Supplementary Material (ESI) for Dalton Transactions

Electronic supplementary information for

Structures, protonation, and electrochemical properties of diiron dithiolate complexes containing pyridyl-phosphine ligands†

Ping Li,[a] Mei Wang,*[a] Lin Chen,[a] Jihong Liu,[a] Zhenbo Zhao,[a] and Licheng Sun*[a,b]

[a] *State Key Laboratory of Fine Chemicals, DUT-KTH Joint Education and Research Centre on Molecular Devices, Dalian University of Technology (DUT), Dalian, 116012, China*
[b] *KTH School of Chemical Science and Engineering, Organic Chemistry, 10044 Stockholm, Sweden*

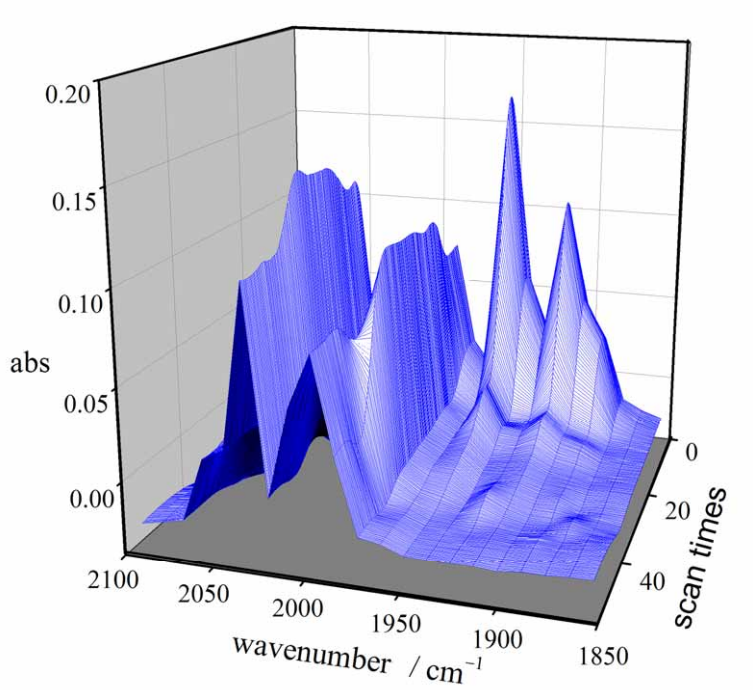

Fig. S1 *React*-IR spectra for the protonation of **4b** in the presence of 0–4 equiv. of HOTf in CH_2Cl_2 at −55 °C.

