

Supporting Information

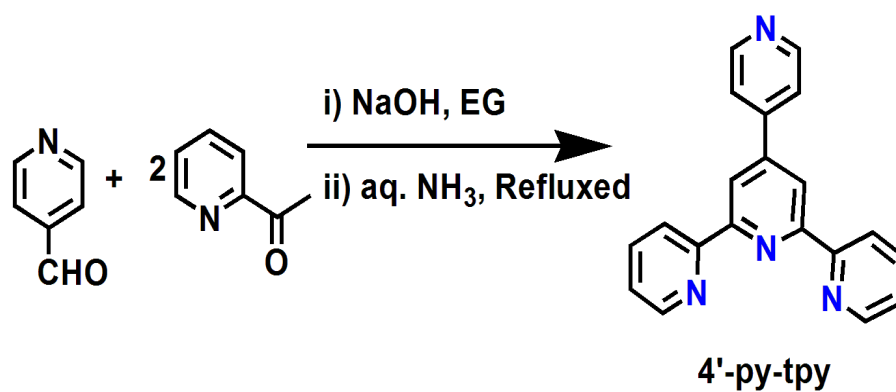
Fe-terpyridyl complex based multiple switches for application in molecular logic gate and circuit

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Scheme S1: Synthetic scheme for 4'-pyridyl-terpyridine (pytpy).

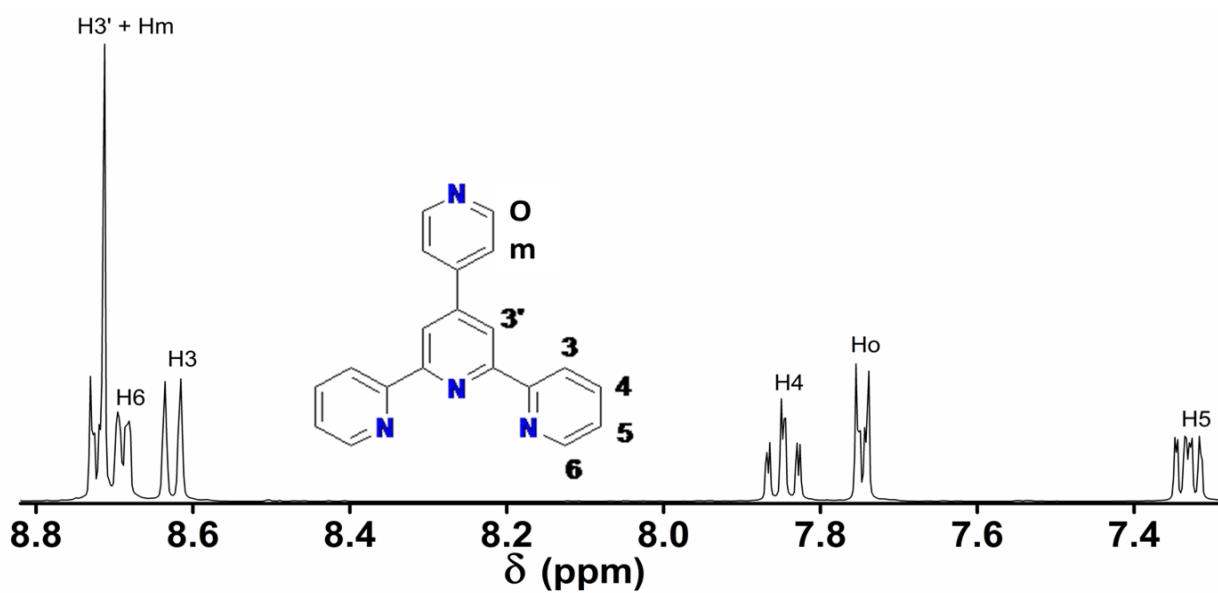
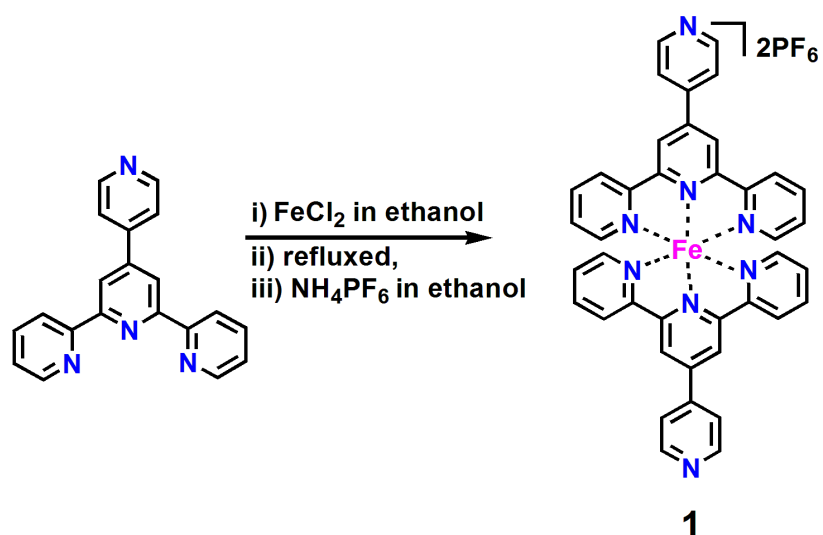


