Supplementary Material (ESI) for Chemical Communications

Supporting Information for:

A Planar Chelating Bitriazole N-heterocyclic Carbene Ligand and its Rhodium(III) and Dirhodium(II) Complexes

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S1. Synthesis and characterization of compounds 3-6

General procedures. All operations were carried out by using standard Schlenk techniques under nitrogen atmosphere. All NMR spectra were recorded at room temperature on Bruker spectrometers operating at 400 or 500 MHz (^{1}H NMR) and 100 or 125 MHz (^{13}C NMR), respectively, and referenced using the residual proton solvent (^{1}H) or solvent (^{13}C) resonance. $[Rh(CO)_2(OAc)]_2$,[1] 4,4'-bi-1,2,4-triazole[2] were prepared according to the method described in the literature, and 1,1'-dimethyl-4,4'-bi-1,2,4-triazolium diiodide (**3-I**)[3] was obtained by a modification of the previously reported procedure. All other reagents were used as received from commercial suppliers and used as received. Microanalyses were carried out by Atlantic Microlabs, Inc. (Norcross, GA). Electrospray mass spectra (ESI-MS) were recorded on a Micromass ZQ instrument using nitrogen as drying agent and nebulizing gas.

Synthesis of 1,1'-dimethyl-4,4'-bi-1,2,4-triazolium diiodide, 3-I. 4,4'-bi-1,2,4-triazole (500 mg, 3.5 mmol) and methyl iodide (2 mL) were dissolved in 10 mL of MeCN in a sealed tube. The mixture was heated at 100ºC for 12h yielding an off-white solid that was filtered and washed with Et_2O. Yield 1.4g (93 %).^{1}H NMR (500 MHz, DMSO-d_6): δ 10.71 (s, 2H, NC*H*N), 9.79 (s, 2H, NC*H*N), 4.37 (s, 6H, C*H*$_3$). ^{13}C NMR (125 MHz, DMSO-d_6): δ 144.42, 144.20 (N*C*HN), 40.41 (N-*C*H$_3$).

Synthesis of 1,1'-dimethyl-4,4'-bi-1,2,4-triazolium tetrafluoroborate, 3-BF$_4$. 4,4'-bi-1,2,4-triazole (300 mg, 2.2 mmol) and trymethyloxonium tetrafluoroborate (718 mg, 4.85 mmol) were placed together in a round bottom flask and dissolved in 10 mL of CH_3CN, the mixture was heated at reflux overnight. The desired salt was collected by filtration, washed several times with CH_2Cl_2 and dried under vacuum. Yield 710 mg (95 %). ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.70 (s, 2H, NC*H*N), 9.74 (s, 2H, NC*H*N), 4.40 (s, 6H, C*H*$_3$). ^{13}C NMR (125 MHz, CD_3CN): 142.9 (N*C*HN), 40.4 (N-*C*H$_3$). Anal. Calc. for $C_6H_{10}N_6B_2F_8$ (339.79): C, 21.21; H, 2.97; N, 24.73. Found: C, 21.20; H, 2.92; N, 24.46.

Synthesis of (bitz)RhI$_3$(CH$_3$CN), 4. A mixture of $[RhCl(cod)]_2$ (100 mg, 0.20 mmol), precursor **3-I** (169 mg, 0.40 mmol) and KI (67 mg, 0.40 mmol) was heated at 50ºC in degassed CH_3CN for

3h under inert atmosphere. The suspension was then filtered through Celite and the solvent removed under high pressure. The crude solid was purified by column chromatography. Elution with a mixture 1:1 CH_2Cl_2/acetone afforded a red band containing compound **4** which was recrystallized in CH_3CN. Suitable crystals for X-ray diffraction studies were grown by slow evaporation of a solution of **3** in CH_3CN. Yield 200 mg (71 %). ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 9.77 (s, 1H, NC*H*N), 9.75 (s, 1H, NC*H*N), 4.54 (s, 3H, N-CH_3), 4.27 (s, 3H, N-CH_3), 3.39 (s, 3H, CH_3CN). ^{13}C NMR (125 MHz, DMSO-d$_6$): δ 166.5 (d, $^1J_{Rh-C}$ = 42.4 Hz, Rh-*C*), 158.2 (d, $^1J_{Rh-C}$= 43.8 Hz, Rh-*C*), 134.3 (N*C*HN), 133.9 (N*C*HN), 116.8 (CH_3*C*N), 42.3 (N-*C*H_3), 38.5 (N-*C*H_3), 28.5 (*C*H_3CN). MS(ESI) m/z (%): 521.3 (100) [M-I-CH_3CN]$^+$. Anal. Calc. for $C_8H_{11}I_3N_7Rh$ (688.84)·CH_3CN: C, 16.45; H, 1.93; N, 15.35. Found: C, 16.14; H, 1.98; N, 15.95.

