Supporting Information

for

Spin crossover behavior in a family of iron(II) zigzag chain coordination polymers

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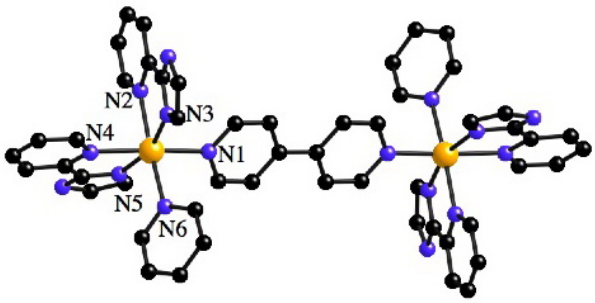
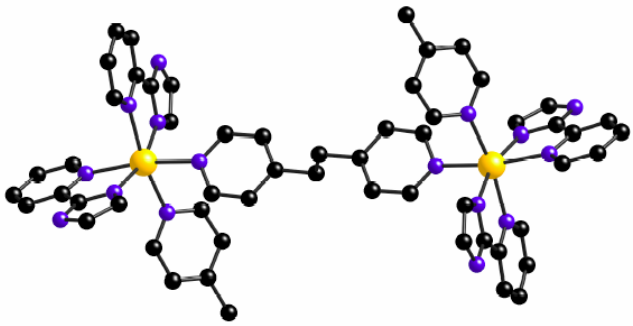
Figure S1. Binuclear fragments of the polymer chains **1** (a), **2** (b) and **3** (c) used in the DFT calculations.

a



b



c

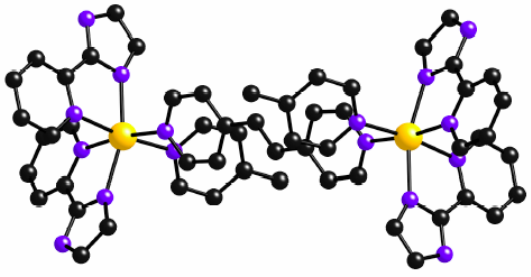


Table S1. Main DFT optimized distances (in Å) for the binuclear fragments of complexes **1**, **2** and **3**. The nitrogen atoms numbering is given in Fig. S1.

	1		***2***		***3***	
	LS	HS	LS	HS	LS	HS
BP86 functional						
Fe-N1	2.000	2.324	2.014	2.278	1.997	2.272
Fe-N2	2.025	2.256	2.022	2.265	2.024	2.272
Fe-N3	1.988	2.173	1.987	2.174	1.985	2.171
Fe-N4	2.035	2.268	2.028	2.280	2.033	2.277
Fe-N5	1.983	2.168	1.981	2.166	1.983	2.165
Fe-N6	2.014	2.209	2.012	2.213	2.014	2.215
Fe-Fe	11.237	11.835	13.544	14.044	13.578	14.094
B3LYP functional						
Fe-N1	2.094	2.344	2.090	2.300	2.082	2.305
Fe-N2	2.082	2.309	2.081	2.316	2.080	2.315
Fe-N3	2.042	2.190	2.042	2.191	2.041	2.190
Fe-N4	2.082	2.314	2.082	2.325	2.082	2.324
Fe-N5	2.034	2.181	2.035	2.182	2.036	2.182
Fe-N6	2.070	2.235	2.071	2.238	2.071	2.238
Fe-Fe	11.361	11.837	13.625	14.035	13.683	14.112