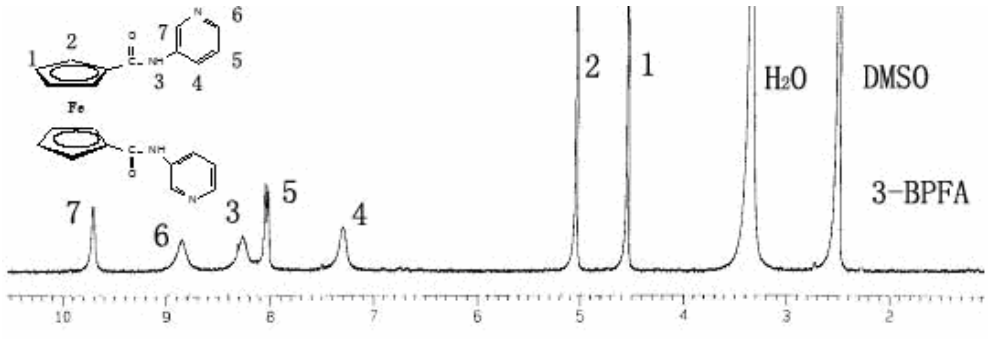
Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2007

Supporting Information

Kai-Ju Wei, Jia Ni, Yong-Shu Xie, Yangzhong Liu and Qing-Liang Liu



Scheme 1. ^{1}H NMR spectra of the ligand **3-BPFA** (300 MHz, DMSO; 298K).

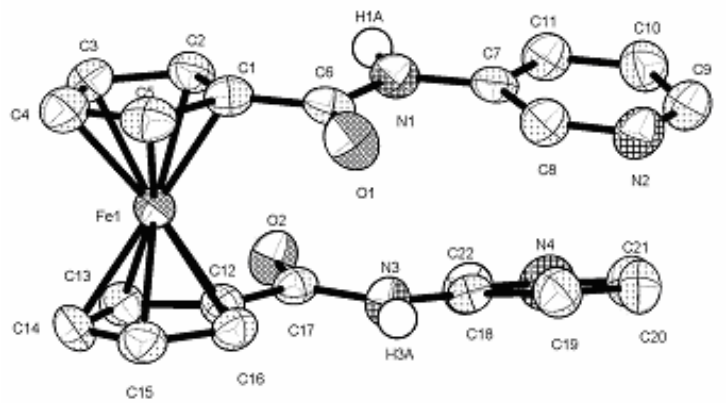


Figure S1. ORTEP diagram showing the structure of **3-BPFA** with 50% thermal ellipsoids probability and the atom-labeling scheme. Hydrogen atoms and water molecules have been omitted for clarity.

Table S1. Hydrogen bonds for ligand **3-BPFA** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠ (DHA)
N(1)-H(1A)···O(2) $^{\#1}$	0.86	2.14	2.97	160
N(3)-H(3A)···N(2) $^{\#2}$	0.86	2.29	3.11	159
O(3)-H(3E)···O(1) $^{\#3}$	0.85	2.03	2.88	179
O(3)-H(3F)···N(4) $^{\#4}$	0.85	1.99	2.84	179

Symmetry transformations used to generate equivalent atoms: (#1) -x+1, y+1/2, -z+1; (#2) -x, y-1/2, -z+1; (#3) x+1, y, z; (#4) x, y, z-1.

This journal is © The Royal Society of Chemistry 2007

Table S2. Selected interatomic distances [Å] and angles [º] for complexes **1-3.**