Fig.S1: ¹H NMR spectrum of 4'-pyridyl terpyridine (pytpy) in CDCl₃.



Scheme S2: Synthetic scheme for preparation of **1**.

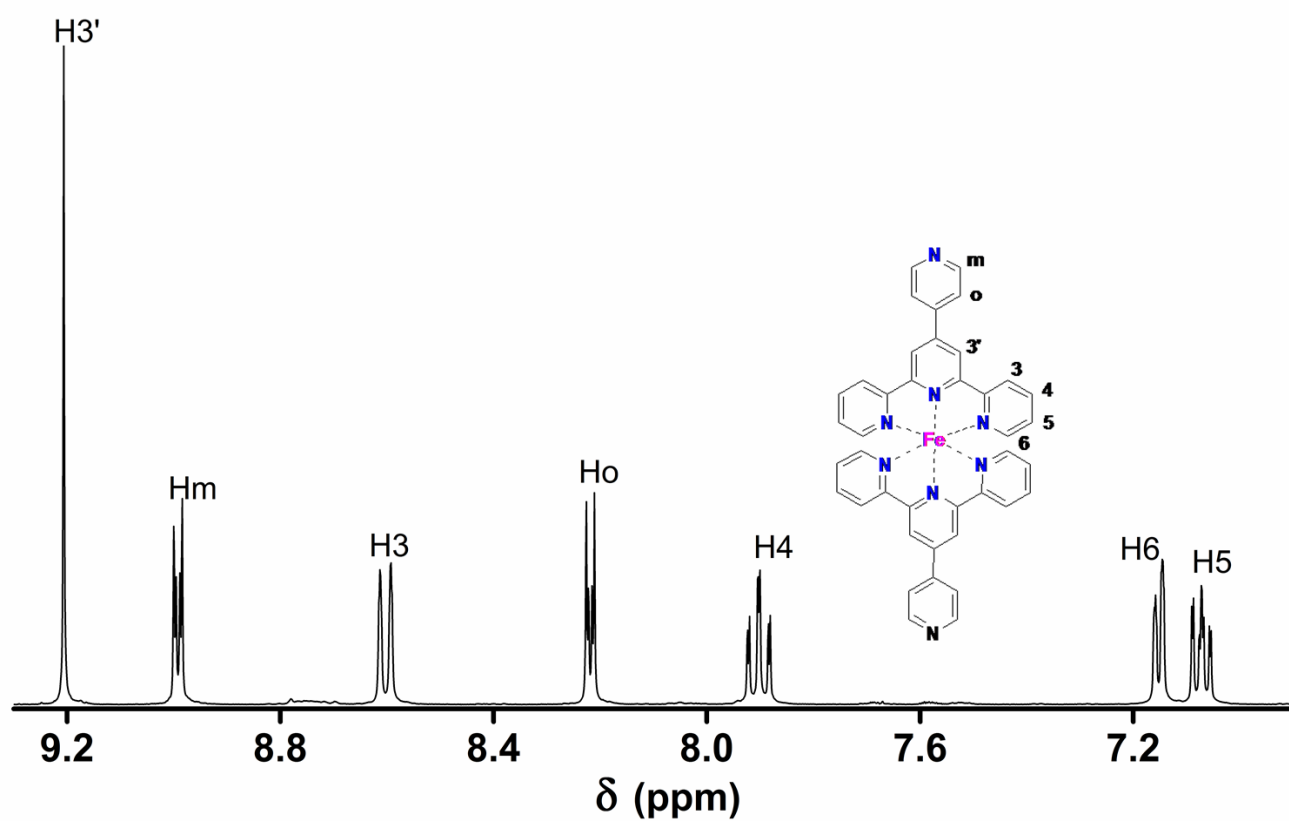


Fig. S2: ^1H NMR spectrum of **1** in CD_3CN . Charge on the metal center (Fe) is +2.

