Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2015

Electronic Supplementary Information

Diiron hexacarbonyl complexes bearing naphthalene-1,8-dithiolate moiety bridge as the mimics of the sub-unit of [FeFe]-hydrogenase: Synthesis, characterisation and electrochemical investigations

Guifen Qian,^b Wei Zhong,^a Zhenhong Wei,^b Hailong Wang,^a Zhiyin Xiao,^a Li

Long^a and Xiaoming Liu*^{a, b}

^a College of Biological and Chemical Engineering, Jiaxing University (Jiaxing 314001, China)

^b School of Chemistry, Nanchang University, Nanchang (Jiangxi 330031, China)

*E-mail: xiaoming.liu@mail.zjxu.edu.cn



Fig. S1 Infrared spectra of diiron hexacarbonyl complexes in DCM.



Fig. S2 UV/Vis spectra of diiron hexacarbonyl complexes (c = 1×10^{-4} mol L⁻¹) in acetonitrile.



Fig. S3 Cyclic voltammograms of complexes **5a**, **5b**, **6a**, **6b**, **7** and **8** (C = 2.86 mmol L^{-1}) on vitreous carbon electrode in 0.1 mol L^{-1} [NBu₄]BF₄ / CH₃CN (dot line) or 0.5 mol L^{-1} [NBu₄]BF₄ / DCM (solid line) solution at a scan rate of 0.1 Vs⁻¹ (298 K, *vs* Fc⁺ / Fc). Blue or red colour is used to distinguish the CVs obtained within various ranges of scanning potentials.



Fig. S4 Cyclic voltammgrams of the disulfides 2a (top) and 2b (bottom) in DCM at a scan rate of 0.1 Vs⁻¹ (298 K, *vs* Fc⁺ / Fc).





Fig. S5 Cyclic voltammogras of the complexes at various scanning rates (Vs⁻¹) in DCM (298 K, *vs* Fc⁺ / Fc).



Fig. S6 Current functions of diiron hexacarbonyl complexes in MeCN.





Fig. S7 Catalytic reduction of proton in MeCN-acetic acid at a scan rate of 0.1 Vs^{-1} (298 K, *vs* Fc⁺ / Fc).



Fig. S8 Cyclic voltammogram of acetic acid (30 mmol L^{-1} , 10 eq. of the diiorn mimics (please refer to Fig. 5)) in MeCN at a scan rate of 0.1 Vs⁻¹ (298 K, *vs* Fc⁺ / Fc).