

Supplementary material

for

Tuning of the lowest excited states in mixed ruthenium(II) polypyridyl complexes having RuN₆ cores by the conformation of the ancillary ligand. Emission from a ³ligand-to-ligand-charge-transfer state

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Table S1 Hydrogen bond dimensions in **1** and **2** (distances, Å; angles, °). A=acceptor, D = donor

	H...A	D...A	D-H...A	symmetry element
In 1				
O(1)- H(1W)... N(63)	2.13	2.901(8)	150	1+x,y,z
O(1)- H(2W)... O(85)	2.29	3.151(13)	177	
O(1)- H(2W)... O(81)	2.56	3.420(12)	175	
N(63)- H(63A)... O(87)	2.20	3.021(9)	161	-1/2+x, 1.5-y, 2-z
N(63)- H(63A)... O(84)	2.52	3.342(8)	161	-1/2+x, 1.5-y, 2-z
N(63)- H(63B)... O(88)	2.11	2.906(9)	154	-1+x, y,z
N(63)- H(63B)... O(83)	2.41	3.158(8)	146	-1+x,y,z
N(73)- H(73B)... O(74)	2.40	3.118(5)	142	1.5-x, y-1/2, z

In 2

N(73)- H(73A)... O(1)	2.20	2.935(10)	143	
N(73)- H(73B)... N(63)	2.36	3.144(11)	152	1+x, y, z
N(63)- H(63B)... O(72)	2.33	2.942(11)	128	
O(1)- H(1W)... O(2)	2.09	2.91(3)	159	1-x, -y, 2-z
O(1)- H(2W)... O(71)	2.22	2.940(10)	140	1-x, -y, 1-z
O(2)- H(4W)... O(74)	2.47	3.30(2)	168	x,y,1+z

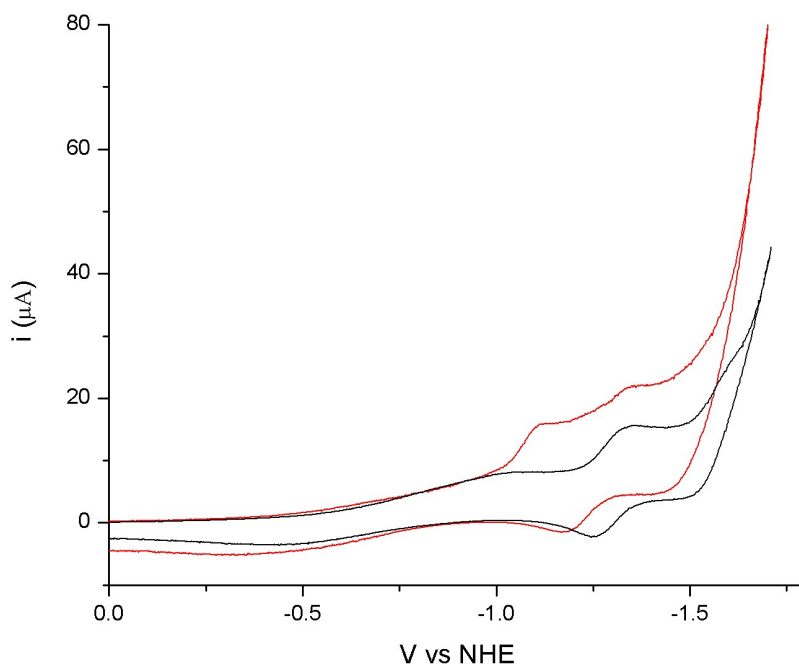


Fig. S1 Cyclic voltammograms (CV)'s of **1** (black) and **2** (red) in acetonitrile 0.1 mol dm⁻³ in TEAP at a Pt electrode on the negative side of NHE. Scan rate = 50 mV s⁻¹. Solute concentration = 1 mmol dm⁻³.

