Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Synthesis and Characterization of 1D Iron(II) Spin Crossover Coordination Polymers with Hysteresis

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Table S1. Crystallographic data of **1**·3 MeOH and **4**·(0.5 bipy)(MeOH).

compound	**1**·3 MeOH	**4**·(0.5 bipy)(2 MeOH)
formula	$C_{33}H_{42}FeN_4O_{11}$	$C_{35}H_{38}FeN_5O_8$
M_r / g mol^{-1}	726.56	712.55
crystal system	monoclinic	triclinic
space group	$P2_1/c$	$P\bar{1}$
a / Å	11.1275(18)	11.1228(9)
b / Å	16.408(2)	11.8129(9)
c / Å	21.317(3)	13.3170(9)
α / °	90	102.269(5)
β / °	115.206(11)	103.440(4)
γ / °	90	95.947(4)
V / Å^3	3521.5(9)	1641.3(2)
Z	4	2
ρ / g cm^{-3}	1.370	1.442
μ / mm^{-1}	0.492	0.521
crystal size	0.23 × 0.07 × 0.03	0.19 × 0.07 × 0.04
T / K	173(3)	173(2)
diffractometer	Oxford XCalibur	KappaCCD
λ (MoK_α) / Å	0.71073	0.71073
θ-range / °	4.22–26.14	3.24–25.19
reflns. collected	12551	10103
indep. reflns. (R_{int})	5806 (0.0487)	5799 (0.072)
mean σ (I) / I	0.1784	0.0993
reflns. with $I \geq 2\sigma$ (I)	2722	3892
x, y (weighting scheme)	0.0082, 0	0.0558, 4.6271
parameters	448	474
restraints	0	31
R (F) (all data)[a]	0.0411 (0.1101)	0.0699 (0.1140)
wR (F^2)[b]	0.0518	0.1853
GooF	0.690	1.064
shift/error$_{max}$	0.001	0.000
max., min. resd. dens. / e Å^{-3}	0.42, −0.38	0.60, −0.73

[a] $R(F) = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR(F^2) = [\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2]^{½}$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [F_o^2 + 2(F_c^2)]/3$.

Figure S1. Plots of the $\chi_M T$ product *vs.* T for the compounds **1**, **2**·(0.3 bpea), **4**·(0.5 bipy)(MeOH) and **2**·(0.5 bpea)(0.5 tol). The green curve of **2**·(0.5 bpea)(0.5 tol) was obtained after heating of the sample to 400 K for one hour.

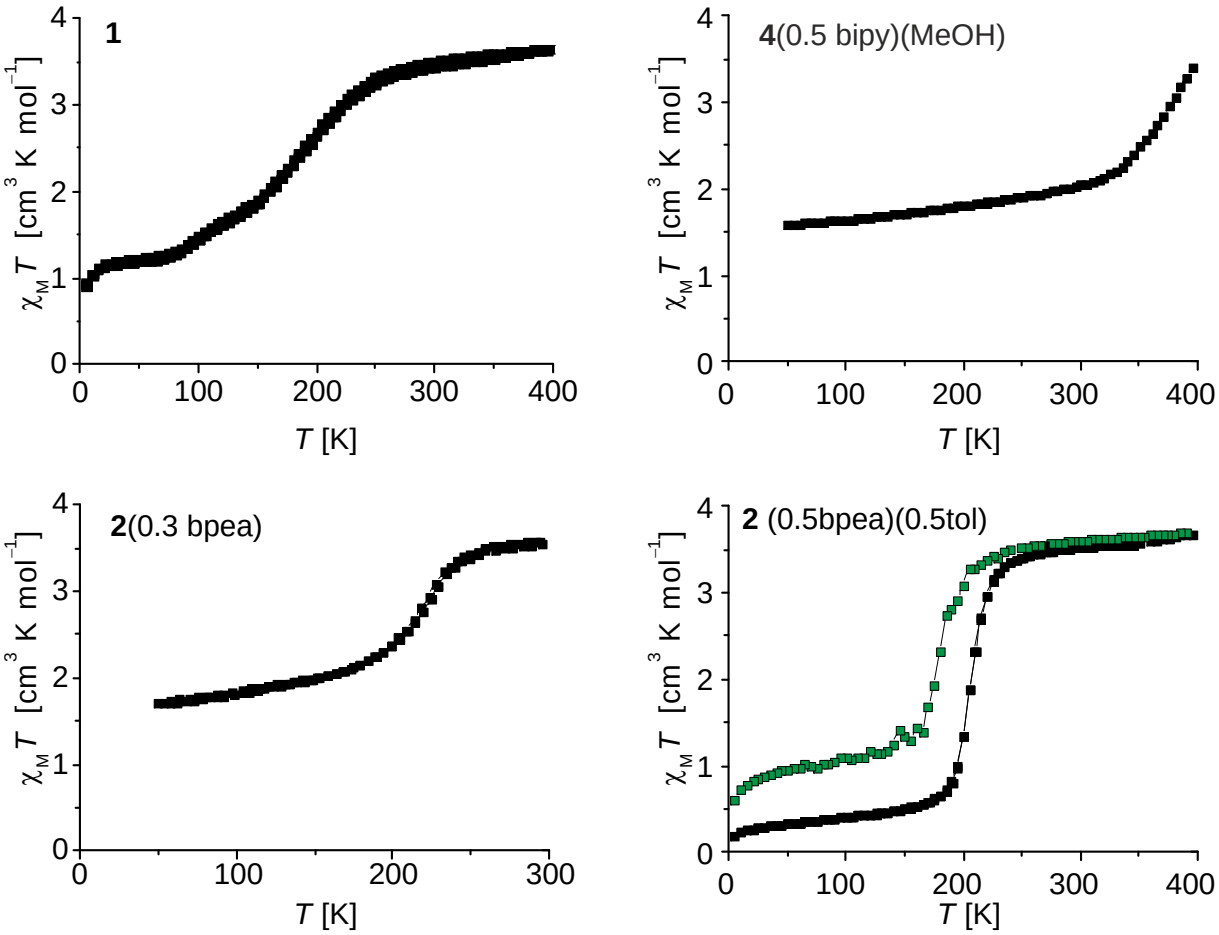

Figure S2. Mössbauer spectrum of the partly oxidised starting material [FeL1a(MeOH)$_2$]. The oxidation product is the corresponding iron(III)-μ-oxido complex. The Mössbauer parameters are δ = 1.004(2) mm/s and ΔE_Q = 2.328(4) mm/s for the iron(II) HS complex and δ = 0.397(3) mm/s and ΔE_Q = 0.768(6) mm/s for the iron(III)-μ-oxido complex.