

Does the Structural Preorganization Contribute to the “Two-Way” Spin Crossover in 1,1'-Di(tetrazol-1-ylo)methane-Based Fe(II) Coordination Polymer Containing Conformationally Labile Adiponitrile Coligand?

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Streszczenie

The reaction between 1,1'-di(tetrazol-1-ylo)methane (1ditz) and iron(II) tetrafluoroborate carried out in the presence of adiponitrile (ADN) afforded the coordination compound $[\text{Fe}_2(\mu\text{-1ditz})_4(\mu\text{-ADN})(\text{ADN})_2](\text{BF}_4)_4 \cdot 2\text{ADN}$. The 1ditz molecules bridge the Fe(II) ions in two directions, resulting in a polymeric layer, whereas adiponitrile molecules join 1ditz-based units, extending the structure into the three-dimensional network. One of the two axial coordination sites of Fe(II) is occupied by monodentately coordinating adiponitrile. Dinitrile can also act as guest molecules occupying the area between the 1ditz-based layers. Cooling from room temperature triggers the structural phase transitions $\text{HS}(P1; a, b, c) \rightarrow \text{HS}(P2; 2a, b, c) \rightarrow \text{LS}(P3; a, b, c)$ (P, phase; HS, high spin; and LS, low spin) associated with the conformational changes of the adiponitrile molecules. In the cooling mode, $T_{1/2}^\downarrow = 160$ K, while in the heating mode $T_{1/2}^\uparrow$ is equal to 185 K. Depending on the further path of change of the temperature, it is possible (i) to perform the same cooling/heating cycle ($T_{1/2}^\downarrow = 160$ K; $T_{1/2}^\uparrow = 185$ K) after the sample is reheated above 240 K or (ii) to execute the cooling with $T_{1/2}^\downarrow = 167$ K after the heating is stopped at 190 K, where the phase with superlattice (P2) does not appear. Both ways are reversible, and they are managed by conformational changes of the adiponitrile molecules.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>

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