Complex **1**			
Cu-N(2)	2.040(4)	Cu-N(4) $^{\#2}$	2.045(3)
Cu-O(3)	2.186(5)		
N(2) -Cu(1)-N(2) $^{\#1}$	167.4(2)	N(2)-Cu(1)-N(4)$^{\#2}$	88.57(13)
N(2)$^{\#1}$-Cu(1)- N(4)$^{\#2}$	90.32(13)	N(2) -Cu(1)- N(4) $^{\#3}$	90.32(13)
N(2)$^{\#1}$-Cu(1)- N(4)$^{\#3}$	88.57(13)	N(4)$^{\#2}$-Cu(1)-N(4) $^{\#3}$	169.85(16)
N(2)-Cu(1)-O(3)	96.30(11)	N(2)$^{\#1}$-Cu(1)-O(3)	96.30(11)
N(4) $^{\#2}$-Cu(1)-O(3)	95.08(8)	N(4) $^{\#3}$-Cu(1)-O(3)	95.08(8)
Symmetry transformations used to generate equivalent atoms: (#1) -x+5/4, y, -z+1/4; (#2) x, -y+1/4, -z+1/4; (#3) -x+5/4, -y+1/4, z.			
Complex **2**			
Ni(1)-N(2)	2.172(7)	Ni(1)-O(3)	2.203(10)
Ni(1)-N(4)$^{\#2}$	2.200(8)	Ni(1)-Cl(1)	2.615(3)
N(2)-Ni(1)-N(2)$^{\#1}$	179.0(4)	N(2)-Ni(1)-N(4)$^{\#2}$	88.9(3)
N(2)$^{\#1}$-Ni(1)-N(4)$^{\#2}$	91.2(3)	N(2)-Ni(1)-N(4)$^{\#3}$	91.2(3)
N(2)$^{\#1}$-Ni(1)-N(4)$^{\#3}$	88.9(3)	N(4)$^{\#2}$-Ni(1)-N(4)$^{\#3}$	177.8(4)
N(2)-Ni(1)-O(3)	90.49(18)	N(2)$^{\#1}$-Ni(1)-O(3)	90.49(18)
N(4)$^{\#2}$-Ni(1)-O(3)	88.92(19)	N(4)$^{\#3}$-Ni(1)-O(3)	88.92(19)
N(2)-Ni(1)-Cl(1)	89.51(18)	N(2)$^{\#1}$-Ni(1)-Cl(1)	89.51(18)
N(4)$^{\#2}$-Ni(1)-Cl(1)	91.08(19)	N(4)$^{\#3}$-Ni(1)-Cl(1)	91.08(19)
O(3)-Ni(1)-Cl(1)	180.000(1)	Ni(1)-Cl(1)-Ni(1)$^{\#3}$	180.000(1)
Symmetry transformations used to generate equivalent atoms: (#1) -x+1/4, y, -z+5/4; (#2) x, -y+1/4, -z+5/4; (#3) -x+1/4, -y+1/4, z.			
Complex **3**			
Co(1)-O(3)	2.125(7)	Co(1)-N(2)	2.162(5)
Co(1)-N(4)$^{\#2}$	2.175(5)	Co(1)-Cl(1)	2.5621(12)
O(3)-Co(1)-N(2)$^{\#1}$	90.64(14)	O(3)-Co(1)-N(2)	90.64(14)
N(2)$^{\#1}$-Co(1)-N(2)	178.7(3)	O(3)-Co(1)-N(4)$^{\#2}$	89.68(14)
N(2)$^{\#1}$-Co(1)-N(4)$^{\#2}$	90.80(18)	N(2)-Co(1)-N(4)$^{\#2}$	89.20(18)
O(3)-Co(1)-N(4)$^{\#3}$	89.68(14)	N(2)$^{\#1}$-Co(1)-N(4)$^{\#3}$	89.20(18)
N(2)-Co(1)-N(4)$^{\#3}$	90.80(18)	N(4)$^{\#2}$-Co(1)-N(4)$^{\#3}$	179.4(3)
O(3)-Co(1)-Cl(1)	180.000(1)	N(2)$^{\#1}$-Co(1)-Cl(1)	89.36(14)
N(2)-Co(1)-Cl(1)	89.36(14)	N(4)$^{\#2}$-Co(1)-Cl(1)	90.32(14)
N(4)$^{\#3}$-Co(1)-Cl(1)	90.32(14)	Co(1)$^{\#3}$-Cl(1)-Co(1)	180.0
Symmetry transformations used to generate equivalent atoms: (#1) -x+9/4, y, -z+1/4; (#2) x, -y+5/4, -z+1/4; (#3) -x+9/4, -y+5/4, z.			

