Sliding polymeric layers and anion displacement coupled with spin crossover in two-dimensional networks of $[Fe(hbtz)_2(CH_3CN)_2](BF_4)_2$.

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Streszczenie

The abrupt high spin (HS)→low spin (LS) transition ($T^{\downarrow}_{1/2}$ =136 K) in $[Fe(hbtz)_2 (CH_3 CN)_2](BF_4)_2$ (hbtz=1,6-di(tetrazol-2-yl)hexane) is finished at 100 K and further thermal treatment influences the spin crossover. Subsequent heating involves a change of the spin state in the same way ($T^{\uparrow}_{1/2}$ =136 K) on cooling. In contrast, cooling below 100 K triggers different behavior and $T^{\uparrow}_{1/2}$ is shifted to 170 K. The extraordinary structural changes that occurred below 100 K are responsible for the observed diversity of properties. A unique feature of the low-temperature phase is the rebuilding of the anion network expressed by a shift of anions inside the polymeric layer at a distance of 1.2 Å as well as the relative shift of neighboring layers at over 4 Å. These structural alterations, connected with a phase transition, become the origin of the strain, which in most cases causes crystal cleaving. In a sample composed from crystals crushed as a result of the phase transition or as a result of mechanical crumbling, the hysteresis loop vanishes; however, annealing the sample allows to its partial restoration. A replacement of acetonitrile by other nitriles leads to preservation of the polymeric structure and spin crossover, but no phase transition follows.

Słowa kluczowe

bridging ligands, 2D coordination networks, Iron, phase transitions, Spin crossover

Adres publiczny

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