

Supplementary material

Tuning the electronic properties of $\text{Fe}_2(\mu\text{-arenedithiolate})(\text{CO})_{6-n}(\text{PMe}_3)_n$ ($n=0, 2$) complexes related to the [Fe-Fe]-hydrogenase active site

Lennart Schwartz^a, Pradyumna S. Singh^a, Lars Eriksson^b, Reiner Lomoth^a, Sascha Ott^{*a}

^aDepartment of Photochemistry and Molecular Science, Uppsala University, Box 523, 751 20 Uppsala, Sweden.

E-mail: Sascha.Ott@fotomol.uu.se

^bDivision of Structural Chemistry, Arrhenius Laboratory, Stockholm University, 106 91 Stockholm, Sweden

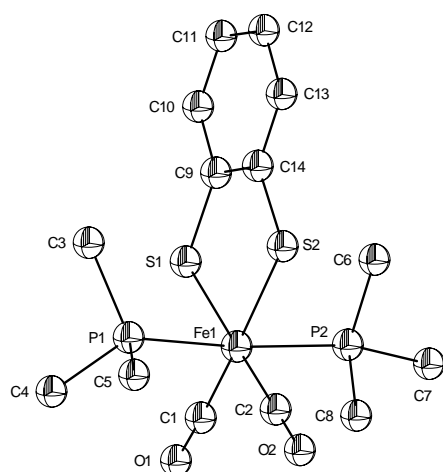


Figure 1. Thermal ellipsoid representations (50% probability) of the molecular structure of $[\text{Fe}(1,2\text{-benzenedithiolate})(\text{CO})_2(\text{PMe}_3)_2]$ (**1c**).

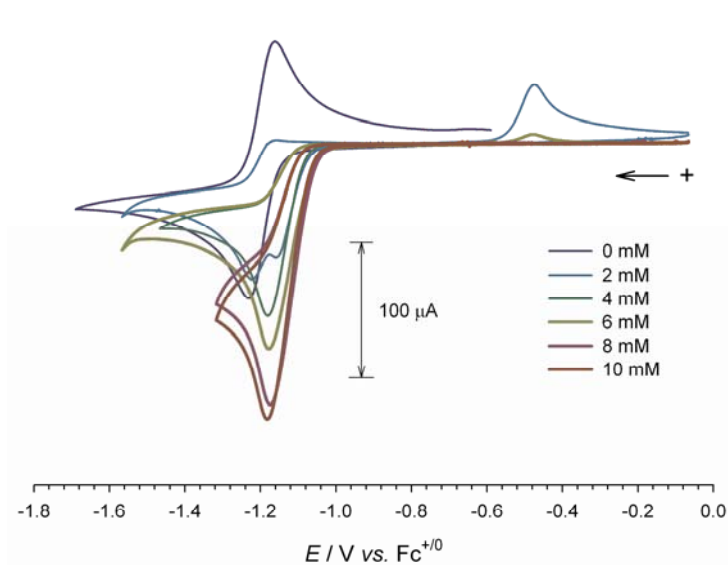


Figure 2. Cyclic voltammograms ($\nu = 100$ mV/s) of complex **3a** (2 mM) on glassy carbon electrode in CH_3CN (0.1 M $(\text{Bu})_4\text{NPF}_6$) solution with trifluoromethanesulfonic acid (0-10 mM).

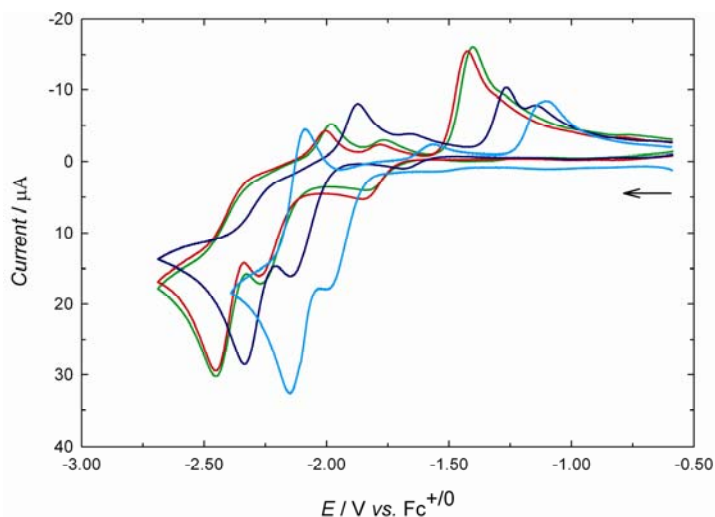


Figure 3. Cyclic voltammograms ($v = 100$ mV/s) of **1c** (1.22 mM, green trace), **2c** (1.13 mM, red trace), **3c** (1.14 mM, blue trace) and **7c** (1.03 mM, cyan trace) in acetonitrile (0.1 M $(\text{Bu})_4\text{NPF}_6$).

Table 1. Cyclic voltammetric data (vs. $\text{Fc}^{+/0}$) for **1c**, **2c**, **3c** and **7c** at $v = 100$ mV/s in MeCN, containing 0.1 M $(\text{Bu})_4\text{NPF}_6$.

	1c	2c	3c	7c
E_p^c (V)	-2.26, -2.45	-2.27, -2.45	-2.15, -2.34)	-2.00, -2.17

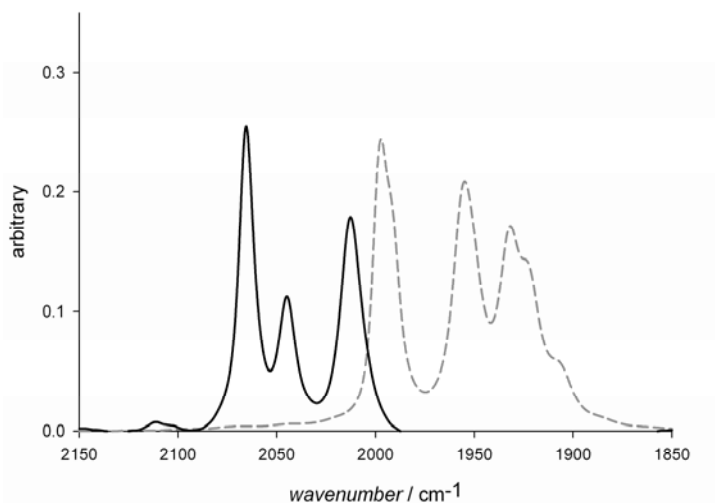


Figure 4. Carbonyl region of the IR spectra obtained for acetonitrile solutions of **3b** (grey, dashed trace) and $[(\mu\text{-H})\mathbf{3b}]^+$, prepared from **3b** with 10 equivalents of trifluoromethanesulfonic acid (black, solid trace).