Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for:

Spin-crossover in a homoleptic cobalt(II) complex containing a redox-active NNO ligand

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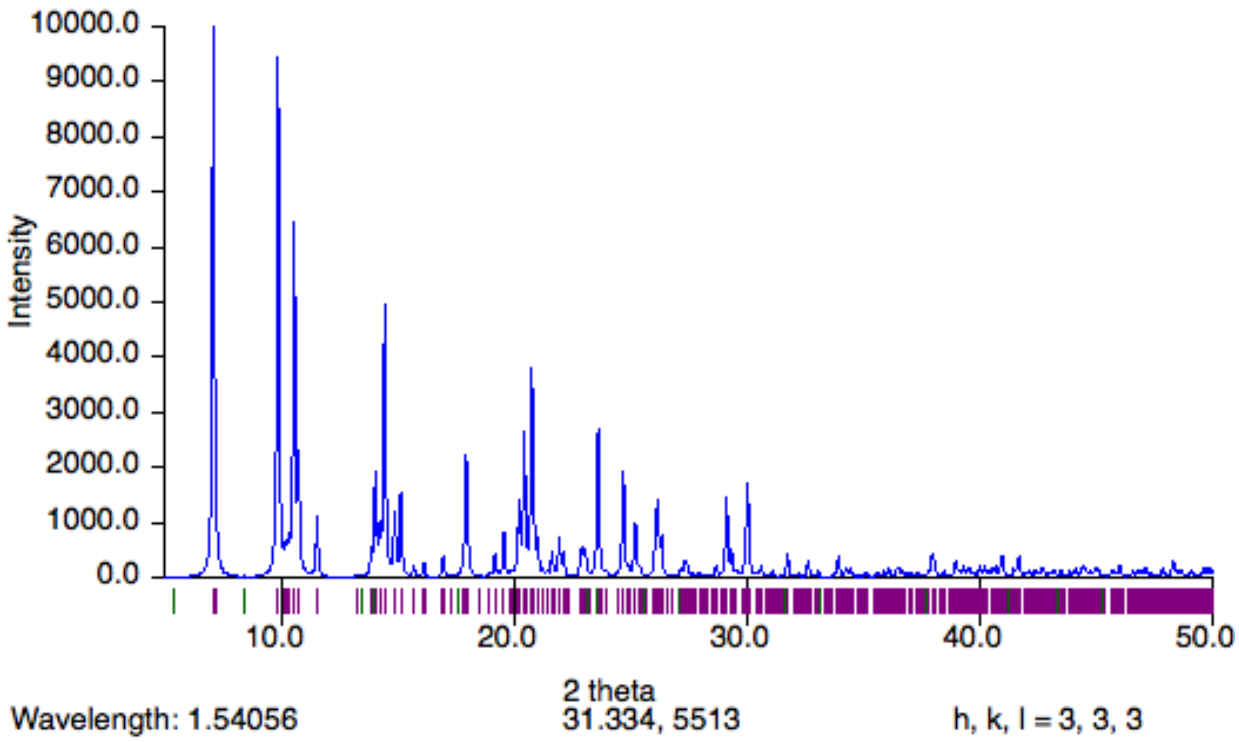

Figure S1. Calculated powder X-ray diffraction pattern for **2**.