Synthesis of *cis*-[(bitz)$_2$RhI$_2$][I], 5. A mixture of [RhCl(cod)]$_2$ (100 mg, 0.20 mmol), precursor **3-I** (334 mg, 0.8 mmol), NaOAc (100 mg), and KI (100 mg) was stirred at room temperature for 48 hours in CH_3CN under inert atmosphere. Afterwards, the suspension was filtered through Celite and the solvent removed under vacuum. The resulting orange residue was washed several times with a mixture 9:1 CH_2Cl_2/CH_3CN, giving the desired compound as a pale yellow solid. Suitable crystals for X-ray diffraction methods were obtained by slow diffusion of Et_2O into a solution of **5** in CH_3CN. Yield 180 mg (55 %). ^{1}H NMR (500 MHz, CD_3CN): δ 9.98 (s, 2H, NC*H*N), 9.75 (s, 2H, NC*H*N), 4.67 (s, 6H, N-CH_3), 3.46 (s, 6H, N-CH_3). ^{13}C NMR (125 MHz, CD_3CN): δ 167.6 (d, $^1J_{Rh-C}$ = 34.9 Hz, Rh-*C*), 162.7 (d, $^1J_{Rh-C}$= 43.6 Hz, Rh-*C*), 135.5 (N*C*HN), 135.0 (N*C*HN), 42.3 (N-*C*H_3), 38.9 (N-*C*H_3). MS(ESI) m/z (%): 685. 3 (80) [M]$^+$, 559.6 (20) [M-I]$^+$. Anal. Calc. for $C_{12}H_{16}I_3N_{12}Rh$ (811.95): C, 17.75; H, 1.99; N, 20.70. Found: C, 17.80; H, 2.05; N, 21.10.

Synthesis of [Rh(μ-bitz)(CH$_3$CN)$_3$]$_2$[BF$_4$]$_4$, 6. [Rh(CO)(OAc)$_2$]$_2$ (75 mg, 0.17 mmol), precursor **3-BF$_4$** (116 mg, 0.34 mmol) and NaOAc (28.2 mg, 0.34 mmol) were placed together in a Schlenk tube and 5 mL of degassed CH_3CN were added. The resulting dark red solution was stirred at room temperature for 12 hours. Afterwards, the suspension was filtered and the solvent removed under high pressure giving a dark orange solid. Compound **6** was obtained as a yellow solid after recrystallization from CH_2Cl_2/Et_2O. Suitable crystals for X-ray diffraction studies were obtained by slow diffusion of Et_2O into a solution of compound **6** in CH_3CN. Yield 134 mg

(70 %). ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.69 (s, 2H, NC*H*N), 9.54 (s, 2H, NC*H*N), 4.49 (s, 6H, N-CH_3), 3.58 (s, 6H, N-CH_3), 2.81 (s, 6H, CH_3CN), 2.35 (s, 6H, CH_3CN). ^{13}C NMR (125 MHz, CD_3CN): δ 161.7 (d, $^{1}J_{Rh\text{-}C}$ = 51.1 Hz, Rh-*C*), 161.1 (d, $^{1}J_{Rh\text{-}C}$ = 53.6, Rh-*C*), 141.4 (N*C*HN), 139.3 (N*C*HN), 42.1 (N-CH_3), 40.1 (N-CH_3). Anal. Calc. for $C_{24}H_{34}B_4F_{16}N_{18}Rh_2$ (1127.69)·$2CH_2Cl_2$: C, 24.07; H, 2.95; N, 19.43. Found: C, 23.44; H, 2.92; N, 20.16.

1 J. M. Wilson, G. J. Sunley, H. Adams, A. Haynes, *J. Organomet. Chem.*, 2005, **690**, 6089.
2 R. K. Bartlett, I. Humphrey, *J. Chem. Soc. (C)* 1967, 1664.
3 M. L. Castellanos, M. Llinas, M. Bruix, J. de Mendoza, M. R. Martin, *J. Chem. Soc. Perkin Trans.*, 1985, 1209.

