Spin transition in a triazine-based Fe(II) complex: variable-temperature structural, thermal, magnetic and spectroscopic studies

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Supplementary Material

Figure S1. Representation of the molecular structure of [Fe(dpyatriz)2(SCN)2] (2), emphasizing the [S···S] interactions between individual molecules, leading to “inorganic wires” protected by an organic shell of dpyatriz ligands.

Figure S2. Infrared spectra of a ground sample of [Fe(dpyatriz)2(SCN)2] (2) and 41K (black) and 300K (red), emphasizing the differences and similarities between the HS and LS forms of the complex.
Figure S3. Isofield magnetization vs field curves of a polycrystalline (black) and ground (blue) sample of \([\text{Fe(dpyatriz)}_2(\text{SCN})_2]\) (2) at 2K, allowing to estimate the residual fraction of the HS form of the complex at this temperature in ca. 3.4 and 6.5 %, respectively. The solid lines are fits to the Brillouin equation.

Figure S4. Relative area of the HS (blue squares) versus LS (red circles) forms of \([\text{Fe(dpyatriz)}_2(\text{SCN})_2]\) (2) at different temperatures, as revealed by Mössbauer spectroscopy, showing a gradual and ca. 70 % complete spin transition.
Figure S5. Plot of the heat capacity at constant pressure, $C_p$, of [Fe(dpyatriz)$_2$(SCN)$_2$] (2) versus $T$ as derived from Differential Scanning Calorimmetry. A heat capacity anomaly is observed, centered near 200K, the temperature where the spin transition of 2 takes place.