This journal is © The Royal Society of Chemistry 2007

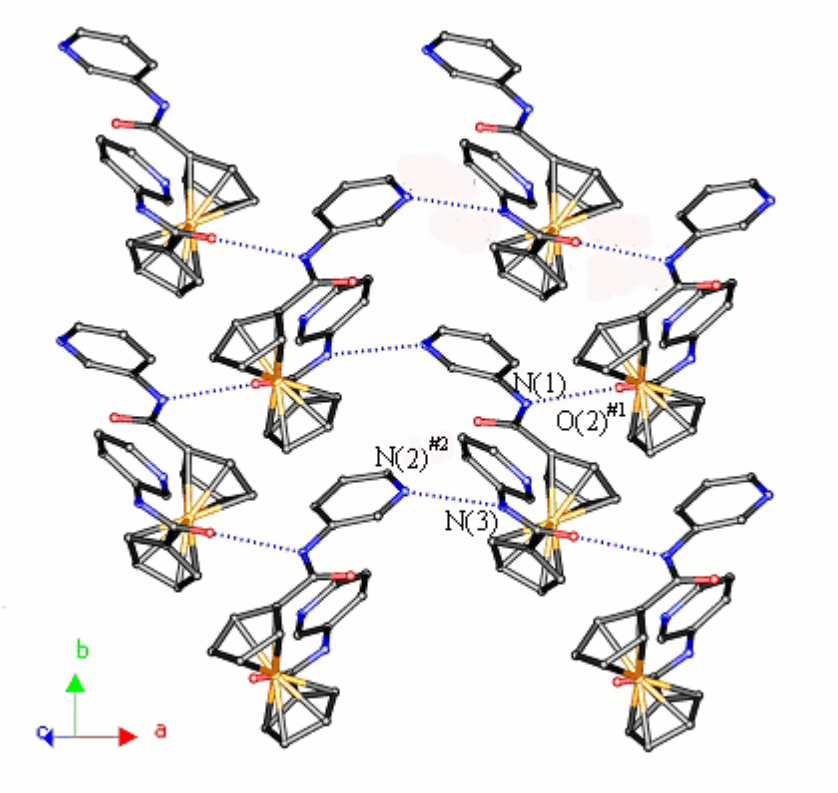


Figure S2. View of the supramolecular adduct **3-BPFA**, showing the hydrogen bonds between N-H donors on **3-BPFA** and the N acceptors on the other moiety. Symmetry transformations used to generate equivalent atoms: (#1) -x+1, y+1/2, -z+1; (#2) -x, y-1/2, -z+1.