S2. Catalytic Experiments

Typical Procedure for Catalytic Transfer Hydrogenation. A mixture of the substrate (0.5 mmol), catalyst (1 or 0.1 mol % *vs*. substrate), ^{t}BuOK (0.05 mmol) and ^{i}PrOH (10 mL) was heated to reflux under inert atmosphere. Aliquots (0.2 mL) were taken at the desired times, quenched with pentane and filtered through a short path of SiO_2. The filtrate was evaporated to dryness (non volatile substrates) and analysed by ^{1}H NMR spectroscopy, using 1,3,5-trimethoxybenzene as internal standard. Table 1 shows selected data for transfer hydrogenation from ^{i}PrOH/^{t}BuOK using complexes **4** and **6** as catalysts.

Table 1. Selected results on catalytic hydrogenation of C=O and C=N groups via hydrogen transfer from ^{i}PrOH/^{t}BuOK at 82ºC

entry	catalyst	substrate	time(h)	cat. loading (mol %)	yield (%)[a]	TON[b]
1	**4**	acetophenone	3	1	>98	98
2	**4**	acetophenone	12	0.1	>98	980
3	**4**	benzophenone	6	1	>98	98
4	**4**	benzophenone	24	0.1	25	250
5	**4**	benzylidene aniline	6	1	90	90
6	**4**	cyclohexanone	48	1	>98	98
7	**4**	cyclohexanone	48	0.1	40	400
8	**6**	acetophenone	4	0.7	>98	140
9	**6**	benzophenone	3.5	0.7	>98	140

[a]Yields were determined by ^{1}H NMR spectroscopy, using 1,3,5-methoxybenzene as internal standard.
[b]TON=(mmol of product)/(mmol of catalyst)

S3. Crystallographic data of compounds 4-6

S3.1 Crystallographic data of compound 4

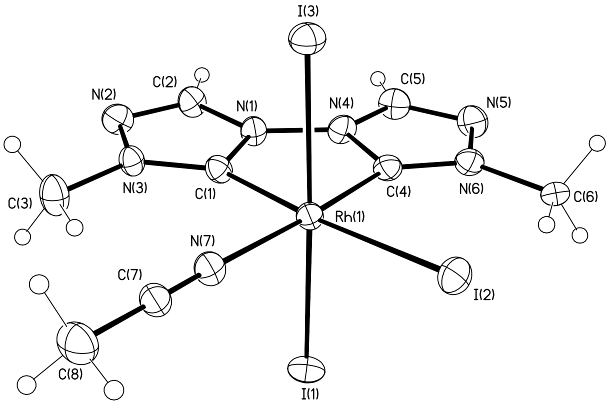

Figure 1. Molecular structure of compound **4**. 30 % probability chosen for the ellipsoids. Selected bond distances (Å) and angles (º): Rh(1)-C(1) 1.977(5), Rh(1)-C(4) 1.976(5), Rh(1)-I(1) 2.6734(7), Rh(1)-I(2) 2.7316(6), Rh(1)-N(7) 2.074(5); and C(1)-Rh(1)-C(4) 79.4(2)

Table 1. Crystal data and structure refinement for compound **4**.

Empirical formula	$C_8 H_{11} I_3 N_7 Rh$	
Formula weight	688.85	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 27.320(6) Å	α= 90°.
	b = 8.2040(16) Å	β= 90°.
	c = 15.373(3) Å	γ = 90°.
Volume	3445.7(12) Å^3	
Z	8	
Density (calculated)	2.656 g/cm^3	
Absorption coefficient	63.65 cm^{-1}	
F(000)	2496	
Crystal size	0.10 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.59 to 28.27°.	
Index ranges	-36<=h<=36, -10<=k<=10, -20<=l<=20	

Reflections collected	7923
Independent reflections	4241 [R(int) = 0.0363]
Completeness to theta = 28.27°	99.3 %
Absorption correction	None
Max. and min. transmission	0.6299 and 0.5686
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4241 / 0 / 173
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0765
R indices (all data)	R1 = 0.0644, wR2 = 0.0832
Largest diff. peak and hole	0.868 and -1.232 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for **4**.

