Electronic Supplementary Material (ESI) for Analytical Methods

Supporting Information

Pyridyl- and Benzimidazole-Based Ruthenium (III) Complex for Selective Chloride Recognition through Fluorescence Spectroscopy

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Table S1: Crystal data and structure refinement for ([Ru(**1**)(Cl)(PPh_3)][PF_6]·2CH_3OH) (**4**)

Identification code	70herbm	
Empirical formula	C39 H42 Cl F6 N3 O4 P2 Ru	
Formula weight	929.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.2059(15) Å	α= 88.423(2)°.
	b = 12.2904(18) Å	β= 79.612(2)°.
	c = 16.590(2) Å	γ = 67.580(2)°.
Volume	1890.2(5) $Å^3$	
Z	2	
Density (calculated)	1.633 Mg/m^3	
Absorption coefficient	0.647 mm^{-1}	
F(000)	948	
Crystal size	0.49 x 0.44 x 0.42 mm^3	
Theta range for data collection	1.25 to 25.00°.	
Index ranges	-12<=h<=12, -14<=k<=14, -19<=l<=19	
Reflections collected	13314	
Independent reflections	6568 [R(int) = 0.0229]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	None	
Max. and min. transmission	0.7729 and 0.7424	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6568 / 17 / 514	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1298	

R indices (all data)	R1 = 0.0523, wR2 = 0.1330
Largest diff. peak and hole	1.271 and -0.877 e.Å^{-3}

Table S2: Selected bond lengths [Å] and angles [°] for the cationic Ru(II) and (III) complexes ([Ru(**1**)(Cl)(PPh_3)]$^+$, ([Ru(**2**)(Cl)(PPh_3)]$^+$ and ([Ru(**3**)(Cl)(H_2O)]$^+$

X-ray structural data of ([Ru(1)(Cl)(PPh_3)]$^+$

Bond distances (Å)

Ru(1)-N(1)	2.070(4)	Ru(1)-N(3)	2.103(4)
Ru(1)-O(1)	2.109(3)	Ru(1)-N(2)	2.245(4)
Ru(1)-P(1)	2.318(12)	Ru(1)-Cl(1)	2.428(12)

Bond Angles (°)

N(1)-Ru(1)-N(3)	97.28(15)	N(1)-Ru(1)-O(1)	80.04(13)
N(3)-Ru(1)-N(2)	101.78(14)	N(1)-Ru(1)-P(1)	95.31(11)
O(1)-Ru(1)-P(1)	87.75(9)	N(1)-Ru(1)-Cl(1)	172.79(11)
O(1)-Ru(1)-Cl(1)	93.67(9)	P(1)-Ru(1)-Cl(1)	87.91(4)
N(3)-Ru(1)-O(1)	176.88(13)	N(1)-Ru(1)-N(2)	84.05(14)
O(1)-Ru(1)-N(2)	76.44(14)	N(3)-Ru(1)-P(1)	94.11(10)
N(2)-Ru(1)-P(1)	164.06(11)	N(3)-Ru(1)-Cl(1)	88.90(11)

Geometry-optimized structural data of ([Ru(2)(Cl)(PPh_3)]$^+$

Bond distances (Å)

Ru(1)-N(1)	2.184	Ru(1)-N(12)	2.221
Ru(1)-Cl(1)	2.504	Ru(1)-P(1)	2.434
Ru(1)-N(12)´	1.196	Ru(1)-N(1)´	2.217

Bond Angles (°)

N(1)-Ru(1)-N(12)	87.77	N(1)-Ru(1)-N(1)´	101.01
N(12)-Ru(1)-N(12)´	80.36	N(1)´-Ru(1)-N(12)´	89.74
N(1)-Ru(1)-P(1)	91.39	N(12)-Ru(1)-P(1)	82.89
N(12)-Ru(1)-P(1)	82.89	(N(12)´-Ru(1)-P(1)	92.96
N(1)´-Ru(1)-P(1)	99.90	N(12)-Ru(1)-Cl(1)	88.56
N(1)-Ru(1)-N(12)´	167.54	N(1)´-Ru(1)-N(12)	164.23
Cl(1)-Ru(1)-P1(1)	178.54		

