New thiocyanato iron(II) complex with 3,5-bis(3-pyridyl)-1,2,4-thiadiazole: synthesis, structure, magnetic and spectral properties.

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Streszczenie

The new iron(II) complex $[Fe(NCS)_2(CH_3OH)_2(bpta)_2]$ (bpta = 3,5-bis(3-pyridyl)-1,2,4-thiadiazole) has been prepared by refluxing $Fe(NCS)_3$ or $Fe(NCS)_2$ with thionicotinamide in methanol solution. It is supposed that the bpta ligand is generated in situ by the oxidative dimerization of thionicotinamide. The complex was characterized by X-ray structural analysis at 150 and 293 K, elemental analysis, spectral and magnetic measurements. The compound crystallizes in the monoclinic $P2_1$ space group, with unit cell parameters at 293 K: a = 7.869(2), b = 17.056(3), c = 12.637(3) Å, β = 102.88(1)°. The crystal structure analysis showed that the iron atom has a distorted octahedral environment with FeN_4O_2 chromophore. Iron atom is coordinated by two nitrogen atoms from NCS^- ions, by two oxygen atoms from methanol molecules in the equatorial plane and by two nitrogen atoms of pyridine rings from dpta ligands in axial positions. The crystal lattice forms 2D supramolecular network which is stabilized by a system of hydrogen bonds and π–π stacking interactions. Variable-temperature magnetic susceptibility data in the temperature range 1.8–300 K show that the octahedral iron(II) is high-spin $S = 2(^5T_{2g})$ and as a result effects due to zero-field splitting are anticipated at low temperatures. Structural parameters and infrared spectra of similar complexes are compared and discussed.

Słowa kluczowe

Iron(II) complex, Thiocyanate complex, Ion, 5-Bis(3-pyridyl)-1, molecule, 4-thiadiazole, Crystal structure, Infrared spectra, Magnetic properties

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