Rh(1)-C(1)	1.977(5)
Rh(1)-C(4)	1.976(5)
Rh(1)-N(7)	2.074(5)
Rh(1)-I(3)	2.6632(6)
Rh(1)-I(1)	2.6734(7)
Rh(1)-I(2)	2.7316(6)
N(1)-C(1)	1.348(6)
N(1)-C(2)	1.358(6)
N(1)-N(4)	1.374(6)
N(2)-C(2)	1.293(7)
N(2)-N(3)	1.369(6)
N(3)-C(1)	1.329(6)
N(3)-C(3)	1.431(7)
N(4)-C(5)	1.347(7)
N(4)-C(4)	1.372(6)
N(5)-C(5)	1.301(7)
N(5)-N(6)	1.393(6)
N(6)-C(4)	1.326(6)
N(6)-C(6)	1.455(6)
N(7)-C(7)	1.128(6)
C(7)-C(8)	1.474(8)
C(1)-Rh(1)-C(4)	79.4(2)
C(1)-Rh(1)-N(7)	96.41(18)
C(4)-Rh(1)-N(7)	175.84(18)
C(1)-Rh(1)-I(3)	85.15(14)
C(4)-Rh(1)-I(3)	87.33(15)
N(7)-Rh(1)-I(3)	92.19(12)
C(1)-Rh(1)-I(1)	88.55(14)
C(4)-Rh(1)-I(1)	88.27(15)
N(7)-Rh(1)-I(1)	91.80(12)
I(3)-Rh(1)-I(1)	172.884(19)
C(1)-Rh(1)-I(2)	176.31(14)
C(4)-Rh(1)-I(2)	98.91(14)
N(7)-Rh(1)-I(2)	85.23(11)
I(3)-Rh(1)-I(2)	91.495(19)
I(1)-Rh(1)-I(2)	94.710(18)
C(1)-N(1)-C(2)	111.3(4)
C(1)-N(1)-N(4)	115.3(4)
C(2)-N(1)-N(4)	133.4(4)
C(2)-N(2)-N(3)	105.7(4)
C(1)-N(3)-N(2)	112.8(4)
C(1)-N(3)-C(3)	127.4(4)
N(2)-N(3)-C(3)	119.8(4)
C(5)-N(4)-N(1)	134.1(4)
C(5)-N(4)-C(4)	110.9(4)
N(1)-N(4)-C(4)	114.8(4)
C(5)-N(5)-N(6)	104.9(4)
C(4)-N(6)-N(5)	112.7(4)
C(4)-N(6)-C(6)	129.7(4)
N(5)-N(6)-C(6)	117.6(4)
C(7)-N(7)-Rh(1)	176.1(4)
N(3)-C(1)-N(1)	102.2(4)
N(3)-C(1)-Rh(1)	142.2(4)
N(1)-C(1)-Rh(1)	115.5(4)
N(2)-C(2)-N(1)	108.0(4)
N(6)-C(4)-N(4)	102.3(4)
N(6)-C(4)-Rh(1)	142.9(4)
N(4)-C(4)-Rh(1)	114.8(4)
N(5)-C(5)-N(4)	109.1(5)
N(7)-C(7)-C(8)	179.6(7)

S3.2 Crystallographic data of compound 5

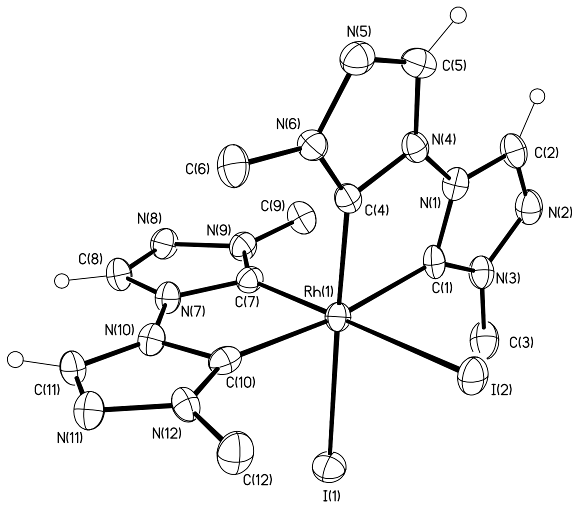

Figure 2. Molecular structure of the cation of **5**. 30 % probability chosen for the ellipsoids. Selected bond distances (Å) and angles (º): Rh(1)-C(4) 2.002(6), Rh(1)-C(1) 2.043(6), Rh(1)-C(7) 1.991(6), Rh(1)-C(10) 2.049(7); and C(4)-Rh(1)-C(1) 78.6(3), C(7)-Rh(1)-C(10) 79.3(2)

Table 1. Crystal data and structure refinement for compound **5**.