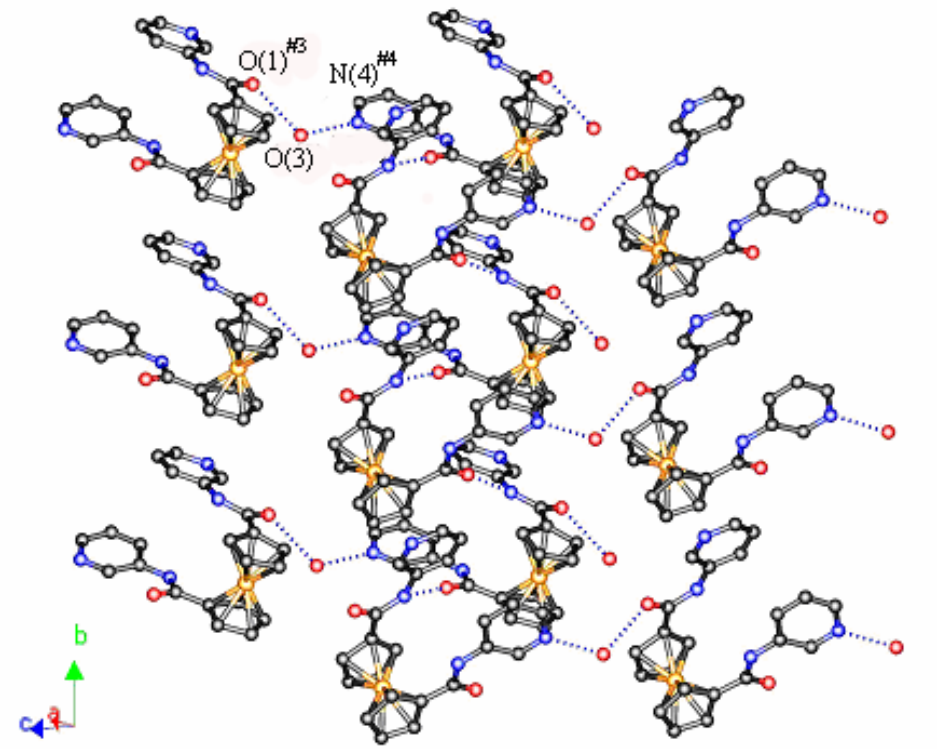


Figure S3. View of the packed structure along *bc* plane in compound **3-BPFA**. Symmetry transformations used to generate equivalent atoms: (#3) x+1, y, z; (#4) x, y, z-1.

This journal is © The Royal Society of Chemistry 2007

Table S3. Hydrogen bonds for **1** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠ (DHA)
N(3)-H(3A)···O(1)	0.86	2.17	2.84	134
N(1)-H(1A)···O(7)$^{\#1}$	0.86	2.17	2.96	154
O(3)-H(3B)···O(8)$^{\#2}$	0.82	1.94	2.71	156
O(8)-H(8A)···O(2)$^{\#3}$	0.82	2.00	2.77	144

Symmetry transformations used to generate equivalent atoms: (#1) x, y, z-1; (#2) -x+5/4, y, -z+1/4; (#3) x-1/2, y+1/2, z.

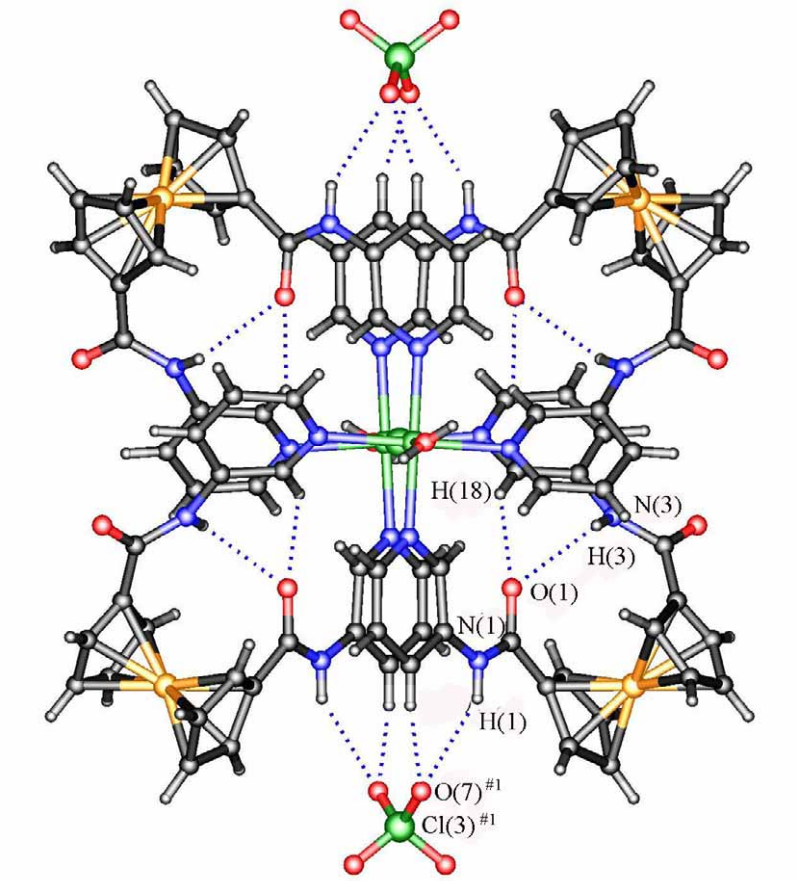


Figure S4. Top view of the pseudo-capsule $[Ni_2(3\text{-BPFA})_4(\mu\text{-Cl})_2(H_2O)_2](ClO_4)_3$, showing multiple N-H···O and C-H···O H-bonding interactions. A ClO_4^- anion is omitted for clarity. Symmetry transformations used to generate equivalent atoms: (#1): -x+1/2, -y+1, -z+3/2.