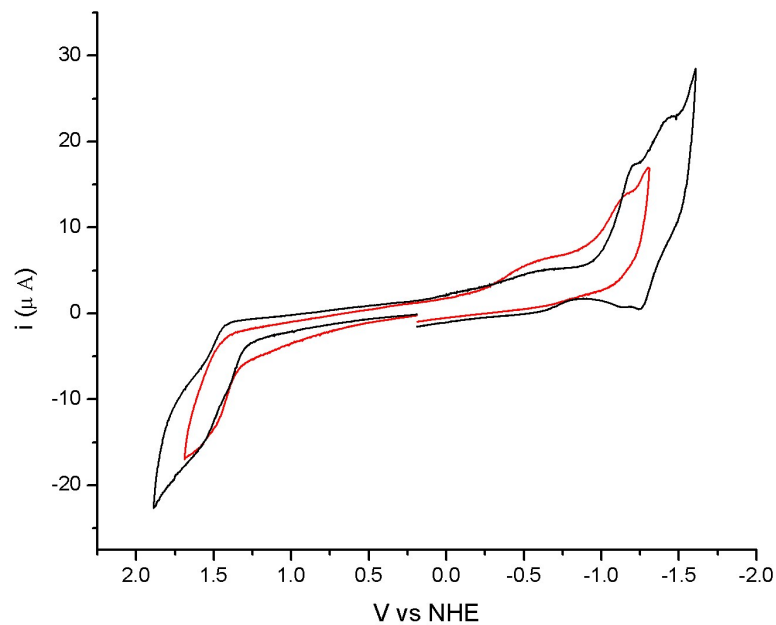


Fig. S2 CV's of **1** (black) and **2** (red) in acetonitrile 0.1 mol dm^{-3} in TEAP at a glassy carbon electrode. Scan rate = 50 mV s^{-1} . Solute concentration = 1 mmol dm^{-3} .

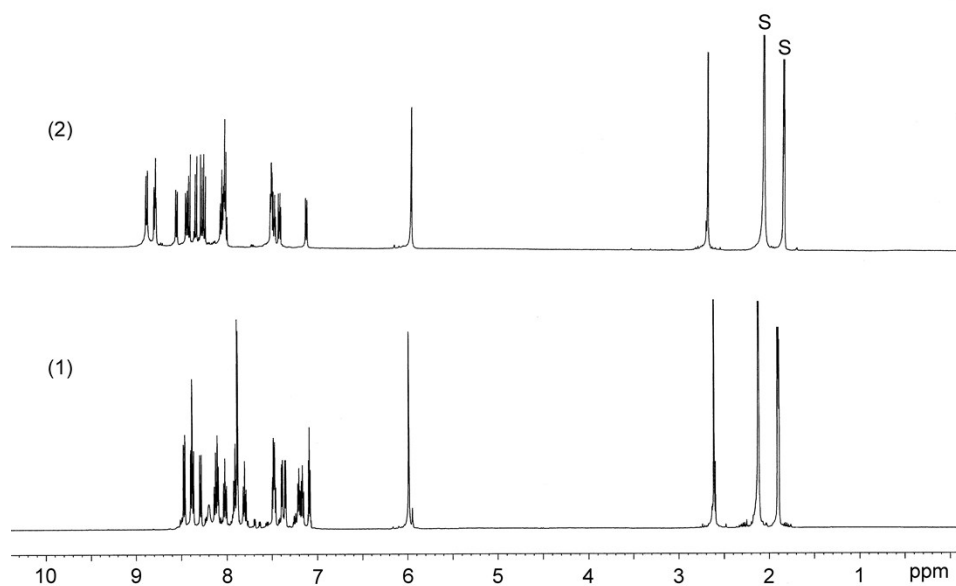


Fig. S3 ^1H NMR of **(1)** and **(2)** in CD_3CN at room temperature. Peaks marked by asterisks are due to the solvent.

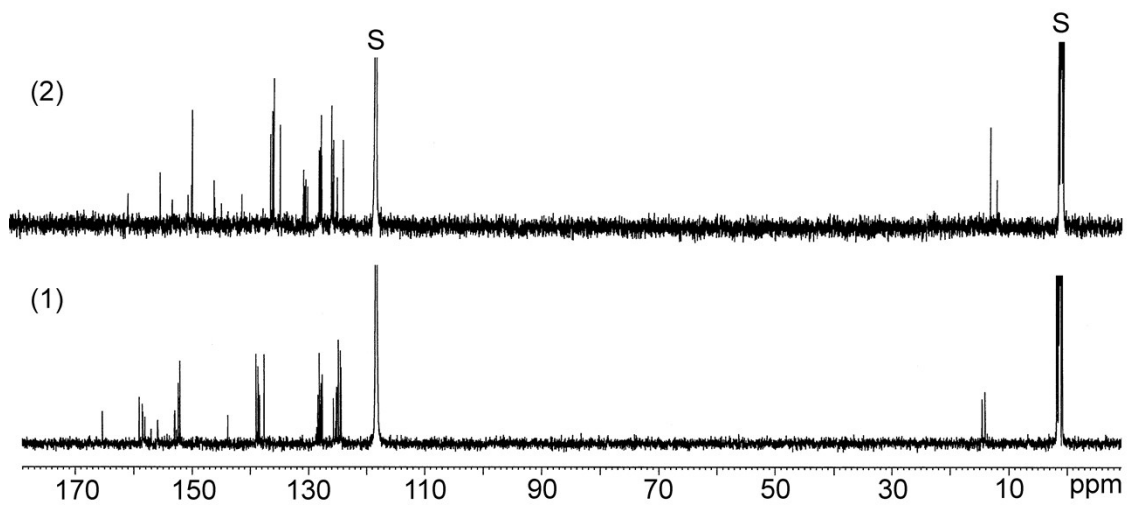


Fig. S4 ^{13}C NMR of (1) and (2) in CD_3CN at room temperature. Peaks marked by asterisks are due to the solvent.