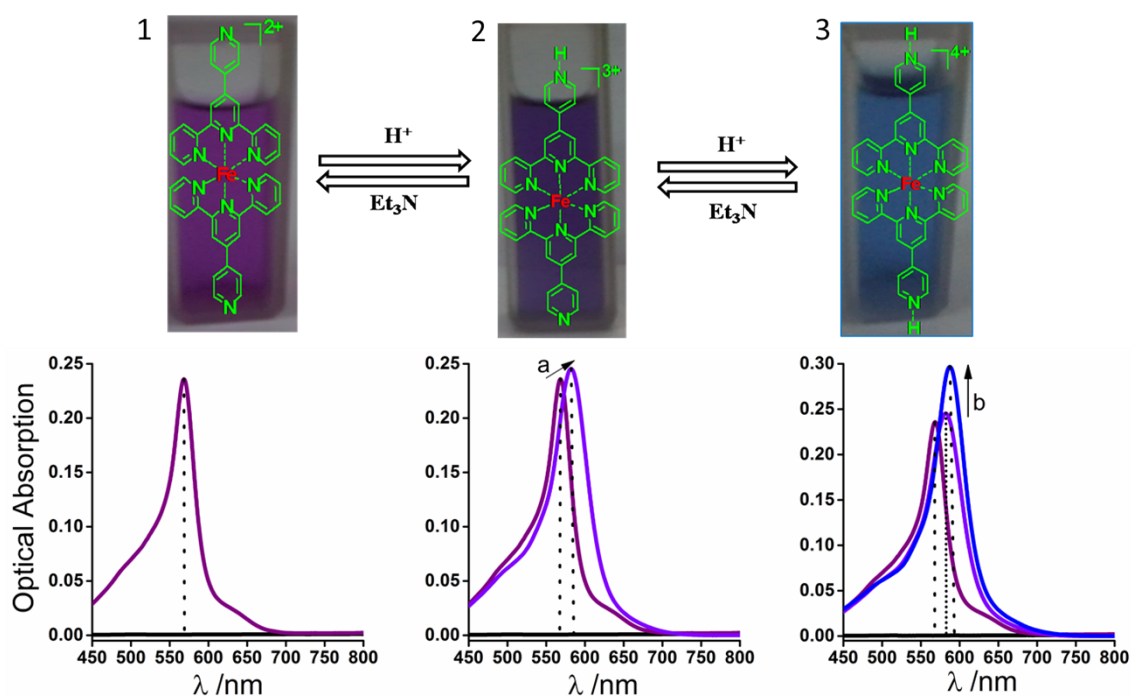


Fig. S3: (1) Native colour of **1** in dry CH_3CN and (below) corresponding UV-Vis spectrum ($^1\text{MLCT}$) with $\lambda_{\text{max}} = 569$ nm; (2) Addition of one eqv. of H^+ to **1** with colour changing from purple to blue and (below) 'a' represents bathochromic shift of 13 nm to 582 nm and increase in molar absorptivity in $^1\text{MLCT}$ of **1**; (3) Addition of another eqv. of H^+ to **1** changed colour to light blue and (below) 'b' represents changes in the UV-Vis spectrum; (4) Excess of H^+ could not produce any further changes. Use of Et_3N leads to original state of **1**. Black line in the UV-Vis spectra represent baseline with dry CH_3CN .

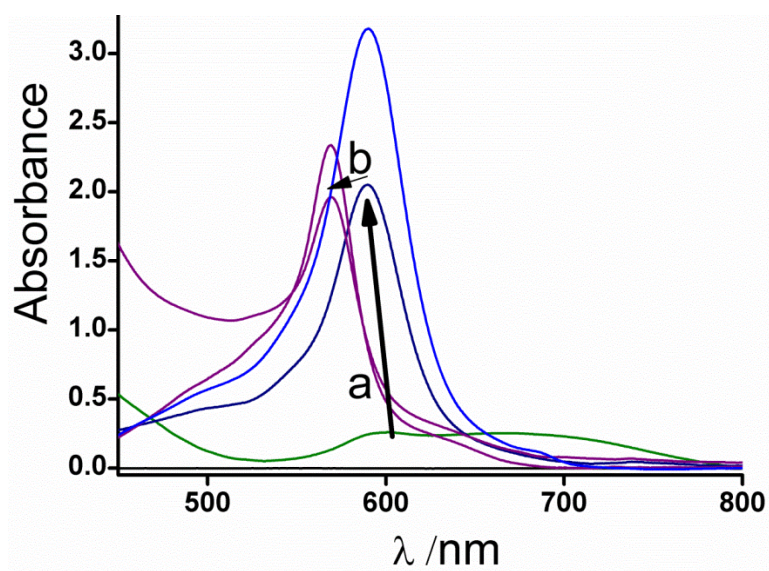


Fig. S4: Representation of getting back to original state of **1** via stepwise addition of a) 5 μL of D.I water: Fe(III) to Fe(II); b) two eqv. of NO^+ : shift the λ_{max} to original value of 569 nm.

