6601	-430	35	1.0
H(5)	1961	6577	-102	37	1.0
H(6)	2964	7967	1957	32	1.0
H(7)	2248	7679	2342	36	1.0
H(8)	2248	5875	3179	40	1.0
H(9)	2963	5046	3342	34	1.0
H(11A)	3618	6437	1908	40	1.0
H(11B)	3638	5499	2707	40	1.0
H(13)	4296	5026	3547	37	1.0
H(14)	4983	4449	3751	50	1.0
H(15)	5519	5679	3933	49	1.0
H(16)	5382	7493	3930	56	1.0
H(17)	4694	8118	3689	46	1.0
H(19)	4279	6234	5392	42	1.0
H(20)	4088	6153	6930	48	1.0
H(21)	3457	6838	7127	46	1.0
H(22)	3028	7700	5803	38	1.0
H(23)	3211	7763	4255	33	1.0
H(25)	3786	8187	1632	97	1.0
H(26)	3736	10125	1230	131	1.0
H(27)	3854	11317	2520	155	1.0
H(28)	3974	10823	4090	124	1.0
H(29)	3973	9059	4515	74	1.0
H(10A)	5245	8005	6243	417	0.5
H(10B)	4764	7806	5980	417	0.5

Table 14: Anisotropic thermal parameters ($Å^2 \times 10^3$) for $[RcCH_2PPh_3]^+[BF_4]^-•0.5CH_2Cl_2$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru	21(1)	24(1)	16(1)	-1(1)	4(1)	1(1)
P	21(1)	28(1)	20(1)	-2(1)	5(1)	3(1)
C(1)	25(3)	33(3)	36(3)	-6(3)	0(3)	-8(3)
C(2)	45(4)	22(3)	21(3)	-1(2)	4(3)	-4(3)
C(3)	36(3)	30(3)	17(3)	-3(2)	7(2)	1(3)
C(4)	45(4)	23(3)	17(3)	2(2)	1(3)	-6(3)
C(5)	32(3)	31(3)	23(3)	-5(3)	-9(2)	3(3)
C(6)	33(3)	25(3)	20(3)	-4(2)	3(2)	-6(2)
C(7)	26(3)	40(4)	22(3)	-8(3)	3(2)	7(3)
C(8)	34(3)	50(4)	19(3)	-7(3)	12(3)	-7(3)
C(9)	31(3)	38(4)	14(3)	-2(2)	1(2)	6(3)
C(10)	25(3)	31(3)	14(2)	-7(2)	3(2)	2(2)
C(11)	26(3)	44(4)	28(3)	-17(3)	2(3)	-2(3)
C(12)	19(3)	35(3)	22(3)	-6(2)	1(2)	4(2)
C(13)	31(3)	34(3)	28(3)	-1(3)	6(3)	5(3)
C(14)	41(4)	51(4)	32(3)	2(3)	6(3)	18(3)
C(15)	25(3)	67(5)	31(3)	2(3)	5(3)	10(3)
C(16)	23(3)	63(5)	53(4)	2(4)	5(3)	0(3)
C(17)	23(3)	40(4)	50(4)	4(3)	3(3)	6(3)
C(18)	27(3)	23(3)	20(3)	-2(2)	8(2)	-1(2)
C(19)	36(3)	46(4)	26(3)	8(3)	12(3)	12(3)
C(20)	48(4)	40(4)	30(3)	7(3)	6(3)	2(3)
C(21)	57(4)	37(4)	25(3)	-5(3)	15(3)	-11(3)
C(22)	38(3)	34(3)	25(3)	-11(3)	13(3)	-7(3)
C(23)	31(3)	25(3)	25(3)	-5(2)	5(2)	0(2)
C(24)	21(3)	42(4)	49(4)	24(3)	11(3)	2(3)
C(25)	61(5)	121(8)	50(5)	54(5)	-16(4)	-37(5)
C(26)	73(7)	142(12)	90(8)	87(8)	-36(6)	-47(8)
C(27)	63(7)	105(11)	205(17)	104(12)	-10(9)	2(7)
C(28)	101(8)	36(5)	194(13)	30(7)	78(9)	16(5)
C(29)	72(6)	30(4)	98(7)	4(4)	55(5)	1(4)
B	30(4)	32(4)	29(3)	1(3)	1(3)	-5(3)
F(1)	62(3)	206(7)	64(3)	-48(4)	20(3)	-60(4)
F(2)	62(4)	428(16)	58(3)	92(6)	12(3)	17(6)
F(3)	101(5)	72(5)	386(15)	-5(7)	103(8)	9(4)
F(4)	62(3)	101(4)	73(3)	-22(3)	37(3)	-19(3)
C(101)	840(140)	66(19)	240(50)	70(20)	360(70)	70(40)
Cl(1)	170(10)	250(14)	302(16)	-45(13)	-69(10)	-56(10)
Cl(2)	320(14)	189(10)	395(18)	0	97(13)	0