Table S4. Hydrogen bonds for **2** [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠ (DHA)
N(3)-H(3)···O(1)	0.86	2.44	3.04	127
C(18)-H(18)···O(1)	0.93	2.37	3.13	139
C(15)-H(15)···O(7) $^{\#1}$	0.93	2.51	3.28	140
N(1)-H(1)···O(7)$^{\#1}$	0.86	2.50	3.27	150

Symmetry transformations used to generate equivalent atoms: (#1): -x+1/2, -y+1, -z+3/2

This journal is © The Royal Society of Chemistry 2007

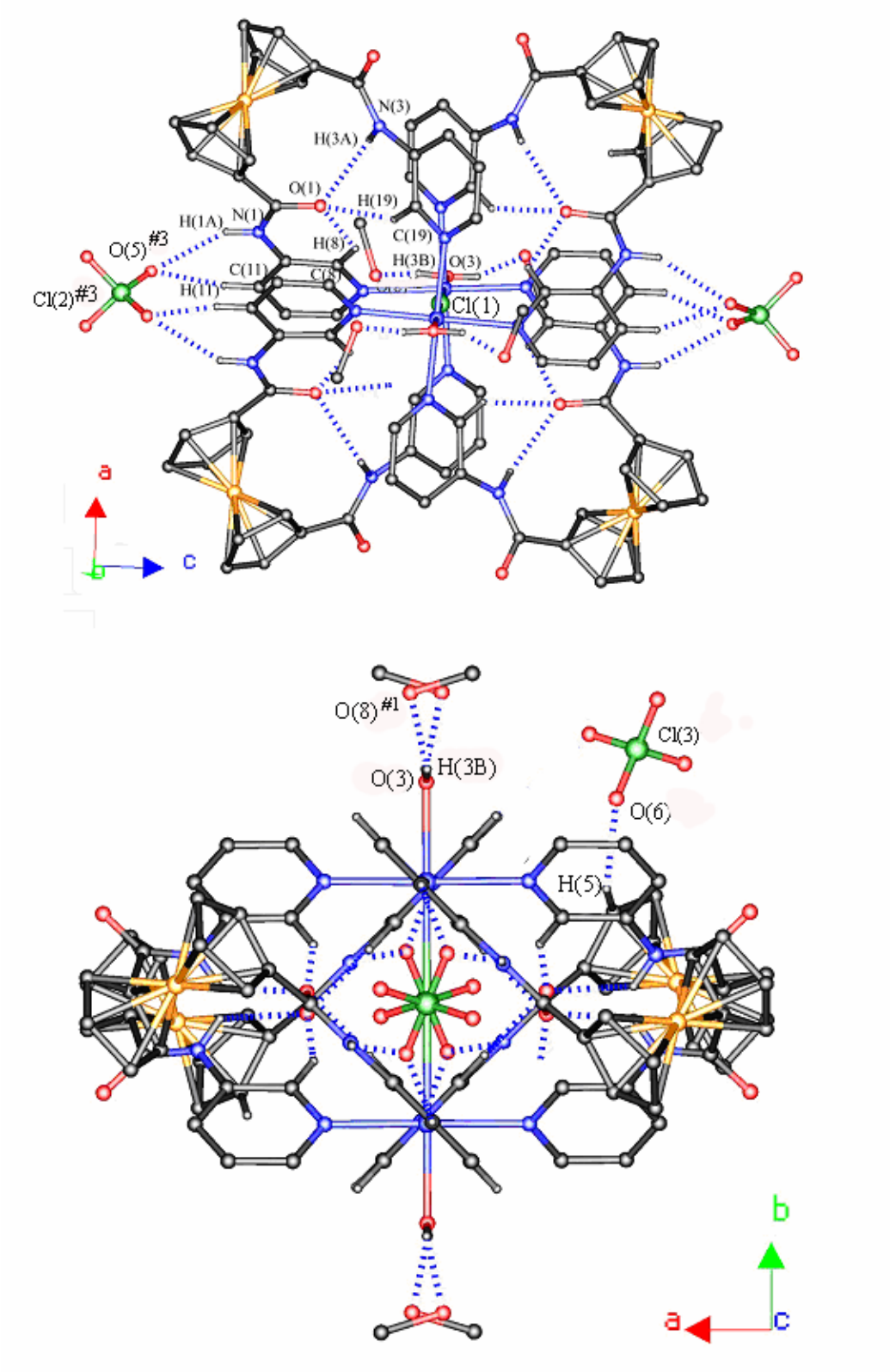


Figure S5. Top and side views of the cage $[Co_2(3\text{-BPFA})_4(\mu\text{-Cl})_2(H_2O)_2](ClO_4)_3\cdot 4CH_3OH$, showing multiple intramolecular N-H···O hydrogen-bonding interactions and intermolecular N-H···O and O-H···O hydrogen-bonding interactions. Hydrogen atoms are omitted for clarity.

