

Ferrocene-appended ligands for use in spin crossover-redox “hybrid” complexes of iron(II) and cobalt(II)

Hayley S. Scott,^a Christopher J. Gartshore,^a Si-Xuan Guo,^a Boujemaa Moubaraki,^a Alan. M. Bond,^a Stuart R. Batten,^a Keith S. Murray^{*a}

ESI – Supporting Information

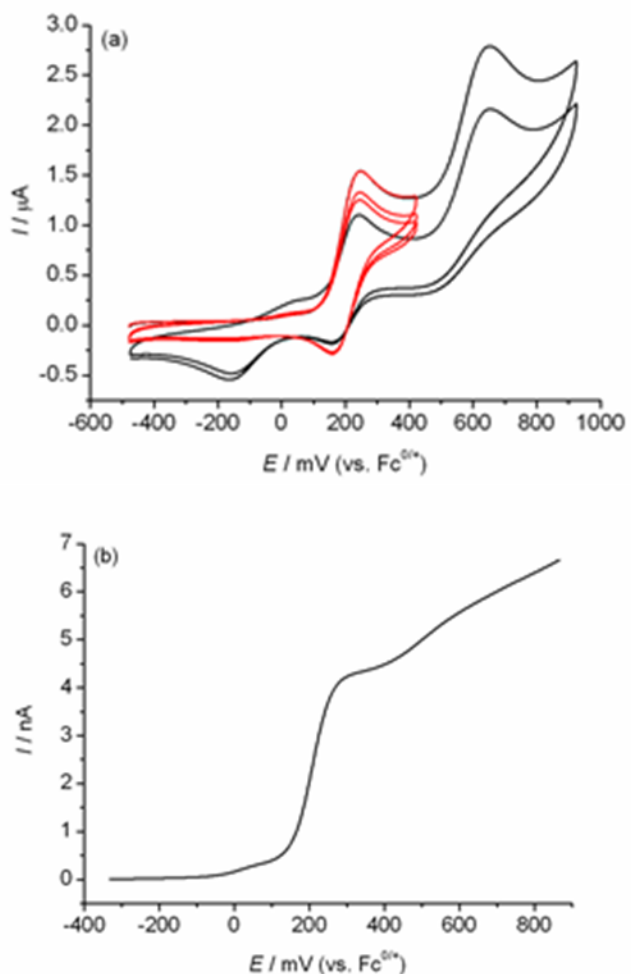


Figure S1. Cyclic (a) and near steady-state (b) voltammograms of 0.5 mM FTP ligand in DMF (0.05 M [Bu₄N][ClO₄]), obtained with a 1 mm dia. glassy carbon disk electrode at a scan rate of 100 mV s⁻¹, and a 36.5 μ m dia. carbon fibre electrode at a scan rate of 5 mV s⁻¹, respectively.

