Supplementary Material (ESI) for Dalton Transactions

Supplementary Data

Weakly Coordinating Counter-ions for Highly Efficient Catalysis of Intramolecular Hydroamination

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Ortep Diagrams and Crystallographic Tables for $[Rh(bpm)(COD)]BAr^F_{24}$ (5a), $[Ir(bim)(CO)_2]BAr^F_{24}$ (10a), and $[Rh(bim)(CO)_2]BAr^F_{24}$ (11a)

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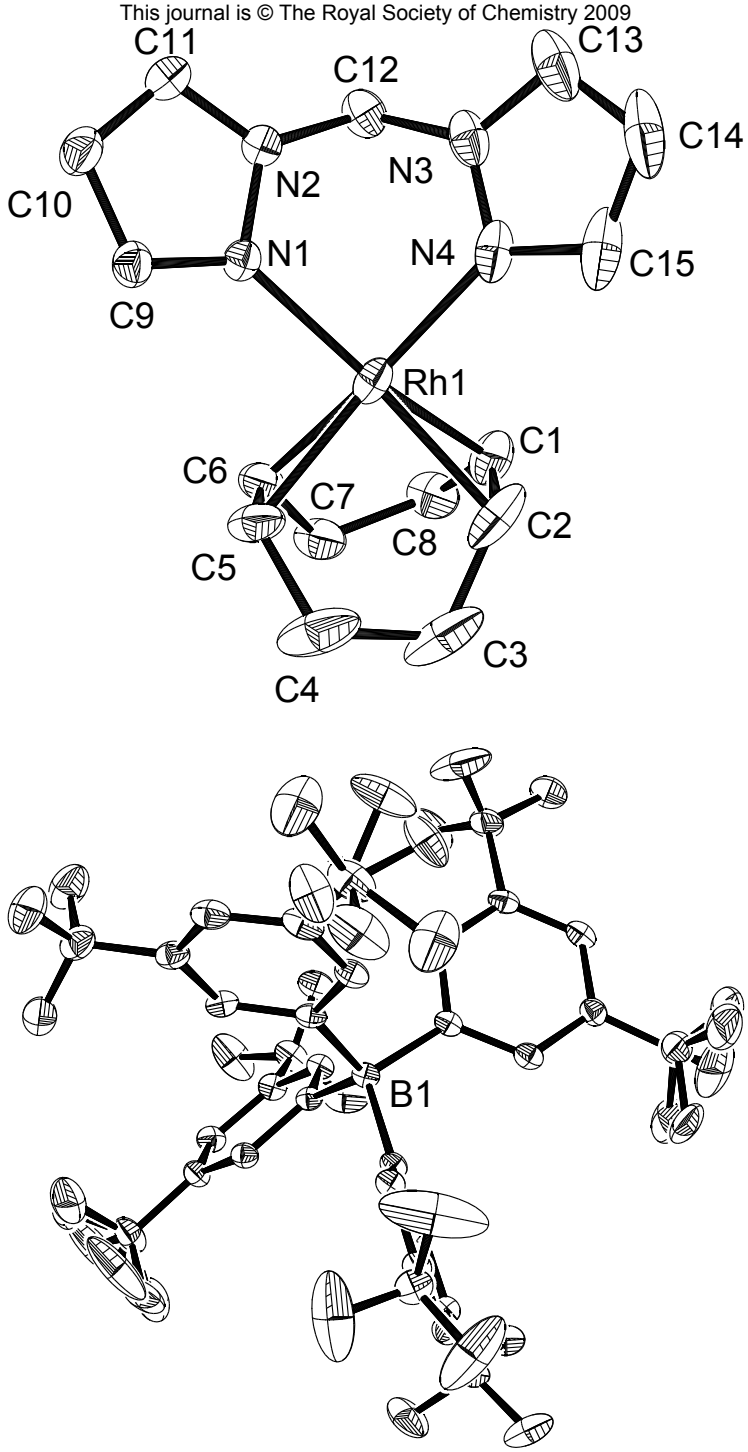
Ortep Diagrams and Crystallographic Tables for [Rh(bpm)(COD)]BAr^{F}_{24} (5a)



ORTEP plot (50% ellipsoids, H-atoms omitted) of cation (top) and anion (bottom). All hydrogen atoms were refined in idealized positions.
Three of the anion´s CF3 groups are twofold disordered each (s.o.f. 0.73 : 0.27, 0.80 : 0.20, 0.73 : 0.27).

Table 1. Crystal data and structure refinement for RH00301.

Identification code	rh00301
Empirical formula	C47 H32 B F24 N4 Rh
Formula weight	1222.49
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.0057(2) A alpha = 68.9120(10) deg.
	b = 13.6112(2) A beta = 69.2710(10) deg.
	c = 15.8258(3) A gamma = 68.3680(10) deg.
Volume	2349.38(7) A^3
Z, Calculated density	2, 1.728 Mg/m^3
Absorption coefficient	0.500 mm^-1
F(000)	1216
Crystal size	0.49 x 0.44 x 0.18 mm
Theta range for data collection	2.73 to 30.00 deg.
Limiting indices	-18<=h<=18, -19<=k<=19, -22<=l<=22
Reflections collected / unique	55288 / 13658 [R(int) = 0.0383]
Completeness to theta = 30.00	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.917 and 0.755
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13658 / 15 / 730
Goodness-of-fit on F^2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.1267
R indices (all data)	R1 = 0.0589, wR2 = 0.1323
Largest diff. peak and hole	1.343 and -1.368 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for RH00301.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Rh(1)	9231(1)	5655(1)	7114(1)	25(1)
N(1)	10105(2)	6631(2)	7193(1)	22(1)
N(2)	9599(2)	7721(2)	7110(1)	22(1)
N(3)	8214(2)	8066(2)	6299(2)	32(1)
N(4)	8437(2)	7051(2)	6203(2)	33(1)
C(1)	7834(2)	4985(3)	7491(2)	38(1)
C(2)	8693(3)	4542(3)	6804(2)	50(1)
C(3)	9479(4)	3376(3)	6987(3)	62(1)
C(4)	10588(3)	3316(3)	7152(3)	60(1)
C(5)	10449(2)	4181(2)	7604(2)	37(1)
C(6)	9566(2)	4438(2)	8370(2)	31(1)
C(7)	8651(2)	3834(2)	8892(2)	36(1)
C(8)	7575(2)	4413(2)	8528(2)	38(1)
C(9)	11154(2)	6470(2)	7259(2)	26(1)
C(10)	11312(2)	7436(2)	7238(2)	31(1)
C(11)	10302(2)	8218(2)	7145(2)	28(1)
C(12)	8401(2)	8167(2)	7111(2)	29(1)
C(13)	7789(3)	8852(3)	5603(2)	47(1)
C(14)	7744(3)	8331(4)	5023(2)	58(1)
C(15)	8146(3)	7232(3)	5417(2)	48(1)
B(1)	4623(2)	1768(2)	7366(2)	17(1)
C(16)	5971(2)	1513(2)	7340(1)	17(1)
C(17)	6278(2)	1210(2)	8184(1)	18(1)
C(18)	7405(2)	984(2)	8209(1)	18(1)
C(19)	8280(2)	1054(2)	7389(2)	19(1)
C(20)	7996(2)	1350(2)	6550(2)	19(1)
C(21)	6865(2)	1583(2)	6519(1)	18(1)
C(22)	7678(2)	701(2)	9128(2)	25(1)
F(22A)	6973(1)	181(1)	9840(1)	29(1)
F(22B)	8740(1)	60(2)	9130(1)	43(1)

F(22C)	7592(2)	1606(2)	9343(1)	46(1)
C(23)	8917(2)	1426(2)	5649(2)	26(1)
F(23A)	9933(2)	811(2)	5765(2)	81(1)
F(23B)	9045(2)	2403(2)	5240(2)	83(1)
F(23C)	8738(2)	1125(4)	5034(2)	108(1)
C(24)	4425(2)	2402(2)	6314(1)	18(1)
C(25)	3877(2)	3517(2)	6031(2)	21(1)
C(26)	3795(2)	4046(2)	5111(2)	24(1)
C(27)	4267(2)	3486(2)	4428(2)	26(1)
C(29)	4866(2)	1836(2)	5614(2)	22(1)
C(30)	3140(2)	5232(2)	4890(2)	30(1)
F(30A)	2006(2)	5355(2)	5217(1)	45(1)
F(30B)	3317(2)	5722(2)	3969(1)	44(1)
F(30C)	3386(2)	5822(1)	5275(1)	45(1)
C(28A)	4797(2)	2373(2)	4691(2)	27(1)
C(31A)	5342(2)	1743(1)	3971(1)	37(1)
F(31A)	5128(2)	815(1)	4248(1)	46(1)
F(31B)	4840(2)	2307(1)	3208(1)	67(1)
F(31C)	6380(2)	1718(1)	3563(1)	58(1)
C(28B)	4797(2)	2373(2)	4691(2)	27(1)
C(31B)	5299(4)	1771(3)	3952(2)	37(1)
F(31D)	6418(4)	842(3)	4179(2)	67(1)
F(31E)	4750(4)	1279(3)	3784(2)	54(2)
F(31F)	5984(4)	2216(3)	3184(2)	43(2)
C(32)	3851(2)	2550(2)	8080(1)	17(1)
C(33)	2870(2)	2377(2)	8791(1)	18(1)
C(34)	2236(2)	3087(2)	9365(2)	20(1)
C(35)	2550(2)	4004(2)	9255(2)	22(1)
C(37)	4164(2)	3475(2)	7995(2)	19(1)
C(38)	1242(2)	2807(2)	10150(2)	28(1)
F(38A)	650(1)	2361(1)	9928(1)	30(1)
F(38B)	488(2)	3682(2)	10440(1)	52(1)
F(38C)	1591(2)	2069(2)	10906(1)	44(1)
C(36A)	3526(2)	4186(2)	8560(2)	21(1)
C(39A)	3923(1)	5156(1)	8431(1)	34(1)
F(39A)	3297(1)	5740(1)	8983(1)	81(1)
F(39B)	3802(1)	5874(1)	7531(1)	56(1)
F(39C)	5001(1)	4992(1)	8229(1)	68(1)
C(36B)	3526(2)	4186(2)	8560(2)	21(1)
C(39B)	3853(5)	5177(3)	8482(5)	34(1)
F(39D)	4127(5)	4998(3)	9380(5)	56(1)
F(39E)	3225(5)	6035(3)	8279(5)	49(2)
F(39F)	4770(5)	5298(3)	7843(5)	81(1)
C(40)	4262(2)	618(2)	7736(1)	17(1)
C(41)	4916(2)	-399(2)	8153(2)	20(1)
C(43)	3459(2)	-1292(2)	8484(2)	21(1)
C(44)	2798(2)	-295(2)	8072(2)	21(1)
C(45)	3195(2)	633(2)	7693(2)	20(1)
C(42A)	4529(2)	-1337(2)	8516(2)	21(1)
C(46A)	5277(2)	-2381(1)	8944(1)	37(1)
F(46A)	4773(2)	-3192(1)	9369(1)	51(1)
F(46B)	6218(2)	-2767(1)	8402(1)	63(1)
F(46C)	5550(2)	-2267(1)	9638(1)	86(1)
C(42B)	4529(2)	-1337(2)	8516(2)	21(1)
C(46B)	5285(4)	-2402(2)	8904(4)	37(1)
F(46D)	4767(4)	-3110(2)	9654(4)	51(1)
F(46E)	6081(4)	-2903(2)	8043(4)	86(1)
F(46F)	6180(4)	-2420(2)	9063(4)	64(3)
C(47)	1609(2)	-180(2)	8070(2)	31(1)
F(47A)	1470(2)	135(2)	7203(2)	68(1)
F(47B)	1289(2)	-1093(1)	8493(2)	44(1)
F(47C)	836(2)	579(2)	8491(2)	67(1)

Table 3. Bond lengths [Å] and angles [deg] for RH00301.

Rh(1)-N(4)	2.096(2)	C(26)-C(30)	1.499(4)
Rh(1)-N(1)	2.0987(19)	C(27)-C(28A)	1.386(4)
Rh(1)-C(5)	2.130(3)	C(29)-C(28A)	1.397(3)
Rh(1)-C(1)	2.133(3)	C(30)-F(30C)	1.340(3)
Rh(1)-C(2)	2.141(3)	C(30)-F(30B)	1.341(3)
Rh(1)-C(6)	2.144(3)	C(30)-F(30A)	1.346(3)
N(1)-C(9)	1.335(3)	C(28A)-C(31A)	1.490(3)
N(1)-N(2)	1.361(3)	C(31A)-F(31C)	1.2670
N(2)-C(11)	1.348(3)	C(31A)-F(31A)	1.2798
N(2)-C(12)	1.449(3)	C(31A)-F(31B)	1.4128
N(3)-C(13)	1.346(4)	C(31B)-F(31E)	1.2825
N(3)-N(4)	1.357(4)	C(31B)-F(31F)	1.3195
N(3)-C(12)	1.449(3)	C(31B)-F(31D)	1.5911
N(4)-C(15)	1.340(3)	C(32)-C(33)	1.401(3)
C(1)-C(2)	1.382(5)	C(32)-C(37)	1.410(3)
C(1)-C(8)	1.514(4)	C(33)-C(34)	1.398(3)
C(2)-C(3)	1.526(6)	C(34)-C(35)	1.388(3)
C(3)-C(4)	1.523(6)	C(34)-C(38)	1.498(3)
C(4)-C(5)	1.512(4)	C(35)-C(36A)	1.389(3)
C(5)-C(6)	1.391(4)	C(37)-C(36A)	1.389(3)
C(6)-C(7)	1.521(4)	C(38)-F(38A)	1.332(3)
C(7)-C(8)	1.531(4)	C(38)-F(38B)	1.343(3)
C(9)-C(10)	1.392(3)	C(38)-F(38C)	1.353(3)
C(10)-C(11)	1.369(4)	C(36A)-C(39A)	1.512(2)
C(13)-C(14)	1.374(6)	C(39A)-F(39A)	1.2568
C(14)-C(15)	1.372(6)	C(39A)-F(39C)	1.2733
B(1)-C(24)	1.640(3)	C(39A)-F(39B)	1.4331
B(1)-C(32)	1.641(3)	C(39B)-F(39E)	1.1603
B(1)-C(40)	1.643(3)	C(39B)-F(39F)	1.2824
B(1)-C(16)	1.645(3)	C(39B)-F(39D)	1.4995
C(16)-C(17)	1.405(3)	C(40)-C(41)	1.396(3)
C(16)-C(21)	1.405(3)	C(40)-C(45)	1.405(3)
C(17)-C(18)	1.394(3)	C(41)-C(42A)	1.398(3)
C(18)-C(19)	1.390(3)	C(43)-C(44)	1.381(3)
C(18)-C(22)	1.500(3)	C(43)-C(42A)	1.389(3)
C(19)-C(20)	1.384(3)	C(44)-C(45)	1.393(3)
C(20)-C(21)	1.401(3)	C(44)-C(47)	1.496(3)
C(20)-C(23)	1.502(3)	C(42A)-C(46A)	1.476(2)
C(22)-F(22B)	1.335(3)	C(46A)-F(46B)	1.2718
C(22)-F(22A)	1.336(3)	C(46A)-F(46A)	1.3371
C(22)-F(22C)	1.344(3)	C(46A)-F(46C)	1.3399
C(23)-F(23B)	1.298(3)	C(46B)-F(46F)	1.2653
C(23)-F(23C)	1.299(3)	C(46B)-F(46D)	1.3715
C(23)-F(23A)	1.314(3)	C(46B)-F(46E)	1.5947
C(24)-C(25)	1.397(3)	C(47)-F(47B)	1.323(3)
C(24)-C(29)	1.409(3)	C(47)-F(47C)	1.333(3)
C(25)-C(26)	1.396(3)	C(47)-F(47A)	1.340(3)
C(26)-C(27)	1.380(3)		

N(4)-Rh(1)-N(1)	87.02(8)	C(25)-C(24)-C(29)	115.61(19)
N(4)-Rh(1)-C(5)	160.65(11)	C(25)-C(24)-B(1)	123.97(18)
N(1)-Rh(1)-C(5)	92.20(9)	C(29)-C(24)-B(1)	120.36(19)
N(4)-Rh(1)-C(1)	90.64(11)	C(26)-C(25)-C(24)	122.4(2)
N(1)-Rh(1)-C(1)	155.34(10)	C(27)-C(26)-C(25)	121.1(2)
C(5)-Rh(1)-C(1)	97.87(12)	C(27)-C(26)-C(30)	120.6(2)
N(4)-Rh(1)-C(2)	94.76(13)	C(25)-C(26)-C(30)	118.2(2)
N(1)-Rh(1)-C(2)	166.91(11)	C(26)-C(27)-C(28A)	117.8(2)
C(5)-Rh(1)-C(2)	81.83(14)	C(28A)-C(29)-C(24)	121.7(2)
C(1)-Rh(1)-C(2)	37.74(13)	F(30C)-C(30)-F(30B)	106.9(2)
N(4)-Rh(1)-C(6)	161.38(10)	F(30C)-C(30)-F(30A)	106.5(2)
N(1)-Rh(1)-C(6)	93.09(9)	F(30B)-C(30)-F(30A)	105.8(2)
C(5)-Rh(1)-C(6)	37.97(11)	F(30C)-C(30)-C(26)	112.8(2)
C(1)-Rh(1)-C(6)	81.52(11)	F(30B)-C(30)-C(26)	113.4(2)
C(2)-Rh(1)-C(6)	89.34(13)	F(30A)-C(30)-C(26)	110.9(2)
C(9)-N(1)-N(2)	104.65(19)	C(27)-C(28A)-C(29)	121.3(2)