Empirical formula	$C_{18} H_{29} I_3 N_{13}$ O Rh	
Formula weight	927.15	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.691(2) Å	α= 90°.
	b = 9.883(2) Å	β= 97.77(3)°.
	c = 26.375(5) Å	γ = 90°.
Volume	3019.4(10) $Å^3$	
Z	4	
Density (calculated)	2.040 g/cm^3	
Absorption coefficient	36.69 cm^{-1}	
F(000)	1760	
Crystal size	0.20 x 0.10 x 0.08 mm^3	
Theta range for data collection	2.20 to 29.06°.	
Index ranges	-15<=h<=15, -13<=k<=13, -35<=l<=35	

Reflections collected	12618
Independent reflections	7790 [R(int) = 0.0379]
Completeness to theta = 29.06°	96.6 %
Absorption correction	None
Max. and min. transmission	0.7579 and 0.5274
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7790 / 0 / 327
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1299
R indices (all data)	R1 = 0.0866, wR2 = 0.1444
Extinction coefficient	0.0038(3)
Largest diff. peak and hole	1.259 and -0.925 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for **5**.

Rh(1)-C(7)	1.991(6)	O(1)-C(16)	1.386(11)
Rh(1)-C(4)	2.002(6)	O(1)-C(17)	1.430(12)
Rh(1)-C(1)	2.043(6)	C(15)-C(16)	1.564(18)
Rh(1)-C(10)	2.049(7)	C(17)-C(18)	1.463(13)
Rh(1)-I(1)	2.7117(10)		
Rh(1)-I(2)	2.7142(7)	C(7)-Rh(1)-C(4)	95.1(2)
N(1)-C(1)	1.325(8)	C(7)-Rh(1)-C(1)	95.3(2)
N(1)-N(4)	1.365(7)	C(4)-Rh(1)-C(1)	78.6(3)
N(1)-C(2)	1.372(8)	C(7)-Rh(1)-C(10)	79.3(2)
N(2)-C(2)	1.306(9)	C(4)-Rh(1)-C(10)	96.3(2)
N(2)-N(3)	1.372(8)	C(1)-Rh(1)-C(10)	172.4(2)
N(3)-C(1)	1.346(8)	C(7)-Rh(1)-I(1)	86.45(17)
N(3)-C(3)	1.460(9)	C(4)-Rh(1)-I(1)	178.40(17)
N(4)-C(4)	1.370(7)	C(1)-Rh(1)-I(1)	100.81(19)
N(4)-C(5)	1.379(8)	C(10)-Rh(1)-I(1)	84.40(16)
N(5)-C(5)	1.281(9)	C(7)-Rh(1)-I(2)	179.44(18)
N(5)-N(6)	1.392(7)	C(4)-Rh(1)-I(2)	85.39(16)
N(6)-C(4)	1.308(8)	C(1)-Rh(1)-I(2)	85.08(17)
N(6)-C(6)	1.459(8)	C(10)-Rh(1)-I(2)	100.32(17)
N(7)-C(8)	1.362(8)	I(1)-Rh(1)-I(2)	93.09(3)
N(7)-C(7)	1.363(8)	C(1)-N(1)-N(4)	117.8(5)
N(7)-N(10)	1.393(7)	C(1)-N(1)-C(2)	112.5(5)
N(8)-C(8)	1.294(9)	N(4)-N(1)-C(2)	129.8(5)
N(8)-N(9)	1.419(7)	C(2)-N(2)-N(3)	105.3(5)
N(9)-C(7)	1.316(8)	C(1)-N(3)-N(2)	113.0(5)
N(9)-C(9)	1.444(8)	C(1)-N(3)-C(3)	128.3(6)
N(10)-C(10)	1.363(8)	N(2)-N(3)-C(3)	118.6(5)
N(10)-C(11)	1.364(8)	N(1)-N(4)-C(4)	114.9(5)
N(11)-C(11)	1.281(9)	N(1)-N(4)-C(5)	135.6(5)
N(11)-N(12)	1.372(7)	C(4)-N(4)-C(5)	109.4(5)
N(12)-C(10)	1.333(8)	C(5)-N(5)-N(6)	104.9(5)
N(12)-C(12)	1.457(8)	C(4)-N(6)-N(5)	113.4(5)
N(13)-C(13)	1.115(10)	C(4)-N(6)-C(6)	128.5(5)
C(13)-C(14)	1.482(13)	N(5)-N(6)-C(6)	117.9(5)