Geometry-optimized structural data of ([Ru(3)(Cl)(H_2O)]$^+$

Bond distances (Å)

Ru(1)-N(1)	2.132	Ru(1)-N(11)	2.211
Ru(1)-N(14)	2.128	Ru(1)-N(24)	2.074
Ru(1)-Cl(1)	2.306	Ru(1)-O(1)	2.204

Bond Angles (°)

N(1)-Ru(1)-N(11)	80.31	N(1)-Ru(1)-N(24)	90.84
N(1)-Ru(1)-C(14)	160.44	N(11)-Ru(1)-N(14)	80.62
N(11)-Ru(1)-N(24)	80.73	N(14)-Ru(1)-N(24)	90.35
N(1)-Ru(1)-Cl(1)	99.08	N(11)-Ru(1)-Cl(1)	178.40
N(14)-Ru(1)-Cl(1)	99.87	N(24)-Ru(1)-Cl(1)	100.73
N(1)-Ru(1)-O(1)	87.30	N(11)-Ru(1)-O(1)	89.52
N(14)-Ru(1)-O(1)	88.23	N(24)-Ru(1)-O(1)	170.24
Cl(1)-Ru(1)-O(1)	88.98		

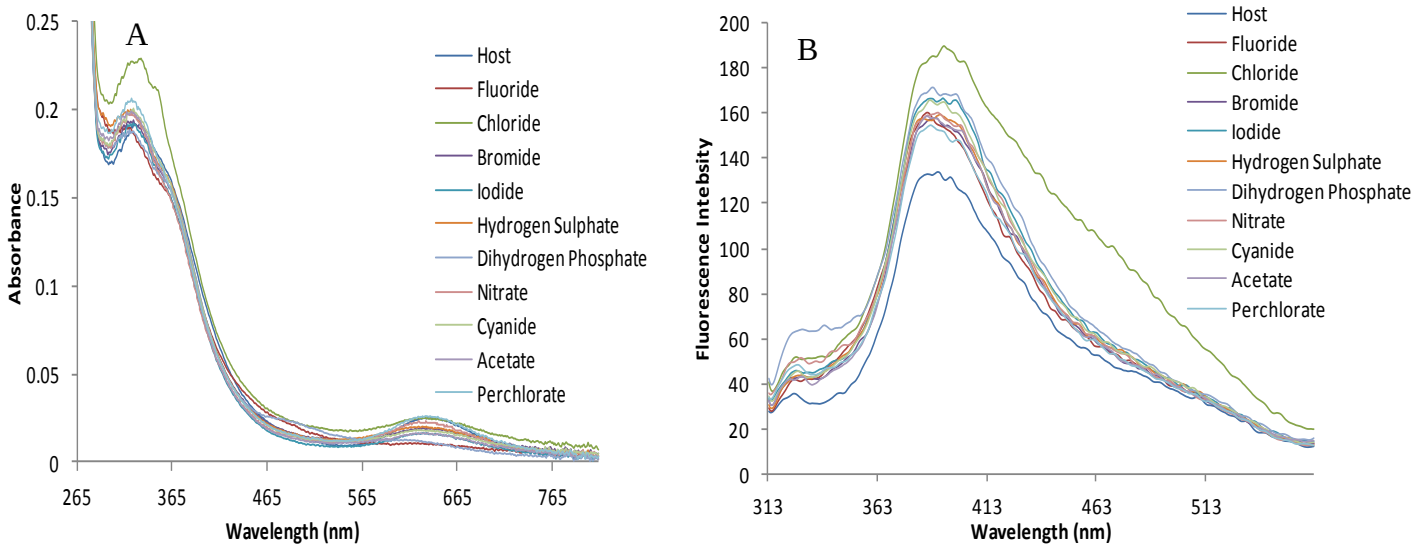

Figure S1: Change in the absorbance and fluorescence intensity of **4** (A & B; 80 µM) upon addition of a particular anion salt (300 µM) in CH_3CN/H_2O (9:1; v/v).