C(9)-N(1)-Rh(1)	135.26(17)	C(27)-C(28A)-C(31A)	119.6(2)
N(2)-N(1)-Rh(1)	119.95(14)	C(29)-C(28A)-C(31A)	119.1(2)
C(11)-N(2)-N(1)	111.53(19)	F(31C)-C(31A)-F(31A)	114.7
C(11)-N(2)-C(12)	128.4(2)	F(31C)-C(31A)-F(31B)	100.6
N(1)-N(2)-C(12)	119.56(19)	F(31A)-C(31A)-F(31B)	102.9
C(13)-N(3)-N(4)	111.5(3)	F(31C)-C(31A)-C(28A)	114.87(11)
C(13)-N(3)-C(12)	129.5(3)	F(31A)-C(31A)-C(28A)	113.19(11)
N(4)-N(3)-C(12)	119.0(2)	F(31B)-C(31A)-C(28A)	108.84(12)
C(15)-N(4)-N(3)	104.6(3)	F(31E)-C(31B)-F(31F)	112.2
C(15)-N(4)-Rh(1)	134.4(3)	F(31E)-C(31B)-F(31D)	104.4
N(3)-N(4)-Rh(1)	120.76(16)	F(31F)-C(31B)-F(31D)	86.7
C(2)-C(1)-C(8)	125.3(3)	C(33)-C(32)-C(37)	115.48(19)
C(2)-C(1)-Rh(1)	71.45(16)	C(33)-C(32)-B(1)	124.85(18)
C(8)-C(1)-Rh(1)	110.00(19)	C(37)-C(32)-B(1)	119.67(18)
C(1)-C(2)-C(3)	124.0(3)	C(34)-C(33)-C(32)	122.12(19)
C(1)-C(2)-Rh(1)	70.81(16)	C(35)-C(34)-C(33)	121.3(2)
C(3)-C(2)-Rh(1)	112.6(2)	C(35)-C(34)-C(38)	119.75(19)
C(4)-C(3)-C(2)	112.5(3)	C(33)-C(34)-C(38)	118.9(2)
C(5)-C(4)-C(3)	112.9(3)	C(34)-C(35)-C(36A)	117.6(2)
C(6)-C(5)-C(4)	124.8(3)	C(36A)-C(37)-C(32)	122.31(19)
C(6)-C(5)-Rh(1)	71.56(15)	F(38A)-C(38)-F(38B)	106.3(2)
C(4)-C(5)-Rh(1)	110.2(3)	F(38A)-C(38)-F(38C)	105.8(2)
C(5)-C(6)-C(7)	123.7(2)	F(38B)-C(38)-F(38C)	106.8(2)
C(5)-C(6)-Rh(1)	70.47(17)	F(38A)-C(38)-C(34)	113.24(19)
C(7)-C(6)-Rh(1)	113.30(18)	F(38B)-C(38)-C(34)	112.9(2)
C(6)-C(7)-C(8)	111.6(2)	F(38C)-C(38)-C(34)	111.3(2)
C(1)-C(8)-C(7)	112.9(2)	C(35)-C(36A)-C(37)	121.2(2)
N(1)-C(9)-C(10)	111.4(2)	C(35)-C(36A)-C(39A)	119.66(19)
C(11)-C(10)-C(9)	105.2(2)	C(37)-C(36A)-C(39A)	119.13(18)
N(2)-C(11)-C(10)	107.2(2)	F(39A)-C(39A)-F(39C)	118.2
N(2)-C(12)-N(3)	110.8(2)	F(39A)-C(39A)-F(39B)	103.4
N(3)-C(13)-C(14)	106.9(3)	F(39C)-C(39A)-F(39B)	94.9
C(15)-C(14)-C(13)	105.6(3)	F(39A)-C(39A)-C(36A)	114.24(10)
N(4)-C(15)-C(14)	111.5(3)	F(39C)-C(39A)-C(36A)	115.91(10)
C(24)-B(1)-C(32)	110.06(17)	F(39B)-C(39A)-C(36A)	106.42(11)
C(24)-B(1)-C(40)	108.68(16)	F(39E)-C(39B)-F(39F)	100.8
C(32)-B(1)-C(40)	110.55(16)	F(39E)-C(39B)-F(39D)	111.4
C(24)-B(1)-C(16)	110.07(16)	F(39F)-C(39B)-F(39D)	104.9
C(32)-B(1)-C(16)	107.20(16)	C(41)-C(40)-C(45)	115.55(19)
C(40)-B(1)-C(16)	110.28(17)	C(41)-C(40)-B(1)	124.70(18)
C(17)-C(16)-C(21)	116.14(19)	C(45)-C(40)-B(1)	119.65(18)
C(17)-C(16)-B(1)	119.39(17)	C(40)-C(41)-C(42A)	122.2(2)
C(21)-C(16)-B(1)	124.47(18)	C(44)-C(43)-C(42A)	117.8(2)
C(18)-C(17)-C(16)	122.13(19)	C(43)-C(44)-C(45)	121.1(2)
C(19)-C(18)-C(17)	121.00(19)	C(43)-C(44)-C(47)	120.2(2)
C(19)-C(18)-C(22)	119.12(19)	C(45)-C(44)-C(47)	118.6(2)
C(17)-C(18)-C(22)	119.84(19)	C(44)-C(45)-C(40)	122.3(2)
C(20)-C(19)-C(18)	117.78(19)	C(43)-C(42A)-C(41)	121.0(2)
C(19)-C(20)-C(21)	121.58(19)	C(43)-C(42A)-C(46A)	120.27(19)
C(19)-C(20)-C(23)	119.5(2)	C(41)-C(42A)-C(46A)	118.76(19)
C(21)-C(20)-C(23)	118.9(2)	F(46B)-C(46A)-F(46A)	105.9
C(20)-C(21)-C(16)	121.4(2)	F(46B)-C(46A)-F(46C)	106.2
F(22B)-C(22)-F(22A)	106.8(2)	F(46A)-C(46A)-F(46C)	103.5
F(22B)-C(22)-F(22C)	106.8(2)	F(46B)-C(46A)-C(42A)	116.40(12)
F(22A)-C(22)-F(22C)	106.3(2)	F(46A)-C(46A)-C(42A)	113.79(11)
F(22B)-C(22)-C(18)	112.8(2)	F(46C)-C(46A)-C(42A)	110.03(11)
F(22A)-C(22)-C(18)	112.53(18)	F(46F)-C(46B)-F(46D)	108.1
F(22C)-C(22)-C(18)	111.29(19)	F(46F)-C(46B)-F(46E)	88.4
F(23B)-C(23)-F(23C)	106.1(3)	F(46D)-C(46B)-F(46E)	114.7
F(23B)-C(23)-F(23A)	104.5(3)	F(47B)-C(47)-F(47C)	106.6(2)
F(23C)-C(23)-F(23A)	106.1(3)	F(47B)-C(47)-F(47A)	105.8(2)
F(23B)-C(23)-C(20)	113.9(2)	F(47C)-C(47)-F(47A)	105.5(3)
F(23C)-C(23)-C(20)	112.8(2)	F(47B)-C(47)-C(44)	114.0(2)
F(23A)-C(23)-C(20)	112.8(2)	F(47C)-C(47)-C(44)	111.8(2)
		F(47A)-C(47)-C(44)	112.6(2)

Table 4. Anisotropic displacement parameters (Å^2 x 10^3) for RH00301.
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
Rh(1)	22(1)	33(1)	25(1)	-14(1)	-2(1)	-12(1)
N(1)	20(1)	25(1)	22(1)	-8(1)	-5(1)	-7(1)
N(2)	21(1)	24(1)	22(1)	-7(1)	-4(1)	-6(1)
N(3)	23(1)	43(1)	26(1)	0(1)	-8(1)	-12(1)
N(4)	28(1)	55(1)	22(1)	-7(1)	-6(1)	-22(1)
C(1)	31(1)	47(2)	46(2)	-12(1)	-9(1)	-23(1)
C(2)	57(2)	71(2)	47(2)	-30(2)	-1(2)	-44(2)
C(3)	66(2)	67(2)	73(3)	-51(2)	15(2)	-39(2)
C(4)	40(2)	48(2)	93(3)	-49(2)	19(2)	-19(1)
C(5)	23(1)	25(1)	63(2)	-21(1)	-2(1)	-6(1)
C(6)	26(1)	21(1)	43(1)	-7(1)	-11(1)	-4(1)
C(7)	29(1)	27(1)	45(2)	-8(1)	-4(1)	-7(1)
C(8)	25(1)	35(1)	47(2)	-6(1)	-2(1)	-12(1)
C(9)	22(1)	29(1)	30(1)	-9(1)	-8(1)	-7(1)
C(10)	26(1)	34(1)	39(1)	-12(1)	-9(1)	-12(1)
C(11)	29(1)	28(1)	30(1)	-9(1)	-6(1)	-12(1)
C(12)	22(1)	33(1)	27(1)	-8(1)	-4(1)	-4(1)
C(13)	28(1)	64(2)	38(2)	14(1)	-15(1)	-19(1)
C(14)	45(2)	102(3)	30(1)	16(2)	-21(1)	-44(2)
C(15)	42(2)	93(3)	23(1)	-6(1)	-8(1)	-43(2)
B(1)	16(1)	21(1)	15(1)	-5(1)	-2(1)	-7(1)
C(16)	17(1)	19(1)	17(1)	-7(1)	-1(1)	-8(1)
C(17)	17(1)	22(1)	17(1)	-7(1)	0(1)	-8(1)
C(18)	20(1)	18(1)	18(1)	-5(1)	-4(1)	-7(1)
C(19)	17(1)	18(1)	23(1)	-7(1)	-3(1)	-6(1)
C(20)	16(1)	20(1)	19(1)	-7(1)	1(1)	-6(1)
C(21)	17(1)	21(1)	17(1)	-7(1)	-1(1)	-7(1)
C(22)	24(1)	31(1)	23(1)	-6(1)	-7(1)	-12(1)
F(22A)	29(1)	38(1)	19(1)	-2(1)	-5(1)	-15(1)
F(22B)	23(1)	67(1)	32(1)	-3(1)	-12(1)	-10(1)
F(22C)	85(1)	43(1)	32(1)	-8(1)	-23(1)	-35(1)
C(23)	18(1)	33(1)	22(1)	-9(1)	2(1)	-8(1)
F(23A)	24(1)	105(2)	39(1)	12(1)	10(1)	14(1)
F(23B)	89(2)	38(1)	59(1)	-2(1)	45(1)	-19(1)
F(23C)	67(2)	251(4)	62(2)	-108(2)	45(1)	-99(2)
C(24)	16(1)	25(1)	16(1)	-7(1)	-2(1)	-9(1)
C(25)	17(1)	28(1)	17(1)	-8(1)	-3(1)	-6(1)
C(26)	22(1)	30(1)	20(1)	-3(1)	-5(1)	-11(1)
C(27)	29(1)	38(1)	17(1)	-4(1)	-5(1)	-18(1)
C(29)	22(1)	28(1)	20(1)	-10(1)	-1(1)	-12(1)
C(30)	33(1)	33(1)	23(1)	-1(1)	-10(1)	-9(1)
F(30A)	29(1)	45(1)	48(1)	-4(1)	-11(1)	-2(1)
F(30B)	56(1)	41(1)	25(1)	6(1)	-16(1)	-11(1)
F(30C)	62(1)	29(1)	51(1)	-6(1)	-32(1)	-8(1)
C(28A)	31(1)	39(1)	17(1)	-12(1)	2(1)	-20(1)
C(31A)	51(2)	48(2)	20(1)	-16(1)	3(1)	-27(1)
F(31A)	65(2)	39(1)	39(1)	-26(1)	8(1)	-26(1)
F(31B)	101(2)	59(2)	36(1)	-30(1)	-33(2)	16(2)
F(31C)	36(2)	75(2)	71(2)	-52(2)	21(1)	-25(2)
C(28B)	31(1)	39(1)	17(1)	-12(1)	2(1)	-20(1)
C(31B)	51(2)	48(2)	20(1)	-16(1)	3(1)	-27(1)
F(31D)	101(2)	59(2)	36(1)	-30(1)	-33(2)	16(2)
F(31E)	57(5)	88(6)	45(4)	-51(4)	14(3)	-43(4)
F(31F)	50(5)	37(4)	31(3)	-16(3)	16(3)	-19(3)
C(32)	17(1)	20(1)	14(1)	-4(1)	-4(1)	-6(1)
C(33)	19(1)	22(1)	14(1)	-6(1)	-1(1)	-8(1)
C(34)	18(1)	25(1)	17(1)	-8(1)	0(1)	-7(1)
C(35)	21(1)	26(1)	22(1)	-12(1)	-4(1)	-5(1)
C(37)	18(1)	21(1)	18(1)	-5(1)	-3(1)	-8(1)
C(38)	29(1)	35(1)	22(1)	-15(1)	5(1)	-15(1)
F(38A)	24(1)	41(1)	29(1)	-13(1)	2(1)	-18(1)

F(38B)	41(1)	54(1)	58(1)	-41(1)	29(1)	-24(1)
F(38C)	49(1)	72(1)	16(1)	-3(1)	-1(1)	-36(1)
C(36A)	22(1)	20(1)	24(1)	-7(1)	-5(1)	-7(1)
C(39A)	25(1)	26(1)	51(2)	-19(1)	2(1)	-10(1)
F(39A)	89(2)	78(2)	90(2)	-70(2)	51(2)	-63(2)
F(39B)	71(2)	37(1)	60(2)	3(1)	-19(1)	-29(1)
F(39C)	31(1)	43(1)	149(3)	-38(2)	-28(2)	-12(1)
C(36B)	22(1)	20(1)	24(1)	-7(1)	-5(1)	-7(1)
C(39B)	25(1)	26(1)	51(2)	-19(1)	2(1)	-10(1)
F(39D)	71(2)	37(1)	60(2)	3(1)	-19(1)	-29(1)
F(39E)	32(4)	17(3)	95(6)	-8(4)	-25(4)	-4(3)
F(39F)	89(2)	78(2)	90(2)	-70(2)	51(2)	-63(2)
C(40)	16(1)	21(1)	14(1)	-8(1)	1(1)	-7(1)
C(41)	17(1)	23(1)	20(1)	-9(1)	0(1)	-8(1)
C(43)	21(1)	24(1)	21(1)	-11(1)	1(1)	-11(1)
C(44)	18(1)	28(1)	21(1)	-11(1)	-2(1)	-10(1)
C(45)	17(1)	24(1)	21(1)	-10(1)	-3(1)	-7(1)
C(42A)	20(1)	20(1)	23(1)	-8(1)	-3(1)	-6(1)
C(46A)	33(1)	25(1)	56(2)	-1(1)	-20(1)	-12(1)
F(46A)	43(1)	26(1)	77(2)	7(1)	-22(1)	-17(1)
F(46B)	25(1)	46(2)	76(2)	-7(1)	4(1)	10(1)
F(46C)	140(4)	35(1)	112(3)	-11(2)	-106(3)	8(2)
C(42B)	20(1)	20(1)	23(1)	-8(1)	-3(1)	-6(1)
C(46B)	33(1)	25(1)	56(2)	-1(1)	-20(1)	-12(1)
F(46D)	43(1)	26(1)	77(2)	7(1)	-22(1)	-17(1)
F(46E)	140(4)	35(1)	112(3)	-11(2)	-106(3)	8(2)
F(46F)	30(4)	29(4)	123(9)	15(4)	-44(5)	-9(3)
C(47)	23(1)	33(1)	43(1)	-11(1)	-8(1)	-13(1)
F(47A)	52(1)	107(2)	55(1)	12(1)	-35(1)	-44(1)
F(47B)	34(1)	38(1)	67(1)	-5(1)	-18(1)	-23(1)
F(47C)	17(1)	61(1)	135(2)	-58(1)	0(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for RH00301.

	x	y	z	U(eq)
H(1)	7369	5707	7298	46
H(2)	8801	4991	6178	60
H(3A)	9072	2905	7543	74
H(3B)	9663	3087	6444	74
H(4A)	10872	2583	7559	72
H(4B)	11171	3403	6545	72
H(5)	11004	4579	7345	45
H(6)	9534	5023	8580	37
H(7A)	8448	3786	9568	43
H(7B)	8958	3079	8819	43
H(8A)	7171	3868	8647	45
H(8B)	7057	4960	8880	45
H(9)	11720	5783	7313	32
H(10)	11979	7533	7279	37
H(11)	10128	8971	7112	33
H(12A)	8147	8950	7107	35
H(12B)	7940	7773	7688	35
H(13)	7563	9620	5528	57
H(14)	7488	8662	4466	70
H(15)	8209	6669	5164	58
H(17)	5699	1158	8756	22
H(19)	9048	904	7405	23
H(21)	6699	1793	5929	22
H(25)	3548	3930	6481	25
H(27)	4229	3851	3798	32
H(29)	5219	1070	5774	27
H(33)	2629	1758	8886	22
H(35)	2114	4490	9642	26
H(37)	4836	3617	7536	23
H(41)	5649	-456	8192	24
H(43)	3190	-1926	8738	25
H(45)	2729	1300	7395	24