Table 15: Bond lengths (Å) for $[RcCH_2PPh_3][BF_4]^-•0.5CH_2Cl_2$

Ru-C(10)	2.158(5)	C(12)-C(13)	1.396(9)
Ru-C(1)	2.160(6)	C(12)-C(17)	1.396(8)
Ru-C(6)	2.166(5)	C(13)-C(14)	1.393(8)
Ru-C(7)	2.173(5)	C(14)-C(15)	1.381(10)
Ru-C(8)	2.173(5)	C(15)-C(16)	1.372(10)
Ru-C(2)	2.174(6)	C(16)-C(17)	1.410(8)
Ru-C(5)	2.175(6)	C(18)-C(19)	1.368(8)
Ru-C(3)	2.176(5)	C(18)-C(23)	1.400(7)
Ru-C(4)	2.183(5)	C(19)-C(20)	1.385(8)
Ru-C(9)	2.190(5)	C(20)-C(21)	1.372(9)
P-C(24)	1.794(7)	C(21)-C(22)	1.387(9)
P-C(12)	1.798(5)	C(22)-C(23)	1.379(7)
P-C(18)	1.802(5)	C(24)-C(25)	1.367(10)

P-C(11)	1.817(6)	C(24)-C(29)	1.395(11)
C(1)-C(5)	1.406(8)	C(25)-C(26)	1.492(16)
C(1)-C(2)	1.421(8)	C(26)-C(27)	1.355(19)
C(2)-C(3)	1.430(8)	C(27)-C(28)	1.290(18)
C(3)-C(4)	1.412(8)	C(28)-C(29)	1.348(11)
C(4)-C(5)	1.437(8)	B-F(2)	1.283(8)
C(6)-C(10)	1.422(8)	B-F(1)	1.315(8)
C(6)-C(7)	1.432(8)	B-F(3)	1.353(10)
C(7)-C(8)	1.422(9)	B-F(4)	1.368(8)
C(8)-C(9)	1.433(8)	C(101)-Cl(1)	1.599(19)
C(9)-C(10)	1.433(8)	C(101)-Cl(2)	1.605(19)
C(10)-C(11)	1.514(7)	Cl(2)-C(101)#1	1.605(19)