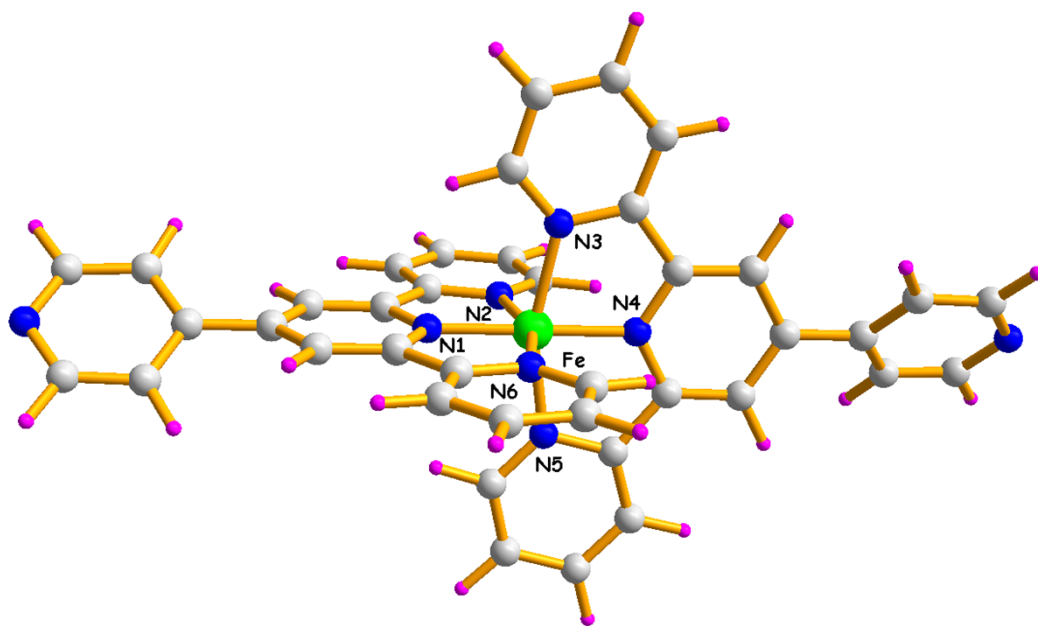


Fig. S5a: DFT-optimized structures of 1^{2+}

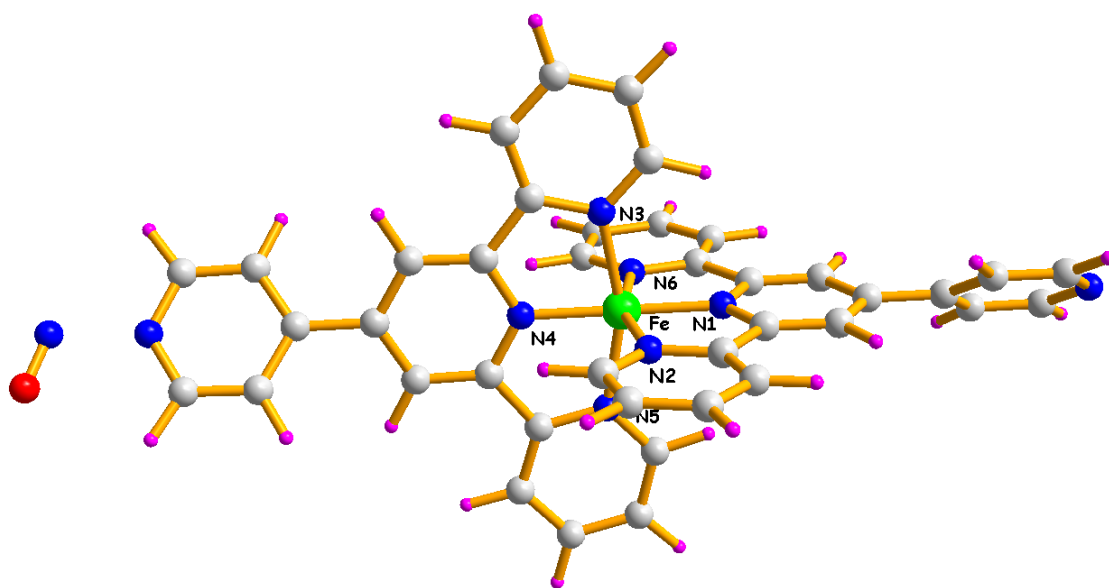


Fig. S5b: DFT-optimized structures of 2^{3+}

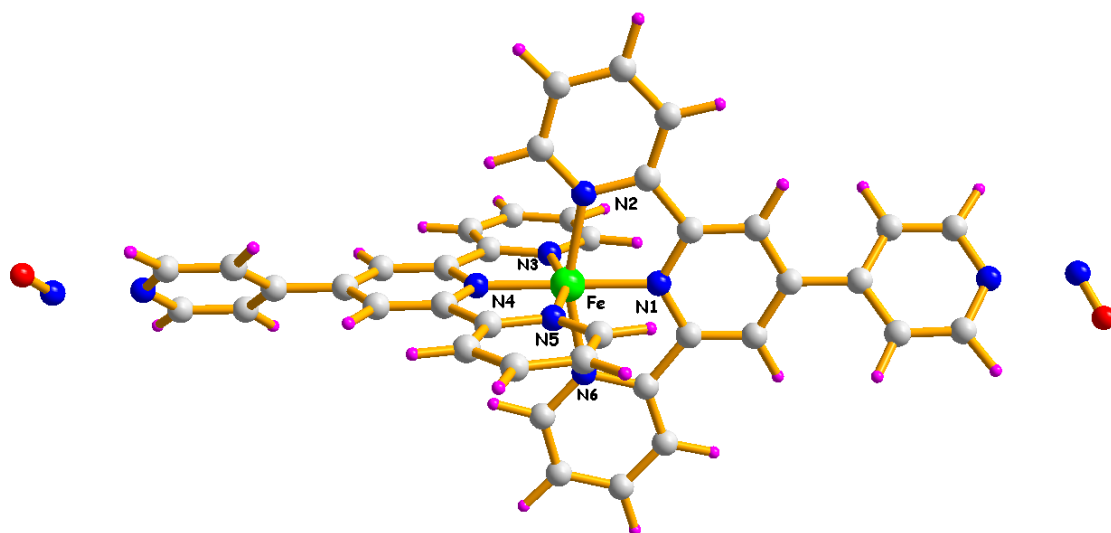


Fig. S5c: DFT-optimized structures of 3^{4+}