C(8)-N(7)-C(7)	111.8(5)	N(2)-C(2)-N(1)	107.3(6)
C(8)-N(7)-N(10)	133.0(5)	N(6)-C(4)-N(4)	103.0(5)
C(7)-N(7)-N(10)	115.2(5)	N(6)-C(4)-Rh(1)	142.2(4)
C(8)-N(8)-N(9)	104.7(5)	N(4)-C(4)-Rh(1)	114.8(4)
C(7)-N(9)-N(8)	112.8(5)	N(5)-C(5)-N(4)	109.3(6)
C(7)-N(9)-C(9)	130.3(6)	N(9)-C(7)-N(7)	102.3(5)
N(8)-N(9)-C(9)	116.9(5)	N(9)-C(7)-Rh(1)	141.8(5)
C(10)-N(10)-C(11)	111.4(6)	N(7)-C(7)-Rh(1)	115.9(4)
C(10)-N(10)-N(7)	116.4(5)	N(8)-C(8)-N(7)	108.5(6)
C(11)-N(10)-N(7)	132.2(5)	N(12)-C(10)-N(10)	100.5(5)
C(11)-N(11)-N(12)	104.9(5)	N(12)-C(10)-Rh(1)	146.2(5)
C(10)-N(12)-N(11)	114.4(5)	N(10)-C(10)-Rh(1)	113.3(4)
C(10)-N(12)-C(12)	127.1(6)	N(11)-C(11)-N(10)	108.7(6)
N(11)-N(12)-C(12)	118.5(5)	N(13)-C(13)-C(14)	177.4(10)
N(1)-C(1)-N(3)	102.0(5)	C(16)-O(1)-C(17)	110.0(9)
N(1)-C(1)-Rh(1)	113.7(4)	O(1)-C(16)-C(15)	107.1(11)
N(3)-C(1)-Rh(1)	144.2(5)	O(1)-C(17)-C(18)	109.7(10)

S3.3 Crystallographic data of compound 6

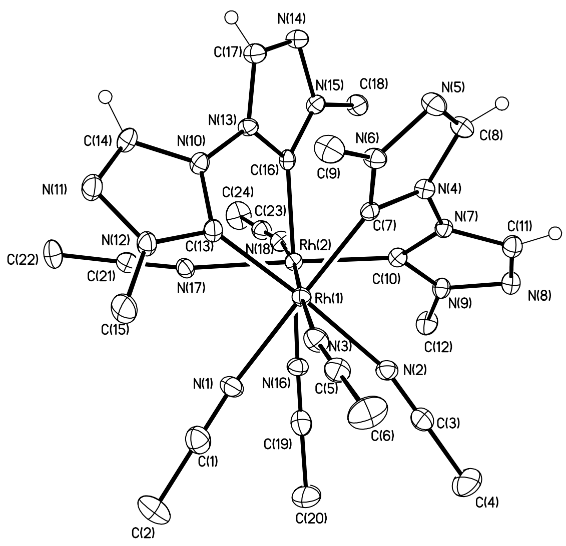

Figure 3. Molecular structure of the cation of **6**. 30 % probability chosen for the ellipsoids. Selected bond distances (Å) and angles (º): Rh(1)-Rh(2) 2.6459(8), Rh(1)-C(7) 1.969(3), Rh(1)-C(13) 1.979(3), Rh(2)-C(16) 1.972(3), Rh(2)-C(10) 1.993(3), Rh(2)-Rh(1)-C(7) 90.90(9), Rh(2)-Rh(1)-C(13) 87.92(9)

Table 1. Crystal data and structure refinement for compound **6**.

Empirical formula	$C_{26} H_{37} B_4 F_{16} N_{19} Rh_2$	
Formula weight	1168.81	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.137(4) Å	α= 90°.
	b = 11.200(2) Å	β= 99.01(3)°.
	c = 19.736(4) Å	γ = 90°.
Volume	4396.3(15) Å^3	
Z	4	
Density (calculated)	1.766 g/cm^3	
Absorption coefficient	8.67 cm^{-1}	
F(000)	2320	
Crystal size	0.15 x 0.15 x 0.08 mm^3	
Theta range for data collection	2.26 to 29.01°.	

Index ranges	-27<=h<=27, -15<=k<=15, -26<=l<=26
Reflections collected	20259
Independent reflections	11606 [R(int) = 0.0453]
Completeness to theta = 29.01°	99.2 %
Absorption correction	None
Max. and min. transmission	0.9339 and 0.8810
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11606 / 0 / 611
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0979
R indices (all data)	R1 = 0.0818, wR2 = 0.1095
Largest diff. peak and hole	0.723 and -0.825 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for **6**.

