

Electronic Supplementary Information for:

Redox and acid–base properties of asymmetric non-heme (hydr)oxo-bridged diiron complexes

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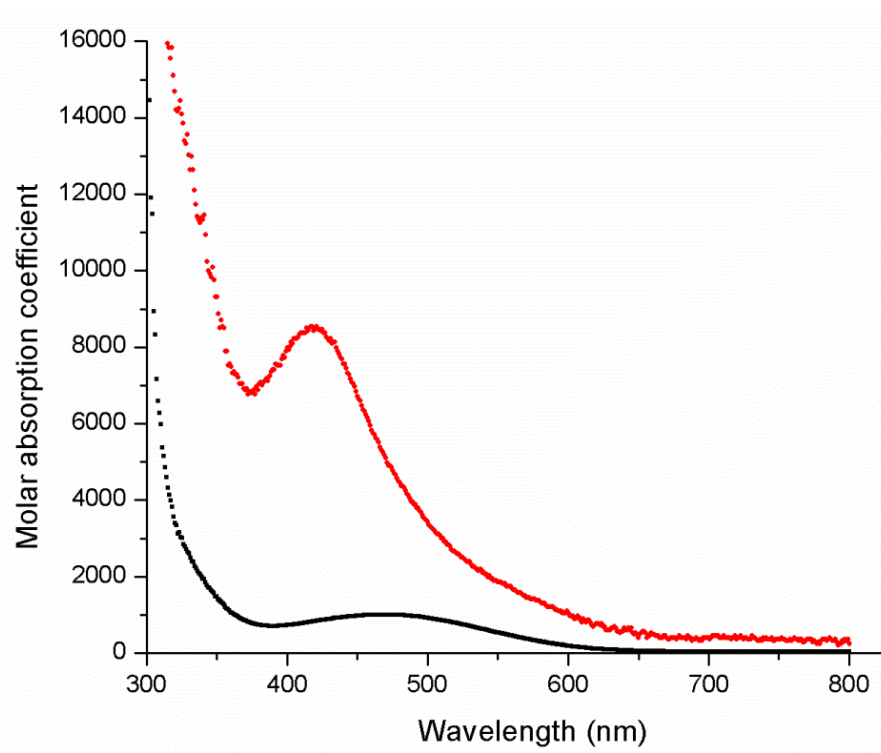


Figure S1. UV-Vis spectrum of [(FeL)₂] (4) in MeCN (λ_{max} at 471 nm, $\epsilon = 1000$) (black) and after exposure to air (λ_{max} at 420 nm, $\epsilon = 8500$), (red).

