

Spin Crossover Quenching by “Racemization” in a Family of *trans*-1,2-Di(tetrazol-1-yl)cyclopentane-Based Fe(II) 1D Coordination Polymers

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Streszczenie

Optically pure (*RR*)- and racemic (*RR/SS*)-*trans*-1,2-di(tetrazol-1-yl)cyclopentane were synthesized and used to prepare homo- and heterochiral Fe(II) coordination compounds. $[\text{Fe}((\text{RR/SS})\text{-C}_7\text{H}_{10}\text{N}_8)_2(\text{CH}_3\text{CN})_2](\text{BF}_4)_2$ (**1A**), $[\text{Fe}((\text{RR/SS})\text{-C}_7\text{H}_{10}\text{N}_8)_2(\text{C}_2\text{H}_5\text{CN})_2](\text{BF}_4)_2$ (**2A**), $[\text{Fe}((\text{RR})\text{-C}_7\text{H}_{10}\text{N}_8)_2(\text{CH}_3\text{CN})_2](\text{BF}_4)_2 \cdot 2\text{CH}_3\text{CN}$ (**1B·solv**), and $[\text{Fe}((\text{RR})\text{-C}_7\text{H}_{10}\text{N}_8)_2(\text{C}_2\text{H}_5\text{CN})_2](\text{BF}_4)_2$ (**2B**) form a family of one-dimensional coordination polymers. Fe(II) cations in these complexes are characterized by a heteroleptic coordination environment: the neighboring metal centers are bridged by two 1,2-di(tetrazol-1-yl)cyclopentane molecules, while the nitrile molecules (acetonitrile or propionitrile, respectively) occupy the axial positions. Independently of the kind of nitrile coligands, an ability to thermally induce spin crossover (SCO) is governed by chirality. **1B·solv** and **2B** exhibit abrupt and complete SCO occurring at $T_{1/2} = 144$ K and $T_{1/2} = 228$ K, respectively. Desolvated form, **1B** (of the same stoichiometry as **2B**), also exhibits SCO ($T_{1/2} = 215$ K). In contrast, an exchange within the polymeric chain of half of the *RR* molecules with the *SS* enantiomeric form results in formation of **1A** and **2A**, which remain in stable high-spin (HS) form down to 10 K. It has been shown that moving from a homochiral to a heterochiral system changes the structure of the polymeric unit (while maintaining the same polymer dimensionality and bridging fashion) that leads to the deep reorganization of the further coordination spheres, including the anion network.

Słowa kluczowe

Anions, Coordination Compounds, Crystals, Ligands, Molecules

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