

Role of Fe–N–C geometry flip-flop in bistability in Fe(tetrazol-2-yl)₄(C₂H₅CN)₂- type core based coordination network.

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Streszczenie

[Fe(ebtz)(2)(C(2)H(5)CN)(2)](ClO(4))(2) was prepared in the reaction of 1,2-di(tetrazol-2-yl)ethane (ebtz) with Fe(ClO(4))(2)·6H(2)O in propionitrile. The compound crystallizes as a one-dimensional (1D) network, where bridging of neighboring iron(II) ions by two ebtz ligand molecules results in formation of a [Fe(ebtz)(2)](∞) polymeric skeleton. The 1D chains are assembled into supramolecular layers with axially coordinated nitrile molecules directed outward. The complex in the high spin (HS) form reveals a very rare feature, namely, a bent geometry of the Fe-N-C(propionitrile) fragment (149.1(3)° at 250 K). The HS to low spin (LS) HS→LS transition triggers reorientation of the propionitrile molecule resulting in accommodation of a typical linear geometry of the Fe-N-C(nitrile) fragment. The switching of the propionitrile molecule orientation in relation to the coordination octahedron is associated with increase of the distance between the supramolecular layers. When the crystal is in the LS phase, raising the temperature does not cause reduction of the distance between supramolecular layers, which contributes to further stabilization of the more linear geometry of Fe-N-C(C(2)H(5)) and the LS form of the complex. Thus, a combination of Fe-N-C(C(2)H(5)) geometry lability and lattice effects contributes to the appearance of hysteretic behavior (T(1/2)(↓) ≈ 112 K, T(1/2)(↑) ≈ 141 K).

Adres publiczny

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<https://www.acs.org/content/acs/en.html>