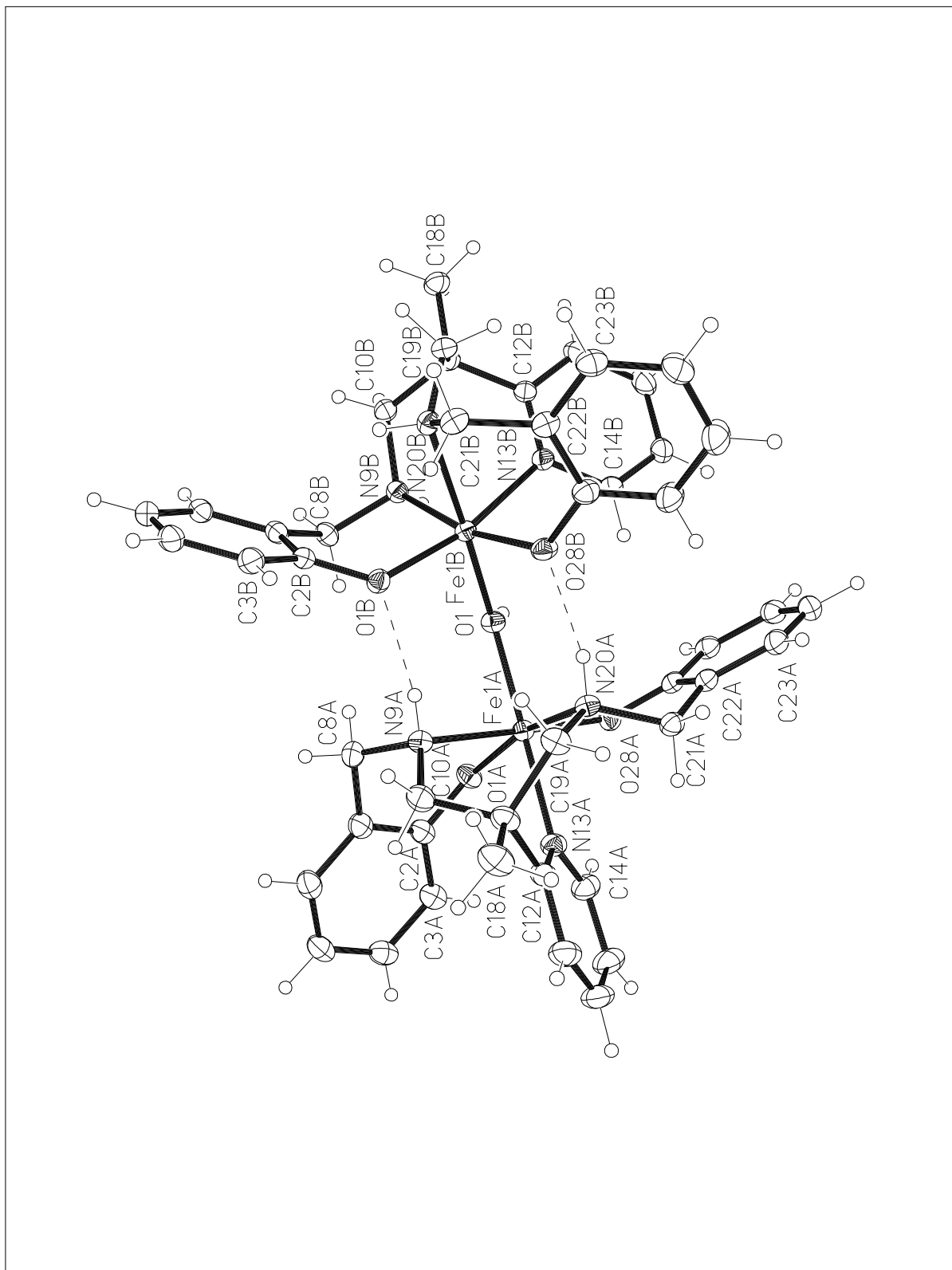


Figure S2. Representation of the X-ray structure of the cationic portion of $[(\text{FeL})_2(\mu\text{-OH})]\text{BPh}_4 \cdot \text{CH}_2\text{Cl}_2$ ($1 \cdot \text{CH}_2\text{Cl}_2$).