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 0.9196 (0.0168) x + 0.5177 (0.0171) y + 14.0805 (0.0092) z = 9.5349 (0.0311)

* 0.0073 (0.0014) N1
* -0.0069 (0.0014) N2
* -0.0051 (0.0016) C9
* 0.0009 (0.0016) C10
* 0.0038 (0.0015) C11
    0.1276 (0.0041) C12
   -0.0741 (0.0040) Rh1

Rms deviation of fitted atoms = 0.0053

10.8737 (0.0108) x + 2.7629 (0.0202) y - 3.4228 (0.0235) z = 9.0008 (0.0328)

Angle to previous plane (with approximate esd) = 53.05 (0.14)

* 0.0036 (0.0016) N3
* -0.0023 (0.0016) N4
* -0.0034 (0.0018) C13
* 0.0019 (0.0019) C14
* 0.0002 (0.0018) C15
   -0.0433 (0.0045) C12
    0.1646 (0.0046) Rh1

Rms deviation of fitted atoms = 0.0026

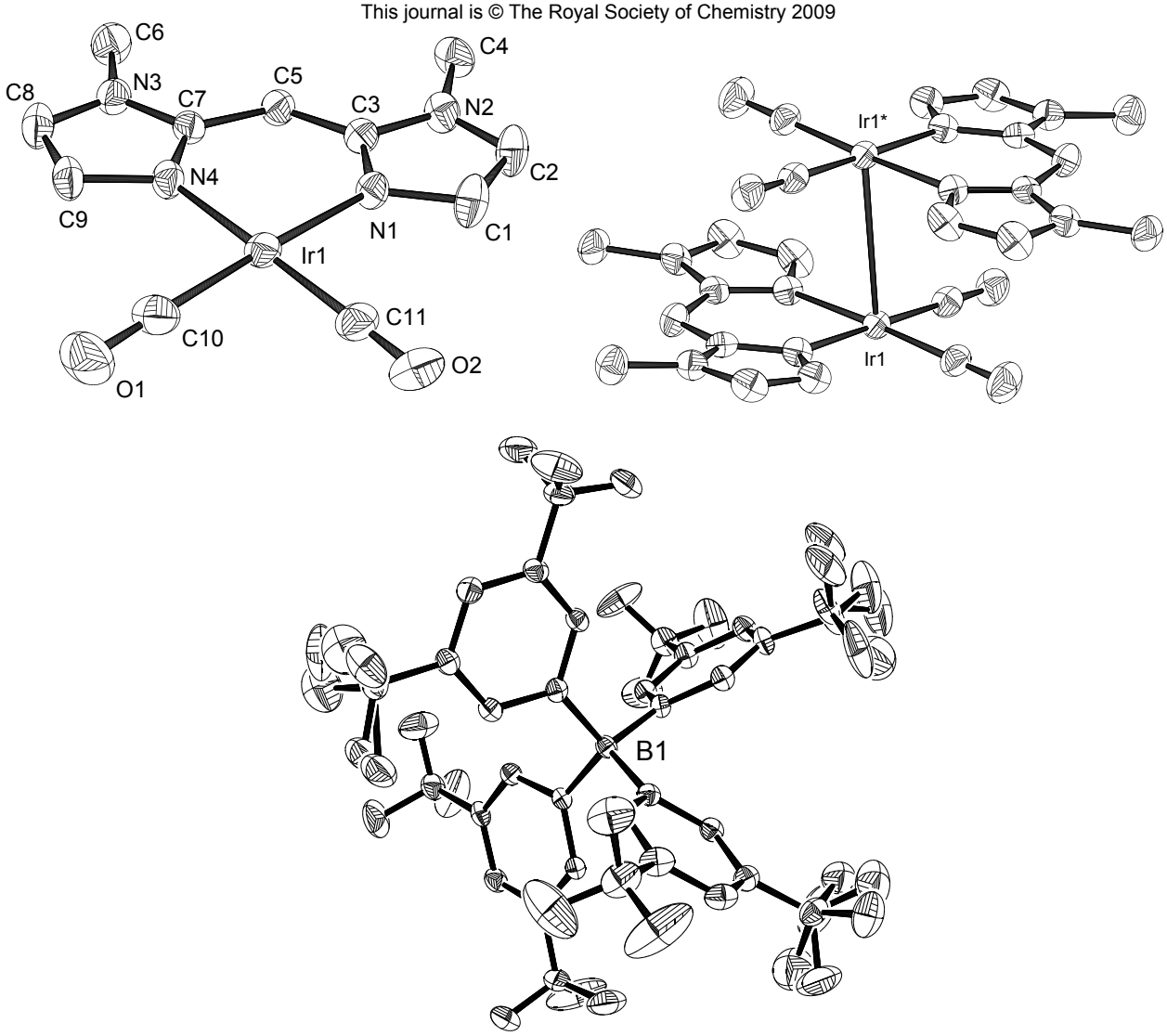
Table 6. Torsion angles [deg] for BH00301.

N(4)-Rh(1)-N(1)-C(9)	-143.9(2)	C(18)-C(19)-C(20)-C(21)	0.6(3)
C(5)-Rh(1)-N(1)-C(9)	16.7(2)	C(18)-C(19)-C(20)-C(23)	-179.44(19)
C(1)-Rh(1)-N(1)-C(9)	131.0(3)	C(19)-C(20)-C(21)-C(16)	-0.8(3)
C(2)-Rh(1)-N(1)-C(9)	-45.7(6)	C(23)-C(20)-C(21)-C(16)	179.3(2)
C(6)-Rh(1)-N(1)-C(9)	54.7(2)	C(17)-C(16)-C(21)-C(20)	0.6(3)
N(4)-Rh(1)-N(1)-N(2)	31.10(17)	B(1)-C(16)-C(21)-C(20)	-179.75(19)
C(5)-Rh(1)-N(1)-N(2)	-168.26(18)	C(19)-C(18)-C(22)-F(22B)	-30.3(3)
C(1)-Rh(1)-N(1)-N(2)	-53.9(3)	C(17)-C(18)-C(22)-F(22B)	152.1(2)
C(2)-Rh(1)-N(1)-N(2)	129.3(5)	C(19)-C(18)-C(22)-F(22A)	-151.1(2)
C(6)-Rh(1)-N(1)-N(2)	-130.26(17)	C(17)-C(18)-C(22)-F(22A)	31.2(3)
C(9)-N(1)-N(2)-C(11)	-1.4(3)	C(19)-C(18)-C(22)-F(22C)	89.7(3)
Rh(1)-N(1)-N(2)-C(11)	-177.81(16)	C(17)-C(18)-C(22)-F(22C)	-88.0(3)
C(9)-N(1)-N(2)-C(12)	-174.2(2)	C(19)-C(20)-C(23)-F(23B)	-93.9(3)
Rh(1)-N(1)-N(2)-C(12)	9.4(3)	C(21)-C(20)-C(23)-F(23B)	86.0(3)
C(13)-N(3)-N(4)-C(15)	0.6(3)	C(19)-C(20)-C(23)-F(23C)	145.1(3)
C(12)-N(3)-N(4)-C(15)	177.9(2)	C(21)-C(20)-C(23)-F(23C)	-34.9(4)
C(13)-N(3)-N(4)-Rh(1)	174.95(18)	C(19)-C(20)-C(23)-F(23A)	24.9(3)
C(12)-N(3)-N(4)-Rh(1)	-7.7(3)	C(21)-C(20)-C(23)-F(23A)	-155.1(3)
N(1)-Rh(1)-N(4)-C(15)	140.3(3)	C(32)-B(1)-C(24)-C(25)	12.4(3)
C(5)-Rh(1)-N(4)-C(15)	52.1(4)	C(40)-B(1)-C(24)-C(25)	133.6(2)
C(1)-Rh(1)-N(4)-C(15)	-64.3(3)	C(16)-B(1)-C(24)-C(25)	-105.5(2)
C(2)-Rh(1)-N(4)-C(15)	-26.7(3)	C(32)-B(1)-C(24)-C(29)	-170.72(18)
C(6)-Rh(1)-N(4)-C(15)	-128.9(3)	C(40)-B(1)-C(24)-C(29)	-49.5(2)
N(1)-Rh(1)-N(4)-N(3)	-32.08(18)	C(16)-B(1)-C(24)-C(29)	71.3(2)
C(5)-Rh(1)-N(4)-N(3)	-120.2(3)	C(29)-C(24)-C(25)-C(26)	-1.6(3)
C(1)-Rh(1)-N(4)-N(3)	123.4(2)	B(1)-C(24)-C(25)-C(26)	175.4(2)
C(2)-Rh(1)-N(4)-N(3)	160.9(2)	C(24)-C(25)-C(26)-C(27)	-0.6(3)
C(6)-Rh(1)-N(4)-N(3)	58.7(4)	C(24)-C(25)-C(26)-C(30)	177.1(2)
N(4)-Rh(1)-C(1)-C(2)	97.0(2)	C(25)-C(26)-C(27)-C(28A)	1.8(3)
N(1)-Rh(1)-C(1)-C(2)	-178.8(2)	C(30)-C(26)-C(27)-C(28A)	-175.9(2)
C(5)-Rh(1)-C(1)-C(2)	-65.6(2)	C(25)-C(24)-C(29)-C(28A)	2.6(3)
C(6)-Rh(1)-C(1)-C(2)	-100.0(2)	B(1)-C(24)-C(29)-C(28A)	-174.5(2)
N(4)-Rh(1)-C(1)-C(8)	-141.2(2)	C(27)-C(26)-C(30)-F(30C)	-137.8(2)
N(1)-Rh(1)-C(1)-C(8)	-57.0(4)	C(25)-C(26)-C(30)-F(30C)	44.5(3)
C(5)-Rh(1)-C(1)-C(8)	56.2(2)	C(27)-C(26)-C(30)-F(30B)	-16.0(3)
C(2)-Rh(1)-C(1)-C(8)	121.8(3)	C(25)-C(26)-C(30)-F(30B)	166.3(2)
C(6)-Rh(1)-C(1)-C(8)	21.8(2)	C(27)-C(26)-C(30)-F(30A)	102.9(3)
C(8)-C(1)-C(2)-C(3)	3.1(5)	C(25)-C(26)-C(30)-F(30A)	-74.9(3)
Rh(1)-C(1)-C(2)-C(3)	104.8(3)	C(26)-C(27)-C(28A)-C(29)	-0.8(4)
C(8)-C(1)-C(2)-Rh(1)	-101.8(3)	C(26)-C(27)-C(28A)-C(31A)	-178.6(2)
N(4)-Rh(1)-C(2)-C(1)	-84.9(2)	C(24)-C(29)-C(28A)-C(27)	-1.5(4)
N(1)-Rh(1)-C(2)-C(1)	177.8(4)	C(24)-C(29)-C(28A)-C(31A)	176.30(19)
C(5)-Rh(1)-C(2)-C(1)	114.3(2)	C(27)-C(28A)-C(31A)-F(31C)	89.0(2)
C(6)-Rh(1)-C(2)-C(1)	76.9(2)	C(29)-C(28A)-C(31A)-F(31C)	-88.9(2)
N(4)-Rh(1)-C(2)-C(3)	155.3(2)	C(27)-C(28A)-C(31A)-F(31A)	-136.56(18)
N(1)-Rh(1)-C(2)-C(3)	58.0(7)	C(29)-C(28A)-C(31A)-F(31A)	45.6(2)
C(5)-Rh(1)-C(2)-C(3)	-5.5(2)	C(27)-C(28A)-C(31A)-F(31B)	-22.8(2)
C(1)-Rh(1)-C(2)-C(3)	-119.8(4)	C(29)-C(28A)-C(31A)-F(31B)	159.33(17)
C(6)-Rh(1)-C(2)-C(3)	-42.9(3)	C(24)-B(1)-C(32)-C(33)	107.9(2)
C(1)-C(2)-C(3)-C(4)	-93.3(4)	C(40)-B(1)-C(32)-C(33)	-12.2(3)
Rh(1)-C(2)-C(3)-C(4)	-11.9(4)	C(16)-B(1)-C(32)-C(33)	-132.4(2)
C(2)-C(3)-C(4)-C(5)	30.8(5)	C(24)-B(1)-C(32)-C(37)	-72.0(2)
C(3)-C(4)-C(5)-C(6)	46.3(5)	C(40)-B(1)-C(32)-C(37)	167.95(18)
C(3)-C(4)-C(5)-Rh(1)	-34.8(4)	C(16)-B(1)-C(32)-C(37)	47.7(2)
N(4)-Rh(1)-C(5)-C(6)	179.5(2)	C(37)-C(32)-C(33)-C(34)	1.2(3)
N(1)-Rh(1)-C(5)-C(6)	92.21(16)	B(1)-C(32)-C(33)-C(34)	-178.7(2)
C(1)-Rh(1)-C(5)-C(6)	-65.22(18)	C(32)-C(33)-C(34)-C(35)	0.0(3)
C(2)-Rh(1)-C(5)-C(6)	-99.50(18)	C(32)-C(33)-C(34)-C(38)	-176.1(2)
N(4)-Rh(1)-C(5)-C(4)	-59.3(4)	C(33)-C(34)-C(35)-C(36A)	-0.6(3)
N(1)-Rh(1)-C(5)-C(4)	-146.6(2)	C(38)-C(34)-C(35)-C(36A)	175.5(2)
C(1)-Rh(1)-C(5)-C(4)	56.0(2)	C(33)-C(32)-C(37)-C(36A)	-1.8(3)
C(2)-Rh(1)-C(5)-C(4)	21.7(2)	B(1)-C(32)-C(37)-C(36A)	178.0(2)
C(6)-Rh(1)-C(5)-C(4)	121.2(3)	C(35)-C(34)-C(38)-F(38A)	145.8(2)
C(4)-C(5)-C(6)-C(7)	3.3(5)	C(33)-C(34)-C(38)-F(38A)	-38.0(3)
Rh(1)-C(5)-C(6)-C(7)	105.5(3)	C(35)-C(34)-C(38)-F(38B)	25.0(3)

C(4)-C(5)-C(6)-Rh(1)	-102.2(4)	C(33)-C(34)-C(38)-F(38B)	-158.8(2)
N(4)-Rh(1)-C(6)-C(5)	-179.4(3)	C(35)-C(34)-C(38)-F(38C)	-95.1(3)
N(1)-Rh(1)-C(6)-C(5)	-89.61(16)	C(33)-C(34)-C(38)-F(38C)	81.1(3)
C(1)-Rh(1)-C(6)-C(5)	114.58(18)	C(34)-C(35)-C(36A)-C(37)	-0.1(3)
C(2)-Rh(1)-C(6)-C(5)	77.52(18)	C(34)-C(35)-C(36A)-C(39A)	-178.27(19)
N(4)-Rh(1)-C(6)-C(7)	61.3(4)	C(32)-C(37)-C(36A)-C(35)	1.3(3)
N(1)-Rh(1)-C(6)-C(7)	151.14(19)	C(32)-C(37)-C(36A)-C(39A)	179.57(18)
C(5)-Rh(1)-C(6)-C(7)	-119.2(3)	C(35)-C(36A)-C(39A)-F(39A)	-0.8(2)
C(1)-Rh(1)-C(6)-C(7)	-4.7(2)	C(37)-C(36A)-C(39A)-F(39A)	-179.06(15)
C(2)-Rh(1)-C(6)-C(7)	-41.7(2)	C(35)-C(36A)-C(39A)-F(39C)	141.81(17)
C(5)-C(6)-C(7)-C(8)	-94.8(3)	C(37)-C(36A)-C(39A)-F(39C)	-36.4(2)
Rh(1)-C(6)-C(7)-C(8)	-13.4(3)	C(35)-C(36A)-C(39A)-F(39B)	-114.24(19)
C(2)-C(1)-C(8)-C(7)	45.0(4)	C(37)-C(36A)-C(39A)-F(39B)	67.5(2)
Rh(1)-C(1)-C(8)-C(7)	-35.9(3)	C(24)-B(1)-C(40)-C(41)	133.2(2)
C(6)-C(7)-C(8)-C(1)	32.5(4)	C(32)-B(1)-C(40)-C(41)	-105.9(2)
N(2)-N(1)-C(9)-C(10)	1.2(3)	C(16)-B(1)-C(40)-C(41)	12.5(3)
Rh(1)-N(1)-C(9)-C(10)	176.77(18)	C(24)-B(1)-C(40)-C(45)	-50.8(2)
N(1)-C(9)-C(10)-C(11)	-0.6(3)	C(32)-B(1)-C(40)-C(45)	70.1(2)
N(1)-N(2)-C(11)-C(10)	1.1(3)	C(16)-B(1)-C(40)-C(45)	-171.51(18)
C(12)-N(2)-C(11)-C(10)	173.1(2)	C(45)-C(40)-C(41)-C(42A)	-0.8(3)
C(9)-C(10)-C(11)-N(2)	-0.3(3)	B(1)-C(40)-C(41)-C(42A)	175.30(19)
C(11)-N(2)-C(12)-N(3)	124.0(3)	C(42A)-C(43)-C(44)-C(45)	0.6(3)
N(1)-N(2)-C(12)-N(3)	-64.6(3)	C(42A)-C(43)-C(44)-C(47)	-176.2(2)
C(13)-N(3)-C(12)-N(2)	-119.8(3)	C(43)-C(44)-C(45)-C(40)	-2.2(3)
N(4)-N(3)-C(12)-N(2)	63.4(3)	C(47)-C(44)-C(45)-C(40)	174.6(2)
N(4)-N(3)-C(13)-C(14)	-0.7(3)	C(41)-C(40)-C(45)-C(44)	2.3(3)
C(12)-N(3)-C(13)-C(14)	-177.7(3)	B(1)-C(40)-C(45)-C(44)	-174.07(19)
N(3)-C(13)-C(14)-C(15)	0.5(3)	C(44)-C(43)-C(42A)-C(41)	0.9(3)
N(3)-N(4)-C(15)-C(14)	-0.3(3)	C(44)-C(43)-C(42A)-C(46A)	-179.73(19)
Rh(1)-N(4)-C(15)-C(14)	-173.5(2)	C(40)-C(41)-C(42A)-C(43)	-0.7(3)
C(13)-C(14)-C(15)-N(4)	-0.2(4)	C(40)-C(41)-C(42A)-C(46A)	179.87(19)
C(24)-B(1)-C(16)-C(17)	165.33(18)	C(43)-C(42A)-C(46A)-F(46B)	116.50(18)
C(32)-B(1)-C(16)-C(17)	45.6(2)	C(41)-C(42A)-C(46A)-F(46B)	-64.1(2)
C(40)-B(1)-C(16)-C(17)	-74.8(2)	C(43)-C(42A)-C(46A)-F(46A)	-7.1(2)
C(24)-B(1)-C(16)-C(21)	-14.3(3)	C(41)-C(42A)-C(46A)-F(46A)	172.29(15)
C(32)-B(1)-C(16)-C(21)	-134.0(2)	C(43)-C(42A)-C(46A)-F(46C)	-122.71(18)
C(40)-B(1)-C(16)-C(21)	105.6(2)	C(41)-C(42A)-C(46A)-F(46C)	56.7(2)
C(21)-C(16)-C(17)-C(18)	-0.4(3)	C(43)-C(44)-C(47)-F(47B)	0.5(3)
B(1)-C(16)-C(17)-C(18)	179.96(19)	C(45)-C(44)-C(47)-F(47B)	-176.4(2)
C(16)-C(17)-C(18)-C(19)	0.3(3)	C(43)-C(44)-C(47)-F(47C)	121.4(3)
C(16)-C(17)-C(18)-C(22)	177.9(2)	C(45)-C(44)-C(47)-F(47C)	-55.4(3)
C(17)-C(18)-C(19)-C(20)	-0.4(3)	C(43)-C(44)-C(47)-F(47A)	-120.0(3)
C(22)-C(18)-C(19)-C(20)	-178.01(19)	C(45)-C(44)-C(47)-F(47A)	63.2(3)

