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Title: Phase transitions associated with conformational changes of ligand and anion reorientation trigger normal and reverse spin crossover : [abstract]

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MS35-P02 | PHASE TRANSITIONS ASSOCIATED WITH CONFORMATIONAL CHANGES OF LIGAND AND ANION REORIENTATION TRIGGER NORMAL AND REVERSE SPIN CROSSOVER

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Spin crossover (SCO) in octahedral complexes of $3d^4$ - $3d^7$ metal ions affects structure of materials because is connected with shortening of Fe-ligand distances at about 0.2\AA . An occurrence of phase transition can trigger reverse SCO depending on high spin \rightarrow low spin (HS \rightarrow LS) transition upon elevation of temperature. Thus structural properties of the material are a crucial factor responsible for occurrence of spin crossover in normal or reverse mode.

Taking into account uncommon properties of ebtr system [1] we have decided to use trifluoromethanesulfonate anion which can be a source of structural lability. The crystal of $[\text{Fe}(\text{ebtr})_2(\text{CH}_3\text{CN})_2](\text{CF}_3\text{SO}_3)_2 \cdot 4\text{CH}_3\text{CN}$ is composed from polymeric layers and area between them is occupied by anions and noncoordinated acetonitriles. At 270K the Fe-N distances are characteristic for HS form. Lowering of temperature triggers HS \rightarrow LS transition, however structural phase transition at 220K involves reversal of direction of SCO and leads to formation of superstructure ($\mathbf{q} = 1/3\mathbf{a}^* + 1/3\mathbf{b}^* - 1/3\mathbf{c}^*$) with Fe-N bond distances characteristic for HS form. During further cooling there occurs subsequent structural phase transition which results in vanishing of superstructure and formation of LS form. In the heating mode two structural phase transitions occurs again, however they are shifted to higher temperatures which results in two types of hysteresis loops: "normal" and "reverse".

[1] M. Weselski, M. Książek, D. Rokosz, A. Dreczko, J. Kusz, R. Bronisz, *Chem. Commun.*, **2018**, 54, 3895.