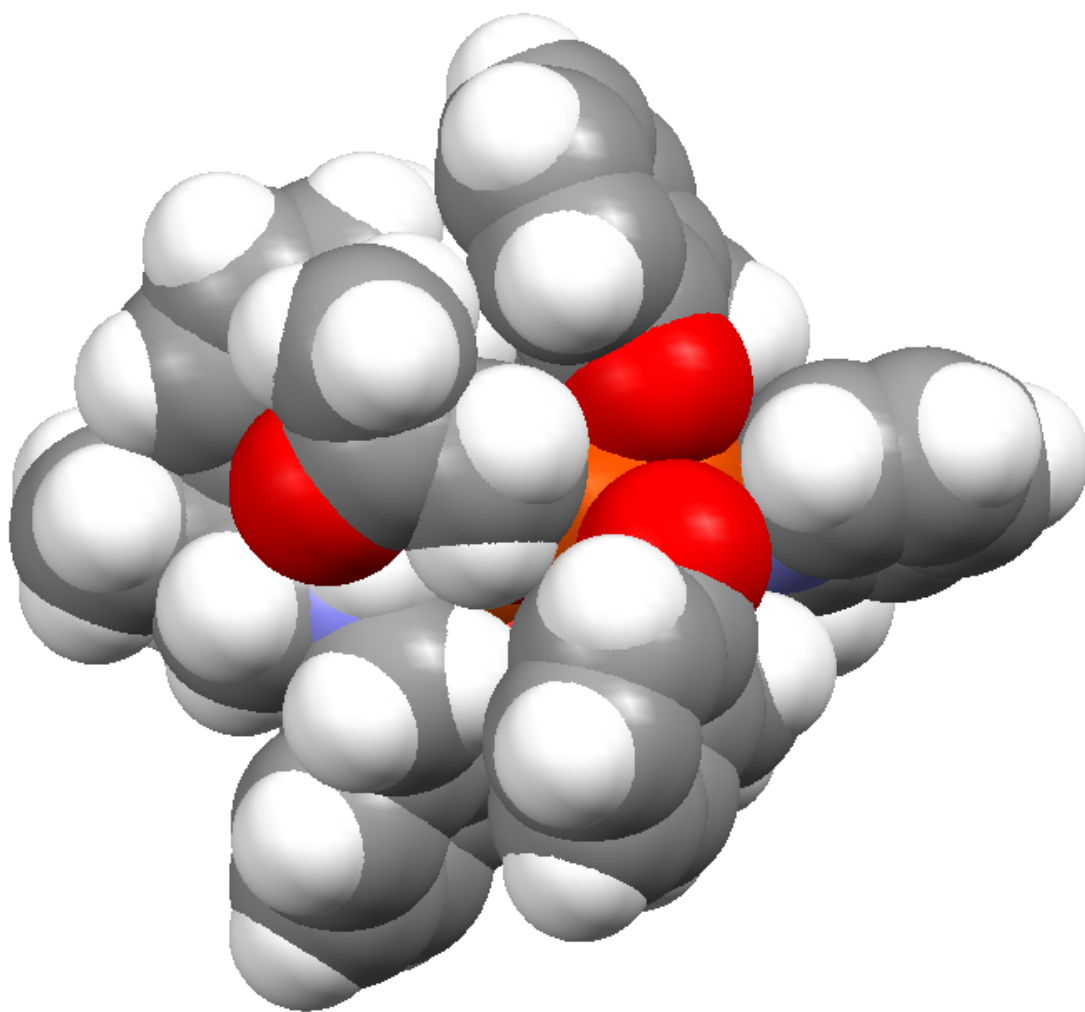


Figure S3. Space-filling representation of $[(\text{FeL})_2(\mu\text{-O})]\cdot(\text{CH}_3)_2\text{CO}$ ($2\cdot(\text{CH}_3)_2\text{CO}$).

