

Supporting information for contribution:

A new family of spin crossover complexes based on $\text{Fe}^{\text{II}}(\text{tetrazolyl})_4(\text{MeCN})_2$ -type core

by

Agata Białońska, Robert Bronisz*, Marek Weselski

from

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383, Wrocław, Poland

Analytical characterization of compound **2**:

Anal calcd for $C_5H_8N_8O$: C, 30.6; H, 4.1; N, 57.1. Found: C, 30.5; H, 4.1.; N, 57.4%. 1H NMR (300 MHz, DMSO- d_6) δ : 9.31 (s, 2H, CH of tetrazol-1-yl), 5.77 (br d, 1H, -CH(OH)-, $^3J=5.6$ Hz), 4.69 (dd, 2H, -CHH-tetrazol-1-yl, $^2J=13.9$ Hz, $^3J=3.2$ Hz), 4.42 (dd, 2H, -CHH-tetrazol-1-yl, $^2J=13.9$ Hz, $^3J=7.9$ Hz), 4.21-4.34 (m, 1H, -CH(OH)-) ppm. ^{13}C NMR (300 MHz, DMSO- d_6) δ : 144.7 (tetrazol-1-yl), 67.1 (-CH(OH)-), 50.9 (-CH $_2$ -) ppm. ESI-MS: m/z 197.1 (LH $^+$).

Analytical characterization of compound **3**:

Anal calcd for $C_5H_8N_8O$: C, 30.6; H, 4.1; N, 57.1. Found: C, 30.7; H, 4.0; N, 57.1.%. 1H NMR (300 MHz, DMSO- d_6) δ : 8.96 (s, 2H, CH of tetrazol-2-yl), 5.66 (d, 1H, -CH(OH)-, $^3J=6.2$ Hz), 4.92 (dd, 2H, -CHH-tetrazol-2-yl, $^2J=13.7$ Hz, $^3J=3.9$ Hz), 4.81 (dd, 2H, -CHH-tetrazol-2-yl, $^2J=13.6$ Hz, $^3J=7.6$ Hz), 4.54-4.66 (m, 1H, -CH(OH)-) ppm. ^{13}C NMR (300 MHz, DMSO- d_6) δ : 153.3 (tetrazol-2-yl), 67.5 (-CH(OH)-), 55.7 (-CH $_2$ -) ppm. ESI-MS: m/z 197.1 (LH $^+$).

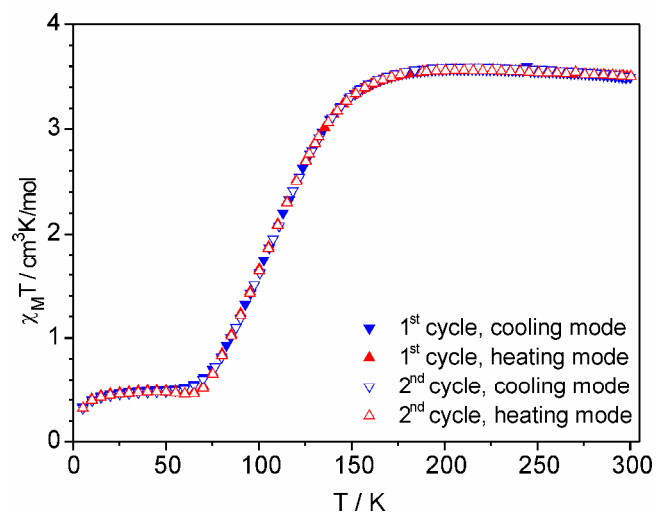


Figure s1. The $\chi_M T(T)$ plot for **4** in cooling and heating modes.