This journal is © The Royal Society of Chemistry 2007

Symmetry transformations used to generate equivalent atoms: (#1): x+1, y, z; (#3): x＋1, y, z－1.

Table S5. Hydrogen bonds for **3** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
N(3)-H(3A)···O(1)	0.86	2.23	2.87	132
C(5)-H(5)···O(6)	0.93	2.49	3.37	157
C(8)-H(8)···O(1)	0.93	2.11	2.73	123
C(19)-H(19)···O(1)	0.93	2.25	3.03	142
O(3)-H(3B)···O(8)$^{\#1}$	0.82	2.07	2.77	143
O(8)-H(8B)···O(2)$^{\#2}$	0.82	2.59	3.29	85
N(1)-H(1A)···O(5)$^{\#3}$	0.86	2.30	3.08	150
C(11)-H(11)···O(5)$^{\#3}$	0.93	2.46	3.23	140

Symmetry transformations used to generate equivalent atoms: (#1): x+1,y,z; (#2): x-1/2, y-1/2, z; (#3): x+1,y,z-1.

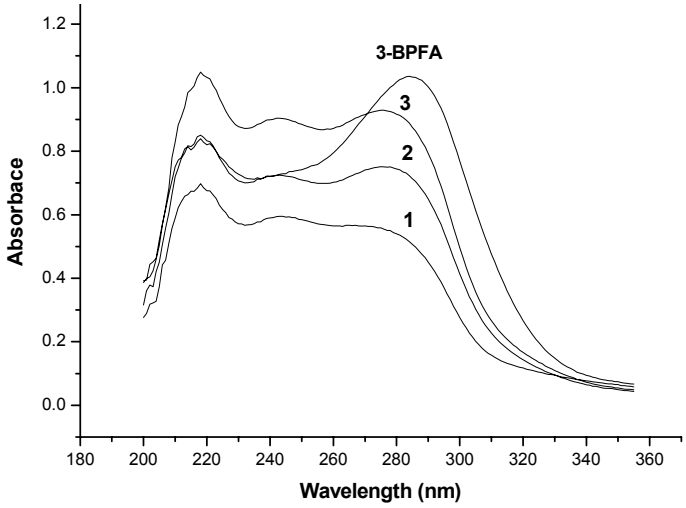
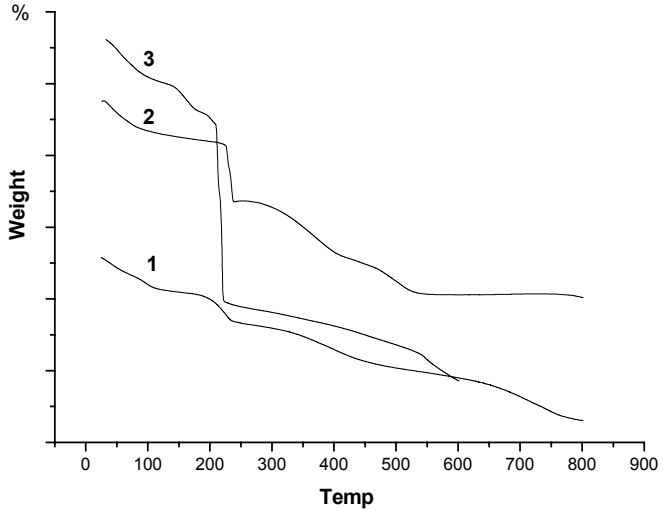