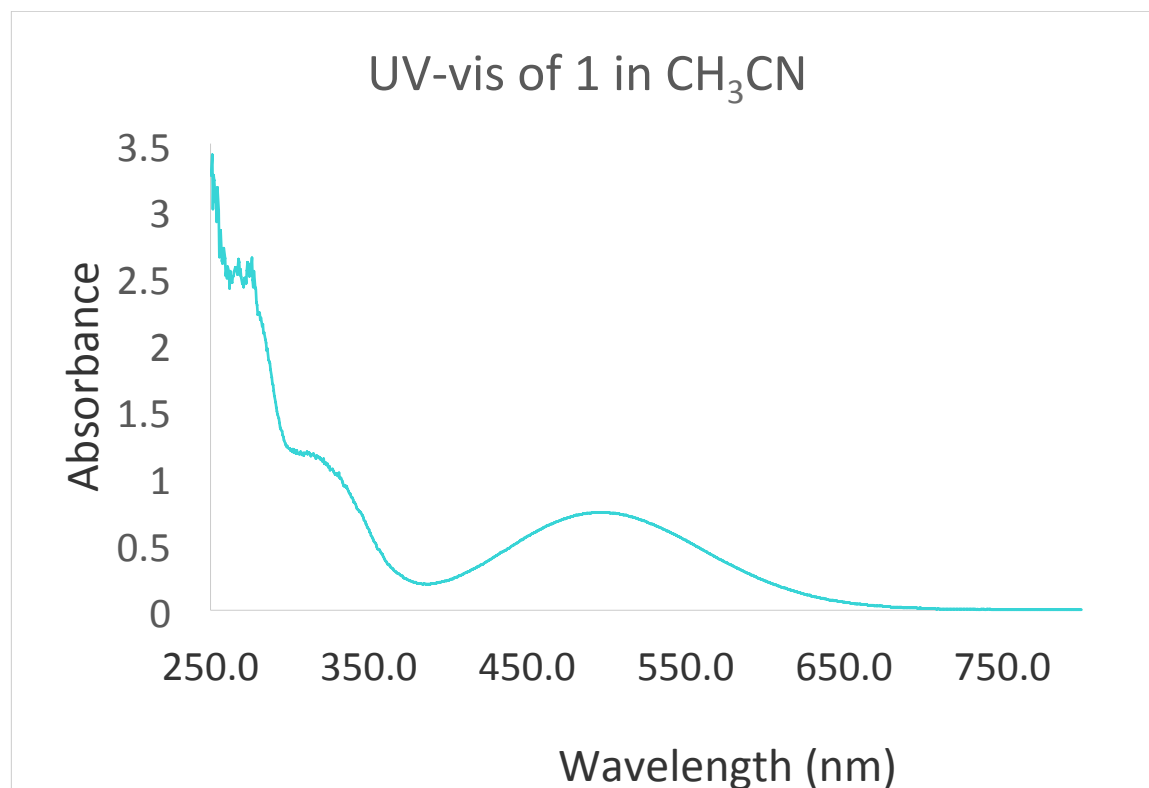


Figure S4. UV-visible spectrum of a CH₃CN solution of **1**.