Supplementary Material (ESI) for Dalton Transactions

Ortep Diagrams and Crystallographic Tables for $[Ir(bim)(CO)_2]BAr^F_{24}$ (10a)



ORTEP plot (50% ellipsoids, H-atoms omitted) of cation (top) and anion (bottom). All hydrogen atoms were refined in idealized positions.
Three of the anion´s CF3 groups are twofold disordered each (s.o.f. 0.24 : 0.76, 0.75 : 0.25, 0.77 : 0.23). The cations form dimers with short Ir-Ir contacts.

Table 1. Crystal data and structure refinement for rh00401.

Identification code	rh00401
Empirical formula	C43 H24 B F24 Ir N4 O2
Formula weight	1287.67
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	a = 12.40560(10) A alpha = 90 deg.
	b = 24.5181(3) A beta = 111.5840(10) deg.
	c = 16.1804(2) A gamma = 90 deg.
Volume	4576.36(9) A^3
Z, Calculated density	4, 1.869 Mg/m^3
Absorption coefficient	3.059 mm^-1
F(000)	2496
Crystal size	0.39 x 0.24 x 0.15 mm
Theta range for data collection	2.71 to 30.00 deg.
Limiting indices	-17<=h<=17, -34<=k<=34, -22<=l<=22
Reflections collected / unique	74647 / 13330 [R(int) = 0.0664]
Completeness to theta = 30.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.638 and 0.425
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13330 / 99 / 727
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.1225
R indices (all data)	R1 = 0.0650, wR2 = 0.1306
Largest diff. peak and hole	2.018 and -1.898 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for rh00401.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ir(1)	9679(1)	121(1)	5858(1)	25(1)
O(1)	7589(4)	830(2)	5047(3)	51(1)
O(2)	11050(4)	1155(2)	6326(2)	41(1)
N(1)	11129(3)	-363(2)	6490(2)	27(1)
N(2)	12294(3)	-1060(2)	6967(3)	32(1)
N(3)	8161(3)	-1446(2)	5341(3)	31(1)
N(4)	8707(3)	-589(2)	5530(2)	27(1)
C(1)	12261(4)	-172(2)	6893(4)	39(1)
C(2)	12978(4)	-604(2)	7187(3)	39(1)
C(3)	11186(4)	-903(2)	6552(3)	26(1)
C(4)	12713(5)	-1625(2)	7137(4)	39(1)
C(5)	10231(4)	-1311(2)	6262(3)	31(1)
C(6)	8196(5)	-2042(2)	5393(4)	43(1)
C(7)	9057(4)	-1106(2)	5717(3)	27(1)
C(8)	7196(4)	-1139(2)	4887(3)	37(1)
C(9)	7526(4)	-614(2)	5002(3)	32(1)
C(10)	8375(5)	558(2)	5350(3)	34(1)
C(11)	10547(4)	758(2)	6165(3)	31(1)
B(1)	9728(4)	1492(2)	8572(3)	19(1)
C(12)	11116(3)	1382(2)	8818(2)	19(1)
C(13)	11751(3)	1035(2)	9523(3)	20(1)
C(14)	12894(3)	889(2)	9682(3)	23(1)
C(15)	13474(3)	1099(2)	9160(3)	25(1)
C(16)	12881(3)	1461(2)	8487(3)	24(1)
C(17)	11727(3)	1599(2)	8318(3)	21(1)
C(18)	13527(4)	495(2)	10403(3)	30(1)
F(18A)	12941(3)	342(2)	10894(3)	63(1)
F(18B)	14530(3)	712(2)	10975(2)	54(1)
F(18C)	13869(4)	53(2)	10095(3)	65(1)
C(19)	13516(4)	1711(2)	7949(3)	30(1)

F(19A)	14295(4)	2012(3)	8426(3)	97(2)
F(19B)	13928(5)	1339(2)	7553(3)	84(2)
F(19C)	12858(3)	2025(2)	7288(2)	54(1)
C(20)	8996(3)	954(2)	8052(2)	19(1)
C(21)	9445(3)	423(2)	8223(3)	21(1)
C(22)	8804(4)	-33(2)	7841(3)	26(1)
C(23)	7653(4)	9(2)	7268(3)	26(1)
C(25)	7831(3)	987(2)	7468(3)	22(1)
C(26)	9340(4)	-584(2)	8099(3)	32(1)
F(26A)	10416(3)	-609(1)	8094(3)	51(1)
F(26B)	9438(4)	-730(2)	8902(2)	62(1)
F(26C)	8779(4)	-979(1)	7528(3)	71(1)
C(24A)	7189(3)	529(2)	7081(3)	25(1)
C(27A)	5973(5)	614(5)	6413(7)	38(1)
F(27A)	5249(5)	822(5)	6835(7)	84(2)
F(27B)	5829(5)	872(5)	5753(7)	82(6)
F(27C)	5476(5)	164(5)	6058(7)	68(2)
C(24B)	7189(3)	529(2)	7081(3)	25(1)
C(27B)	5914(2)	608(1)	6540(2)	38(1)
F(27D)	5203(2)	461(1)	6877(2)	84(2)
F(27E)	5750(2)	1101(1)	6067(2)	70(2)
F(27F)	5627(2)	188(1)	5793(2)	68(2)
C(28)	9366(3)	2028(2)	7921(3)	19(1)
C(29)	9373(4)	2556(2)	8231(3)	24(1)
C(30)	9197(4)	3012(2)	7691(3)	29(1)
C(31)	8982(4)	2962(2)	6791(3)	28(1)
C(33)	9142(3)	1985(2)	6998(3)	21(1)
C(34)	9258(5)	3563(2)	8110(4)	42(1)
F(34A)	8515(3)	3608(1)	8530(2)	48(1)
F(34B)	9069(6)	3972(1)	7559(3)	95(2)
F(34C)	10311(4)	3663(2)	8739(4)	85(2)
C(32A)	8960(3)	2436(2)	6455(3)	25(1)
C(35A)	8723(3)	2362(1)	5493(2)	29(1)
F(35A)	9081(3)	1886(1)	5279(2)	71(2)
F(35B)	7634(3)	2373(1)	4979(2)	71(2)
F(35C)	9228(3)	2715(1)	5150(2)	79(2)
C(32B)	8960(3)	2436(2)	6455(3)	25(1)
C(35B)	8680(7)	2380(3)	5485(2)	29(1)
F(35D)	8418(7)	1844(3)	5211(2)	48(3)
F(35E)	7815(7)	2675(3)	4972(2)	49(3)
F(35F)	9728(7)	2356(3)	5379(2)	67(4)
C(36)	9432(3)	1610(2)	9459(3)	19(1)
C(37)	8410(3)	1428(2)	9548(3)	20(1)
C(38)	8119(3)	1571(2)	10271(3)	23(1)
C(39)	8839(3)	1903(2)	10944(3)	24(1)
C(41)	10164(3)	1936(2)	10161(3)	21(1)
C(42)	7021(4)	1368(2)	10350(3)	32(1)
F(42A)	7213(3)	1012(2)	11014(2)	51(1)
F(42B)	6326(3)	1112(2)	9617(2)	49(1)
F(42C)	6407(3)	1770(2)	10518(3)	57(1)
C(40A)	9866(3)	2082(2)	10879(3)	22(1)
C(43A)	10628(2)	2445(1)	11600(2)	29(1)
F(43A)	11462(2)	2676(1)	11430(2)	51(1)
F(43B)	11089(2)	2197(1)	12362(2)	77(2)
F(43C)	10033(2)	2872(1)	11757(2)	49(1)
C(40B)	9866(3)	2082(2)	10879(3)	22(1)
C(43B)	10703(8)	2422(4)	11597(6)	29(1)
F(43D)	11343(8)	2818(4)	11180(6)	51(1)
F(43E)	11651(8)	2120(4)	12201(6)	69(5)
F(43F)	10261(8)	2682(4)	12075(6)	71(6)

Table 3. Bond lengths [Å] and angles [deg] for rh00401.

Ir(1)-C(11)	1.857(5)	C(25)-C(24A)	1.386(6)
Ir(1)-C(10)	1.861(5)	C(26)-F(26B)	1.310(6)
Ir(1)-N(4)	2.073(4)	C(26)-F(26A)	1.339(6)
Ir(1)-N(1)	2.082(4)	C(26)-F(26C)	1.342(6)
Ir(1)-Ir(1)#1	3.2120(3)	C(24A)-C(27A)	1.513(5)
O(1)-C(10)	1.132(6)	C(27A)-F(27B)	1.1980
O(2)-C(11)	1.135(6)	C(27A)-F(27C)	1.2912
N(1)-C(3)	1.329(6)	C(27A)-F(27A)	1.4084
N(1)-C(1)	1.393(6)	C(27B)-F(27D)	1.2492
N(2)-C(3)	1.345(6)	C(27B)-F(27E)	1.4043
N(2)-C(2)	1.369(7)	C(27B)-F(27F)	1.5270
N(2)-C(4)	1.469(7)	C(28)-C(29)	1.386(6)
N(3)-C(7)	1.344(6)	C(28)-C(33)	1.419(6)
N(3)-C(8)	1.375(7)	C(29)-C(30)	1.387(6)
N(3)-C(6)	1.462(7)	C(30)-C(31)	1.385(7)
N(4)-C(7)	1.337(6)	C(30)-C(34)	1.501(7)
N(4)-C(9)	1.400(6)	C(31)-C(32A)	1.399(6)
C(1)-C(2)	1.352(8)	C(33)-C(32A)	1.376(6)
C(3)-C(5)	1.488(7)	C(34)-F(34B)	1.304(6)
C(5)-C(7)	1.486(6)	C(34)-F(34A)	1.337(6)
C(8)-C(9)	1.343(8)	C(34)-F(34C)	1.350(7)
B(1)-C(36)	1.632(6)	C(32A)-C(35A)	1.485(5)
B(1)-C(28)	1.641(6)	C(35A)-F(35B)	1.3007
B(1)-C(12)	1.642(6)	C(35A)-F(35C)	1.3056
B(1)-C(20)	1.646(6)	C(35A)-F(35A)	1.3398
C(12)-C(17)	1.400(5)	C(35B)-F(35E)	1.3083
C(12)-C(13)	1.410(5)	C(35B)-F(35F)	1.3728
C(13)-C(14)	1.392(5)	C(35B)-F(35D)	1.3859
C(14)-C(15)	1.394(6)	C(36)-C(37)	1.401(5)
C(14)-C(18)	1.495(6)	C(36)-C(41)	1.413(5)
C(15)-C(16)	1.386(6)	C(37)-C(38)	1.391(6)
C(16)-C(17)	1.396(5)	C(38)-C(39)	1.389(6)
C(16)-C(19)	1.503(6)	C(38)-C(42)	1.499(6)
C(18)-F(18A)	1.313(6)	C(39)-C(40A)	1.387(6)
C(18)-F(18C)	1.326(6)	C(41)-C(40A)	1.388(6)
C(18)-F(18B)	1.356(5)	C(42)-F(42C)	1.332(6)
C(19)-F(19A)	1.308(6)	C(42)-F(42A)	1.336(6)
C(19)-F(19B)	1.321(6)	C(42)-F(42B)	1.339(6)
C(19)-F(19C)	1.327(6)	C(40A)-C(43A)	1.496(4)
C(20)-C(21)	1.404(5)	C(43A)-F(43A)	1.2942
C(20)-C(25)	1.407(5)	C(43A)-F(43B)	1.3028
C(21)-C(22)	1.380(6)	C(43A)-F(43C)	1.3589
C(22)-C(23)	1.391(6)	C(43B)-F(43F)	1.2726
C(22)-C(26)	1.496(6)	C(43B)-F(43E)	1.4281
C(23)-C(24A)	1.386(6)	C(43B)-F(43D)	1.5556

C(11)-Ir(1)-C(10)	87.6(2)	C(24A)-C(25)-C(20)	122.3(4)
C(11)-Ir(1)-N(4)	179.26(17)	F(26B)-C(26)-F(26A)	105.3(4)
C(10)-Ir(1)-N(4)	92.4(2)	F(26B)-C(26)-F(26C)	108.8(4)
C(11)-Ir(1)-N(1)	92.07(18)	F(26A)-C(26)-F(26C)	103.3(4)
C(10)-Ir(1)-N(1)	177.00(18)	F(26B)-C(26)-C(22)	113.1(4)
N(4)-Ir(1)-N(1)	87.89(15)	F(26A)-C(26)-C(22)	112.3(4)
C(11)-Ir(1)-Ir(1)#1	94.79(14)	F(26C)-C(26)-C(22)	113.3(4)
C(10)-Ir(1)-Ir(1)#1	100.18(15)	C(23)-C(24A)-C(25)	121.6(4)
N(4)-Ir(1)-Ir(1)#1	85.94(10)	C(23)-C(24A)-C(27A)	120.5(6)
N(1)-Ir(1)-Ir(1)#1	82.81(10)	C(25)-C(24A)-C(27A)	117.8(6)
C(3)-N(1)-C(1)	106.4(4)	F(27B)-C(27A)-F(27C)	99.5
C(3)-N(1)-Ir(1)	128.1(3)	F(27B)-C(27A)-F(27A)	109.2
C(1)-N(1)-Ir(1)	125.4(3)	F(27C)-C(27A)-F(27A)	103.8
C(3)-N(2)-C(2)	108.5(4)	F(27B)-C(27A)-C(24A)	119.5(6)
C(3)-N(2)-C(4)	126.1(4)	F(27C)-C(27A)-C(24A)	112.8(5)
C(2)-N(2)-C(4)	125.3(4)	F(27A)-C(27A)-C(24A)	110.5(5)
C(7)-N(3)-C(8)	108.4(4)	F(27D)-C(27B)-F(27E)	120.2
C(7)-N(3)-C(6)	126.3(4)	F(27D)-C(27B)-F(27F)	98.9
C(8)-N(3)-C(6)	125.3(4)	F(27E)-C(27B)-F(27F)	101.8