Figure S6. UV-visible absorption spectra at ambient temperature in MeOH (4×10^{-5} M) for the ligand **3-BPFA** and in MeOH (1×10^{-5} M) complexes **1-3**.



This journal is © The Royal Society of Chemistry 2007

Figure S7. Thermogravimetric analysis of complexes **1-3**.

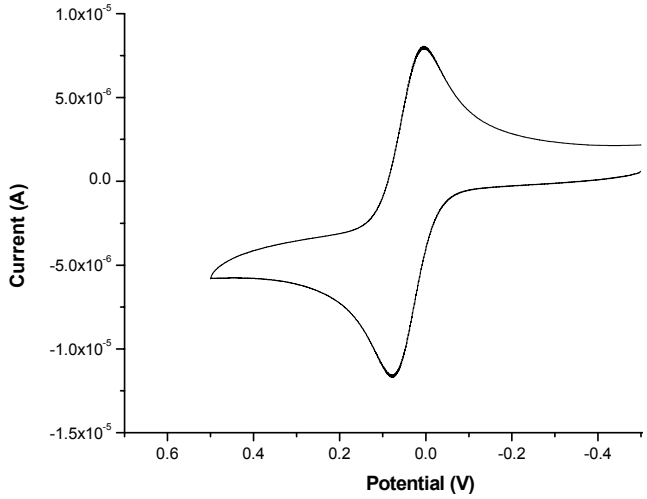


Figure S8. Cyclic voltammogram of **Ferrocene** in acetonitril/0.1 M tetrabutylammonium hexafluorophosphate; concentration of **Ferrocene**: 0.5 x 10^{-3} M. Scan rate of 50 mV/s.

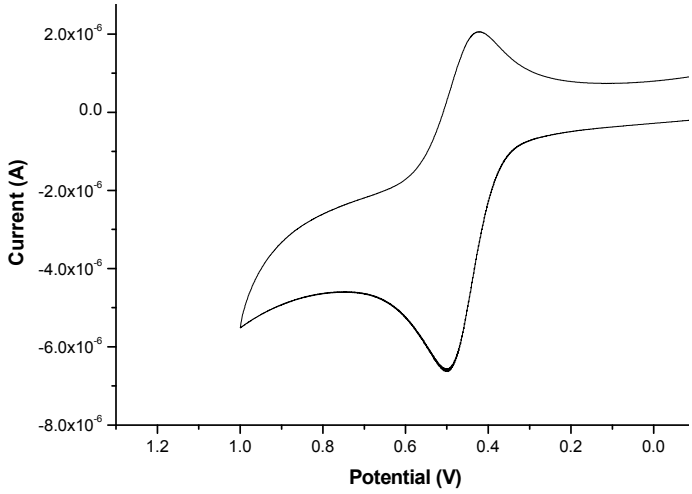


Figure S9. Cyclic voltammogram of **3-BPFA** in acetonitril/0.1 M tetrabutylammonium hexafluorophosphate; concentration of **3-BPFA**: 0.5 x 10^{-3} M. Scan rate of 50 mV/s.