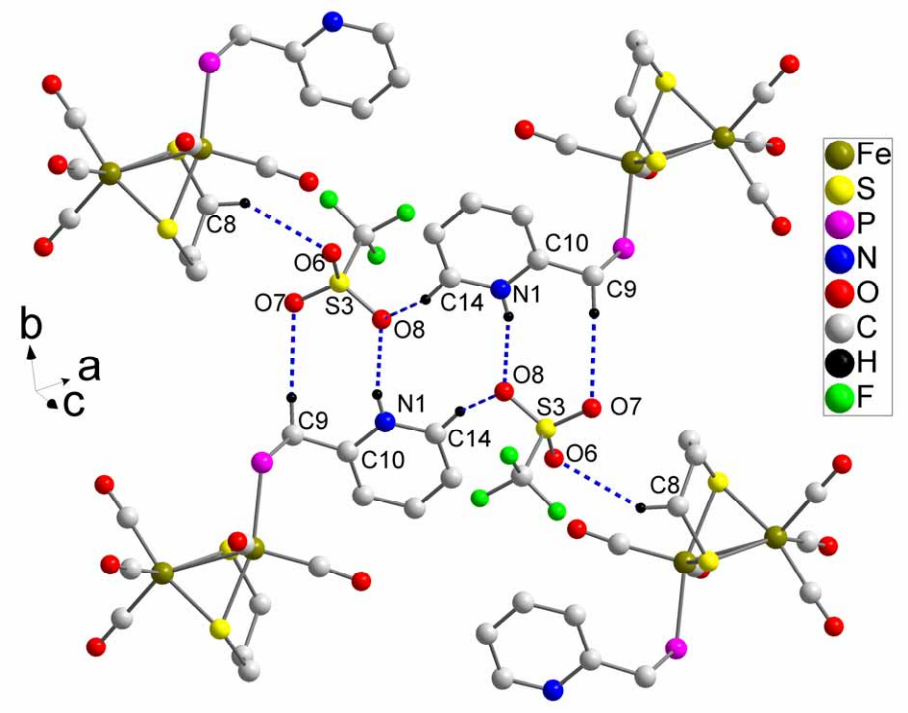

Fig. S2 Packing diagram showing the hydrogen bonds in [**3a**H_N][OTf]. Unrelated H atoms and phenyl groups are omitted for clarity.

Table S1 Geometric parameters for the hydrogen bonds in the packing diagrams of complex [**3a**H_N][OTf]

D–H···A	D–H	H···A	D···A	D–H···A
N(1)–H(1)···O(8)	0.78	1.98	2.7338	160
C(8)–H(8A)···O(6)	0.97	2.59	3.4322	146
C(9)–H(9A)···O(7)	0.97	2.46	3.4247	175
C(14)–H(14A)···O(8)	0.93	2.45	3.2404	142

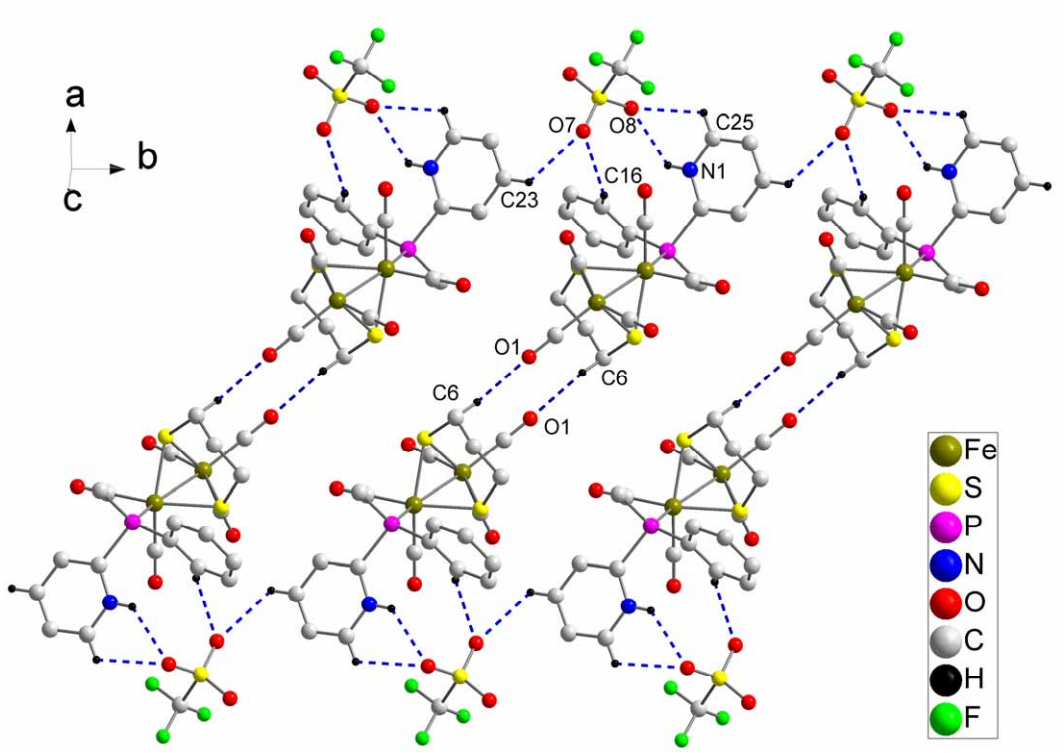

Fig. S3 Packing diagram showing the hydrogen bonds in [**3b**H_N][OTf]. Unrelated H atoms and phenyl groups are omitted for clarity.