C(7)-N(4)-C(9)	106.1(4)	C(29)-C(28)-C(33)	115.0(4)
C(7)-N(4)-Ir(1)	128.9(3)	C(29)-C(28)-B(1)	123.5(4)
C(9)-N(4)-Ir(1)	125.0(3)	C(33)-C(28)-B(1)	121.2(3)
C(2)-C(1)-N(1)	108.8(5)	C(28)-C(29)-C(30)	123.2(4)
C(1)-C(2)-N(2)	106.5(4)	C(31)-C(30)-C(29)	121.0(4)
N(1)-C(3)-N(2)	109.9(4)	C(31)-C(30)-C(34)	120.8(4)
N(1)-C(3)-C(5)	129.3(4)	C(29)-C(30)-C(34)	118.2(4)
N(2)-C(3)-C(5)	120.8(4)	C(30)-C(31)-C(32A)	117.3(4)
C(7)-C(5)-C(3)	116.8(4)	C(32A)-C(33)-C(28)	122.4(4)
N(4)-C(7)-N(3)	109.9(4)	F(34B)-C(34)-F(34A)	107.5(5)
N(4)-C(7)-C(5)	128.5(4)	F(34B)-C(34)-F(34C)	104.9(6)
N(3)-C(7)-C(5)	121.7(4)	F(34A)-C(34)-F(34C)	105.0(5)
C(9)-C(8)-N(3)	106.8(4)	F(34B)-C(34)-C(30)	114.6(5)
C(8)-C(9)-N(4)	108.9(4)	F(34A)-C(34)-C(30)	111.9(4)
O(1)-C(10)-Ir(1)	179.1(6)	F(34C)-C(34)-C(30)	112.2(5)
O(2)-C(11)-Ir(1)	177.5(5)	C(33)-C(32A)-C(31)	121.2(4)
C(36)-B(1)-C(28)	109.0(3)	C(33)-C(32A)-C(35A)	119.7(4)
C(36)-B(1)-C(12)	111.8(3)	C(31)-C(32A)-C(35A)	119.2(4)
C(28)-B(1)-C(12)	107.5(3)	F(35B)-C(35A)-F(35C)	105.3
C(36)-B(1)-C(20)	109.4(3)	F(35B)-C(35A)-F(35A)	102.5
C(28)-B(1)-C(20)	110.1(3)	F(35C)-C(35A)-F(35A)	102.2
C(12)-B(1)-C(20)	109.0(3)	F(35B)-C(35A)-C(32A)	115.26(19)
C(17)-C(12)-C(13)	115.9(4)	F(35C)-C(35A)-C(32A)	115.1(2)
C(17)-C(12)-B(1)	122.8(3)	F(35A)-C(35A)-C(32A)	114.8(2)
C(13)-C(12)-B(1)	121.2(3)	F(35E)-C(35B)-F(35F)	122.5
C(14)-C(13)-C(12)	122.1(4)	F(35E)-C(35B)-F(35D)	106.3
C(13)-C(14)-C(15)	120.7(4)	F(35F)-C(35B)-F(35D)	92.4
C(13)-C(14)-C(18)	121.1(4)	C(37)-C(36)-C(41)	115.8(4)
C(15)-C(14)-C(18)	118.2(4)	C(37)-C(36)-B(1)	122.6(3)
C(16)-C(15)-C(14)	118.0(4)	C(41)-C(36)-B(1)	121.5(3)
C(15)-C(16)-C(17)	121.2(4)	C(38)-C(37)-C(36)	122.1(4)
C(15)-C(16)-C(19)	118.4(4)	C(39)-C(38)-C(37)	121.0(4)
C(17)-C(16)-C(19)	120.4(4)	C(39)-C(38)-C(42)	118.1(4)
C(16)-C(17)-C(12)	121.9(4)	C(37)-C(38)-C(42)	120.9(4)
F(18A)-C(18)-F(18C)	108.6(5)	C(40A)-C(39)-C(38)	118.0(4)
F(18A)-C(18)-F(18B)	105.8(4)	C(40A)-C(41)-C(36)	121.9(4)
F(18C)-C(18)-F(18B)	103.7(4)	F(42C)-C(42)-F(42A)	105.4(4)
F(18A)-C(18)-C(14)	114.1(4)	F(42C)-C(42)-F(42B)	107.3(4)
F(18C)-C(18)-C(14)	112.5(4)	F(42A)-C(42)-F(42B)	105.8(4)
F(18B)-C(18)-C(14)	111.4(4)	F(42C)-C(42)-C(38)	112.3(4)
F(19A)-C(19)-F(19B)	106.8(5)	F(42A)-C(42)-C(38)	112.7(4)
F(19A)-C(19)-F(19C)	106.2(5)	F(42B)-C(42)-C(38)	112.9(4)
F(19B)-C(19)-F(19C)	104.0(4)	C(39)-C(40A)-C(41)	121.1(4)
F(19A)-C(19)-C(16)	113.0(4)	C(39)-C(40A)-C(43A)	117.6(3)
F(19B)-C(19)-C(16)	112.2(4)	C(41)-C(40A)-C(43A)	121.2(3)
F(19C)-C(19)-C(16)	113.9(4)	F(43A)-C(43A)-F(43B)	107.3
C(21)-C(20)-C(25)	114.9(4)	F(43A)-C(43A)-F(43C)	103.6
C(21)-C(20)-B(1)	122.5(3)	F(43B)-C(43A)-F(43C)	105.2
C(25)-C(20)-B(1)	122.3(3)	F(43A)-C(43A)-C(40A)	114.88(19)
C(22)-C(21)-C(20)	122.8(4)	F(43B)-C(43A)-C(40A)	113.1(2)
C(21)-C(22)-C(23)	121.3(4)	F(43C)-C(43A)-C(40A)	111.95(19)
C(21)-C(22)-C(26)	118.9(4)	F(43F)-C(43B)-F(43E)	105.9
C(23)-C(22)-C(26)	119.6(4)	F(43F)-C(43B)-F(43D)	110.7
C(24A)-C(23)-C(22)	117.0(4)	F(43E)-C(43B)-F(43D)	101.4

Table 4. Anisotropic displacement parameters (Å^2 x 10^3) for rh00401.
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
Ir(1)	27(1)	28(1)	19(1)	0(1)	6(1)	4(1)
O(1)	48(2)	51(2)	48(2)	6(2)	12(2)	21(2)
O(2)	52(2)	32(2)	38(2)	-11(2)	15(2)	-3(2)
N(1)	23(2)	34(2)	19(2)	2(2)	2(1)	3(2)
N(2)	27(2)	39(2)	24(2)	9(2)	4(2)	5(2)
N(3)	28(2)	33(2)	31(2)	-2(2)	10(2)	-4(2)
N(4)	22(2)	34(2)	22(2)	3(2)	5(1)	1(2)
C(1)	28(2)	46(3)	31(2)	7(2)	-1(2)	-8(2)
C(2)	22(2)	50(3)	33(2)	8(2)	-4(2)	-1(2)
C(3)	26(2)	34(2)	17(2)	4(2)	6(2)	3(2)
C(4)	34(2)	42(3)	37(3)	9(2)	8(2)	16(2)
C(5)	28(2)	29(2)	33(2)	-2(2)	6(2)	4(2)
C(6)	41(3)	32(3)	54(3)	-5(2)	14(3)	-5(2)
C(7)	23(2)	35(2)	23(2)	-2(2)	10(2)	0(2)
C(8)	23(2)	48(3)	34(2)	2(2)	5(2)	-5(2)
C(9)	21(2)	42(3)	30(2)	4(2)	4(2)	3(2)
C(10)	40(3)	34(2)	29(2)	0(2)	13(2)	9(2)
C(11)	33(2)	34(2)	22(2)	-5(2)	7(2)	3(2)
B(1)	16(2)	17(2)	22(2)	0(2)	5(2)	1(2)
C(12)	17(2)	20(2)	19(2)	-1(1)	5(1)	-3(1)
C(13)	18(2)	21(2)	21(2)	0(1)	6(1)	0(1)
C(14)	15(2)	27(2)	23(2)	-3(2)	2(1)	1(2)
C(15)	16(2)	32(2)	27(2)	-1(2)	6(2)	1(2)
C(16)	19(2)	30(2)	23(2)	-4(2)	10(2)	-4(2)
C(17)	18(2)	23(2)	18(2)	-2(1)	5(1)	-2(1)
C(18)	20(2)	34(2)	30(2)	4(2)	4(2)	3(2)
F(18A)	33(2)	96(3)	61(2)	52(2)	19(2)	19(2)
F(18B)	34(2)	57(2)	46(2)	12(2)	-13(1)	-2(2)
F(18C)	102(3)	36(2)	49(2)	5(2)	17(2)	33(2)
C(19)	21(2)	39(3)	30(2)	3(2)	12(2)	-4(2)
F(19A)	75(3)	172(5)	40(2)	-8(3)	17(2)	-91(3)
F(19B)	132(4)	62(3)	115(4)	24(3)	110(4)	27(3)
F(19C)	38(2)	72(2)	61(2)	33(2)	26(2)	3(2)
C(20)	18(2)	18(2)	18(2)	-1(1)	4(1)	0(1)
C(21)	20(2)	17(2)	23(2)	2(1)	6(1)	1(1)
C(22)	26(2)	20(2)	28(2)	2(2)	7(2)	3(2)
C(23)	24(2)	22(2)	30(2)	-3(2)	7(2)	-2(2)
C(25)	22(2)	18(2)	25(2)	1(2)	7(2)	3(2)
C(26)	34(2)	20(2)	39(2)	0(2)	10(2)	2(2)
F(26A)	52(2)	38(2)	74(2)	17(2)	38(2)	24(2)
F(26B)	101(3)	49(2)	60(2)	34(2)	58(2)	42(2)
F(26C)	74(3)	24(2)	85(3)	-11(2)	-6(2)	7(2)
C(24A)	18(2)	26(2)	26(2)	-3(2)	2(2)	1(2)
C(27A)	23(2)	32(2)	45(3)	-4(2)	-4(2)	-3(2)
F(27A)	18(2)	139(7)	89(4)	2(5)	11(2)	1(3)
F(27B)	74(7)	79(7)	82(7)	9(5)	17(5)	-11(5)
F(27C)	52(2)	72(2)	58(3)	-30(2)	-7(2)	13(2)
C(24B)	18(2)	26(2)	26(2)	-3(2)	2(2)	1(2)
C(27B)	23(2)	32(2)	45(3)	-4(2)	-4(2)	-3(2)
F(27D)	18(2)	139(7)	89(4)	2(5)	11(2)	1(3)
F(27E)	43(2)	40(2)	82(3)	-1(2)	-31(2)	12(2)
F(27F)	52(2)	72(2)	58(3)	-30(2)	-7(2)	13(2)
C(28)	16(2)	19(2)	22(2)	3(1)	7(1)	2(1)
C(29)	25(2)	23(2)	27(2)	1(2)	12(2)	1(2)
C(30)	36(2)	17(2)	40(2)	2(2)	20(2)	5(2)
C(31)	27(2)	22(2)	38(2)	10(2)	16(2)	7(2)
C(33)	18(2)	19(2)	25(2)	2(1)	6(1)	2(1)
C(34)	61(3)	26(2)	44(3)	2(2)	25(3)	4(2)
F(34A)	67(2)	34(2)	58(2)	-9(2)	41(2)	4(2)
F(34B)	215(6)	22(2)	82(3)	8(2)	97(4)	17(3)
F(34C)	62(3)	52(2)	131(4)	-51(3)	25(3)	-13(2)

C(32A)	19(2)	29(2)	26(2)	6(2)	8(2)	7(2)
C(35A)	32(2)	30(2)	27(2)	8(2)	12(2)	8(2)
F(35A)	103(4)	68(3)	42(2)	7(2)	27(2)	40(3)
F(35B)	53(3)	114(4)	43(2)	-9(3)	14(2)	12(3)
F(35C)	115(4)	86(3)	48(3)	-1(2)	43(3)	-52(3)
C(32B)	19(2)	29(2)	26(2)	6(2)	8(2)	7(2)
C(35B)	32(2)	30(2)	27(2)	8(2)	12(2)	8(2)
F(35D)	53(5)	47(5)	42(5)	2(4)	16(4)	-12(4)
F(35E)	59(5)	38(5)	40(5)	8(4)	6(4)	22(4)
F(35F)	63(6)	82(6)	60(6)	0(5)	28(4)	6(5)
C(36)	19(2)	17(2)	20(2)	3(1)	5(1)	3(1)
C(37)	15(2)	21(2)	23(2)	1(1)	4(1)	0(1)
C(38)	17(2)	25(2)	26(2)	4(2)	7(2)	3(2)
C(39)	21(2)	31(2)	24(2)	0(2)	10(2)	6(2)
C(41)	18(2)	19(2)	24(2)	0(2)	7(1)	0(1)
C(42)	23(2)	40(3)	36(2)	3(2)	15(2)	-1(2)
F(42A)	36(2)	67(2)	52(2)	25(2)	18(2)	-6(2)
F(42B)	26(1)	78(3)	44(2)	-11(2)	14(1)	-18(2)
F(42C)	36(2)	53(2)	96(3)	-5(2)	42(2)	4(2)
C(40A)	20(2)	21(2)	24(2)	0(2)	6(2)	2(1)
C(43A)	30(2)	30(2)	26(2)	-8(2)	9(2)	-2(2)
F(43A)	46(2)	63(2)	51(2)	-25(2)	25(2)	-25(2)
F(43B)	103(4)	51(3)	40(2)	1(2)	-16(2)	-18(3)
F(43C)	39(2)	39(2)	71(3)	-30(2)	20(2)	-5(2)
C(40B)	20(2)	21(2)	24(2)	0(2)	6(2)	2(1)
C(43B)	30(2)	30(2)	26(2)	-8(2)	9(2)	-2(2)
F(43D)	46(2)	63(2)	51(2)	-25(2)	25(2)	-25(2)
F(43E)	58(6)	68(7)	72(7)	-10(5)	14(5)	4(5)
F(43F)	64(7)	74(8)	76(7)	-18(5)	27(5)	7(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for rh00401.

	x	y	z	U(eq)
H(1)	12491	200	6951	46
H(2)	13795	-593	7487	47
H(4A)	12193	-1838	7344	58
H(4B)	13496	-1629	7592	58
H(4C)	12729	-1786	6587	58
H(5A)	10442	-1597	5917	37
H(5B)	10187	-1488	6799	37
H(6A)	8833	-2177	5229	65
H(6B)	7461	-2191	4983	65
H(6C)	8317	-2156	6001	65
H(8)	6442	-1273	4555	44
H(9)	7037	-309	4765	39
H(13)	11386	895	9902	24
H(15)	14252	998	9262	30
H(17)	11346	1846	7850	25
H(21)	10225	376	8619	25
H(23)	7204	-306	7016	31
H(25)	7473	1335	7335	26
H(29)	9504	2607	8842	29
H(31)	8853	3274	6418	33
H(33)	9117	1634	6746	25
H(37)	7899	1200	9099	25
H(39)	8634	2005	11433	29
H(41)	10880	2060	10142	25

Table 6. Torsion angles [deg] for rh0401.