Rh(1)-C(7)	1.969(3)	N(13)-C(17)	1.354(4)
Rh(1)-C(13)	1.979(3)	N(13)-C(16)	1.366(4)
Rh(1)-N(1)	2.072(3)	N(14)-C(17)	1.297(4)
Rh(1)-N(2)	2.079(3)	N(14)-N(15)	1.381(4)
Rh(1)-N(3)	2.164(3)	N(15)-C(16)	1.334(4)
Rh(1)-Rh(2)	2.6459(8)	N(15)-C(18)	1.462(4)
Rh(2)-C(16)	1.972(3)	N(16)-C(19)	1.128(4)
Rh(2)-C(10)	1.993(3)	N(17)-C(21)	1.128(4)
Rh(2)-N(16)	2.073(3)	N(18)-C(23)	1.129(4)
Rh(2)-N(17)	2.076(3)	C(1)-C(2)	1.481(5)
Rh(2)-N(18)	2.171(3)	C(3)-C(4)	1.454(5)
N(1)-C(1)	1.130(4)	C(5)-C(6)	1.462(5)
N(2)-C(3)	1.118(4)	C(19)-C(20)	1.468(6)
N(3)-C(5)	1.116(4)	C(21)-C(22)	1.456(5)
N(4)-C(7)	1.360(4)	C(23)-C(24)	1.466(5)
N(4)-C(8)	1.364(4)	B(1)-F(3)	1.362(6)
N(4)-N(7)	1.375(3)	B(1)-F(4)	1.373(6)
N(5)-C(8)	1.293(4)	B(1)-F(2)	1.384(6)
N(5)-N(6)	1.392(4)	B(1)-F(1)	1.392(6)
N(6)-C(7)	1.332(4)	B(2)-F(5)	1.338(6)
N(6)-C(9)	1.463(4)	B(2)-F(7)	1.378(6)
N(7)-C(11)	1.360(4)	B(2)-F(8)	1.379(6)
N(7)-C(10)	1.371(4)	B(2)-F(6)	1.389(6)
N(8)-C(11)	1.302(4)	B(3)-F(12)	1.372(5)
N(8)-N(9)	1.384(4)	B(3)-F(10)	1.375(5)
N(9)-C(10)	1.338(4)	B(3)-F(11)	1.378(5)
N(9)-C(12)	1.456(4)	B(3)-F(9)	1.396(5)
N(10)-C(13)	1.371(4)	B(4)-F(15)	1.331(6)
N(10)-C(14)	1.372(4)	B(4)-F(14)	1.369(5)
N(10)-N(13)	1.381(3)	B(4)-F(16)	1.378(6)
N(11)-C(14)	1.286(4)	B(4)-F(13)	1.382(5)
N(11)-N(12)	1.384(4)	C(25)-C(26)	1.468(6)
N(12)-C(13)	1.329(4)	C(26)-N(19)	1.099(5)
N(12)-C(15)	1.464(4)		