Table S2 Geometric parameters for the hydrogen bonds in the packing diagrams of complex [**3b**H_N][OTf]

D–H···A	D–H	H···A	D···A	D–H···A
N(1)–H(1)···O(8)	0.84	2.28	2.8729	128
C(6)–H(6B)···O(1)	0.97	2.58	3.2828	129
C(16)–H(16A)···O(7)	0.93	2.53	3.2712	137
C(23)–H(23A)···O(7)	0.93	2.57	3.1229	119
C(25)–H(25A)···O(8)	0.93	2.45	2.9653	115

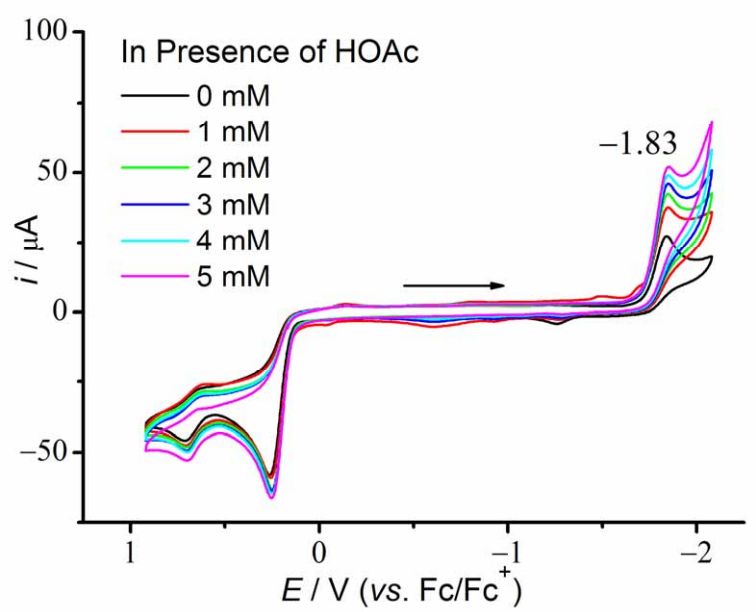

Fig. S4 Cyclic voltammograms of complex **3b** (1 mM) in the presence of HOAc.

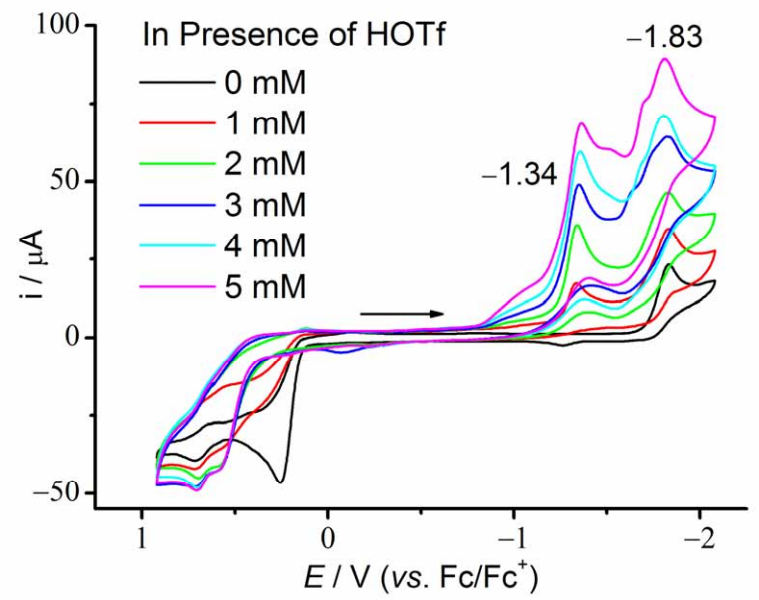

Fig. S5 Cyclic voltammograms of complex **3b** (1 mM) in the presence of HOTf.