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High spin and spin-crossover two-dimensional coordination polymers containing $Fe^{II}(tetrazol\text{-}2\text{-}yl)_4(solv)_2$(solv=ethanol, acetonitrile) cores linked by flexible/elastic spacers.

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Streszczenie

1,6-Di(tetrazol-2-yl)hexane (1, hbtz) in the reaction with Fe(ClO(4))(2).6H(2)O performed in acetonitrile or ethanol forms complexes {[Fe(hbtz)(2)(CH(3)CN)(2)](ClO(4))(2)}(infinity) (2) and {[Fe(hbtz)(2)(C(2)H(5)OH)(2)](ClO(4))(2)}(infinity) (3), respectively. Both compounds crystallize in the triclinic system and P1 space group. In 2 and 3 the basal plane of the coordination octahedron is formed by four tetrazole rings coordinated through N4 nitrogen atoms. The coordination spheres in 2 and 3 are completed by axially coordinated CH(3)CN or C(2)H(5)OH molecules, respectively. In 2 and 3 ligand molecules bridge neighboring iron(II) ions in two directions resulting in two-dimensional (2D) networks. 3 is paramagnetic in the range 5-300 K whereas 2 undergoes the thermally induced HS <==> LS transition (SCO) with T(1/2) (upward arrow) = T(1/2)(downward arrow) = 128 K. Both complexes have very similar architecture with (4,4) network topology; however, the temperature dependence of ligand bridge parameters in 2 differs markedly from the ones observed for 3. In 2 a lowering of temperature from 293 to 100 K causes a reduction of the distances between bridged iron(II) ions at 0.26 and 0.30 A accompanied by the shortening of the distances between N4,N4' donor atoms at about 0.04 and 0.09 A indicating elasticity of the ligand molecules. In 3 at 250 K iron(II) ions are linked by ordered and disordered over two positions hbtz bridges. Cooling to 100 K involves a shortening of Fe...Fe and N4...N4' distances of the ordered bridge at 0.09 and 0.07 A, respectively. The previously disordered bridge is ordered at 100 K, and only one conformer is present. In this case conformational changes enable a reduction of Fe...Fe and N4...N4' distances at about 0.14 and 0.14 A, respectively.

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