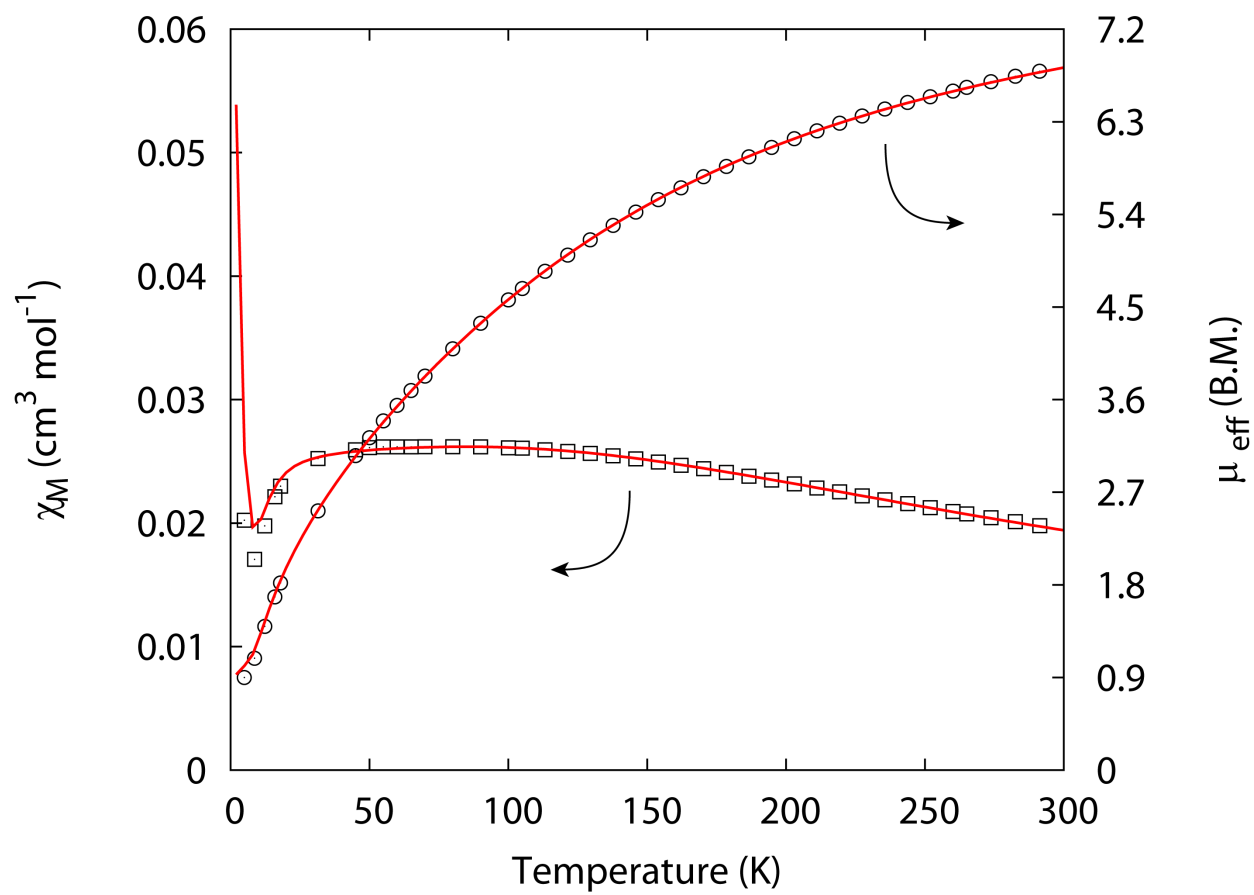


Figure S5. Plot of molar susceptibility vs. temperature for crystalline $1 \cdot \text{CH}_2\text{Cl}_2$.

