



Tetrazol-2-yl as a donor group for incorporation of a Spin-crossover function based on Fe(II) ions into a coordination network.

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The coordination polymer $\{[\text{Fe}(\text{pbtz})_3](\text{ClO}_4)_2 \cdot 2\text{EtOH}\}_\infty$ (**1**) has been prepared in a reaction between $\text{Fe}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ and 1,3-di(tetrazol-2-yl)propane (pbtz). The formation of the second product $\{[\text{Fe}(\text{pbtz})_3](\text{ClO}_4)_2\}_\infty$ (**2**) was also noticed. Both complexes crystallize in the $R3$ space group. The single-crystal X-ray diffraction study of **1** (295, 90 and 230 K) revealed that the 2-substituted tetrazole rings (2tz) coordinate monodentately to the metal ions, forming $\text{Fe}(\text{2tz})_6$ cores. There are two crystallographically independent iron(II) ions in **1**. At 295 K the Fe–N4 bond lengths are equal to 2.173(5) and 2.196(5) Å for Fe1 and 2.176(5) and 2.190(4) Å for Fe2. The pbtz ligand molecules act as N4,N4' connectors, bridging central atoms in the three directions, which leads to the formation of the 3D network. The crystal lattice of **1** is solvated by ethanol molecules. At 295 K the solvent and ligand molecules are disordered. The results of temperature-dependent magnetic susceptibility measurements (5–300 K), and the single-crystal X-ray diffraction studies (90 K) have exhibited that **1** undergoes the thermally induced spin transition $\text{HS} \leftrightarrow \text{LS}$ (SCO). The $\chi_M T(T)$ dependence shows in the range 200–75 K gradual SCO. Below 75 K the transition is finished and ~20% of the HS fraction is present in the sample. The $\text{HS} \rightarrow \text{LS}$ transition is accompanied by a shortening of the Fe–N bonds of 0.15 Å. At 90 K the ligand molecules are ordered. The presence of **2** in the reaction product was disclosed accidentally, and only the X-ray diffraction studies (250, 90 K) were performed. Also in **2** iron(II) ions serve as topological nodes of the 3D network. Despite the same network topology, **2** crystallizes without ethanol molecules solvating the crystal lattice. The pbtz molecules bridge the neighboring iron(II) ions, coordinating through N4,N4' atoms of the 2-substituted tetrazole rings forming the $\text{Fe}(\text{2tz})_6$ cores. At 250 K the Fe–N bond lengths are equal to 2.208(5) and 2.218(5) Å. In contrast to **1**, the cooling of the crystal of **2** from 250 to 90 K does not involve the shortening of the Fe–N bond lengths. At this temperature, the Fe–N distances remain characteristic for the HS form of the complex and are equal to 2.203(3) and 2.208(3) Å.

Słowa kluczowe

Ligands, Crystal structure, Molecules, Ions, Quantum mechanics

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