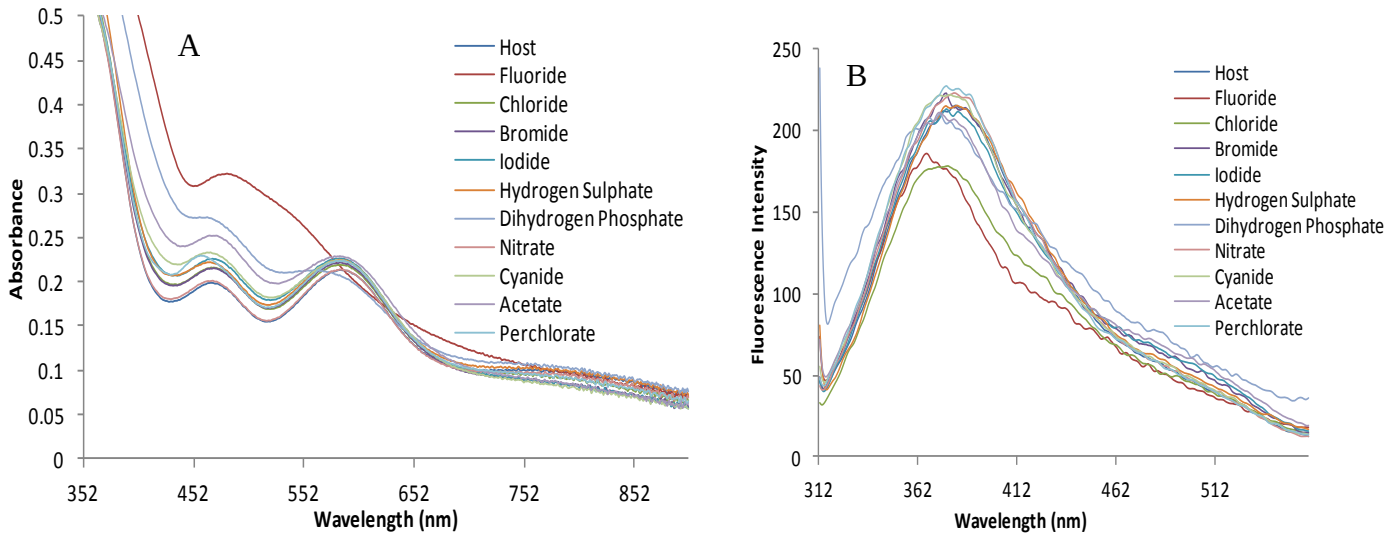

Figure S2: Change in the absorbance and fluorescence intensity of **5** (A & B; 80 µM) upon addition of a particular anion salt (300 µM) in CH_3CN/H_2O (9:1; v/v).