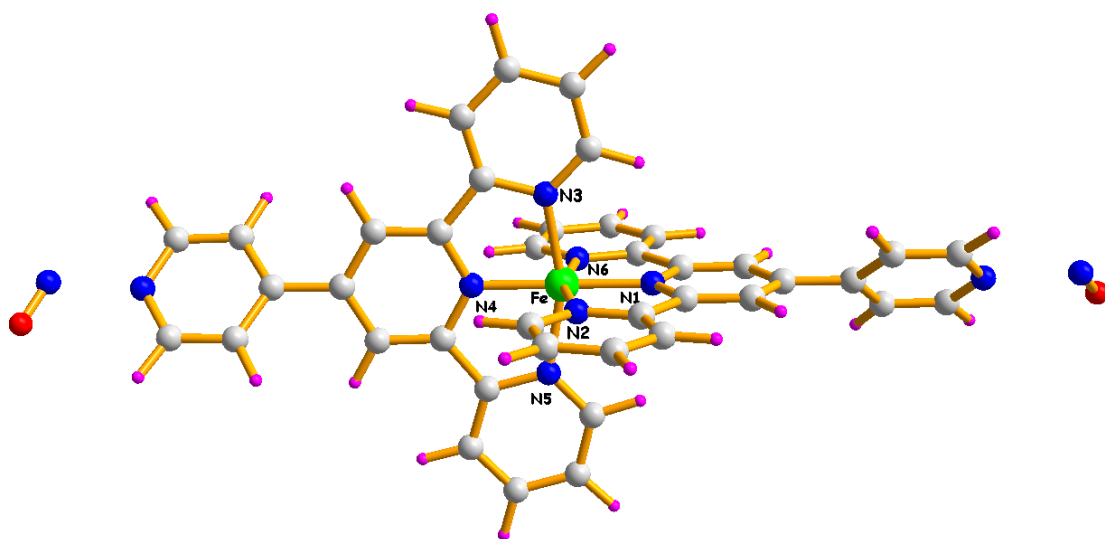


Fig. S5d: DFT-optimized structures of 4^{5+}

Table S1

	2 ⁺	3 ⁺ (NO)	4 ⁺ (NO) ₂	5 ⁺ (NO) ₂
Fe–N2	2.0371	2.0415	2.0420	2.0099
Fe–N1	1.9176	1.9236	1.9267	1.9271
Fe–N6	2.0372	2.0414	2.0421	2.0100
Fe–N5	2.0371	2.0337	2.0420	2.0099
Fe–N4	1.9175	1.9143	1.9265	1.9271
Fe–N3	2.0371	2.0336	2.0421	2.0100
N–NO	-	1.8619	1.9147	2.0438
N–O	-	1.1220	1.1165	1.1054
∠O–N··N	-	110.951	111.141	112.360
N–NO	-	-	1.9144	2.0438
N–O	-	-	1.1166	1.1055
∠O–N··N	-	-	111.097	112.362