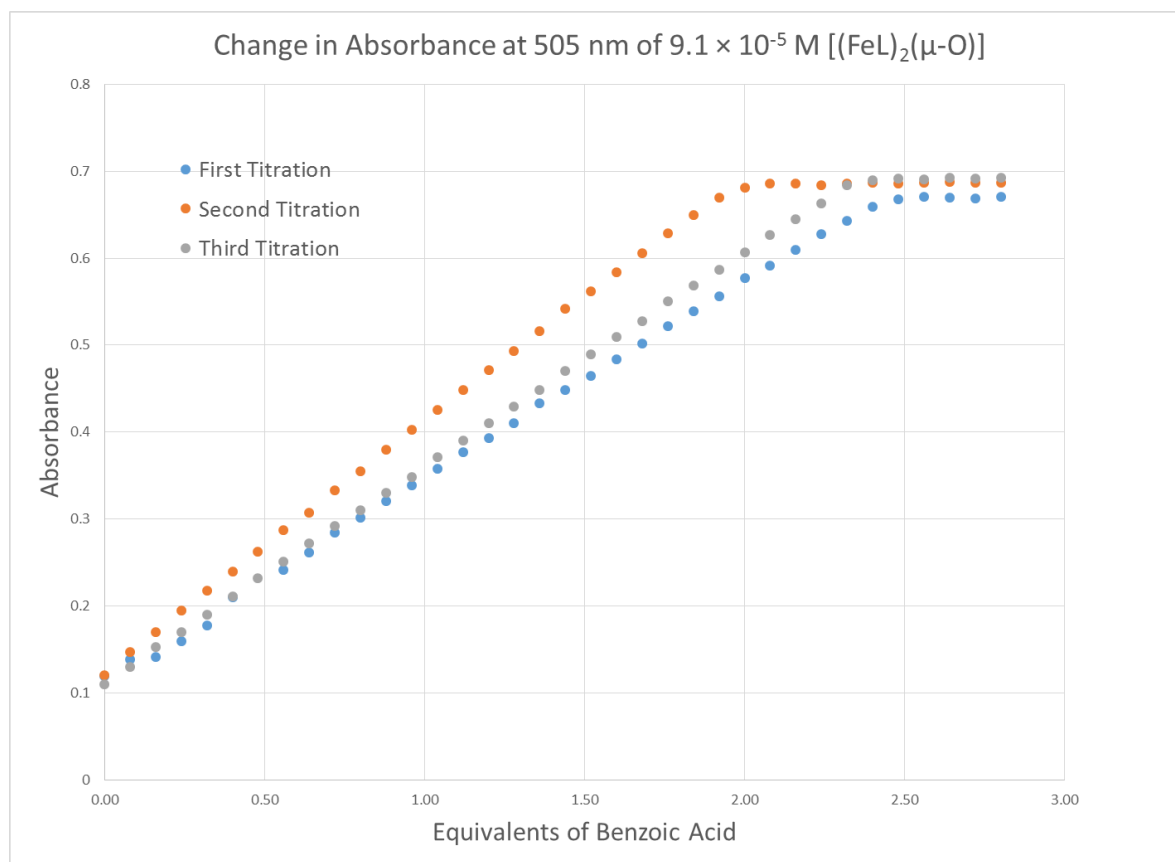


Figure S6. Change in absorbance at 505 nm of 9.1×10^{-5} M **2** with addition of benzoic acid (9.1×10^{-4} M) in acetonitrile.

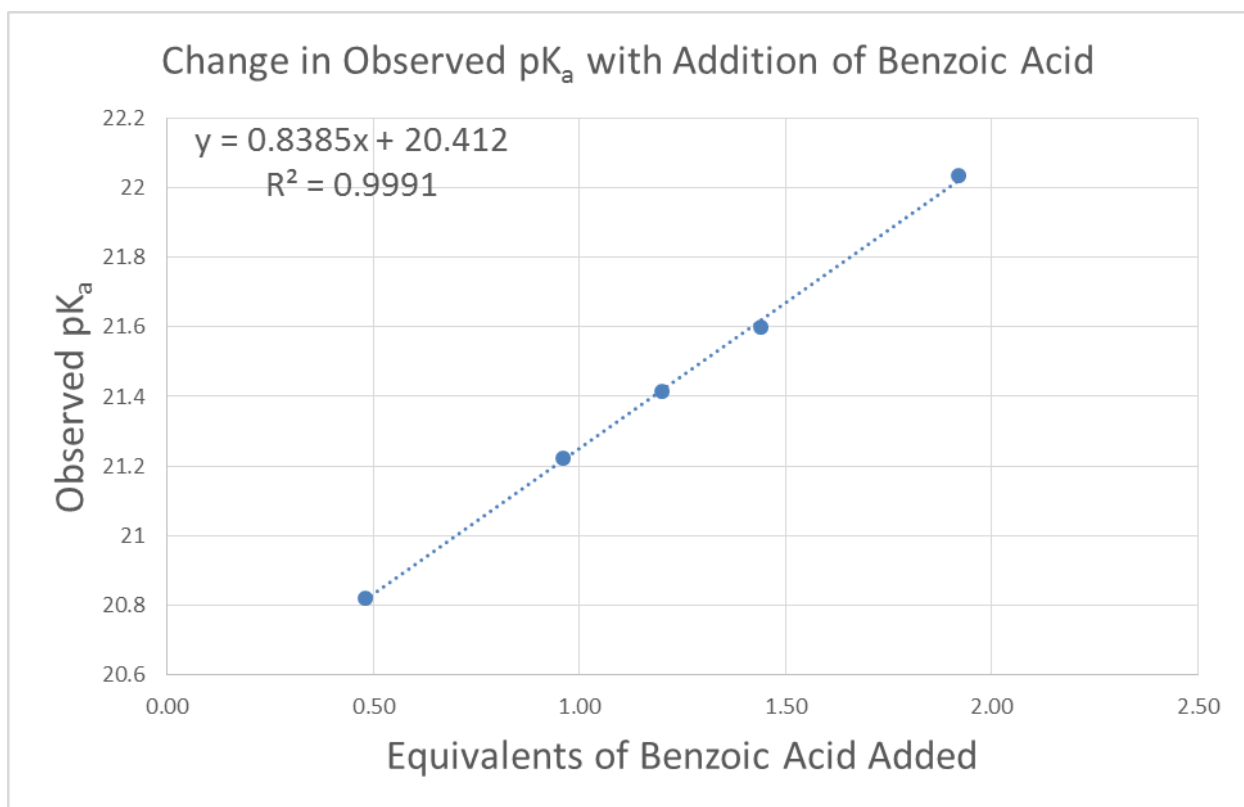


Figure S7. Change in calculated pK_a value for **2** as more equivalents of benzoic acid are added. The theoretical value if no benzoic acid were present can be estimated from the y-intercept; 20.4 in this case.