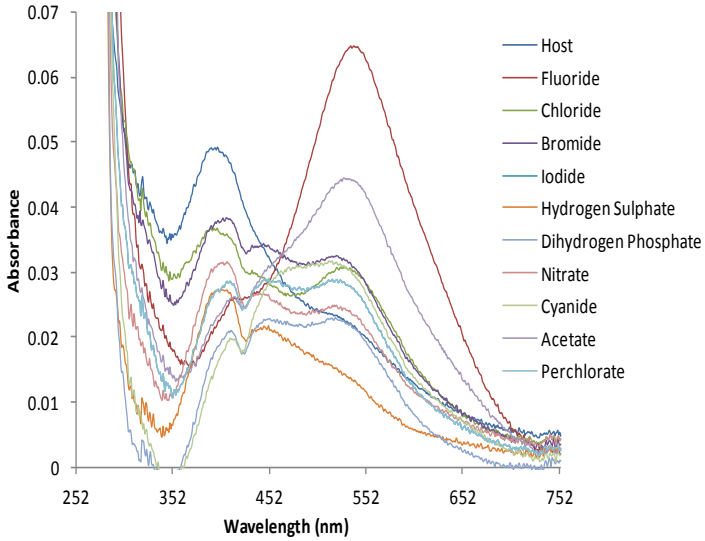

Figure S3: Change in the UV-Visible absorbance profile **6** (80 µM) upon addition of a particular anion salt (300 µM) in CH_3CN/H_2O (9:1; v/v).

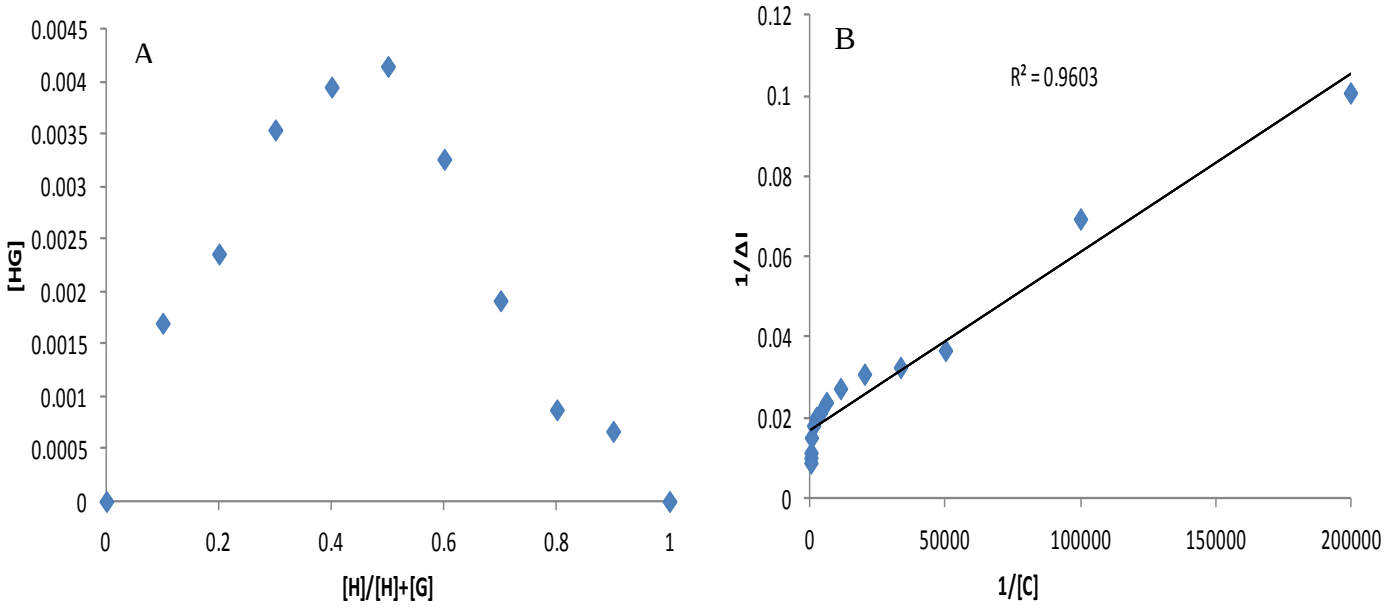

Figure S4: (A) Job's plot showing that the stoichiometry between receptor **6** and chloride is 1:1. The concentration of [HG] was calculated using the equation $[HG]=\Delta I/I_o \times [H]$; (B) Benesi-Hildebrand plot for the determination of the stability constant of the complex formed between receptor **6** (80 μM) and chloride.