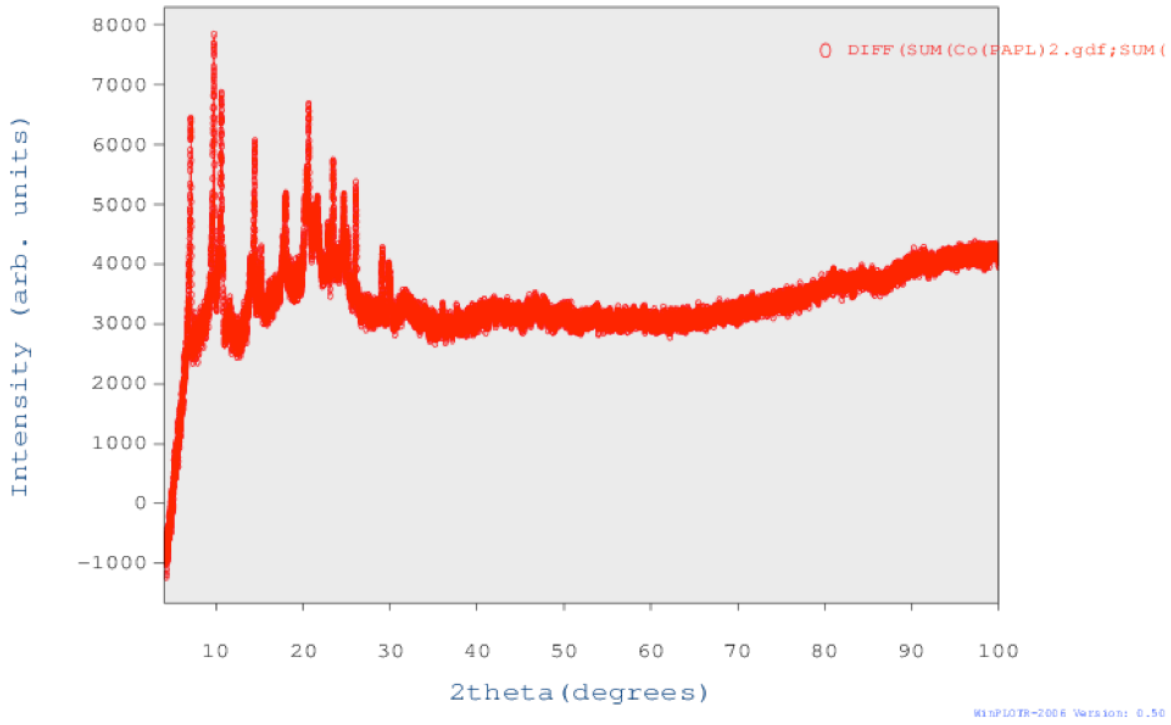

Figure S2. Experimental powder X-ray diffraction pattern for **2**.

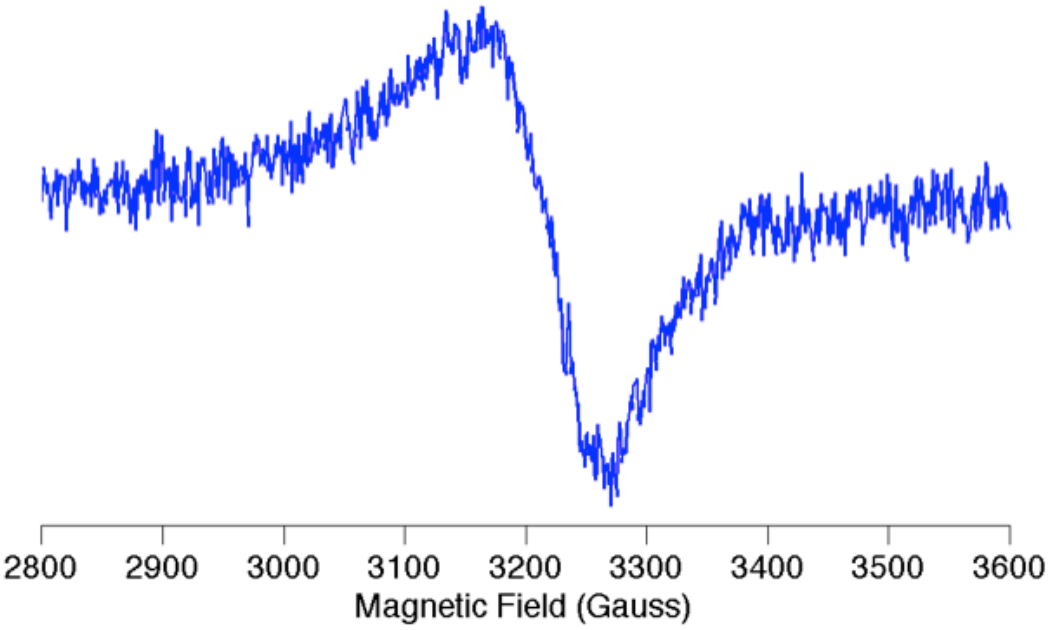

Figure S3. EPR spectrum of **2** at 100 K (powder).

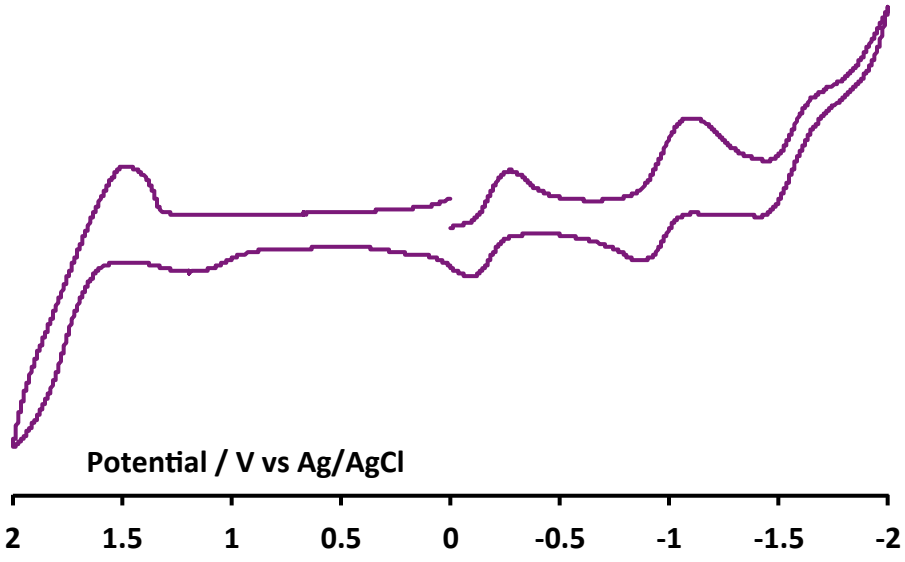

Figure S4. CV of **2** in CH_2Cl_2 containing ~0.5 M Bu_4NPF_6. Scan rate 100 mV/s.

