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# 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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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 $[Fe_2(\mu\text{-}1ditz)_4(\mu\text{-}ADN)(ADN)_2](BF_4)_4 \cdot 2ADN$. 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 HS($P1$; $a$, $b$, $c$) → HS($P2$; $2a$, $b$, $c$) → 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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