Spin crossover in iron(II) complexes with 2,6-bis(1H-imidazole-2-yl)-4-chloropyridine

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Table 1S. Parameters of the local atomic surrounding of Fe in coordination compounds. *R* is the interatomic distance, *N* is the coordination number, σ^2 is the Debye-Waller factor, *R*-factor is the coefficient characterizing the quality of the fit

Compound		***R*** **/ Å**	***N***	σ^2 / Å^{-2}	ΔE_0 / eV	***R*-factor**
$[FeL_2]SO_4 \cdot 5H_2O$	Fe(1) – N(1)	1.95 ± 0.037	4.4 ± 0.97	0.008 ± 0.003	0.2 ± 5.3	0.0056
	Fe(1) – N(2)	2.14 ± 0.089	1.6 ± 0.35			
	Fe(1) – C(1)	2.85 ± 0.060	7 ± 1.8	0.015 ± 0.006		
	Fe(1) – C(2)	3.23 ± 0.074	5 ± 1.3			
$[FeL_2](NO_3)_2 \cdot 2H_2O$	Fe(1) – N(1)	1.99 ± 0.060	1.2 ± 0.61	0.006 ± 0.003	4.2 ± 3.1	0.0190
	Fe(1) – N(2)	2.16 ± 0.025	4.8 ± 2.4			
	Fe(1) – C(1)	3.02 ± 0.041	6 ± 1.6	0.009 ± 0.003		
	Fe(1) – C(2)	3.41 ± 0.032	6 ± 1.6			

$[FeL_2]Cl_2 \cdot 3H_2O$	Fe(1) – N(1)	1.99 ± 0.048	1.3 ± 0.65	0.006 ± 0.003	4 ± 2.9	0.0200
	Fe(1) – N(2)	2.17 ± 0.024	4.7 ± 2.4			
	Fe(1) – C(1)	3.03 ± 0.040	6 ± 1.4	0.010 ± 0.003		
	Fe(1) – C(2)	3.41 ± 0.034	6 ± 1.4			

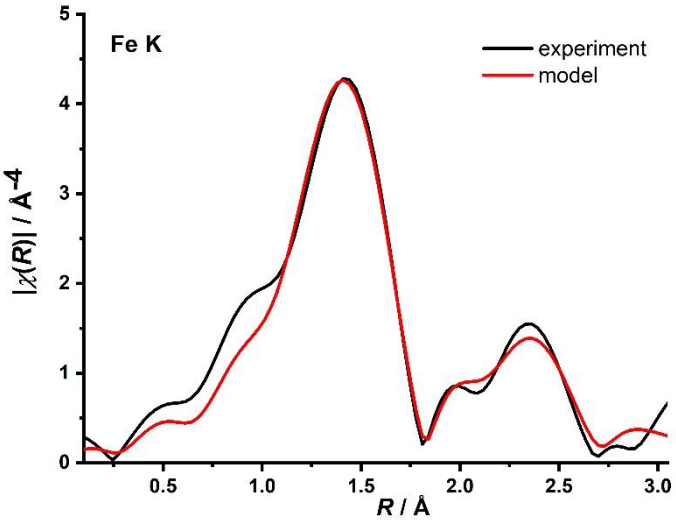

Fig. 1S. Fourier transformed Fe K-edge EXAFS spectrum (without phase correction) of $[FeL_2]SO_4 \cdot 5H_2O$ (*R*-range = 1.0 – 3.0 Å, *k*-range = 3.0-11.0 $Å^{-1}$).

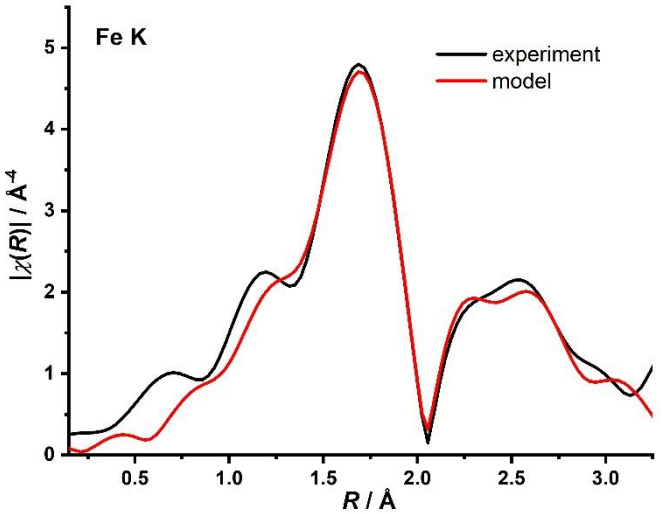

Fig. 2S. Fourier transformed Fe K-edge EXAFS spectrum (without phase correction) of $[FeL_2](NO_3)_2 \cdot 2H_2O$ (*R*- range = 1.0 – 3.2 Å, *k*- range = 2.8-11.2 $Å^{-1}$).

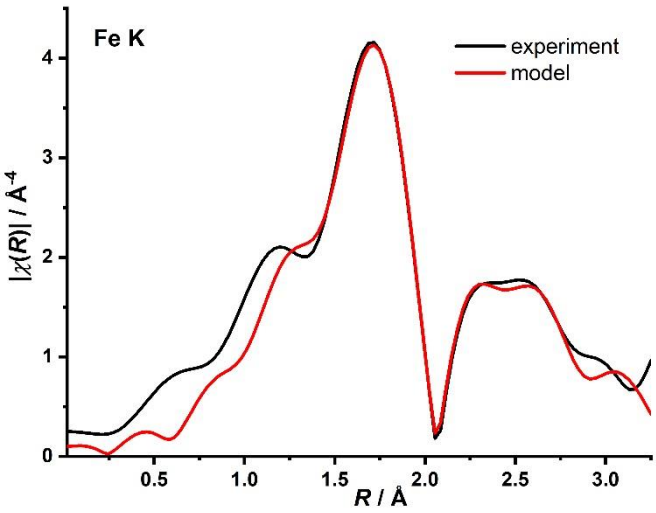

Fig. 3S. Fourier transformed Fe K-edge EXAFS spectrum (without phase correction) of $[FeL_2]Cl_2 \cdot 3H_2O$ (*R*- range = 1.0 – 3.2 Å, *k*- range = 2.8-11.2 $Å^{-1}$).