

Evidence of ligand elasticity occurring in temperature-, light-, and pressure-induced spin crossover in 1D coordination polymers [Fe(3ditz)₃]X₂ (X = ClO₄⁻, BF₄⁻).

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The complexes [M(**3ditz**)₃]X₂ [X = ClO₄⁻, M = Fe^{II} (**1**), Zn^{II} (**2**); X = BF₄⁻, M = Fe^{II} (**3**), Zn^{II} (**4**); **3ditz** = 1,3-di(tetrazol-1-yl)propane] were prepared. Disorder of the propylene chain in **3ditz** is not affected by thermally induced spin crossover in **1** ($T_{1/2\downarrow} = 149$ K, $T_{1/2\uparrow} = 150$ K) and **3** ($T_{1/2\downarrow} = 158$, $T_{1/2\uparrow} = 161$ K). Low-spin to high-spin (LS→HS) switching triggered by laser-light irradiation (520 nm) also does not influence the disorder of the ligand, leading to restoration of the initial HS phase. Pressurization of crystals results in a reduction of the Fe–N distances by about 0.19 Å, which indicates practically complete spin crossover (SCO). Also, in this case, the disorder of the ligand remains unchanged, although thermally and pressure-induced SCO is accompanied by different changes of **3ditz** molecules. Upon thermally induced SCO, perturbation resulting from the reduction of the Fe–N distances is accompanied by a slight elongation of the bridging ligand. In contrast, in the range 0.25–0.55 GPa, the pressure-induced SCO is associated with shrinkage of the **3ditz** molecule. Further elevation of pressure results in the inversion of structural changes and – similar to temperature-induced spin crossover – a slight elongation of the ligand molecule takes place.

Słowa kluczowe

N ligands, Iron, Spin crossover, structure elucidation

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