Table 16: Bond angles (°) for $[RcCH_2PPh_3][BF_4]^-•0.5CH_2Cl_2$

C(10)-Ru-C(1)	164.6(2)	C(2)-C(3)-Ru	70.7(3)
C(10)-Ru-C(6)	38.4(2)	C(3)-C(4)-C(5)	108.1(5)
C(1)-Ru-C(6)	155.4(2)	C(3)-C(4)-Ru	70.8(3)
C(10)-Ru-C(7)	64.4(2)	C(5)-C(4)-Ru	70.5(3)
C(1)-Ru-C(7)	122.7(2)	C(1)-C(5)-C(4)	107.3(5)
C(6)-Ru-C(7)	38.5(2)	C(1)-C(5)-Ru	70.5(3)
C(10)-Ru-C(8)	64.2(2)	C(4)-C(5)-Ru	71.1(3)
C(1)-Ru-C(8)	111.8(2)	C(10)-C(6)-C(7)	108.0(5)
C(6)-Ru-C(8)	64.1(2)	C(10)-C(6)-Ru	70.5(3)
C(7)-Ru-C(8)	38.2(2)	C(7)-C(6)-Ru	71.0(3)
C(10)-Ru-C(2)	129.8(2)	C(8)-C(7)-C(6)	107.6(5)
C(1)-Ru-C(2)	38.3(2)	C(8)-C(7)-Ru	70.9(3)
C(6)-Ru-C(2)	165.0(2)	C(6)-C(7)-Ru	70.5(3)
C(7)-Ru-C(2)	155.2(2)	C(7)-C(8)-C(9)	108.8(5)
C(8)-Ru-C(2)	123.4(2)	C(7)-C(8)-Ru	70.9(3)
C(10)-Ru-C(5)	156.5(2)	C(9)-C(8)-Ru	71.4(3)
C(1)-Ru-C(5)	37.8(2)	C(10)-C(9)-C(8)	107.0(5)
C(6)-Ru-C(5)	123.5(2)	C(10)-C(9)-Ru	69.6(3)
C(7)-Ru-C(5)	111.4(2)	C(8)-C(9)-Ru	70.2(3)
C(8)-Ru-C(5)	128.2(2)	C(6)-C(10)-C(9)	108.6(5)
C(2)-Ru-C(5)	64.0(2)	C(6)-C(10)-C(11)	127.6(5)
C(10)-Ru-C(3)	113.2(2)	C(9)-C(10)-C(11)	123.7(5)
C(1)-Ru-C(3)	63.9(2)	C(6)-C(10)-Ru	71.1(3)
C(6)-Ru-C(3)	129.8(2)	C(9)-C(10)-Ru	72.0(3)
C(7)-Ru-C(3)	164.4(2)	C(11)-C(10)-Ru	126.4(3)
C(8)-Ru-C(3)	156.5(2)	C(10)-C(11)-P	112.1(4)
C(2)-Ru-C(3)	38.4(2)	C(13)-C(12)-C(17)	121.2(5)
C(5)-Ru-C(3)	64.0(2)	C(13)-C(12)-P	119.3(4)
C(10)-Ru-C(4)	124.4(2)	C(17)-C(12)-P	119.5(5)
C(1)-Ru-C(4)	63.6(2)	C(14)-C(13)-C(12)	118.7(6)
C(6)-Ru-C(4)	112.9(2)	C(15)-C(14)-C(13)	120.9(7)
C(7)-Ru-C(4)	129.3(2)	C(16)-C(15)-C(14)	120.2(6)
C(8)-Ru-C(4)	163.8(2)	C(15)-C(16)-C(17)	120.8(6)
C(2)-Ru-C(4)	63.8(2)	C(12)-C(17)-C(16)	118.2(6)
C(5)-Ru-C(4)	38.5(2)	C(19)-C(18)-C(23)	120.0(5)
C(3)-Ru-C(4)	37.8(2)	C(19)-C(18)-P	121.0(4)
C(10)-Ru-C(9)	38.5(2)	C(23)-C(18)-P	119.0(4)
C(1)-Ru-C(9)	129.1(2)	C(18)-C(19)-C(20)	120.1(6)
C(6)-Ru-C(9)	64.3(2)	C(21)-C(20)-C(19)	120.4(6)
C(7)-Ru-C(9)	64.3(2)	C(20)-C(21)-C(22)	119.8(5)
C(8)-Ru-C(9)	38.4(2)	C(23)-C(22)-C(21)	120.2(6)
C(2)-Ru-C(9)	112.5(2)	C(22)-C(23)-C(18)	119.5(5)
C(5)-Ru-C(9)	163.3(2)	C(25)-C(24)-C(29)	120.0(8)
C(3)-Ru-C(9)	124.5(2)	C(25)-C(24)-P	120.3(7)

C(4)-Ru-C(9)	156.8(2)	C(29)-C(24)-P	119.7(5)
C(24)-P-C(12)	109.1(3)	C(24)-C(25)-C(26)	116.5(10)
C(24)-P-C(18)	107.8(3)	C(27)-C(26)-C(25)	117.5(10)
C(12)-P-C(18)	109.2(3)	C(28)-C(27)-C(26)	124.1(13)
C(24)-P-C(11)	110.3(3)	C(27)-C(28)-C(29)	120.4(14)
C(12)-P-C(11)	109.4(3)	C(28)-C(29)-C(24)	121.4(10)
C(18)-P-C(11)	111.0(3)	F(2)-B-F(1)	113.5(7)
C(5)-C(1)-C(2)	109.3(5)	F(2)-B-F(3)	102.2(9)
C(5)-C(1)-Ru	71.7(3)	F(1)-B-F(3)	106.3(7)
C(2)-C(1)-Ru	71.4(3)	F(2)-B-F(4)	112.1(7)
C(1)-C(2)-C(3)	107.1(5)	F(1)-B-F(4)	115.9(6)
C(1)-C(2)-Ru	70.3(3)	F(3)-B-F(4)	105.3(6)
C(3)-C(2)-Ru	70.9(3)	Cl(1)-C(101)-Cl(2)	131(2)
C(4)-C(3)-C(2)	108.2(5)	C(101)#1-Cl(2)-C(101)	133(3)
C(4)-C(3)-Ru	71.4(3)		