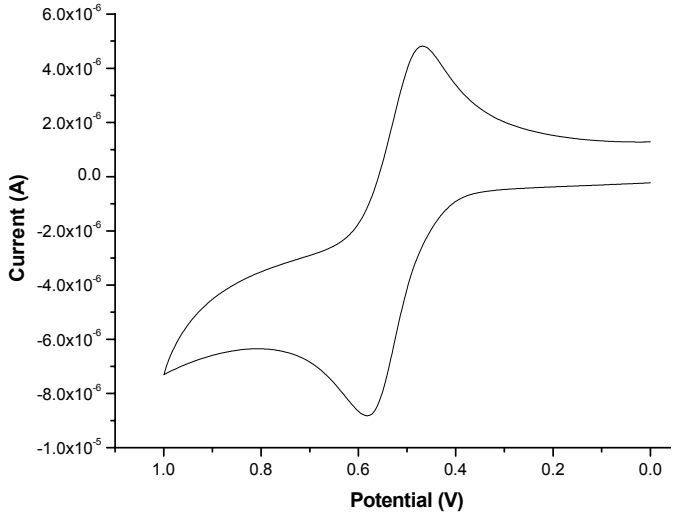


Figure S10. Cyclic voltammogram of **1** in acetonitril/0.1 M tetrabutylammonium

This journal is © The Royal Society of Chemistry 2007

hexafluorophosphate; concentration of **1**: 0.5 x 10^{-3} M. Scan rate of 50 mV/s.

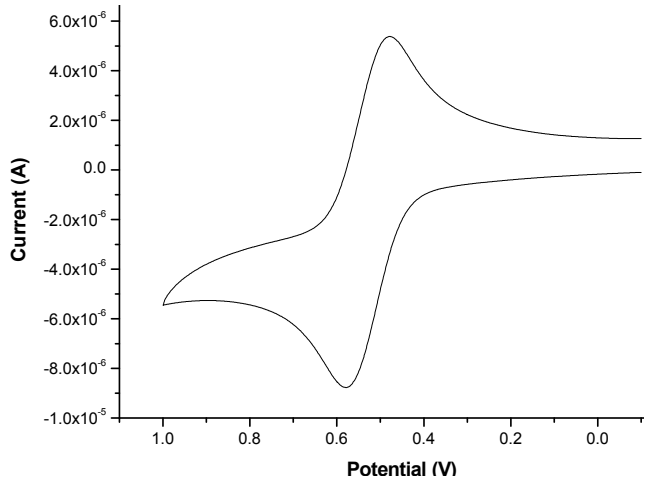


Figure S11. Cyclic voltammogram of **2** in acetonitril/0.1 M tetrabutylammonium hexafluorophosphate; concentration of **2**: 0.5 x 10^{-3} M. Scan rate of 50 mV/s.

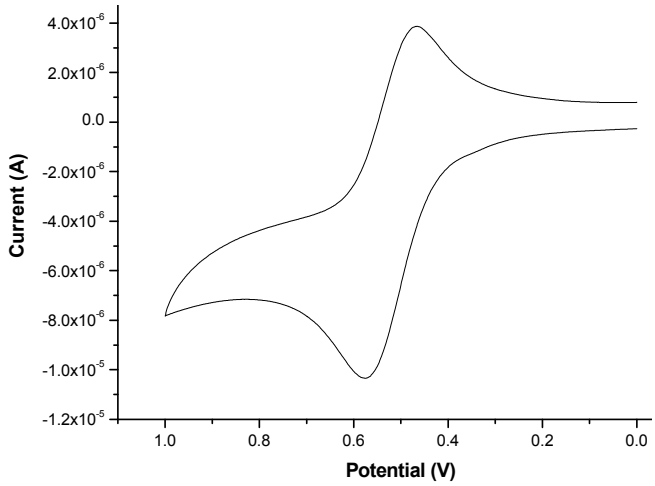


Figure S12. Cyclic voltammogram of **3** in acetonitril/0.1 M tetrabutylammonium hexafluorophosphate; concentration of **3**: 0.5 x 10^{-3} M. Scan rate of 50 mV/s.