

Supplementary Materials: Hydrogenase Biomimetics with Redox-Active Ligands: Synthesis, Structure, and Electrocatalytic Studies on $[\text{Fe}_2(\text{CO})_4(\kappa^2\text{-dppn})(\mu\text{-edt})]$ (edt = Ethanedithiolate; dppn = 1,8-bis(Diphenylphosphino)Naphthalene)

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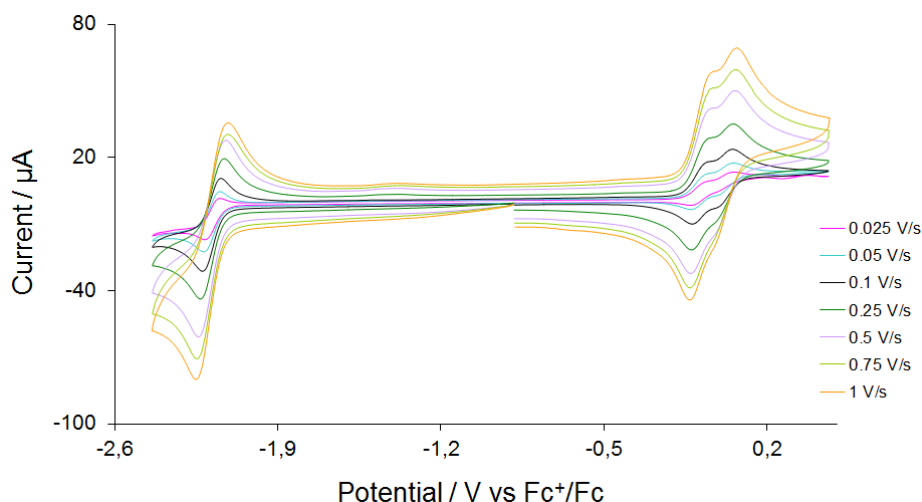


Figure S1. CVs of $[\text{Fe}_2(\text{CO})_4(\kappa^2\text{-dppn})(\mu\text{-edt})]$ (3) at various scan rates as shown in the legend (in MeCN, 1 mM solution, supporting electrolyte $[\text{NBu}_4][\text{PF}_6]$, scan rate $0.1 \text{ V}\cdot\text{s}^{-1}$, glassy carbon electrode, potential vs Fc^+/Fc).

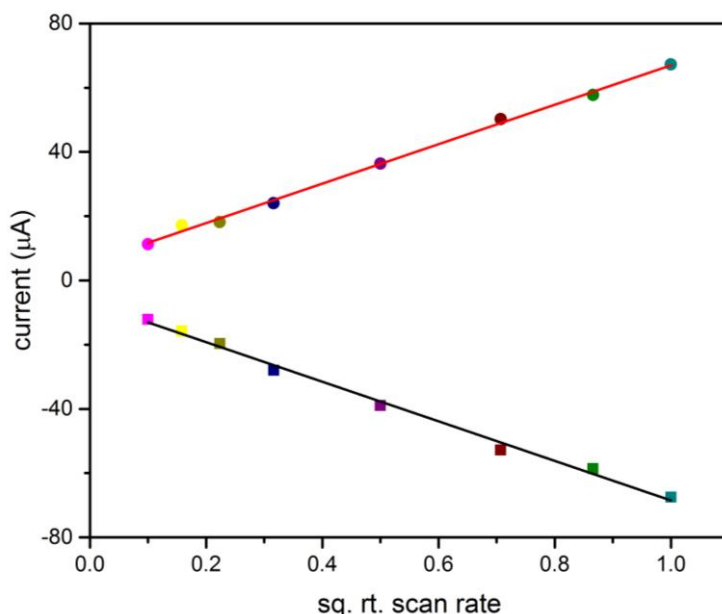


Figure S2. Scan rate dependence of the cathodic and anodic peak currents for the reduction of $[\text{Fe}_2(\text{CO})_4(\kappa^2\text{-dppn})(\mu\text{-edt})]$ (3) in MeCN (1 mM solution, supporting electrolyte $[\text{NBu}_4][\text{PF}_6]$, glassy carbon electrode, potential vs Fc^+/Fc). Lines show best linear fit of data.