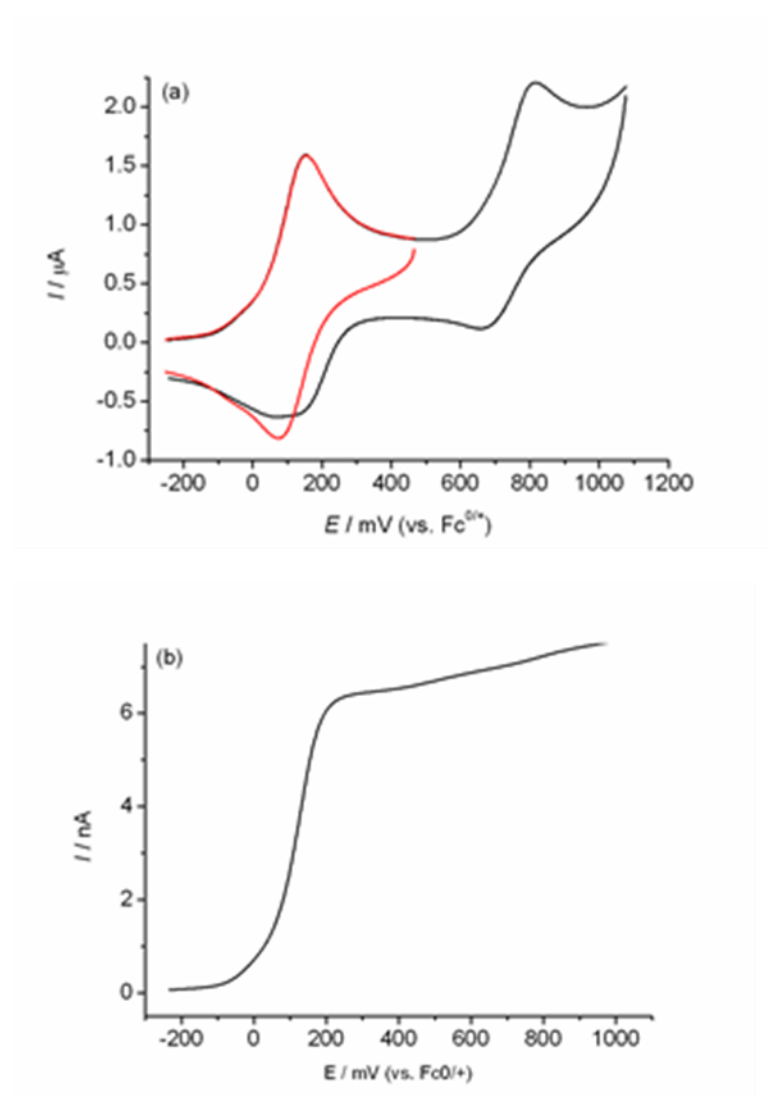


Figure S2. Cyclic (a) and near steady-state (b) voltammograms of 0.5 mM FTTP in MeCN (0.05 M [Bu₄N][ClO₄]), obtained with a 1 mm dia. glassy carbon disk electrode at a scan rate of 100 mV s⁻¹ and a 36.5 μ m dia. carbon fibre electrode at a scan rate of 5 mV s⁻¹, respectively.

Table S1. Selected bond lengths and angles for complexes **1-3** at 100 K.

Bond(s)	1		2		3
<i>Lengths (Å)</i>					
N(1)-Fe(1)	2.100(2)	N(1)-Co(1)	1.876(3)	N(1)-Fe(1)	1.984(5)
N(2)-Fe(1)	2.214(2)	N(2)-Co(1)	1.918(3)	N(2)-Fe(1)	1.883(5)
N(3)-Fe(1)	2.191(2)	N(3)-Co(1)	2.020(3)	N(3)-Fe(1)	1.972(5)
N(1')-Fe(1)	2.100(2)	N(4)-Co(1)	2.024(3)	N(4)-Fe(1)	1.969(5)
N(2')-Fe(1)	2.214(2)	N(5)-Co(1)	2.128(3)	N(5)-Fe(1)	1.889(5)
N(3')-Fe(1)	2.191(2)	N(6)-Co(1)	2.138(3)	N(6)-Fe(1)	1.982(5)
<i>Angles (°)</i>					
N(1)-Fe-N(2)	90.53(9)	N(1)-Co-N(2)	80.75(12)	N(1)-Fe-N(2)	80.92(19)
N(1)-Fe-N(3)	86.07(9)	N(1)-Co-N(3)	161.23(11)	N(1)-Fe-N(3)	161.7(2)
N(1')-Fe-N(1)	180	N(1)-Co-N(4)	92.01(11)	N(1)-Fe-N(4)	90.02(19)
N(1)-Fe-N(2')	89.47(9)	N(1)-Co-N(5)	101.23(11)	N(1)-Fe-N(5)	98.59(19)
N(1)-Fe-N(3')	93.93(9)	N(1)-Co-N(6)	88.14(11)	N(1)-Fe-N(6)	92.92(19)
N(2)-Fe-N(3)	76.16(8)	N(2)-Co-N(3)	80.82(12)	N(2)-Fe-N(3)	80.85(19)
N(1')-Fe-N(2)	89.47(9)	N(2)-Co-N(4)	95.87(11)	N(2)-Fe-N(4)	101.7(2)
N(2)-Fe-N(2')	180	N(2)-Co-N(5)	174.88(11)	N(2)-Fe-N(5)	177.20(19)
N(3')-Fe-N(2)	103.84(8)	N(2)-Co-N(6)	106.12(11)	N(2)-Fe-N(6)	96.56(19)
N(1')-Fe-N(3)	93.93(9)	N(3)-Co-N(4)	93.36(11)	N(3)-Fe-N(4)	92.9(2)
N(2')-Fe-N(3)	103.84(8)	N(3)-Co-N(5)	97.44(11)	N(3)-Fe-N(5)	99.7(2)
N(3')-Fe-N(3)	180	N(3)-Co-N(6)	93.58(11)	N(3)-Fe-N(6)	89.9(2)
N(1')-Fe-N(2')	90.53(9)	N(4)-Co-N(5)	79.38(11)	N(4)-Fe-N(5)	81.1(2)
N(1')-Fe-N(3')	86.07(9)	N(4)-Co-N(6)	157.73(11)	N(4)-Fe-N(6)	161.8(2)
N(3')-Fe-N(2')	76.16(8)	N(5)-Co-N(6)	78.75(11)	N(5)-Fe-N(6)	80.70(19)