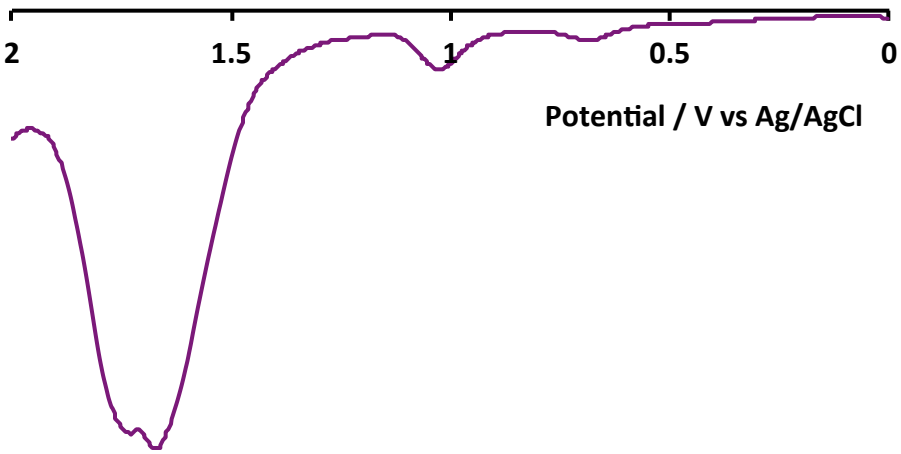

Figure S5. Anodic differential pulse voltammogram of **2** in CH_2Cl_2. Scan rate 25 mV/s.

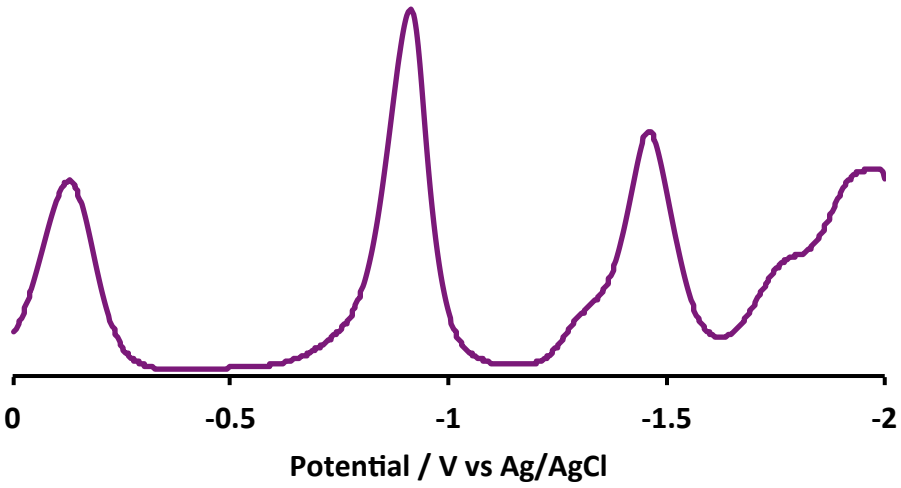

Figure S6. Cathodic differential pulse voltammogram of **2** in CH_2Cl_2. Scan rate 25 mV/s.

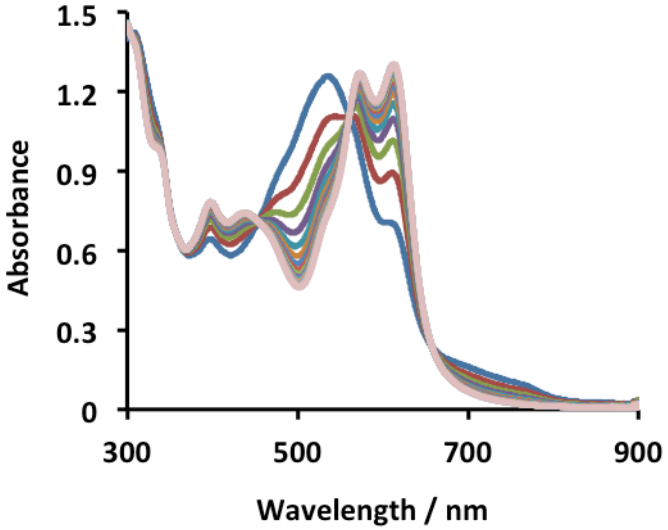

Figure S7. UV-visible spectrum of **2** in $CHCl_3$ (blue trace) followed by titration with ethanol (the final spectrum of the titration is the peach trace).

Table S1. Experimental coordinate bond distances (147 K) compared with DFT calculated [B3LYP/6-31G(d,p)] distances for the doublet spin state isomer.

Bond	Experimental distance (Å) [147(2) K structure]	Calculated distance (Å) (doublet spin state)
Co(1)-N(1) (N_{azo})	1.9127(17)	1.951
Co(1)-N(4) (N_{azo})	1.8651(17)	1.864
Co(1)-N(3) (N_{py})	2.0479(18)	2.143
Co(1)-N(6) (N_{py})	1.9685(18)	1.956
Co(1)-O(1)	2.1224(16)	2.147
Co(1)-O(2)	1.9982(15)	1.954