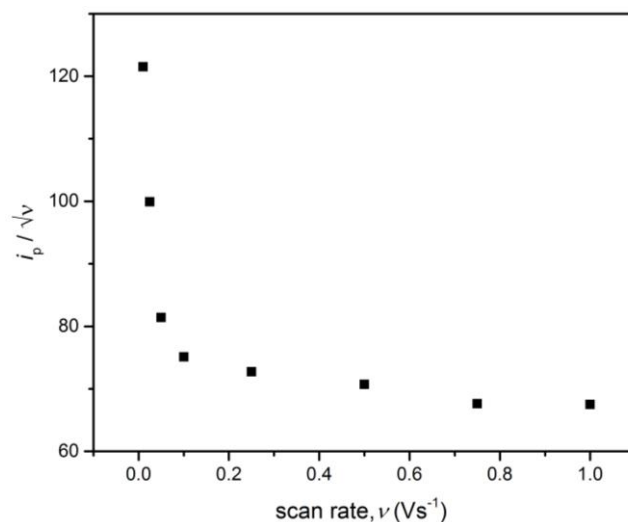


Figure S3. Scan rate (ν) dependence of the current function ($i_p/\sqrt{\nu}$) for the reduction of $[\text{Fe}_2(\text{CO})_4(\kappa^2\text{-dppn})(\mu\text{-edt})]$ (**3**) (1 mM solution in MeCN, supporting electrolyte $[\text{NBu}_4][\text{PF}_6]$, glassy carbon electrode, potential vs Fc^+/Fc).

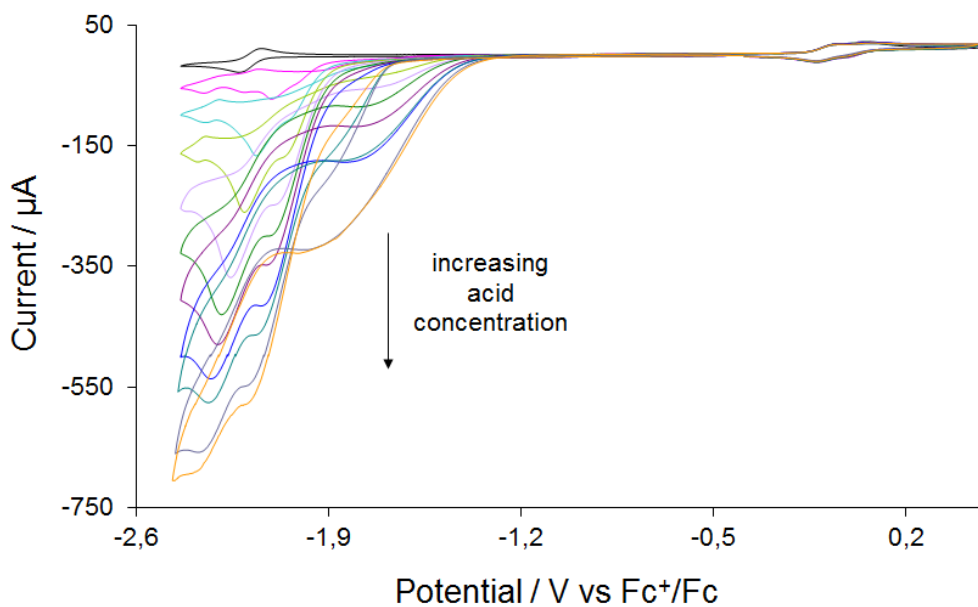


Figure S4. CVs of $[\text{Fe}_2(\text{CO})_4(\kappa^2\text{-dppn})(\mu\text{-edt})]$ (**3**) in the absence of acid and in the presence of 1–10 equivalents of $\text{CF}_3\text{CO}_2\text{H}$ (in MeCN, 1 mM solution, supporting electrolyte $[\text{NBu}_4][\text{PF}_6]$, scan rate $0.1 \text{ V}\cdot\text{s}^{-1}$, glassy carbon electrode, potential vs Fc^+/Fc).