C(11)-Ir(1)-N(1)-C(3)	-179.8(4)	C(20)-C(21)-C(22)-C(26)	-177.0(4)
N(4)-Ir(1)-N(1)-C(3)	0.9(4)	C(21)-C(22)-C(23)-C(24A)	1.6(7)
Ir(1)#1-Ir(1)-N(1)-C(3)	-85.3(4)	C(26)-C(22)-C(23)-C(24A)	177.4(4)
C(11)-Ir(1)-N(1)-C(1)	-3.8(4)	C(21)-C(20)-C(25)-C(24A)	-1.2(6)
N(4)-Ir(1)-N(1)-C(1)	177.0(4)	B(1)-C(20)-C(25)-C(24A)	-175.1(4)
Ir(1)#1-Ir(1)-N(1)-C(1)	90.8(4)	C(21)-C(22)-C(26)-F(26B)	72.5(6)
C(10)-Ir(1)-N(4)-C(7)	-177.2(4)	C(23)-C(22)-C(26)-F(26B)	-103.4(6)
N(1)-Ir(1)-N(4)-C(7)	-0.2(4)	C(21)-C(22)-C(26)-F(26A)	-46.6(6)
Ir(1)#1-Ir(1)-N(4)-C(7)	82.7(4)	C(23)-C(22)-C(26)-F(26A)	137.5(5)
C(10)-Ir(1)-N(4)-C(9)	7.1(4)	C(21)-C(22)-C(26)-F(26C)	-163.1(5)
N(1)-Ir(1)-N(4)-C(9)	-175.9(4)	C(23)-C(22)-C(26)-F(26C)	21.0(7)
Ir(1)#1-Ir(1)-N(4)-C(9)	-93.0(4)	C(22)-C(23)-C(24A)-C(25)	-2.0(7)
C(3)-N(1)-C(1)-C(2)	0.3(6)	C(22)-C(23)-C(24A)-C(27A)	175.5(7)
Ir(1)-N(1)-C(1)-C(2)	-176.5(3)	C(20)-C(25)-C(24A)-C(23)	1.8(7)
N(1)-C(1)-C(2)-N(2)	0.0(6)	C(20)-C(25)-C(24A)-C(27A)	-175.7(7)
C(3)-N(2)-C(2)-C(1)	-0.3(6)	C(23)-C(24A)-C(27A)-F(27B)	-117.3(5)
C(4)-N(2)-C(2)-C(1)	178.1(5)	C(25)-C(24A)-C(27A)-F(27B)	60.2(6)
C(1)-N(1)-C(3)-N(2)	-0.5(5)	C(23)-C(24A)-C(27A)-F(27C)	-1.1(7)
Ir(1)-N(1)-C(3)-N(2)	176.2(3)	C(25)-C(24A)-C(27A)-F(27C)	176.5(3)
C(1)-N(1)-C(3)-C(5)	177.6(5)	C(23)-C(24A)-C(27A)-F(27A)	114.7(5)
Ir(1)-N(1)-C(3)-C(5)	-5.7(7)	C(25)-C(24A)-C(27A)-F(27A)	-67.8(6)
C(2)-N(2)-C(3)-N(1)	0.5(5)	C(36)-B(1)-C(28)-C(29)	29.0(5)
C(4)-N(2)-C(3)-N(1)	-177.9(4)	C(12)-B(1)-C(28)-C(29)	-92.4(4)
C(2)-N(2)-C(3)-C(5)	-177.8(4)	C(20)-B(1)-C(28)-C(29)	149.0(4)
C(4)-N(2)-C(3)-C(5)	3.8(7)	C(36)-B(1)-C(28)-C(33)	-157.9(3)
N(1)-C(3)-C(5)-C(7)	9.1(7)	C(12)-B(1)-C(28)-C(33)	80.7(4)
N(2)-C(3)-C(5)-C(7)	-173.0(4)	C(20)-B(1)-C(28)-C(33)	-37.9(5)
C(9)-N(4)-C(7)-N(3)	-0.4(5)	C(33)-C(28)-C(29)-C(30)	-1.2(6)
Ir(1)-N(4)-C(7)-N(3)	-176.7(3)	B(1)-C(28)-C(29)-C(30)	172.3(4)
C(9)-N(4)-C(7)-C(5)	-179.4(4)	C(28)-C(29)-C(30)-C(31)	1.1(7)
Ir(1)-N(4)-C(7)-C(5)	4.2(7)	C(28)-C(29)-C(30)-C(34)	-178.3(4)
C(8)-N(3)-C(7)-N(4)	0.6(5)	C(29)-C(30)-C(31)-C(32A)	-0.6(7)
C(6)-N(3)-C(7)-N(4)	179.9(5)	C(34)-C(30)-C(31)-C(32A)	178.8(4)
C(8)-N(3)-C(7)-C(5)	179.7(4)	C(29)-C(28)-C(33)-C(32A)	0.8(6)
C(6)-N(3)-C(7)-C(5)	-1.0(7)	B(1)-C(28)-C(33)-C(32A)	-172.8(4)
C(3)-C(5)-C(7)-N(4)	-8.3(7)	C(31)-C(30)-C(34)-F(34B)	1.5(8)
C(3)-C(5)-C(7)-N(3)	172.8(4)	C(29)-C(30)-C(34)-F(34B)	-179.2(5)
C(7)-N(3)-C(8)-C(9)	-0.5(6)	C(31)-C(30)-C(34)-F(34A)	124.2(5)
C(6)-N(3)-C(8)-C(9)	-179.9(5)	C(29)-C(30)-C(34)-F(34A)	-56.4(7)
N(3)-C(8)-C(9)-N(4)	0.3(6)	C(31)-C(30)-C(34)-F(34C)	-118.1(6)
C(7)-N(4)-C(9)-C(8)	0.1(5)	C(29)-C(30)-C(34)-F(34C)	61.3(7)
Ir(1)-N(4)-C(9)-C(8)	176.6(3)	C(28)-C(33)-C(32A)-C(31)	-0.4(6)
C(36)-B(1)-C(12)-C(17)	-138.4(4)	C(28)-C(33)-C(32A)-C(35A)	-179.6(3)
C(28)-B(1)-C(12)-C(17)	-18.8(5)	C(30)-C(31)-C(32A)-C(33)	0.2(6)
C(20)-B(1)-C(12)-C(17)	100.6(4)	C(30)-C(31)-C(32A)-C(35A)	179.5(4)
C(36)-B(1)-C(12)-C(13)	45.4(5)	C(33)-C(32A)-C(35A)-F(35B)	97.3(3)
C(28)-B(1)-C(12)-C(13)	165.0(3)	C(31)-C(32A)-C(35A)-F(35B)	-81.9(4)
C(20)-B(1)-C(12)-C(13)	-75.7(4)	C(33)-C(32A)-C(35A)-F(35C)	-139.8(3)
C(17)-C(12)-C(13)-C(14)	-3.6(6)	C(31)-C(32A)-C(35A)-F(35C)	40.9(4)
B(1)-C(12)-C(13)-C(14)	172.8(4)	C(33)-C(32A)-C(35A)-F(35A)	-21.5(4)
C(12)-C(13)-C(14)-C(15)	2.2(6)	C(31)-C(32A)-C(35A)-F(35A)	159.3(3)
C(12)-C(13)-C(14)-C(18)	-176.6(4)	C(28)-B(1)-C(36)-C(37)	97.3(4)
C(13)-C(14)-C(15)-C(16)	0.6(6)	C(12)-B(1)-C(36)-C(37)	-143.9(4)
C(18)-C(14)-C(15)-C(16)	179.5(4)	C(20)-B(1)-C(36)-C(37)	-23.1(5)
C(14)-C(15)-C(16)-C(17)	-1.8(6)	C(28)-B(1)-C(36)-C(41)	-78.3(4)
C(14)-C(15)-C(16)-C(19)	177.1(4)	C(12)-B(1)-C(36)-C(41)	40.5(5)
C(15)-C(16)-C(17)-C(12)	0.2(6)	C(20)-B(1)-C(36)-C(41)	161.3(3)
C(19)-C(16)-C(17)-C(12)	-178.6(4)	C(41)-C(36)-C(37)-C(38)	1.5(6)
C(13)-C(12)-C(17)-C(16)	2.4(6)	B(1)-C(36)-C(37)-C(38)	-174.3(4)
B(1)-C(12)-C(17)-C(16)	-174.0(4)	C(36)-C(37)-C(38)-C(39)	0.0(6)
C(13)-C(14)-C(18)-F(18A)	-4.9(6)	C(36)-C(37)-C(38)-C(42)	-179.8(4)
C(15)-C(14)-C(18)-F(18A)	176.3(4)	C(37)-C(38)-C(39)-C(40A)	-1.0(6)
C(13)-C(14)-C(18)-F(18C)	119.4(5)	C(42)-C(38)-C(39)-C(40A)	178.8(4)
C(15)-C(14)-C(18)-F(18C)	-59.5(6)	C(37)-C(36)-C(41)-C(40A)	-2.1(6)
C(13)-C(14)-C(18)-F(18B)	-124.6(4)	B(1)-C(36)-C(41)-C(40A)	173.8(4)

C(15)-C(14)-C(18)-F(18B)	56.5(6)	C(39)-C(38)-C(42)-F(42C)	50.5(6)
C(15)-C(16)-C(19)-F(19A)	-62.5(6)	C(37)-C(38)-C(42)-F(42C)	-129.8(5)
C(17)-C(16)-C(19)-F(19A)	116.4(5)	C(39)-C(38)-C(42)-F(42A)	-68.3(6)
C(15)-C(16)-C(19)-F(19B)	58.3(6)	C(37)-C(38)-C(42)-F(42A)	111.4(5)
C(17)-C(16)-C(19)-F(19B)	-122.8(5)	C(39)-C(38)-C(42)-F(42B)	171.9(4)
C(15)-C(16)-C(19)-F(19C)	176.2(4)	C(37)-C(38)-C(42)-F(42B)	-8.3(6)
C(17)-C(16)-C(19)-F(19C)	-4.9(6)	C(38)-C(39)-C(40A)-C(41)	0.4(6)
C(36)-B(1)-C(20)-C(21)	-91.0(4)	C(38)-C(39)-C(40A)-C(43A)	179.2(4)
C(28)-B(1)-C(20)-C(21)	149.2(4)	C(36)-C(41)-C(40A)-C(39)	1.2(6)
C(12)-B(1)-C(20)-C(21)	31.5(5)	C(36)-C(41)-C(40A)-C(43A)	-177.6(3)
C(36)-B(1)-C(20)-C(25)	82.5(4)	C(39)-C(40A)-C(43A)-F(43A)	-168.3(3)
C(28)-B(1)-C(20)-C(25)	-37.3(5)	C(41)-C(40A)-C(43A)-F(43A)	10.5(4)
C(12)-B(1)-C(20)-C(25)	-155.0(4)	C(39)-C(40A)-C(43A)-F(43B)	68.0(4)
C(25)-C(20)-C(21)-C(22)	0.9(6)	C(41)-C(40A)-C(43A)-F(43B)	-113.1(3)
B(1)-C(20)-C(21)-C(22)	174.8(4)	C(39)-C(40A)-C(43A)-F(43C)	-50.6(4)
C(20)-C(21)-C(22)-C(23)	-1.2(7)	C(41)-C(40A)-C(43A)-F(43C)	128.3(3)

Least-squares planes (x,y,z in Cartesian coordinates) and deviations from them
(* indicates atom used to define plane)

- 5.8861 (0.0275) x + 1.1582 (0.0639) y + 16.0495 (0.0049) z = 3.8250 (0.0352)

*	-0.0021 (0.0029)	N1
*	-0.0020 (0.0029)	N2
*	0.0008 (0.0032)	C1
*	0.0007 (0.0032)	C2
*	0.0026 (0.0027)	C3
	-0.0418 (0.0086)	C4
	0.0505 (0.0085)	C5
	-0.1069 (0.0078)	Ir1

Rms deviation of fitted atoms = 0.0018

- 6.4010 (0.0102) x + 1.2682 (0.0234) y + 15.9360 (0.0027) z = 3.1595 (0.0118)

Angle to previous plane (with approximate esd) = 2.76 (0.18)

*	0.0127 (0.0028)	N1
*	-0.0604 (0.0024)	N2
*	-0.0553 (0.0024)	N3
*	0.0044 (0.0028)	N4
*	0.1036 (0.0038)	C5
*	-0.0050 (0.0018)	Ir1

Rms deviation of fitted atoms = 0.0542

- 7.0440 (0.0252) x + 1.0031 (0.0568) y + 15.7495 (0.0092) z = 2.5153 (0.0267)

Angle to previous plane (with approximate esd) = 3.57 (0.18)

*	0.0029 (0.0028)	N3
*	0.0013 (0.0027)	N4
*	-0.0026 (0.0027)	C7
*	-0.0021 (0.0030)	C8
*	0.0005 (0.0030)	C9
	-0.0003 (0.0090)	C6
	-0.0955 (0.0075)	Ir1

Rms deviation of fitted atoms = 0.0021

- 6.2781 (0.0173) x + 1.0246 (0.0355) y + 15.9739 (0.0041) z = 3.3183 (0.0194)

Angle to previous plane (with approximate esd) = 4.20 (0.20)

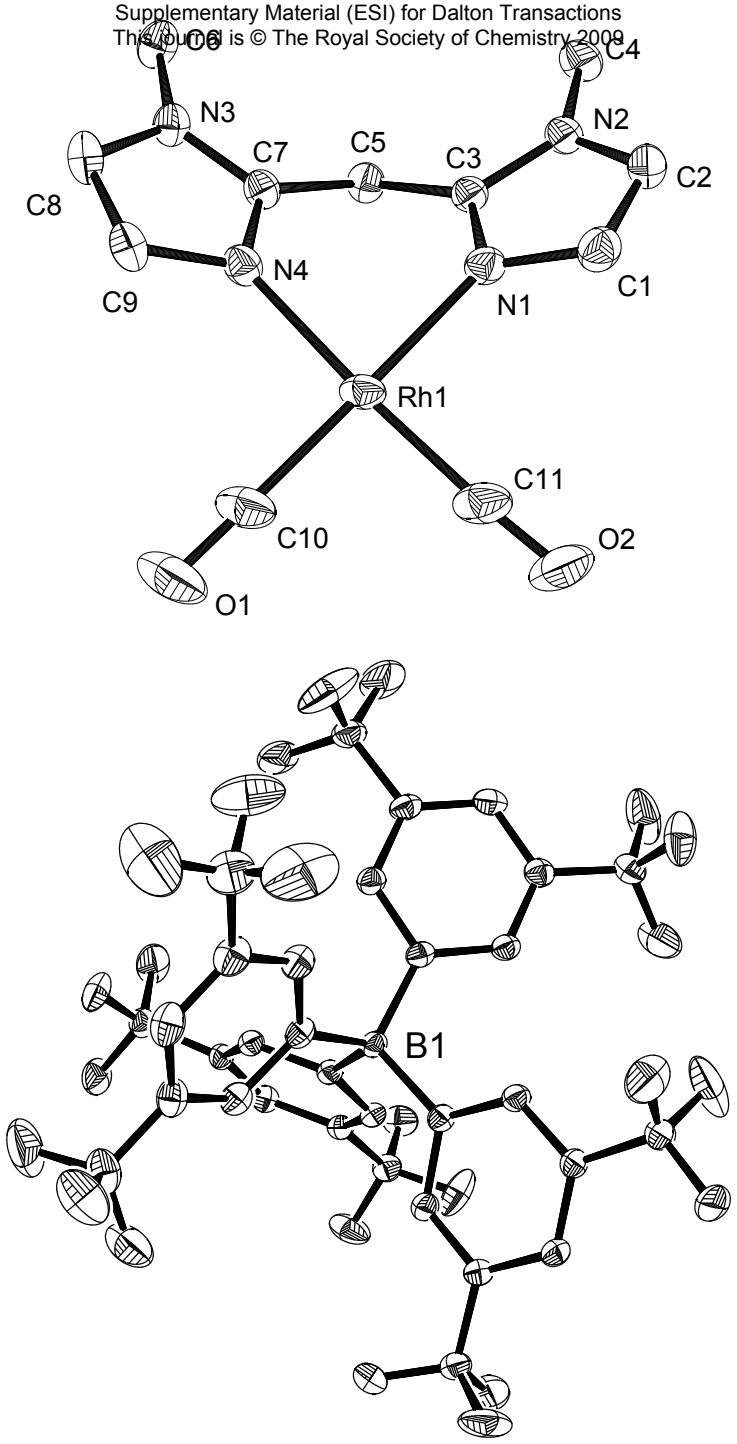
*	0.0241 (0.0020)	N1
*	-0.0120 (0.0020)	N4
*	0.0270 (0.0022)	C10
*	-0.0136 (0.0022)	C11
*	-0.0255 (0.0017)	Ir1

Rms deviation of fitted atoms = 0.0214

Supplementary Material (ESI) for Dalton Transactions

Ortep Diagrams and Crystallographic Tables for

$[Rh(bim)(CO)_2]BAr^F_{24}$ (11a)



ORTEP plot (50% ellipsoids, H-atoms omitted) of cation (top) and anion (bottom).
All hydrogen atoms were refined in idealized positions.
The asym. unit bears ½ dichloromethane molecule which is twofold disordered (s.o.f. 0.23 : 0.27).

Table 1. Crystal data and structure refinement for rh00502.

Identification code	rh00502
Empirical formula	C43.50 H25 B Cl F24 N4 O2 Rh
Formula weight	1240.84
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/n
Unit cell dimensions	a = 13.1291(3) A alpha = 90 deg.
	b = 25.6224(6) A beta = 113.0720(10) deg.
	c = 15.3207(4) A gamma = 90 deg.
Volume	4741.6(2) A^3
Z, Calculated density	4, 1.738 Mg/m^3
Absorption coefficient	0.554 mm^-1
F(000)	2452
Crystal size	0.39 x 0.32 x 0.24 mm
Theta range for data collection	2.73 to 30.00 deg.
Limiting indices	-18<=h<=18, -33<=k<=36, -21<=l<=21
Reflections collected / unique	75612 / 13785 [R(int) = 0.0649]
Completeness to theta = 30.00	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.874 and 0.731
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13785 / 5 / 702
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1030
R indices (all data)	R1 = 0.0608, wR2 = 0.1102
Largest diff. peak and hole	0.861 and -1.116 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for rh00502.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Rh(1)	4667(1)	2469(1)	1056(1)	23(1)
O(1)	2611(2)	2377(1)	1448(2)	55(1)
O(2)	5634(2)	3285(1)	2550(1)	50(1)
N(1)	6090(1)	2493(1)	786(1)	23(1)
N(2)	7537(1)	2198(1)	562(1)	23(1)
N(3)	4257(1)	1218(1)	-803(1)	23(1)
N(4)	4157(1)	1894(1)	37(1)	23(1)
C(1)	6794(2)	2907(1)	855(2)	27(1)
C(2)	7689(2)	2726(1)	716(2)	27(1)
C(3)	6556(2)	2071(1)	601(1)	20(1)
C(4)	8344(2)	1842(1)	438(2)	29(1)
C(5)	6063(2)	1534(1)	449(2)	23(1)
C(6)	4674(2)	761(1)	-1134(2)	29(1)
C(7)	4834(2)	1552(1)	-109(1)	21(1)
C(8)	3155(2)	1355(1)	-1118(2)	27(1)
C(9)	3097(2)	1772(1)	-599(2)	26(1)
C(10)	3386(2)	2419(1)	1301(2)	35(1)
C(11)	5235(2)	2977(1)	1988(2)	35(1)
B(1)	1340(2)	1015(1)	2811(2)	18(1)
C(12)	679(2)	1530(1)	2948(1)	19(1)
C(13)	-279(2)	1468(1)	3140(1)	21(1)
C(14)	-930(2)	1889(1)	3176(1)	24(1)
C(15)	-657(2)	2397(1)	3034(2)	25(1)
C(16)	277(2)	2468(1)	2831(1)	23(1)
C(17)	920(2)	2044(1)	2780(1)	21(1)
C(18)	-1946(2)	1784(1)	3372(2)	29(1)
F(18A)	-1718(1)	1680(1)	4266(1)	65(1)
F(18B)	-2521(1)	1379(1)	2879(1)	53(1)
F(18C)	-2651(1)	2184(1)	3137(2)	64(1)
C(19)	611(2)	3010(1)	2686(2)	27(1)