Table S2

M.Os	Energy (eV)			
	2 ⁺	3 ⁺	3 ⁺ (NO)	4 ⁺ (NO) ₂
HOMO	-10.94	-12.1	-15.03	-18.52
LUMO	-7.55	-11.82	-12.95	-14.89

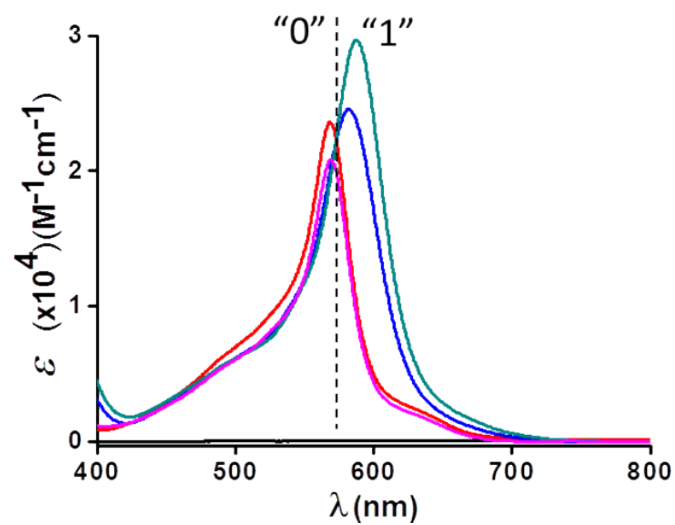


Fig. S6: Change in UV-Vis spectra of **1** upon exposing to different chemical inputs. (a) MLCT spectra of **1** (red line), (b) after addition of one eqv H⁺ (blue line), (c) after addition of two eqv H⁺ (grey line), (d) with more than two equivalent of Et₃N (pink line) and acetonitrile baseline (black line).

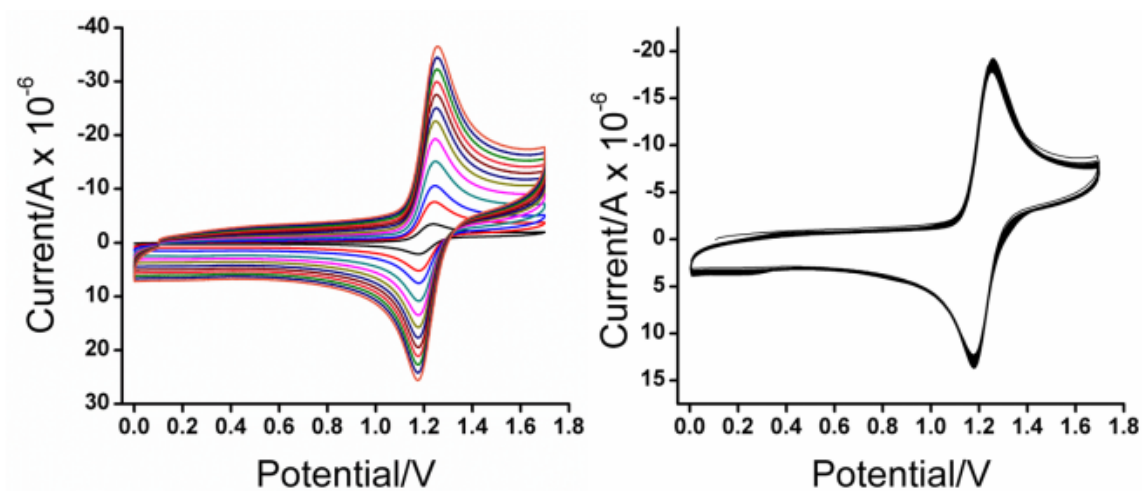


Fig. S7: (Left) cyclic voltammogram of **1** in dry CH₃CN at scan rates 10 mV s⁻¹ to 1000 mV s⁻¹. (Right) cyclic voltammograms of **1** recorded for 300 cycles at a scan rate of 300 mV s⁻¹ under the identical conditions.