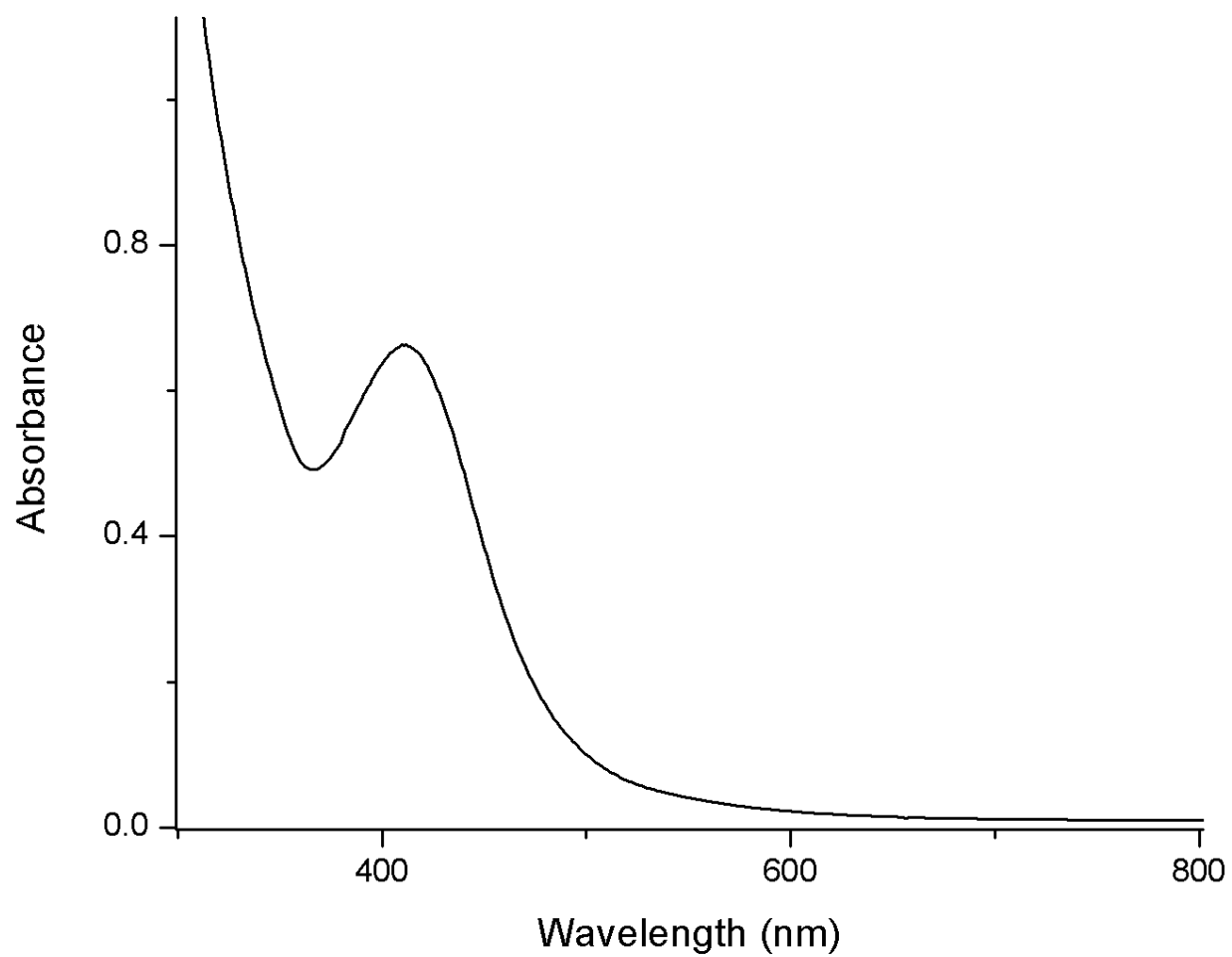


Figure S8. UV-visible spectrum of $\text{CoCp}_2\text{BPh}_4$ ($0.9 \times 10^{-3} \text{ M}$) in MeCN . Molar absorptivity at 412 nm = $262 \text{ M}^{-1}\text{cm}^{-1}$.