F(19A)	-265(1)	3327(1)	2310(2)	58(1)
F(19B)	1134(2)	3036(1)	2122(2)	65(1)
F(19C)	1236(1)	3241(1)	3502(1)	48(1)
C(20)	2599(2)	1142(1)	2891(1)	18(1)
C(21)	3269(2)	1522(1)	3509(1)	20(1)
C(22)	4357(2)	1612(1)	3612(1)	20(1)
C(23)	4848(2)	1310(1)	3134(1)	21(1)
C(24)	4217(2)	916(1)	2546(1)	20(1)
C(25)	3114(2)	842(1)	2414(1)	20(1)
C(26)	4970(2)	2056(1)	4230(2)	28(1)
F(26A)	5007(2)	2020(1)	5110(1)	57(1)
F(26B)	4471(2)	2510(1)	3905(2)	67(1)
F(26C)	6011(1)	2102(1)	4313(1)	44(1)
C(27)	4727(2)	571(1)	2038(2)	26(1)
F(27A)	4286(1)	95(1)	1875(1)	35(1)
F(27B)	4588(1)	759(1)	1177(1)	44(1)
F(27C)	5815(1)	513(1)	2508(1)	52(1)
C(28)	530(2)	805(1)	1750(1)	17(1)
C(29)	595(2)	1004(1)	921(1)	19(1)
C(30)	-175(2)	873(1)	22(1)	19(1)
C(31)	-1050(2)	537(1)	-85(1)	21(1)
C(32)	-1135(2)	340(1)	727(1)	19(1)
C(33)	-358(2)	469(1)	1625(1)	18(1)
C(34)	-108(2)	1107(1)	-850(1)	23(1)
F(34A)	-64(1)	745(1)	-1465(1)	39(1)
F(34B)	-1002(1)	1398(1)	-1336(1)	32(1)
F(34C)	764(1)	1419(1)	-652(1)	44(1)
C(35)	-2102(2)	0(1)	617(2)	23(1)
F(35A)	-2022(1)	-230(1)	1426(1)	33(1)
F(35B)	-2259(1)	-384(1)	-20(1)	34(1)
F(35C)	-3055(1)	274(1)	307(1)	44(1)
C(36)	1497(2)	565(1)	3615(1)	21(1)
C(37)	1763(2)	50(1)	3464(1)	23(1)
C(38)	1996(2)	-336(1)	4147(2)	27(1)
C(39)	1939(2)	-230(1)	5022(2)	32(1)
C(40)	1669(2)	270(1)	5183(2)	30(1)
C(41)	1466(2)	662(1)	4503(1)	26(1)
C(42)	2275(2)	-877(1)	3950(2)	35(1)
F(42A)	2620(2)	-899(1)	3238(1)	54(1)
F(42B)	1421(2)	-1201(1)	3718(2)	65(1)
F(42C)	3077(2)	-1091(1)	4707(1)	54(1)
C(43)	1599(3)	399(1)	6110(2)	44(1)
F(43A)	760(2)	714(1)	6021(1)	74(1)
F(43B)	2454(2)	675(1)	6680(1)	87(1)
F(43C)	1507(3)	-10(1)	6585(2)	120(1)
Cl(1)	5129(5)	9621(4)	3980(5)	114(2)
C(1S)	5210(40)	9765(11)	5092(18)	114(2)
Cl(2)	4662(7)	10366(4)	5110(7)	114(2)
Cl(3)	5465(4)	9230(3)	4070(4)	114(2)
C(2S)	5235(18)	9809(8)	4369(15)	114(2)
Cl(4)	5154(6)	9840(3)	5393(5)	114(2)

Table 3. Bond lengths [Å] and angles [deg] for rh00502.

Rh(1)-C(11)	1.859(3)	C(22)-C(26)	1.496(3)
Rh(1)-C(10)	1.867(2)	C(23)-C(24)	1.391(3)
Rh(1)-N(4)	2.0594(18)	C(24)-C(25)	1.394(3)
Rh(1)-N(1)	2.0661(17)	C(24)-C(27)	1.498(3)
O(1)-C(10)	1.129(3)	C(26)-F(26C)	1.328(2)
O(2)-C(11)	1.133(3)	C(26)-F(26B)	1.332(3)
N(1)-C(3)	1.327(2)	C(26)-F(26A)	1.334(3)
N(1)-C(1)	1.383(3)	C(27)-F(27C)	1.333(2)
N(2)-C(3)	1.352(2)	C(27)-F(27A)	1.333(3)
N(2)-C(2)	1.373(3)	C(27)-F(27B)	1.348(3)
N(2)-C(4)	1.465(3)	C(28)-C(33)	1.401(3)
N(3)-C(7)	1.344(3)	C(28)-C(29)	1.401(3)
N(3)-C(8)	1.380(3)	C(29)-C(30)	1.392(3)
N(3)-C(6)	1.464(3)	C(30)-C(31)	1.393(3)
N(4)-C(7)	1.328(3)	C(30)-C(34)	1.498(3)
N(4)-C(9)	1.386(3)	C(31)-C(32)	1.386(3)
C(1)-C(2)	1.355(3)	C(32)-C(33)	1.394(3)
C(3)-C(5)	1.499(3)	C(32)-C(35)	1.494(3)
C(5)-C(7)	1.502(3)	C(34)-F(34C)	1.332(2)
C(8)-C(9)	1.351(3)	C(34)-F(34A)	1.338(2)
B(1)-C(12)	1.639(3)	C(34)-F(34B)	1.343(2)
B(1)-C(36)	1.640(3)	C(35)-F(35A)	1.338(2)
B(1)-C(20)	1.641(3)	C(35)-F(35B)	1.343(2)
B(1)-C(28)	1.646(3)	C(35)-F(35C)	1.348(2)
C(12)-C(17)	1.402(3)	C(36)-C(41)	1.399(3)
C(12)-C(13)	1.407(3)	C(36)-C(37)	1.406(3)
C(13)-C(14)	1.391(3)	C(37)-C(38)	1.386(3)
C(14)-C(15)	1.388(3)	C(38)-C(39)	1.398(3)
C(14)-C(18)	1.502(3)	C(38)-C(42)	1.495(3)
C(15)-C(16)	1.390(3)	C(39)-C(40)	1.376(4)
C(16)-C(17)	1.396(3)	C(40)-C(41)	1.397(3)
C(16)-C(19)	1.500(3)	C(40)-C(43)	1.496(3)
C(18)-F(18A)	1.310(3)	C(42)-F(42B)	1.327(3)
C(18)-F(18B)	1.331(3)	C(42)-F(42A)	1.337(3)
C(18)-F(18C)	1.332(3)	C(42)-F(42C)	1.340(3)
C(19)-F(19B)	1.299(3)	C(43)-F(43C)	1.307(4)
C(19)-F(19C)	1.335(3)	C(43)-F(43B)	1.325(4)
C(19)-F(19A)	1.354(3)	C(43)-F(43A)	1.328(4)
C(20)-C(21)	1.402(3)	Cl(1)-C(1S)	1.704(16)
C(20)-C(25)	1.404(3)	C(1S)-Cl(2)	1.704(16)
C(21)-C(22)	1.394(3)	Cl(3)-C(2S)	1.615(13)
C(22)-C(23)	1.384(3)	C(2S)-Cl(4)	1.615(13)

C(11)-Rh(1)-C(10)	90.91(11)	C(22)-C(23)-C(24)	117.72(17)
C(11)-Rh(1)-N(4)	175.74(8)	C(23)-C(24)-C(25)	120.98(18)
C(10)-Rh(1)-N(4)	92.98(10)	C(23)-C(24)-C(27)	119.37(17)
C(11)-Rh(1)-N(1)	90.62(9)	C(25)-C(24)-C(27)	119.64(18)
C(10)-Rh(1)-N(1)	177.72(9)	C(24)-C(25)-C(20)	122.28(18)
N(4)-Rh(1)-N(1)	85.43(7)	F(26C)-C(26)-F(26B)	107.1(2)
C(3)-N(1)-C(1)	106.86(17)	F(26C)-C(26)-F(26A)	106.29(18)
C(3)-N(1)-Rh(1)	123.18(14)	F(26B)-C(26)-F(26A)	104.8(2)
C(1)-N(1)-Rh(1)	129.61(14)	F(26C)-C(26)-C(22)	114.02(17)
C(3)-N(2)-C(2)	107.81(17)	F(26B)-C(26)-C(22)	111.33(18)
C(3)-N(2)-C(4)	127.19(18)	F(26A)-C(26)-C(22)	112.67(19)
C(2)-N(2)-C(4)	124.90(17)	F(27C)-C(27)-F(27A)	107.00(18)
C(7)-N(3)-C(8)	107.67(17)	F(27C)-C(27)-F(27B)	105.96(18)
C(7)-N(3)-C(6)	127.69(17)	F(27A)-C(27)-F(27B)	105.09(17)
C(8)-N(3)-C(6)	124.47(18)	F(27C)-C(27)-C(24)	112.91(18)
C(7)-N(4)-C(9)	106.66(17)	F(27A)-C(27)-C(24)	112.81(17)
C(7)-N(4)-Rh(1)	124.05(14)	F(27B)-C(27)-C(24)	112.47(18)
C(9)-N(4)-Rh(1)	129.28(14)	C(33)-C(28)-C(29)	116.27(17)
C(2)-C(1)-N(1)	108.72(19)	C(33)-C(28)-B(1)	121.12(16)
C(1)-C(2)-N(2)	106.72(18)	C(29)-C(28)-B(1)	122.09(16)
N(1)-C(3)-N(2)	109.89(18)	C(30)-C(29)-C(28)	122.00(17)
N(1)-C(3)-C(5)	125.01(17)	C(29)-C(30)-C(31)	120.75(17)

N(2)-C(3)-C(5)	125.10(17)	C(29)-C(30)-C(34)	120.80(17)
C(3)-C(5)-C(7)	111.37(16)	C(31)-C(30)-C(34)	118.41(17)
N(4)-C(7)-N(3)	110.26(17)	C(32)-C(31)-C(30)	118.14(17)
N(4)-C(7)-C(5)	124.36(18)	C(31)-C(32)-C(33)	120.94(17)
N(3)-C(7)-C(5)	125.35(18)	C(31)-C(32)-C(35)	118.37(17)
C(9)-C(8)-N(3)	106.76(18)	C(33)-C(32)-C(35)	120.66(18)
C(8)-C(9)-N(4)	108.65(18)	C(32)-C(33)-C(28)	121.90(17)
O(1)-C(10)-Rh(1)	178.6(3)	F(34C)-C(34)-F(34A)	107.81(18)
O(2)-C(11)-Rh(1)	176.3(2)	F(34C)-C(34)-F(34B)	106.14(17)
C(12)-B(1)-C(36)	112.80(16)	F(34A)-C(34)-F(34B)	105.28(16)
C(12)-B(1)-C(20)	113.48(15)	F(34C)-C(34)-C(30)	112.58(17)
C(36)-B(1)-C(20)	104.92(15)	F(34A)-C(34)-C(30)	112.65(17)
C(12)-B(1)-C(28)	102.69(15)	F(34B)-C(34)-C(30)	111.88(16)
C(36)-B(1)-C(28)	110.79(15)	F(35A)-C(35)-F(35B)	106.51(16)
C(20)-B(1)-C(28)	112.39(15)	F(35A)-C(35)-F(35C)	106.33(17)
C(17)-C(12)-C(13)	115.37(18)	F(35B)-C(35)-F(35C)	105.57(16)
C(17)-C(12)-B(1)	124.38(16)	F(35A)-C(35)-C(32)	113.41(16)
C(13)-C(12)-B(1)	119.84(17)	F(35B)-C(35)-C(32)	112.93(17)
C(14)-C(13)-C(12)	122.30(19)	F(35C)-C(35)-C(32)	111.52(17)
C(15)-C(14)-C(13)	121.32(18)	C(41)-C(36)-C(37)	115.60(19)
C(15)-C(14)-C(18)	120.15(19)	C(41)-C(36)-B(1)	124.14(19)
C(13)-C(14)-C(18)	118.5(2)	C(37)-C(36)-B(1)	120.09(17)
C(14)-C(15)-C(16)	117.54(19)	C(38)-C(37)-C(36)	122.76(19)
C(15)-C(16)-C(17)	121.10(19)	C(37)-C(38)-C(39)	120.4(2)
C(15)-C(16)-C(19)	119.34(19)	C(37)-C(38)-C(42)	120.6(2)
C(17)-C(16)-C(19)	119.56(19)	C(39)-C(38)-C(42)	119.0(2)
C(16)-C(17)-C(12)	122.33(18)	C(40)-C(39)-C(38)	117.9(2)
F(18A)-C(18)-F(18B)	106.3(2)	C(39)-C(40)-C(41)	121.5(2)
F(18A)-C(18)-F(18C)	106.9(2)	C(39)-C(40)-C(43)	119.5(2)
F(18B)-C(18)-F(18C)	105.48(19)	C(41)-C(40)-C(43)	119.0(2)
F(18A)-C(18)-C(14)	112.88(18)	C(40)-C(41)-C(36)	121.8(2)
F(18B)-C(18)-C(14)	112.11(18)	F(42B)-C(42)-F(42A)	106.0(2)
F(18C)-C(18)-C(14)	112.7(2)	F(42B)-C(42)-F(42C)	105.7(2)
F(19B)-C(19)-F(19C)	108.0(2)	F(42A)-C(42)-F(42C)	106.7(2)
F(19B)-C(19)-F(19A)	105.6(2)	F(42B)-C(42)-C(38)	112.7(2)
F(19C)-C(19)-F(19A)	103.42(18)	F(42A)-C(42)-C(38)	113.1(2)
F(19B)-C(19)-C(16)	113.99(18)	F(42C)-C(42)-C(38)	112.1(2)
F(19C)-C(19)-C(16)	112.29(18)	F(43C)-C(43)-F(43B)	107.5(3)
F(19A)-C(19)-C(16)	112.77(18)	F(43C)-C(43)-F(43A)	106.9(3)
C(21)-C(20)-C(25)	115.40(17)	F(43B)-C(43)-F(43A)	101.4(3)
C(21)-C(20)-B(1)	122.44(16)	F(43C)-C(43)-C(40)	113.9(3)
C(25)-C(20)-B(1)	121.88(16)	F(43B)-C(43)-C(40)	113.1(2)
C(22)-C(21)-C(20)	122.42(18)	F(43A)-C(43)-C(40)	113.2(2)
C(23)-C(22)-C(21)	121.08(18)	Cl(1)-C(1S)-Cl(2)	110.4(15)
C(23)-C(22)-C(26)	120.83(17)	Cl(4)-C(2S)-Cl(3)	114.3(16)
C(21)-C(22)-C(26)	118.06(17)		

Table 6. Torsion angles [deg] for rh00502.

C(11)-Rh(1)-N(1)-C(3)	140.85(18)	C(26)-C(22)-C(23)-C(24)	-177.79(19)
N(4)-Rh(1)-N(1)-C(3)	-37.53(16)	C(22)-C(23)-C(24)-C(25)	2.6(3)
C(11)-Rh(1)-N(1)-C(1)	-31.4(2)	C(22)-C(23)-C(24)-C(27)	-178.31(19)
N(4)-Rh(1)-N(1)-C(1)	150.18(19)	C(23)-C(24)-C(25)-C(20)	-2.8(3)
C(10)-Rh(1)-N(4)-C(7)	-144.53(18)	C(27)-C(24)-C(25)-C(20)	178.10(19)
N(1)-Rh(1)-N(4)-C(7)	33.82(17)	C(21)-C(20)-C(25)-C(24)	0.1(3)
C(10)-Rh(1)-N(4)-C(9)	33.70(19)	B(1)-C(20)-C(25)-C(24)	-173.88(18)
N(1)-Rh(1)-N(4)-C(9)	-147.95(18)	C(23)-C(22)-C(26)-F(26C)	-4.1(3)
C(3)-N(1)-C(1)-C(2)	-0.4(2)	C(21)-C(22)-C(26)-F(26C)	177.84(19)
Rh(1)-N(1)-C(1)-C(2)	172.88(15)	C(23)-C(22)-C(26)-F(26B)	117.3(2)
N(1)-C(1)-C(2)-N(2)	-0.1(2)	C(21)-C(22)-C(26)-F(26B)	-60.8(3)
C(3)-N(2)-C(2)-C(1)	0.6(2)	C(23)-C(22)-C(26)-F(26A)	-125.3(2)
C(4)-N(2)-C(2)-C(1)	-176.0(2)	C(21)-C(22)-C(26)-F(26A)	56.6(3)
C(1)-N(1)-C(3)-N(2)	0.8(2)	C(23)-C(24)-C(27)-F(27C)	29.4(3)
Rh(1)-N(1)-C(3)-N(2)	-173.03(13)	C(25)-C(24)-C(27)-F(27C)	-151.4(2)
C(1)-N(1)-C(3)-C(5)	-178.62(19)	C(23)-C(24)-C(27)-F(27A)	150.90(19)
Rh(1)-N(1)-C(3)-C(5)	7.6(3)	C(25)-C(24)-C(27)-F(27A)	-30.0(3)