C(7)-Rh(1)-C(13)	90.07(13)	C(8)-N(5)-N(6)	103.9(3)
C(7)-Rh(1)-N(1)	178.79(12)	C(7)-N(6)-N(5)	113.8(3)
C(13)-Rh(1)-N(1)	90.55(13)	C(7)-N(6)-C(9)	130.2(3)
C(7)-Rh(1)-N(2)	93.99(11)	N(5)-N(6)-C(9)	116.0(3)
C(13)-Rh(1)-N(2)	175.43(12)	C(11)-N(7)-C(10)	110.6(3)
N(1)-Rh(1)-N(2)	85.43(11)	C(11)-N(7)-N(4)	123.6(3)
C(7)-Rh(1)-N(3)	90.76(12)	C(10)-N(7)-N(4)	125.5(2)
C(13)-Rh(1)-N(3)	97.74(12)	C(11)-N(8)-N(9)	104.0(3)
N(1)-Rh(1)-N(3)	88.13(11)	C(10)-N(9)-N(8)	114.1(3)
N(2)-Rh(1)-N(3)	84.31(10)	C(10)-N(9)-C(12)	129.7(3)
C(7)-Rh(1)-Rh(2)	90.90(9)	N(8)-N(9)-C(12)	116.3(3)
C(13)-Rh(1)-Rh(2)	87.92(9)	C(13)-N(10)-C(14)	110.0(3)
N(1)-Rh(1)-Rh(2)	90.16(8)	C(13)-N(10)-N(13)	125.6(2)
N(2)-Rh(1)-Rh(2)	89.93(7)	C(14)-N(10)-N(13)	124.3(3)
N(3)-Rh(1)-Rh(2)	174.10(8)	C(14)-N(11)-N(12)	104.6(3)
C(16)-Rh(2)-C(10)	90.99(12)	C(13)-N(12)-N(11)	113.9(3)
C(16)-Rh(2)-N(16)	178.23(11)	C(13)-N(12)-C(15)	129.0(3)
C(10)-Rh(2)-N(16)	90.32(12)	N(11)-N(12)-C(15)	117.0(3)
C(16)-Rh(2)-N(17)	89.79(11)	C(17)-N(13)-C(16)	111.0(3)
C(10)-Rh(2)-N(17)	178.08(11)	C(17)-N(13)-N(10)	124.1(3)
N(16)-Rh(2)-N(17)	88.86(11)	C(16)-N(13)-N(10)	124.6(2)
C(16)-Rh(2)-N(18)	91.53(11)	C(17)-N(14)-N(15)	104.1(3)
C(10)-Rh(2)-N(18)	97.44(11)	C(16)-N(15)-N(14)	114.2(3)
N(16)-Rh(2)-N(18)	89.47(11)	C(16)-N(15)-C(18)	128.1(3)
N(17)-Rh(2)-N(18)	84.30(10)	N(14)-N(15)-C(18)	117.6(2)
C(16)-Rh(2)-Rh(1)	90.97(9)	C(19)-N(16)-Rh(2)	178.4(3)
C(10)-Rh(2)-Rh(1)	86.58(9)	C(21)-N(17)-Rh(2)	168.9(3)
N(16)-Rh(2)-Rh(1)	87.92(8)	C(23)-N(18)-Rh(2)	165.9(3)
N(17)-Rh(2)-Rh(1)	91.65(7)	N(1)-C(1)-C(2)	179.9(5)
N(18)-Rh(2)-Rh(1)	175.22(8)	N(2)-C(3)-C(4)	178.5(4)
C(1)-N(1)-Rh(1)	168.7(3)	N(3)-C(5)-C(6)	179.5(4)
C(3)-N(2)-Rh(1)	166.3(3)	N(6)-C(7)-N(4)	101.9(3)
C(5)-N(3)-Rh(1)	167.3(3)	N(6)-C(7)-Rh(1)	131.3(2)
C(7)-N(4)-C(8)	110.6(3)	N(4)-C(7)-Rh(1)	126.8(2)
C(7)-N(4)-N(7)	123.4(3)	N(5)-C(8)-N(4)	109.9(3)
C(8)-N(4)-N(7)	125.5(3)	N(9)-C(10)-N(7)	101.5(3)

N(9)-C(10)-Rh(2)	129.9(2)	F(2)-B(1)-F(1)	108.5(5)
N(7)-C(10)-Rh(2)	128.1(2)	F(5)-B(2)-F(7)	109.8(5)
N(8)-C(11)-N(7)	109.7(3)	F(5)-B(2)-F(8)	110.3(4)
N(12)-C(13)-N(10)	101.9(3)	F(7)-B(2)-F(8)	109.8(4)
N(12)-C(13)-Rh(1)	129.6(2)	F(5)-B(2)-F(6)	111.2(4)
N(10)-C(13)-Rh(1)	128.1(2)	F(7)-B(2)-F(6)	107.7(4)
N(11)-C(14)-N(10)	109.6(3)	F(8)-B(2)-F(6)	108.0(4)
N(15)-C(16)-N(13)	101.2(3)	F(12)-B(3)-F(10)	109.3(3)
N(15)-C(16)-Rh(2)	132.6(2)	F(12)-B(3)-F(11)	109.4(4)
N(13)-C(16)-Rh(2)	126.2(2)	F(10)-B(3)-F(11)	110.0(4)
N(14)-C(17)-N(13)	109.5(3)	F(12)-B(3)-F(9)	109.8(3)
N(16)-C(19)-C(20)	177.5(4)	F(10)-B(3)-F(9)	108.6(3)
N(17)-C(21)-C(22)	178.9(4)	F(11)-B(3)-F(9)	109.8(3)
N(18)-C(23)-C(24)	179.2(4)	F(15)-B(4)-F(14)	110.9(4)
F(3)-B(1)-F(4)	111.4(4)	F(15)-B(4)-F(16)	112.2(4)
F(3)-B(1)-F(2)	109.9(5)	F(14)-B(4)-F(16)	109.4(4)
F(4)-B(1)-F(2)	110.1(4)	F(15)-B(4)-F(13)	109.3(4)
F(3)-B(1)-F(1)	108.8(4)	F(14)-B(4)-F(13)	108.2(4)
F(4)-B(1)-F(1)	108.1(5)	F(16)-B(4)-F(13)	106.8(4)