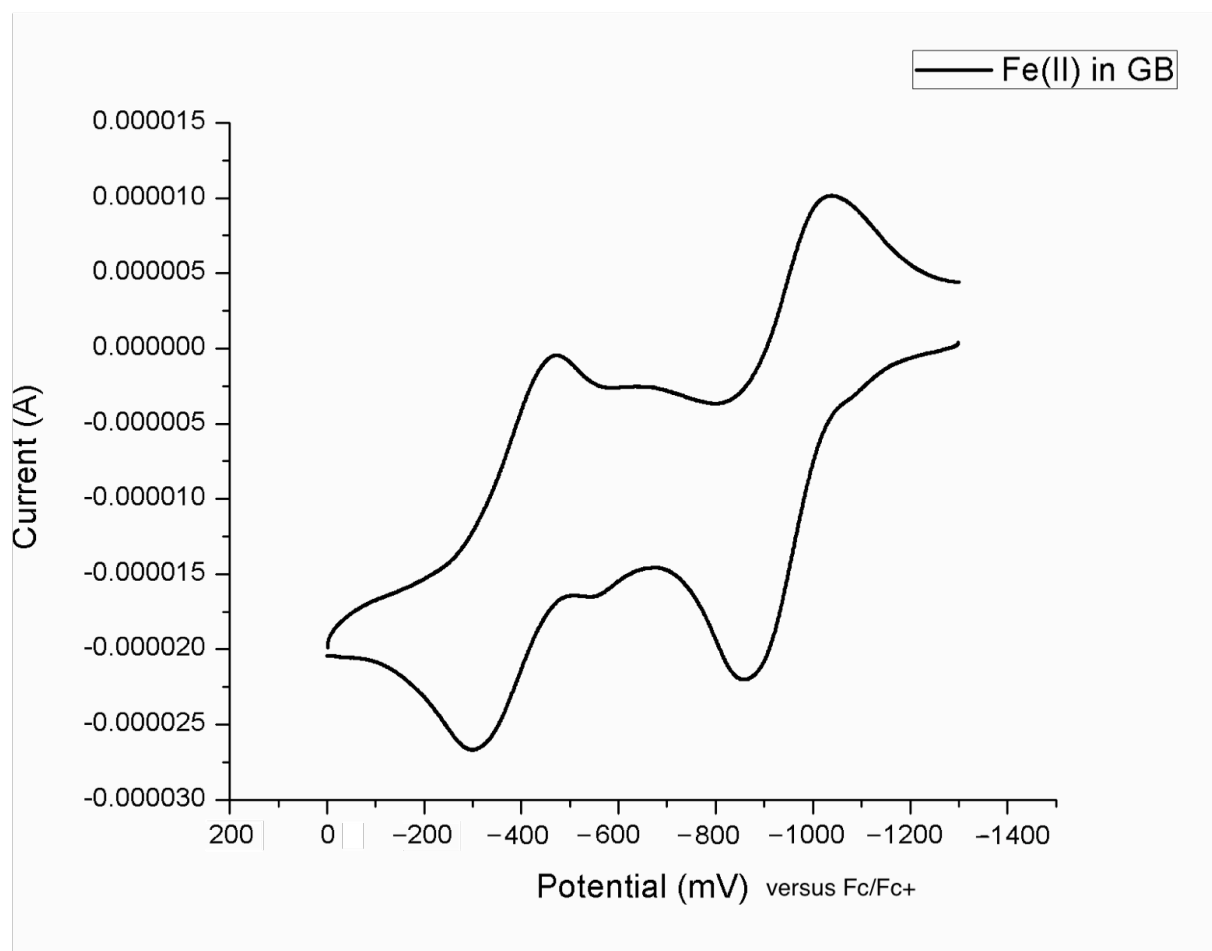


Figure S9. Cyclic voltammogram (scan rate = 100 mV s⁻¹; 0.1 M TBAPF₆ supporting electrolyte) of a 1 mM solution of **4** in CH₃CN.