C(2)-N(2)-C(3)-N(1)	0.8(2)	C(23)-C(24)-C(27)-F(27B)	-90.4(2)
C(4)-N(2)-C(3)-N(1)	175.63(19)	C(25)-C(24)-C(27)-F(27B)	88.7(2)
C(2)-N(2)-C(3)-C(5)	178.52(19)	C(12)-B(1)-C(28)-C(33)	-86.3(2)
C(4)-N(2)-C(3)-C(5)	-5.0(3)	C(36)-B(1)-C(28)-C(33)	34.4(2)
N(1)-C(3)-C(5)-C(7)	38.8(3)	C(20)-B(1)-C(28)-C(33)	151.44(17)
N(2)-C(3)-C(5)-C(7)	-140.5(2)	C(12)-B(1)-C(28)-C(29)	85.1(2)
C(9)-N(4)-C(7)-N(3)	-0.1(2)	C(36)-B(1)-C(28)-C(29)	-154.17(17)
Rh(1)-N(4)-C(7)-N(3)	178.45(13)	C(20)-B(1)-C(28)-C(29)	-37.2(2)
C(9)-N(4)-C(7)-C(5)	-178.41(19)	C(33)-C(28)-C(29)-C(30)	-0.3(3)
Rh(1)-N(4)-C(7)-C(5)	0.2(3)	B(1)-C(28)-C(29)-C(30)	-172.06(17)
C(8)-N(3)-C(7)-N(4)	0.1(2)	C(28)-C(29)-C(30)-C(31)	0.2(3)
C(6)-N(3)-C(7)-N(4)	-175.25(19)	C(28)-C(29)-C(30)-C(34)	177.76(18)
C(8)-N(3)-C(7)-C(5)	178.38(19)	C(29)-C(30)-C(31)-C(32)	0.4(3)
C(6)-N(3)-C(7)-C(5)	3.0(3)	C(34)-C(30)-C(31)-C(32)	-177.28(18)
C(3)-C(5)-C(7)-N(4)	-43.1(3)	C(30)-C(31)-C(32)-C(33)	-0.8(3)
C(3)-C(5)-C(7)-N(3)	138.8(2)	C(30)-C(31)-C(32)-C(35)	177.05(17)
C(7)-N(3)-C(8)-C(9)	0.0(2)	C(31)-C(32)-C(33)-C(28)	0.7(3)
C(6)-N(3)-C(8)-C(9)	175.5(2)	C(35)-C(32)-C(33)-C(28)	-177.09(18)
N(3)-C(8)-C(9)-N(4)	0.0(2)	C(29)-C(28)-C(33)-C(32)	-0.2(3)
C(7)-N(4)-C(9)-C(8)	0.1(2)	B(1)-C(28)-C(33)-C(32)	171.71(17)
Rh(1)-N(4)-C(9)-C(8)	-178.38(15)	C(29)-C(30)-C(34)-F(34C)	2.4(3)
C(36)-B(1)-C(12)-C(17)	143.12(18)	C(31)-C(30)-C(34)-F(34C)	-179.91(18)
C(20)-B(1)-C(12)-C(17)	24.0(3)	C(29)-C(30)-C(34)-F(34A)	124.6(2)
C(28)-B(1)-C(12)-C(17)	-97.6(2)	C(31)-C(30)-C(34)-F(34A)	-57.7(2)
C(36)-B(1)-C(12)-C(13)	-44.6(2)	C(29)-C(30)-C(34)-F(34B)	-117.0(2)
C(20)-B(1)-C(12)-C(13)	-163.78(17)	C(31)-C(30)-C(34)-F(34B)	60.6(2)
C(28)-B(1)-C(12)-C(13)	74.7(2)	C(31)-C(32)-C(35)-F(35A)	170.80(18)
C(17)-C(12)-C(13)-C(14)	-1.0(3)	C(33)-C(32)-C(35)-F(35A)	-11.3(3)
B(1)-C(12)-C(13)-C(14)	-173.93(18)	C(31)-C(32)-C(35)-F(35B)	49.5(2)
C(12)-C(13)-C(14)-C(15)	-0.8(3)	C(33)-C(32)-C(35)-F(35B)	-132.61(19)
C(12)-C(13)-C(14)-C(18)	179.16(18)	C(31)-C(32)-C(35)-F(35C)	-69.2(2)
C(13)-C(14)-C(15)-C(16)	1.6(3)	C(33)-C(32)-C(35)-F(35C)	108.7(2)
C(18)-C(14)-C(15)-C(16)	-178.43(19)	C(12)-B(1)-C(36)-C(41)	-22.5(2)
C(14)-C(15)-C(16)-C(17)	-0.5(3)	C(20)-B(1)-C(36)-C(41)	101.5(2)
C(14)-C(15)-C(16)-C(19)	-179.21(19)	C(28)-B(1)-C(36)-C(41)	-136.98(18)
C(15)-C(16)-C(17)-C(12)	-1.5(3)	C(12)-B(1)-C(36)-C(37)	162.52(16)
C(19)-C(16)-C(17)-C(12)	177.30(18)	C(20)-B(1)-C(36)-C(37)	-73.5(2)
C(13)-C(12)-C(17)-C(16)	2.1(3)	C(28)-B(1)-C(36)-C(37)	48.0(2)
B(1)-C(12)-C(17)-C(16)	174.68(18)	C(41)-C(36)-C(37)-C(38)	-0.9(3)
C(15)-C(14)-C(18)-F(18A)	-104.0(3)	B(1)-C(36)-C(37)-C(38)	174.50(18)
C(13)-C(14)-C(18)-F(18A)	76.0(3)	C(36)-C(37)-C(38)-C(39)	2.1(3)
C(15)-C(14)-C(18)-F(18B)	136.1(2)	C(36)-C(37)-C(38)-C(42)	-179.95(19)
C(13)-C(14)-C(18)-F(18B)	-43.9(3)	C(37)-C(38)-C(39)-C(40)	-1.3(3)
C(15)-C(14)-C(18)-F(18C)	17.2(3)	C(42)-C(38)-C(39)-C(40)	-179.3(2)
C(13)-C(14)-C(18)-F(18C)	-162.8(2)	C(38)-C(39)-C(40)-C(41)	-0.6(3)
C(15)-C(16)-C(19)-F(19B)	-151.3(2)	C(38)-C(39)-C(40)-C(43)	179.9(2)
C(17)-C(16)-C(19)-F(19B)	29.9(3)	C(39)-C(40)-C(41)-C(36)	1.8(3)
C(15)-C(16)-C(19)-F(19C)	85.4(2)	C(43)-C(40)-C(41)-C(36)	-178.7(2)
C(17)-C(16)-C(19)-F(19C)	-93.4(2)	C(37)-C(36)-C(41)-C(40)	-1.0(3)
C(15)-C(16)-C(19)-F(19A)	-30.9(3)	B(1)-C(36)-C(41)-C(40)	-176.19(19)
C(17)-C(16)-C(19)-F(19A)	150.3(2)	C(37)-C(38)-C(42)-F(42B)	-99.8(3)
C(12)-B(1)-C(20)-C(21)	34.8(2)	C(39)-C(38)-C(42)-F(42B)	78.2(3)
C(36)-B(1)-C(20)-C(21)	-88.7(2)	C(37)-C(38)-C(42)-F(42A)	20.5(3)
C(28)-B(1)-C(20)-C(21)	150.80(18)	C(39)-C(38)-C(42)-F(42A)	-161.6(2)
C(12)-B(1)-C(20)-C(25)	-151.64(18)	C(37)-C(38)-C(42)-F(42C)	141.1(2)
C(36)-B(1)-C(20)-C(25)	84.8(2)	C(39)-C(38)-C(42)-F(42C)	-40.9(3)
C(28)-B(1)-C(20)-C(25)	-35.7(2)	C(39)-C(40)-C(43)-F(43C)	-17.8(4)
C(25)-C(20)-C(21)-C(22)	2.7(3)	C(41)-C(40)-C(43)-F(43C)	162.7(3)
B(1)-C(20)-C(21)-C(22)	176.66(18)	C(39)-C(40)-C(43)-F(43B)	105.3(3)
C(20)-C(21)-C(22)-C(23)	-3.0(3)	C(41)-C(40)-C(43)-F(43B)	-74.3(3)
C(20)-C(21)-C(22)-C(26)	175.09(19)	C(39)-C(40)-C(43)-F(43A)	-140.1(3)
C(21)-C(22)-C(23)-C(24)	0.2(3)	C(41)-C(40)-C(43)-F(43A)	40.4(3)

Table 4. Anisotropic displacement parameters (Å^2 x 10^3) for rh00502. 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
Rh(1)	22(1)	28(1)	21(1)	-1(1)	11(1)	7(1)
O(1)	39(1)	86(2)	52(1)	9(1)	32(1)	14(1)
O(2)	37(1)	70(1)	38(1)	-28(1)	9(1)	8(1)
N(1)	22(1)	22(1)	24(1)	-3(1)	10(1)	2(1)
N(2)	19(1)	26(1)	23(1)	-2(1)	9(1)	0(1)
N(3)	21(1)	19(1)	27(1)	0(1)	8(1)	0(1)
N(4)	20(1)	22(1)	28(1)	0(1)	11(1)	1(1)
C(1)	30(1)	23(1)	29(1)	-4(1)	11(1)	-1(1)
C(2)	25(1)	28(1)	27(1)	-2(1)	10(1)	-5(1)
C(3)	18(1)	23(1)	20(1)	-2(1)	7(1)	1(1)
C(4)	19(1)	37(1)	33(1)	-1(1)	12(1)	5(1)
C(5)	19(1)	22(1)	26(1)	-1(1)	8(1)	3(1)
C(6)	29(1)	19(1)	34(1)	-5(1)	8(1)	2(1)
C(7)	20(1)	19(1)	24(1)	2(1)	9(1)	0(1)
C(8)	19(1)	22(1)	35(1)	3(1)	6(1)	-3(1)
C(9)	18(1)	25(1)	34(1)	3(1)	10(1)	-1(1)
C(10)	32(1)	48(2)	30(1)	5(1)	17(1)	14(1)
C(11)	27(1)	50(2)	28(1)	-6(1)	10(1)	14(1)
B(1)	16(1)	20(1)	20(1)	-2(1)	7(1)	-2(1)
C(12)	15(1)	25(1)	16(1)	-3(1)	6(1)	-2(1)
C(13)	19(1)	25(1)	21(1)	-4(1)	8(1)	-3(1)
C(14)	17(1)	33(1)	22(1)	-5(1)	9(1)	-2(1)
C(15)	21(1)	30(1)	24(1)	-6(1)	9(1)	3(1)
C(16)	23(1)	25(1)	19(1)	-3(1)	7(1)	-1(1)
C(17)	18(1)	25(1)	20(1)	-3(1)	8(1)	-1(1)
C(18)	22(1)	36(1)	33(1)	-8(1)	14(1)	-2(1)
F(18A)	37(1)	134(2)	32(1)	-2(1)	21(1)	-20(1)
F(18B)	31(1)	64(1)	73(1)	-33(1)	32(1)	-21(1)
F(18C)	40(1)	55(1)	117(2)	11(1)	52(1)	15(1)
C(19)	30(1)	25(1)	25(1)	-4(1)	11(1)	1(1)
F(19A)	38(1)	25(1)	88(1)	3(1)	-1(1)	4(1)
F(19B)	131(2)	26(1)	80(1)	7(1)	86(1)	6(1)
F(19C)	56(1)	42(1)	33(1)	-2(1)	5(1)	-23(1)
C(20)	17(1)	20(1)	17(1)	0(1)	6(1)	-1(1)
C(21)	18(1)	22(1)	21(1)	-2(1)	8(1)	-1(1)
C(22)	16(1)	21(1)	23(1)	-2(1)	6(1)	-2(1)
C(23)	16(1)	23(1)	25(1)	0(1)	9(1)	0(1)
C(24)	18(1)	22(1)	21(1)	0(1)	9(1)	1(1)
C(25)	17(1)	21(1)	21(1)	-1(1)	7(1)	-2(1)
C(26)	19(1)	26(1)	39(1)	-10(1)	11(1)	-4(1)
F(26A)	57(1)	80(1)	44(1)	-37(1)	29(1)	-37(1)
F(26B)	47(1)	24(1)	99(2)	-16(1)	-5(1)	2(1)
F(26C)	24(1)	47(1)	66(1)	-27(1)	22(1)	-17(1)
C(27)	21(1)	27(1)	33(1)	-6(1)	14(1)	-2(1)
F(27A)	40(1)	24(1)	48(1)	-9(1)	26(1)	0(1)
F(27B)	63(1)	42(1)	43(1)	-3(1)	40(1)	-2(1)
F(27C)	19(1)	66(1)	66(1)	-33(1)	11(1)	7(1)
C(28)	16(1)	18(1)	19(1)	-1(1)	7(1)	0(1)
C(29)	16(1)	20(1)	23(1)	-1(1)	9(1)	-1(1)
C(30)	20(1)	19(1)	19(1)	1(1)	9(1)	2(1)
C(31)	18(1)	23(1)	19(1)	-2(1)	5(1)	-1(1)
C(32)	16(1)	18(1)	24(1)	-2(1)	7(1)	-1(1)
C(33)	17(1)	19(1)	19(1)	1(1)	8(1)	0(1)
C(34)	24(1)	26(1)	21(1)	2(1)	9(1)	1(1)
F(34A)	65(1)	34(1)	28(1)	4(1)	27(1)	17(1)
F(34B)	35(1)	33(1)	28(1)	10(1)	13(1)	11(1)
F(34C)	36(1)	66(1)	28(1)	11(1)	10(1)	-21(1)
C(35)	19(1)	23(1)	26(1)	-1(1)	7(1)	-2(1)
F(35A)	33(1)	39(1)	29(1)	-1(1)	13(1)	-17(1)
F(35B)	35(1)	34(1)	33(1)	-12(1)	13(1)	-16(1)
F(35C)	17(1)	36(1)	73(1)	5(1)	12(1)	1(1)

C(36)	14(1)	26(1)	19(1)	9(1)	4(1)	-4(1)
C(37)	19(1)	28(1)	20(1)	0(1)	5(1)	-2(1)
C(38)	23(1)	26(1)	26(1)	3(1)	4(1)	-3(1)
C(39)	33(1)	34(1)	24(1)	6(1)	6(1)	-6(1)
C(40)	33(1)	39(1)	18(1)	1(1)	9(1)	-6(1)
C(41)	26(1)	30(1)	21(1)	-2(1)	9(1)	-4(1)
C(42)	36(1)	28(1)	33(1)	5(1)	5(1)	0(1)
F(42A)	85(1)	34(1)	52(1)	5(1)	36(1)	17(1)
F(42B)	52(1)	31(1)	101(2)	-10(1)	17(1)	-13(1)
F(42C)	59(1)	41(1)	43(1)	7(1)	0(1)	18(1)
C(43)	55(2)	53(2)	25(1)	2(1)	18(1)	0(1)
F(43A)	77(1)	117(2)	43(1)	1(1)	38(1)	20(1)
F(43B)	71(1)	150(2)	35(1)	-39(1)	16(1)	-22(1)
F(43C)	275(4)	61(1)	68(2)	11(1)	116(2)	-3(2)
Cl(1)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)
C(1S)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)
Cl(2)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)
Cl(3)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)
C(2S)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)
Cl(4)	61(1)	152(4)	106(2)	53(2)	7(2)	-33(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for rh00502.

	x	y	z	U(eq)
H(1)	6672	3259	980	33
H(2)	8302	2925	723	32
H(4A)	8538	1569	924	44
H(4B)	9011	2037	500	44
H(4C)	8021	1682	-193	44
H(5A)	6219	1368	1071	27
H(5B)	6412	1320	104	27
H(6A)	5358	854	-1212	43
H(6B)	4118	645	-1745	43
H(6C)	4825	479	-668	43
H(8)	2552	1189	-1606	32
H(9)	2440	1951	-660	31
H(13)	-487	1127	3249	26
H(15)	-1093	2684	3074	30
H(17)	1543	2107	2625	25
H(21)	2971	1726	3870	24
H(23)	5590	1371	3206	25
H(25)	2696	579	1986	24
H(29)	1183	1234	974	23
H(31)	-1574	446	-697	25
H(33)	-432	324	2168	22
H(37)	1784	-36	2868	28
H(39)	2083	-494	5491	38
H(41)	1302	1005	4646	31
H(1S1)	5996	9759	5543	137
H(1S2)	4806	9498	5296	137
H(2S1)	5836	10043	4373	137
H(2S2)	4533	9940	3882	137

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

1.1817 (0.0135) x - 4.3280 (0.0276) y + 13.2942 (0.0078) z = 0.6823 (0.0115)

*	0.0031 (0.0013)	N1
*	0.0040 (0.0012)	N2
*	-0.0006 (0.0013)	C1
*	-0.0021 (0.0013)	C2
*	-0.0045 (0.0012)	C3
	-0.0335 (0.0036)	C5
	0.2043 (0.0034)	Rh1

Rms deviation of fitted atoms = 0.0032

5.6367 (0.0157) x + 15.1787 (0.0164) y - 12.1867 (0.0076) z = 5.1967 (0.0062)

Angle to previous plane (with approximate esd) = 43.07 (0.08)

*	0.0304 (0.0017)	N3
*	-0.0234 (0.0012)	N4
*	-0.0239 (0.0010)	C6
*	0.0158 (0.0013)	C7
*	0.0011 (0.0007)	C8
	0.0032 (0.0039)	C5
	-0.1047 (0.0030)	Rh1

Rms deviation of fitted atoms = 0.0215

- 2.1676 (0.0101) x + 17.9682 (0.0146) y - 8.7840 (0.0098) z = 2.4748 (0.0065)

Angle to previous plane (with approximate esd) = 35.18 (0.08)

*	-0.0053 (0.0011)	N1
*	-0.0053 (0.0011)	N4
*	-0.0062 (0.0011)	C10
*	-0.0060 (0.0011)	C11
*	0.0228 (0.0009)	Rh1

Rms deviation of fitted atoms = 0.0114